COMPUTATIONAL AND EXPERIMENTAL ANALYSIS OF THE FLOW IN AN ANNUlar CENTRIFUGAL CONTACTOR

by

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For Brooke,
always.
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ABSTRACT

The annular centrifugal contactor has been developed for solvent extraction processes for recycling used nuclear fuel. The compact size and high efficiency of these contactors have made them the choice for advanced reprocessing schemes and a key equipment for a proposed future advanced fuel cycle facility. While a sufficient base of experience exists to facilitate successful operation of current contactor technology, a more complete understanding of the fluid flow within the contactor would enable further advancements in design and operation of future units and greater confidence for use of such contactors in a variety of other solvent extraction applications. This research effort has coupled computational fluid dynamics modeling with a variety of experimental measurements and observations to provide a valid detailed analysis of the flow within the centrifugal contactor. CFD modeling of the free surface flow in the annular mixing zone using the Volume of Fluid (VOF) volume tracking method combined with Large Eddy Simulation (LES) of turbulence was found to have very good agreement with the experimental measurements and observations. A detailed study of the flow and mixing for different housing vane geometries was performed and it was found that the four straight mixing vane geometry had greater mixing for the flow rate simulated and more predictable operation over a range of low to moderate flow rates. The separation zone was also modeled providing a useful description of the flow in this region and identifying critical design features. It is anticipated that this work will form a foundation for additional efforts at improving the design and operation of centrifugal contactors and provide a framework for progress towards simulation of solvent extraction processes.
Part I

Background
Chapter 1

Introduction and Background

With the resurgence of interest in nuclear power in recent years there has been a corresponding increased interest in spent nuclear fuel reprocessing. Several past and current government initiatives have focused on research and development of advanced reprocessing schemes for implementation in future closed fuel cycle strategies. The Advanced Fuel Cycle Initiative (AFCI) program began in 2003 as the successor to the Accelerator Transmutation of Waste (ATW) and Advanced Accelerator Applications (AAA) programs. The stated goals of the AFCI program and the advanced reprocessing research that it has funded are to:

- Improve waste management and geologic disposal
- Enable energy recovery from spent fuel and more effective uranium use
- Enhance proliferation resistance
- Provide competitive economics
- Provide excellent safety

The AFCI program has funded the development of the UREX+ advanced reprocessing technology which is based on annular centrifugal contactors and has been demonstrated at the lab-scale at Argonne National Laboratory (ANL). This process has been designed to meet the goals outlined by the AFCI program including enhanced proliferation resistance compared to current reprocessing technologies.

Building upon these previous programs, President George W. Bush and the U.S. Department of Energy (DOE) unveiled in February 2006 the Global Nuclear Energy Partnership (GNEP) for
furthering the effort to implement a closed nuclear fuel cycle.\textsuperscript{[3]} This program builds on the groundwork of the AFCI program and has similar goals, namely, to:

- Reduce America’s dependence on foreign sources of fossil fuels and encourage economic growth
- Improve our environment
- Recycle nuclear fuel using new proliferation-resistant technologies to recover more energy and reduce waste
- Encourage prosperity growth and clean development around the world
- Utilize the latest technologies to reduce the risk of nuclear proliferation worldwide

It is proposed that these overarching goals will be implemented according to the following specific strategy:

- A new generation of nuclear power plants in the United States
- New recycling technologies that enhance proliferation resistance while extracting more energy and producing less waste
- An aggressive plan to manage spent nuclear fuel in the United States, including permanent geologic disposal at Yucca Mountain
- Advanced Burner Reactors that recycle nuclear fuel

Under the GNEP framework it is planned to construct an engineering scale advanced fuel cycle facility (AFCF) based on the UREX+ aqueous reprocessing scheme using annular centrifugal contactors. The centrifugal contactor is key to the success of these advanced reprocessing schemes and will be the foundation of the solvent extraction processes for the AFCF as planned under the GNEP initiative. Thus, centrifugal contactors are, and will be, integral to the successful future implementation of advanced spent fuel reprocessing.

While a sufficient base of experience exists to facilitate successful operation of current contactor technology, a more complete understanding of the fluid flow within the contactor would enable further advancements in design and operation of future units. This project has been aimed at performing a detailed analysis of the flow in the annular centrifugal contactor through the application
of computational fluid dynamics (CFD) modeling supported by necessary experimental observations. These simulations provide both qualitative and quantitative description of the flow within the contactor and enable greater understanding of, and confidence in, current contactor designs. Further, this work forms a basis for implementing contactor design improvements and evaluating designs which would be used in pilot and full-scale operational facilities.

This work is outlined as follows: the motivations and contextual setting, relevant background research, and basis for approaching the contactor problem are presented in Chapter 1. Details regarding the computational and experimental methods used in this project are set forth in Chapters 2 and 3, respectively. The following chapters comprise the main body of research that makes up this work which is divided into separate analyses of the two main regions of the centrifugal contactor, namely, the Mixing Zone (Part II) and the Separation Zone (Part III). The last chapter (Chapter 8) summarizes this work and the main conclusions which can be drawn therefrom and outlines ideas for some potential future directions of research in this area.

1.1 Spent Nuclear Fuel Reprocessing

Solvent extraction processes have been the keystone to the reprocessing of spent nuclear fuel since the beginning of the nuclear era.\textsuperscript{4} Solvent extraction, also called liquid–liquid extraction, refers to processes which incorporate the selective extraction of a solute from one liquid phase to another. This is done by mixing and subsequent separation of two immiscible fluids, typically an aqueous phase and an organic phase, by which the desired species is transferred between phases. The Plutonium URanium EXtraction (PUREX) process was originally developed for plutonium production for nuclear weapons in the 1940s and was based on selective extraction of plutonium and uranium by tri-butyl phosphate (TBP). Of course, as the military goal was plutonium production rather than the creation of an overall environmentally friendly, optimized process, the Defense PUREX process generated large quantities of high-level liquid waste (HLLW). Modification of the PUREX process for commercial use as a recycle scheme for power reactor fuel of necessity involved internal clean-up and recycle of process solvents and the ultimate solidification of residual high-level waste (primarily fission products) in a stable form by vitrification in borosilicate glass
as well as the collection and sequestration of volatile products in the spent fuel. This PUREX process has been used commercially throughout the subsequent decades in the UK, France, Russia, and Japan. The Rokkasho reprocessing facility in Japan was set to begin commercial operation at the end of 2007 and is primarily based on a French plant design which employs pulse columns and mixer settlers using the PUREX process.\[^5\] Use of the PUREX process for commercial reprocessing in the U.S. was officially ruled out by an Executive Order issued by President Jimmy Carter in April 1977 (this ban was later overturned by President Reagan). One stated driver for President Carter’s policy decision—as well as the more recent U.S. policies and programs outlined above—was the concern over proliferation of nuclear weapons materials and technology.

More recently, advanced reprocessing schemes have been developed which are aimed at enhancing the proliferation resistance of spent fuel reprocessing. In particular, the UREX+ process has been developed and demonstrated\[^2\] as part of the AFCI program as mentioned previously. The UREX+ process is actually a suite of processes which can be tailored for the extraction of various critical chemical species as desired. The current preferred formulation is referred to as UREX+1a and involves uranium extraction (for volume reduction), extraction of cesium and strontium (short-term heat production), and the group extraction of transuraneics (TRU, long-term heat and radiotoxicity). This process is preferred for proliferation reasons as it produces no pure plutonium product, rather the plutonium remains mixed with the other TRU elements. With the UREX+ process (specifically the UREX+1a process), it is proposed that the uranium (which is approximately 94% of the total volume) could be separated and disposed of as a low-level waste or stored for recycle in future fast reactors. The Cs/Sr would be placed in short-term storage and allowed to decay and the TRU product could be burned in an Advanced Burner Reactor which would be designed and constructed for that purpose as part of GNEP. The UREX+ process has been designed to meet stringent product specifications\[^2\] that the high efficiency of the annular centrifugal contactor makes possible. While the UREX+ process has been primarily developed by Argonne and other national laboratories, industry groups have also proposed alternative processes, such as the NUEx process (proposed for GNEP by EnergySolutions), which could also take advantage of the potential space savings and added efficiency from using centrifugal contactors.\[^6\]
1.2 Annular Centrifugal Contactors

Among the many types of process equipment which are applicable to solvent extraction,[7–9] liquid–liquid extraction columns (originally packed and later pulsed columns) and mixer-settlers have traditionally been used for spent fuel reprocessing.[10] The annular centrifugal contactor has several important advantages over these other types of equipment.[11–13] Centrifugal contactors are compact and have a relatively short fluid residence time and small liquid volume hold-up resulting in reduced solvent exposure to radiation, and consequently, decreased solvent degradation. This can be particularly necessary for processes which employ sensitive or expensive solvents and/or extractants.[14,15] Their small size also reduces physical space requirements, improves criticality safety, and results in quick startup and shutdown. Despite the short residence time and small size, contactors also have very high extraction efficiency and high throughput. Yarbro and Schreiber[16] give a good overview of the process intensification benefits of the centrifugal contactor as compared to other equipment. Further, annular centrifugal contactors can operate over a wide range of organic to aqueous flow ratios (O/A) making them a versatile piece of equipment for a wide range of solvent extraction processes.

The initial design of the annular centrifugal contactor was made at Argonne National Laboratory (ANL) by modification of a Savannah River Laboratory (SRL) contactor as described by Bernstein et al.[17,18] Groups in Japan[13] and China[19] have also developed annular centrifugal contactors based on the ANL design. Others have also developed similar equipment based on the same principles.[20,21] A cross–section for a generalized ANL contactor is shown in Figure 1.1. Contactors are typically referred to by the diameter of the rotor. Hence, a 2 cm contactor is an annular centrifugal contactor with a 2 cm diameter rotor. While contactors were originally developed for use in spent fuel reprocessing they have application to liquid-liquid extraction used in many areas of chemical processing such as pharmaceutical production[23] as well as for oil-water separations.[24]
Figure 1.1: Sketch of the cross-section of an annular centrifugal contactor with the main components labeled. Figure taken from Leonard et al. 2002.\textsuperscript{[22]}
1.2.1 Operation

For solvent extraction processes using a mix/settle stage-wise extraction type of equipment (as opposed to a continuous column), the key to successful operation is to achieve efficient mixing of two immiscible fluids by creating small droplets with a large total surface area for good extraction followed by quick separation of the two phases. The annular centrifugal contactor is able to combine both the mixing and separation zones in a compact device. Flows of immiscible liquids enter through tangential ports into the annular mixing region where the dispersion begins to form as the fluids are mixed by shear induced by the spinning rotor. Radially oriented vanes below the rotor break the rotation of the dispersion and force the liquid into the hollow rotor which then acts as a centrifuge separating the two phases and pumping the liquid upward. The separated phases then flow over their respective weirs and out the exit lines flowing by gravity to successive stages or collection vessels. In this way the contactor acts as a mixer, a centrifuge, and a pump. Contactors can be set up in a linear bank of multiple units with countercurrent flow requiring no interstage pumps. Figure 1.2 shows a bank of twenty-four 2 cm annular centrifugal contactors that were designed and built at ANL for use in their hot cell facility and have been used in the development of the UREX+ process.

During contactor operation, it is possible for the entire mixing zone to become flooded making the stage inoperable and requiring the processes to be halted. Contactor flooding most often is a result of a rotor stopping to spin for some reason (such as motor failure) but can also occur as a result of the build-up of particulates or the formation and accumulation of other liquid phases (‘third phases’) in the contactor. Under some conditions, even though the contactor is still operating it is also possible for the liquid height in the annulus to fill the mixing zone and overflow into the light phase collector ring. On the other hand, if the total flow rate to a contactor is too low, poor mixing and even complete loss of fluid–rotor contact can occur. Thus, coupled design of both the process flowsheet AND the process equipment are critical to ensuring efficient operation of each contactor stage and high efficiency for the overall process.
1.2.2 Design

Extensive experimental work was performed throughout the 1980s by ANL researchers which enabled successful design and operation of contactors which could be used for a range of input compositions and flow rates. Specific effort was also made to improve low flow rate operation in smaller contactor units. The key design features of the annular centrifugal contactor have been described by one of the chief investigators.\textsuperscript{[11,12]} Some of the important design characteristics include:

**Stationary vanes beneath the rotor** These break the rotation of the fluid and direct the flow inward toward the rotor inlet. The design and orientation of these vanes has a large impact on annular liquid level, degree of mixing, and contactor throughput. The ANL contactors have been designed using eight straight, radially oriented vanes. A similar commercial contactor design, originally based on the ANL contactor, employs curved vanes.\textsuperscript{[25]} Curved vanes were also tested as part of the original contactor development at ANL.\textsuperscript{[18]}
**Small rotor inlet relative to light phase weir**  This ensures that the contactor is able to pump fluids up through the rotor (fully pumping). If a wider rotor inlet is used, the rotor becomes *partially pumping* and the necessary pressure to pump the fluids upward is made up by increased annular liquid level.

**Axial vanes inside the rotor**  These are required to accelerate the fluid entering the rotor and keep it spinning at a steady rate.

**Diverter disk just inside rotor**  The diverter disk is used to increase throughput by directing the flow of dispersion coming into the rotor radially outward into the middle portion of the separation zone. The diverter disk is similar to the inlet baffle used in the gravity settling zone of some mixer settlers which was shown to reduce entrainment and stabilize the dispersion band.\(^{[26]}\)

**Appropriate organic and aqueous weir radii**  The relative weir radii are very critical to the rotor design and ensure that for a given O/A flow ratio the band of separating fluid in the rotor remains between the light phase weir and the heavy phase underflow such that there is no other phase carryover. Previous ANL contactor designs have included an air-controlled aqueous weir which allowed dynamic adjustment of the effective aqueous weir radius to allow optimum operation over the widest range of O/A flow ratios;\(^{[18]}\) however, this feature was abandoned for simplicity in design. Specifically, it was found that the rotary seals needed for introduction of the compressed air to the upper weir were problematic.

In regards to the weir dimensions, it is important to recognize at this point that the inlet flow rates of the liquid phases to a given stage in a bank of contactors is often defined by a specified O/A flow ratio for the given process section (i.e. extraction, strip, scrub). For equipment dedicated to a specific process, it would be desirable to be able to optimize the contactors for each section of the process for the given process parameters in that section. For equipment to be used for testing of various processes, however, it is desirable to be able to have a versatile contactor that can operate over a wide range of process conditions.

Other parameters which are important to contactor design are:
• Rotor to housing gap (also called the Couette gap or annular gap)
• Vane to rotor gap
• Vane height and shape
• Inlet orientation (tangential versus perpendicular)
• Collector ring design
• Rotor length sufficient to achieve phase separation for the desired rotor speed
• Well-balanced rotor and stable support frame design to minimize vibrations

The rotor to housing gap is perhaps one of the most important parameters affecting the flow in the annulus and the degree of mixing. More important than the absolute value of the gap is the radius ratio \( \eta \) which is the ratio of the inner radius \( r_i \) to the outer radius \( r_o \) (\( \eta < 1 \)). The flow patterns in different size units are similar for similar values of \( \eta \). ANL researchers found that larger contactor units tended to have a higher extraction efficiency and it was determined that this was due to a larger radius ratio (narrower relative gap size) in these units.

Beyond these relatively standard design features, there are various possible additions. The following section (Section 1.2.3) reviews the U.S. patents which have been given for contactors, but a few additional design features presented in the literature are mentioned here. Centrifugal contactors are typically constructed entirely of stainless steel; however, Zhou et al. have reported the development of a contactor constructed of composite materials.\(^{[27]}\) Recall that the rotor is the only moving part of the centrifugal contactor resulting in relatively simple remote operation and maintenance. Typically, the rotor and its motor are attached in a single assembly which can be easily lifted out of the contactor housing and a replacement inserted. Others have reported magnetic coupling between the motor and rotor\(^{[13,28]}\) allowing independent replacement of the motor and no need for bearings. Contactor flooding was mentioned previously as a problematic occurrence during multistage operation. Duan et al. have reported the development of a centrifugal contactor that employs an overflow structure design which allows the contactor cascade to continue operation though a single stage becomes inoperable.\(^{[19]}\) While the contactor has the specific advantage of a short fluid residence time which decreases solvent degradation, for some processes with slower extraction kinetics a longer residence time or lower flow rate may be required necessitating further
design considerations. Potential design changes that might facilitate better low flow rate operation include such things as modification of the annular gap, the housing vanes, or somehow increasing the volume of the mixing region under the rotor.

1.2.3 Review of Contactor Patents

This section will give a brief review of the various U.S. patents which have been awarded in regards to the design of annular centrifugal contactors. To the author’s knowledge, there is no original patent for the annular type contactor as developed by ANL. Even so, virtually all the patents described here embody modifications based upon this original development.

While not specifically for an annular type contactor, Kashihara et al. proposed a modification to the weir exit ports such that the position of the interface between the two fluids within the rotor can be changed. This is not a dynamic method as with the air-controlled aqueous weir, but is a simple construction which is intended to give greater freedom in optimizing the location of the liquid–liquid interface within the separation zone for a given O/A ratio without physically changing the weir dimensions.

As mentioned above, often the inlet flow rates of the liquid phases to the contactor are defined by the specified O/A flow ratio for a given section of the process. Nemoto et al. presented a modification to the upper section of the rotor in order to allow recirculation of a portion of one or both phases to change the effective flow ratio within a given stage. As with the invention of Kashihara et al., the purpose of this modification is to alter the position of the dispersion band within the rotor and thus change the effective weir radii.

A June 1991 patent by Jubin and Randolph of Oak Ridge National Laboratory presents novel modifications aimed at improving flow in the mixing region. Specifically, the inventors attempt to address the problem of poor mixing at low flow rates and flooding at high flow rates. Helical vanes are added to the lower portion of the housing near the bottom of the rotor in order to direct the flow upward and maintain adequate liquid height in the annulus. To guard against flooding of the mixing zone, slightly steeper helical vanes are attached to the side of the housing above the flow inlets to direct the flow of liquid downward if the annular liquid height reaches this point.
The patent explicitly lists a preferred annular gap of 0.73 cm for a rotor radius of 2.75 cm—giving a radius ratio $\eta = 0.79$. This invention also employs the use of more tangentially oriented flow inlets. In regards to mixing, it is also stated that the introduction of air into the process streams and entrainment that occurs with inadequate liquid volume in the mixing zone has a negative effect on operation. Incidentally, Jubin also has a patent for a contactor modified for end stage operation to mitigate contactor flooding if a stage becomes inoperable.\footnote{Jubin also has a patent for a contactor modified for end stage operation to mitigate contactor flooding if a stage becomes inoperable.}

The standard annular centrifugal contactor was modified for application as a high temperature pyrocontactor for liquid–liquid extraction using immiscible liquid salts and liquid metals by Chow and Leonard.\footnote{Chow and Leonard.} Due to the added mass of the process materials, a shaft running down the axis of the rotor and supported by a bearing at the base of the housing was added to minimize rotor vibration. Vertical vanes attached to the side of the rotor and corresponding baffles attached to the housing were also included to increase mixing in the annular region. A stationary horizontal baffle is also include to reduce splashing in the annulus. The patent also states that the rotor bottom should be tapered at $10^\circ$ relative to the horizontal to ensure fluid-rotor contact at low liquid flow rates. While this added rotor design feature is briefly mentioned elsewhere and shown in the drawings for several other patents,\footnote{As the primary application of annular centrifugal contactor technology is the processing of used nuclear fuel, nuclear criticality is an important consideration. For engineering scale contactors this is less problematic, but for plant scale contactors it can be a serious concern and one that ultimately limits the size of the unit. To mitigate this issue, Ogino and Washiya have proposed introduction of neutron absorbing media into the rotor and the housing of the contactor. A cylinder of neutron absorbing material can be included along the axis of the rotor either suspended from the rotor or extending up from the housing. The latter configuration can also incorporate a secondary support for the rotor. While not specifically pointed out in the patent, this configuration is nice strictly from a design perspective as it moves the lower support bearing axially up into the rotor where it would be away from the process streams.} it is explicitly described here but not included as a specific claim of the given patent.

As the primary application of annular centrifugal contactor technology is the processing of used nuclear fuel, nuclear criticality\footnote{Criticality is characterized by the attainment of a neutron multiplication factor $k$ of $\geq 1$ marking the initiation of a self-sustaining nuclear reaction.} is an important consideration. For engineering scale contactors this is less problematic, but for plant scale contactors it can be a serious concern and one that ultimately limits the size of the unit. To mitigate this issue, Ogino and Washiya have proposed introduction of neutron absorbing media into the rotor and the housing of the contactor. A cylinder of neutron absorbing material can be included along the axis of the rotor either suspended from the rotor or extending up from the housing. The latter configuration can also incorporate a secondary support for the rotor. While not specifically pointed out in the patent, this configuration is nice strictly from a design perspective as it moves the lower support bearing axially up into the rotor where it would be away from the process streams.
likely be within the air core (see Section 1.2.5.2) rather than submerged in the process fluids were it positioned at the base of the housing as in other designs that employ a lower bearing.\[^{25,33}\] Ogino et al. have also patented a contactor with a non-contact, magnetically coupled motor and rotor as cited previously.\[^{28}\]

While the centrifugal contactor was primarily developed as a device for solvent extraction, it has also been employed for use solely as a separator. A patent was issued to Meikrantz in September 1990 for demonstration of the application of a standard centrifugal contactor with no modification as a “centrifugal separator”.\[^{24}\] Though described thus as a separator, this appears to be the first patent issued for an annular centrifugal contactor; however, it only predates that of Jubin and Randolph\[^{32}\] by several months. Note that both of these patents were assigned to the United States Department of Energy. Further modifications to the “centrifugal separator” are embodied in various subsequent patents issued to Costner Industries Nevada, Inc.\[^{25,35–38}\] As mixing is not desired if the purpose of the equipment is merely for separation of previously mixed liquids (e.g. oil–water separation for environmental cleanup), a stationary sleeve which slides up into the annulus and shields the fluid from contacting the spinning rotor was designed.\[^{36}\] A clean-in-place rotor\[^{37}\] and an easily disassembled rotor assembly\[^{38}\] were also developed.

Meikrantz et al. later also received a patent for a complete centrifugal separator apparatus.\[^{25,35}\] This design employs unique housing vanes which are curved in the direction of rotation and direct the flow toward the axis of the rotor “with significantly less turbulence.” Similar vanes were tested as part of the original annular centrifugal contactor development.\[^{18}\] While not specifically noted in the text of this Meikrantz et al. patent, the diagrams also show phase outlets with a downward slope which would help in drawing fluid from the collector rings. In regards to unit scaling, it is mentioned that a rotor height to diameter ratio of about 2.4 should be preserved; no details are given in regards to the scaling of the mixing zone. The details of this ‘centrifugal separator’ design are important for centrifugal extraction in that the same commercially available ‘separator’ units are now being evaluated for use as solvent extraction units.\[^{22,39–41}\] Moreover, process units manufactured by CINC are already being employed at the plant scale for the removal of cesium from tank waste at Savannah River using the CSSX process.\[^{15}\] The research reported in this
dissertation also employs a CINC-designed centrifugal contactor as the basis for the experiments and modeling.

A very recent patent which presents a substantial redesign of the annular centrifugal contactor has been issued to Rivalier et al. of the French Atomic Energy Commission (CEA).\textsuperscript{[42]} While this design departs significantly from the ‘standard’ ANL-type annular centrifugal contactor design, it is described here as it highlights some of the problematic points of the ‘standard’ configuration. The fundamental change in this design is the shift in the location of the annular mixing zone from outside the rotor to a separate cylindrical section below the rotor (Figure 1.3). The issue of proper balancing to reduce vibration on this longer rotor/mixing shaft assembly is not addressed. This configuration harkens back to the original Savannah River design with the paddle mixing region extending below the rotor; however, in this case an annular mixing cylinder is used. While this configuration sacrifices some of the compactness of the standard contactor, several advantages of this modification are outlined in the patent. It allows different radii to be used for the mixing and separating regions. This is beneficial because one might like to have a larger radius for separation than for mixing. Also, because the flow continues along the same vertical axis from the mixing zone directly into the separation zone, there is no need for stationary housing vanes and the corresponding loss of energy associated with redirecting the flow toward the rotor inlet and then re-accelerating the flow within the rotor zone. Another key difference with this design is that the removal of air from the mixing zone is a stated goal; this is primarily accomplished by attempting to prevent communication of air from above the weirs down into the mixing zone. It is specifically noted that air in the mixing zone reduces mass transfer efficiency between the liquid phases. It is claimed that removal of air from the mixing zone also facilitates a consistent volume of liquid in the mixing zone (which would result in more constant fluid-rotor contact). Communication between the sections above the upper and lower weirs is also enabled resulting in a reduction in the ‘uncertainty of the position of the interface.’ In general it appears that this design has several advantageous features which could be evaluated as part of a future study.
Figure 1.3: Alternative contactor configuration as proposed by researchers at the French Atomic Energy Commission (CEA). Figure taken from Rivalier et al. 2006 patent.\cite{42}
1.2.4 Modeling

Prior to this project, there has been no detailed study of the fluid dynamics of the centrifugal contactor. While some useful models have been developed, particularly by researchers at ANL, the effort has primarily focused on descriptive correlation of experimental data; analytical methods were also implemented where possible. As one product of previous modeling efforts, the dimensionless dispersion number was developed in order to predict the maximum throughput of a contactor for a given set of immiscible fluids and a fixed rotor speed.\[^{43, 44}\] Significant effort was also put forth in the development of a computational model which could aid in the design of contactor weirs by calculating the necessary weir sizes given the properties of the two phases. A descriptive model for the height of the liquid in the annulus as a function of rotor speed was also developed. This model corresponded well with experimental data for low flow rates and for low to moderate rotor rotational speeds. For the region of moderate to high flow rates and high rotational speed, which is nearly always the region of actual operation, a correlation of the experimental data was made which predicts a linearly increase in liquid height with increasing rotor speed.\[^{22}\] The experimental data, however, appear to show a relatively constant liquid height regardless of rotor speed for the fully pumping rotor (see Figure 1.4).

It is apparent from Figure 1.4 that one area to which improved contactor modeling could contribute is the capability of predicting the liquid height in the annulus for a given set of conditions. Such knowledge is critical to optimized design and operation of the contactor. While the throughput of a given contactor is typically limited by the capacity for complete separation of the two phases within the rotor such that there is minimal other-phase contamination in the respective outlets, another limiting case is if the dispersion in the annulus fills the mixing zone and overflows into the organic collector ring. Even if the liquid height under nominal conditions is acceptable, flow transients and changes in liquid height due to phase inversion\[^{2}\] make the annular liquid height an important factor during operation. Further, it appears that the majority of mixing occurs in the annulus (as opposed to underneath the rotor) with the result that a greater liquid height results in more efficient mixing. Issues related to mixing will be discussed in greater detail in Section 1.3.

\[^{2}\] dispersed phase becomes continuous phase and visa versa
Figure 1.4: Plot of annular liquid height as a function of flow rate in a 5-cm contactor using eight straight vanes and water showing comparison of experimental correlation with data. The rotor rotational speed was 3600 RPM.\textsuperscript{[22]}

is critically important to understand the factors which effect the annular liquid height and computational fluid dynamics (CFD) modeling is a valuable tool for doing this.

For spent fuel processing operations the maximum contactor size is limited by uncertainty about the disposition of particulates in the contactor which results in size restrictions due to nuclear criticality concerns. Typically, feed streams are filtered to remove particulates remaining from incomplete dissolution of the spent fuel. It is also possible, however, for precipitates or colloidal products to form during processing.\textsuperscript{[45, 46]} Application of CFD modeling to contactors could also ultimately provide a means for analyzing the flow of particulates and lead to better understanding of potential criticality limits.

To the author’s knowledge, aside from the application of CFD to the annular centrifugal contactor as conducted herein the only attempt at modeling the flow in the contactor via CFD is a 2006 study by a group at Los Alamos National Laboratory (LANL).\textsuperscript{[47]} That work, however, considered only a simplified version of the flow inside the rotor looking mainly at the degree of phase separation for various rotation speeds. A review paper on centrifugal contactor technology by Vedantam
and Joshi\textsuperscript{[48]} also points out the need for detailed research and analysis of the flow in both the mixing and separation zones of the contactor. The computational fluid dynamics modeling performed under this current project has focused primarily on flow in the mixing zone (Part II) as it is the less well understood of the two contactor regions; informative simulations of flow in the separation zone were also performed (Chapter 7).

1.2.5 Hydrodynamics

There are distinctly different flow characteristics in the two major zones of the contactor, namely, the annular mixing zone and the separation zone. The flow in the annular mixing zone could also be further delineated by the different characteristics of the flow in the annular region and the flow underneath the rotor.

1.2.5.1 Mixing Zone

The flow in the annulus of the mixing zone is similar to Taylor-Couette flow which is a well known flow pattern formed for flow in an annulus between a rotating inner cylinder and a stationary outer cylinder. Taylor-Couette flow can be characterized by the dimensionless Taylor number ($Ta$)\textsuperscript{[49]} which is a ratio of the centrifugal forces to the viscous forces and can be defined according to Equation 1.1 where $\Delta r$ is the gap width ($\Delta r = r_o - r_i$), $\Omega$ is the rotational speed, and $\nu$ the kinematic viscosity.

$$
Ta = \frac{r_i(\Delta r)^3 \Omega^2}{\nu^2} \quad [1.1]
$$

$$
Re = \frac{(r_i \Omega) \Delta r}{\nu} \quad [1.2]
$$

Equation 1.1 is equivalent to $Ta = Re^2 (1 - \eta)/\eta$ where the Reynolds number ($Re$) is defined by Equation 1.2 and $\eta$ again is the radius ratio. Depending on both the Taylor and Reynolds numbers of the flow there are different characteristic flow regimes.\textsuperscript{[50]} For flow in a 5 cm annular centrifugal contactor with a gap size of 0.63 cm ($\eta = 0.801$) and operating at 3000 RPM the corresponding Taylor and Reynolds numbers are $Ta = 6.2 \times 10^8$ and $Re = 5 \times 10^4$. In the absence of a free
surface, flow of this magnitude is in the turbulent Taylor vortex (TTV) regime which is true for all $Re \gtrsim 1.3 \times 10^3$ (corresponding to $Ta \gtrsim 5 \times 10^5$).\textsuperscript{[50–52]}

There have been numerous experimental and numerical\textsuperscript{[53]} studies over several decades analyzing turbulent Taylor vortex flow (TTV). Koschmieder\textsuperscript{[54]} examined high TTV flow for two different radius ratios and determined that the vortex spacing for turbulent Taylor vortices was greater than that for laminar vortices. Lathrop et al.\textsuperscript{[51]} explored the torque scaling for turbulent Taylor vortex flow with increasing Reynolds numbers up to $1.2 \times 10^6$. It has also been shown that the combination of axial flow with Taylor vortex flow introduces several different flow regimes.\textsuperscript{[55]} For low Taylor numbers, Gu and Fahidy\textsuperscript{[56]} showed experimentally that the introduction of axial flow causes overlapping and mixing between neighboring Taylor vortices. Wereley and Lueptow\textsuperscript{[57]} have analyzed the flow field of Taylor-Couette flow with axial flow (also called Taylor-Couette-Poiseuille flow) using Particle Image Velocimetry (PIV) for low to moderate Taylor numbers and observed mixing between neighboring toroids to be more significant with increasing rotation rate.

While the flow in the annulus of a centrifugal contactor is similar to turbulent Taylor vortex flow with axial flow, the contactor is different from other Taylor-Couette flow equipment in that it is not liquid full; rather, one end is ‘open’ to air. The flow from the inlets into the annular region can be by droplets or rivulets down the housing wall or rotor depending on operational conditions. Thus, the free surface effects dominate the annular flow and differentiate it from standard closed system Taylor-Couette flow. The effect of an upper free surface on Taylor-Couette flow between vertically oriented concentric cylinders has been primarily studied for low to moderate Taylor numbers.\textsuperscript{[58–60]} Mujica and Lathrop\textsuperscript{[61]} have experimentally observed the instabilities of turbulent free-surface flow in an annular device for high Reynolds numbers ($Re \sim 10^6$) and have observed large-scale ‘gravity-wave’ oscillations in liquid height. However, these observations were for an ‘annular’ device (essentially a spinning rod in a tank) with a very small radius ratio (large gap) of $\eta = 0.128$ and would thus be substantially different from standard Taylor-Couette flow with a relatively narrow gap. The recent review of centrifugal contactor technology that was cited previously interestingly also fails to recognize the importance of free surface flow and air entrainment.
for common contactor designs and, despite being a review of annular centrifugal contactors, focuses more generally on traditional turbulent Taylor-Couette Vortex flow in more standard closed concentric cylinder devices.\cite{48}

Somewhat related to free surface flow, various researchers have looked at the effect of air bubbles and their distribution in turbulent Taylor-Couette flow. It has been shown that bubbles migrate toward the inner cylinder and are most stably located in rings along the regions of outflow between toroidal vortices.\cite{62–65} Numerical studies have also been able to predict this behavior.\cite{65–67} Batten et al.\cite{68} developed a method of using the average bubble distribution to identify the location of Taylor cells. One effect of bubbles on Taylor-Couette flow is the reduction of drag and corresponding decrease in energy dissipation.\cite{69} This is important as energy dissipation is a key measure of the mixing intensity in a given device as will be discussed in Section 1.3.

Atkhen et al.\cite{65} have observed the fluid mechanics of a long rotor, contactor apparatus with radial vanes beneath the rotor directing the flow toward an axial exit (see also Tison 1996\cite{70} and Atkhen 1998\cite{71}). This device, however, has a very long aspect ratio (total height relative to annular gap). Hydrodynamic observations were made with a liquid height of \( \sim 50 \text{ cm} \) and annular gaps of 0.5 cm and 1.0 cm. Thus, for this system, the effect of the free surface was observed in the formation and distribution of air bubbles throughout the annulus. It was observed that at higher rotation speeds (\( Ta > 5 \times 10^4 \)) spatial and temporal defects due to free surface agitation led to elimination of stable Taylor vortices. Note that this is approximately an order of magnitude lower than the transition to fully turbulent Taylor vortex flow and several orders of magnitude lower than the Taylor number in typical contactor flow.

The flow of two immiscible fluids in a Taylor-Couette device has also been studied in recent years primarily with application to low shear, laminar liquid–liquid extraction.\cite{72} Campero and Vigil\cite{73} have examined the various flow patterns for liquid–liquid Taylor-Couette-Poiseuille flow for the water-kerosene system among other phase pairs. Zhu and Vigil\cite{74} have used the kerosene-water system for both experimental and numerical studies of banded liquid-liquid flow which consists of alternating aqueous-rich and organic-rich vortices and occurs for high rotation rates. None of these studies included the effects of a free surface.
While physical measurements of the flow field (velocities, turbulence values, etc.) in an annular centrifugal contactor have not been performed, the flow in the annulus of an actual contactor has been observed experimentally both by ANL and others through the use of a transparent contactor housing. It has been observed that the flow in the annulus is in general very oscillatory and the liquid level appears to be much higher near the housing wall (outer cylinder) than at the rotor. Thus, it appears that the fluid–rotor contact is not continuous but intermittent and that the free surface is indeed an important feature of the flow. Detailed experimental observations have been performed as a critical supporting part of this study and are outlined in Chapter 3.

### 1.2.5.2 Separation Zone

The flow in the separation zone of the contactor is considerably more simple than that in the mixing zone and better lends itself to simple correlation (see Leonard et al.[75]). Specifically, the maximum throughput of a contactor is by design limited to the separation capacity of the inside of the rotor and can be characterized by the dispersion number \[^{[43,44]} N_{Di} \] which is given by:

\[
N_{Di} = \frac{1}{t_B} \sqrt{\frac{\Delta Z}{a}} \tag{1.3}
\]

for batch systems where \(\Delta Z\) is the initial dispersion thickness, \(t_B\) is the time for the dispersion to break, and \(a\) is the acceleration. For gravity settling, \(a\) is simply the acceleration due to gravity \(g\). For continuous flow systems, the dispersion number is given by:

\[
N_{Di} = \frac{\dot{q}}{V} \sqrt{\frac{\Delta Z}{a}} \tag{1.4}
\]

where \(\dot{q}\) is the volumetric flow rate and \(V\) is the volume of the dispersion band. For a centrifugal settler operating in continuous flow such as is the case for the separating zone of the contactor, the volume-average acceleration is given by:

\[
\bar{a} = \tau \Omega^2 \tag{1.5}
\]
where $\bar{r}$ is:

$$
\bar{r} = \frac{\int_{r_{d,i}}^{r_{d,o}} r^2 dr}{\int_{r_{d,i}}^{r_{d,o}} 2\pi r dr} = \frac{2}{3} \left( \frac{r_{d,o}^3 - r_{d,i}^3}{r_{d,o}^2 - r_{d,i}^2} \right) 
$$

[1.6]

for $r_{d,i}$ and $r_{d,o}$ being the inner and outer radii of the dispersion band, respectively, and the dispersion number can be written as:

$$
N_{Di} = \frac{\dot{q}}{V} \sqrt{\frac{\Delta Z}{\bar{r} \Omega^2}}
$$

[1.7]

Since it has been determined that the dispersion number for a given immiscible liquid pair is the same for both batch gravity settling and continuous operation, batch tests can be used to determine the dispersion number which can then be inserted into Equation 1.7 to determine the throughput $\dot{q}$ for a given separation zone geometry ($\Delta Z$ and $\bar{r}$) and rotor speed.$^{[44]}$

A useful test for experimental characterization of the flow in the rotor was developed by Leonard and is referred to as the ‘zero-point flow test.’ The purpose of this test is to measure the single-phase flow rate at which flow just begins to come out the less dense phase exit. A model has been developed which accounts for the height of the flow over each weir$^{[7,75]}$ as well as the volume of fluid and pressure distribution in the separation zone and can predict the zero-point flow rate. CFD prediction of the zero-point flow rate and comparison with the experimentally measured values$^{[22]}$ will provide a method for validation of a CFD-based separation zone model versus the experimental data and previous correlations.

In terms of the actual flow regimes in the separation zone of the contactor, it is likely that the flow is laminar for most of the separation zone except near the rotor inlet where it is accelerated by the vanes within the rotor. As cited previously, a group at Los Alamos National Laboratory (LANL) has used an in-house CFD code to predict the flow and phase separation in a simplified rotor under various conditions.$^{[47]}$ This study considered only laminar flow and did not account for the core of air which develops within the spinning rotor. Chapter 7 of this book presents the results of the flow analysis of the separation zone.
1.2.6 Process and Stage Efficiency

Two values which are critical to process analysis and design are the distribution coefficients of each component and the overall organic to aqueous flow ratio \((O/A)\).\(^{76,77}\) The distribution coefficient, or ‘D-value’, is defined as ratio of the equilibrium species concentration in the organic phase divided by that in the aqueous phase and can be a function of temperature and pH. The product of the \(O/A\) flow ratio and the distribution coefficient gives the extraction factor, that is:

\[
E = (O/A) \cdot D_i
\]  \hspace{1cm} [1.8]

The extraction factor for a given extraction stage is the ratio of the moles of a component leaving in the organic phase versus the moles of the same component leaving in the aqueous phase. Thus, \(E > 1.0\) means that the component is being concentrated in the organic phase. For a specific phase pair system (i.e. 0.1 M \(\text{HNO}_3\) in water and 30\% TBP in n-dodecane) the D-value is fixed (assuming constant temperature). Thus, the extraction factor \(E\) can be set by selection of the \(O/A\) flow ratio such that \(E \gg 1\) for extraction and \(E \ll 1\) for stripping. The process solvent composition can also be modified to ensure adequate extraction factors for a moderate range of \(O/A\) flow ratios. However, unlike other liquid–liquid processing equipment which may require a \(O/A\) ratio near 1 for adequate operation, the centrifugal contactor has been shown to operate efficiently for \(O/A\) ratios ranging from 0.01 to 33.\(^{76}\)

The overall decontamination factor \(DF\) for a given species in a bank of \(n\) contactors is the component concentration in the aqueous feed \(c_{i,\text{feed}}\) divided by the concentration in the aqueous effluent \(c_{i,\text{effl}}\) from the section and as a first approximation can be given by:

\[
DF = \frac{c_{i,\text{feed}}}{c_{i,\text{effl}}} \approx E^n
\]  \hspace{1cm} [1.9]

where \(E\) is the extraction factor according to Equation 1.8. We can define the overall cascade efficiency \(\eta_o\) as:

\[
\eta_o = \frac{n}{N}
\]  \hspace{1cm} [1.10]

or the total number of theoretical stages \(n\) needed to achieve a given \(D.F.\) at a specified extraction factor divided by the actual number of stages needed \(N\). Thus, for a desired decontamination factor
of $10^5$ and with an extraction factor $E = 2.0$, the required number of 90% efficient stages is:

$$N = \frac{\ln(10^5)}{\ln(2)} \frac{1}{\eta_o} \approx 19 \text{ stages}$$ \[1.11\]

Individual stage efficiency in a liquid–liquid extraction device is commonly defined in terms of the concentration of the desired species $i$ as:

$$\eta_{MD} = \frac{c_{i,\text{in}} - c_{i,\text{out}}}{c_{i,\text{in}} - c_{i,\text{equil}}}$$ \[1.12\]

or the actual amount of solute extracted divided by the maximum amount which could be extracted based on the equilibrium distribution ratio of the solute in the two phases. This is called the Murphree efficiency based on the dispersed phase. The quantities $\eta_o$ and $\eta_{MD}$ are not equivalent but can be related (assuming a constant distribution coefficient) for a countercurrent cascade by:

$$\eta_o = \frac{\ln[1 + \eta_{MD}(1/E - 1)]}{\ln(1/E)}$$ \[1.13\]

If other phase entrainment is significant, it is possible to also account for its deleterious effects on stage efficiency.

For the case of a completely back-mixed continuous phase (concentration in continuous phase is the same everywhere as the exit concentration) and an unmixed dispersed phase, the Murphree efficiency is related to the mass transfer coefficient $K_D$ according to:

$$\eta_{MD} = 1 - \exp\left(\frac{-K_D a V}{Q_D}\right) = 1 - \exp(N_{OD})$$ \[1.14\]

where $a$ is the specific surface area [m$^2$/m$^3$], $V$ is the total liquid volume, and $Q_D$ is the dispersed phase volumetric flow rate. The quantity $N_{OD}$ is the number of dispersed phase transfer units.$^9$ The assumption of a completely back-mixed continuous phase is common and has been shown to be valid experimentally.$^{79}$ Thus, the stage efficiency increases as the droplet surface area is increased and it is clear that $\eta_{MD} \to 1$ as $a \to \infty$.

In physical terms, the extraction efficiency of a given stage depends on the mixing efficiency and fluid residence time in the mixing zone. Efficient mixing results in a fine dispersion of small droplets with a large surface area for enhanced mass transfer. In general, the annular liquid height
appears to play a large role in the mixing efficiency and consequent overall extraction efficiency as most of the mixing occurs in the annulus rather than under the rotor. Factors which effect mixing and encourage the generation of small droplets will be discussed in the next section.
1.3 Fluid Mixing

Fluid mixing is a critical part of nearly all chemical and engineering processes and has been the subject of significant research over many years and is still an important topic today. In regards to liquid–liquid mixing in centrifugal contactors, understanding the forces which govern the breakup and dispersion of droplets is key to predicting overall operational efficiency based on droplet size distributions, interfacial area for mass transfer, and mass transfer rates.\textsuperscript{[80]} The following section will discuss the role of energy dissipation in mixing, the formation and distribution of droplets, and a method for approximating the overall stage efficiency from these quantities. While much of the previous research has focused on impeller mixing in stirred tanks, the physical principles are applicable to liquid–liquid mixing in centrifugal contactors.

1.3.1 Droplet Breakup and the Role of Turbulent Energy Dissipation

Many theories regarding droplet breakup in liquid–liquid dispersions have been based on the early theories and studies of Kolmogorov and Hinze. Hinze\textsuperscript{[81]} argued that droplet breakup occurs when the relative magnitude of the forces acting to deform a droplet exceed the restoring forces. Restoring forces include interfacial tension ($\sigma$) and internal viscous stresses. Internal viscous stresses are primarily important for small droplets with high viscosity and are typically negligible for gas bubbles. The primary deforming forces are the turbulent stresses which are the viscous shear stress ($\tau$) and turbulent pressure fluctuations. These deforming forces are generated by turbulent eddies with a characteristic length scale of the same order or smaller than the droplet size. It is generally assumed that eddies larger than the droplet cause bulk motion of the droplet rather than its distortion.\textsuperscript{[82]} Hinze\textsuperscript{[81]} suggested that the deformation of fluid particles could be described by two dimensionless groups representing these two forces affecting droplet stability. These are the Weber number $We$ (ratio of inertial forces and interfacial tension) and the viscosity group $Vi$ (also called the Ohnesorge number $Oh$) and are defined as:

\begin{align*}
    We &= \frac{\tau d}{\sigma} \\
    Vi &= \frac{\mu_d}{\sqrt{\rho_d d \sigma}}
\end{align*}

\textsuperscript{[1.15]} \textsuperscript{[1.16]}
where \( d \) is the droplet diameter, and \( \mu_d \) and \( \rho_d \) are the dispersed phase viscosity and density (denoted by the subscript \( d \)). At some critical value of the Weber number \( W e_{crit} \), droplet breakup would occur and Hinze proposed that the overall deformation process could be described by:

\[
W e_{crit} = c_1[1 + f(Vi)]
\]  

[1.17]

For droplet deformation dominated by dynamic local pressure fluctuations, the corresponding stress generated by eddies in the continuous phase (denoted by subscript \( c \)) with a length scale \( \lambda \) is given by:

\[
\tau \propto \rho_c \bar{u}_\lambda^2/2
\]

[1.18]

For homogeneous, isotropic turbulence in the inertial subrange \(^{4}\), the fluctuating component of velocity \(^5\) \( \bar{u}_\lambda^2 \) is proportional to the turbulent energy dissipation rate \( \varepsilon \).

\[
\bar{u}_\lambda^2 = c_2(\varepsilon \lambda)^{2/3} \approx 2.0(\varepsilon \lambda)^{2/3}
\]

[1.19]

Assuming that the characteristic eddy length scale of interest \( \lambda \approx d_{max} \), that is, deformation of droplets are caused primarily by the dynamic pressure fluctuations of eddies with a similar size, \( W e_{crit} \) can be written as:

\[
W e_{crit} = \frac{\rho_c \varepsilon^{2/3} d_{max}^{5/3}}{\sigma}
\]

[1.20]

For the case of \( Vi \ll 1 \) (negligible internal viscous stresses) the maximum stable droplet diameter is then given by:

\[
d_{max} = c_3 \left( \frac{\sigma}{\rho_c} \right)^{3/5} \varepsilon^{-2/5}
\]

[1.21]

Haas\(^{[83,84]}\) experimentally determined the value of \( c_3 \) in Equation 1.21 to be \( c_3 = 1.2 \) for data from three different liquid–liquid mixing devices (including an annular mixer) along with data from Davies.\(^{[85]}\) There was agreement for a wide range (\( \sim 10^4 \)) of energy dissipation rates.

---

\(^3\)Note that throughout this and following sections, generic empirical constants will be numbered \( c_1, c_2, c_3, \ldots \) and so on to avoid confusion.

\(^4\)Range of scales in which turbulent energy is transported between large, energy-containing scales to small, energy-dissipating scales.

\(^5\)Assumes the measured velocity is the sum of a mean component and a fluctuating component \( u = \bar{u} + u' \). This is described later in Section 2.1.2.
Calabrese et al.\textsuperscript{[86]} derived a version of Equation 1.17 including the effects of internal viscous stress as:

\[ We_{crit} = c_4[1 + c_5 N_{Vi}] \]  \hspace{1cm} [1.22]

where \( N_{Vi} \) is a different form of the viscosity group given by:

\[ N_{Vi} = \left( \frac{\rho_c}{\rho_d} \right)^{1/2} \frac{\mu_d (\varepsilon d_{max})^{1/3}}{\sigma} \]  \hspace{1cm} [1.23]

From the above discussion it is clear that the maximum stable droplet size can be determined simply from the fluid properties and the turbulent energy dissipation rate \( \varepsilon \). It should be noted that these equations consider only dilute dispersions where coalescence is negligible. Calabrese et al.\textsuperscript{[87]} discusses corrections for finite dispersed phase volume fractions. Time also has a role in droplet breakup and the maximum stable drop size. A recent study by Andersson and Andersson\textsuperscript{[82]} using high speed digital photography provided detailed observation of the dynamics of droplet and bubble breakup including measurement of the mean breakup time. It was found that the average breakup time was approximately 1/2 to 2/3 of the turbulent time scale as given by the turbulent kinetic energy divided by the dissipation rate \( (k/\varepsilon) \). In particular, dodecane droplets dispersed in water were found to have an average breakup time of 4.2 ms in a flow with \( \varepsilon = 8.54 \text{ m}^2/\text{s}^3 \) and a corresponding turbulent time scale of 7.5 ms (average \( \varepsilon \) measurements from particle image velocimetry (PIV), see Andersson and Andersson\textsuperscript{[88]}). From these long eddy time scales it is concluded that eddies of the same size as (and up to three times larger than)\textsuperscript{[89]} droplets are responsible for droplet stretching and breakup. This conclusion was for droplets near the equilibrium size. For droplets larger than the equilibrium size, smaller eddies are responsible for over 90\% of the total breakup rate.\textsuperscript{[89]}

Energy dissipation in typical mixing vessels is inhomogeneously distributed. For example, in stirred mixing vessels the energy dissipation in the impeller region can be approximately 100 times the average \( (\varepsilon / \bar{\varepsilon} \sim 100) \).\textsuperscript{[90]} While the average power dissipated per unit mass \( (\bar{\varepsilon} = P/\rho V \) where \( P \) is power and \( V \) is volume) is often used to characterize a given mixer and for device scaling, it is the local dissipation, specifically the maximum dissipation rate \( \varepsilon_{max} \), which has been shown to be the dominant factor for mixing.\textsuperscript{[90–93]} The effect of the main flow field is also important to
the overall mixing in determining the amount of time that the fluid spends in the regions of high dissipation.

The average energy dissipation ($\bar{\varepsilon}$) can be easily gotten experimentally from torque measurements on the mixing shaft (rotor of contactor); however, experimentally measuring the local energy dissipation is more difficult. Some techniques for approximating the turbulent energy dissipation from experimental measurements will be discussed in the following section. CFD has the significant advantage that among many other quantities including the instantaneous and/or mean flow field, the turbulence dissipation rate (and its spatial and temporal distribution) can be calculated directly and thus provide greater insight into mixing. The difficulty arises in making a useful comparison of CFD predictions of local turbulent energy dissipation with adequately approximated experimental values. Details regarding how the local dissipation rate is calculated using CFD will be given in Section 2.1

### 1.3.2 Experimental Approximation of the Dissipation Rate

It is theoretically possible to calculate $\varepsilon$ directly from its definition. Dissipation is defined as being proportional to the product of the fluctuating rate of strain tensor $s'_{ij}$ according to:

$$\varepsilon \equiv 2\nu \langle s'_{ij} s'_{ij} \rangle = \nu \left\langle \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \frac{\partial u'_j}{\partial x_i} \right\rangle$$

[1.24]

where $\nu$ is the kinematic viscosity and $u'_i$ again denotes fluctuating component of the instantaneous velocity $u_i$ ($u_i = \bar{u}_i + u'_i$). The above equation, however, requires fine spatial resolution of all three components of the fluctuating velocity ($u'$) and their gradients. Experimental measurements with accuracy of this magnitude is ordinarily not possible and therefore some approximation method is required. Kresta and Wood 1993 and Sheng et al. 2000 provide review and comparison of various methods for approximate calculation methods for $\varepsilon$ based on experimental measurements.

For isotropic turbulence, the dissipation rate can be approximated by:

$$\varepsilon = 15\nu \frac{u'^2}{\lambda^2}$$

[1.25]
where $\lambda$ is the Taylor micro-scale. Equation 1.25 is commonly rewritten using dimensional arguments to be:

$$\varepsilon = A \frac{u'_{3}}{\ell}$$  \[1.26\]

where $\ell$ is the integral length scale and $A$ is a constant of order 1. The constant $A$ is actually equal to 1 for perfectly isotropic turbulence. If the integral time scale $\tau_{E}$ (given by $\tau_{E,1} = u'_{1}/\ell$) is used instead of the length scale, the above equation becomes:

$$\varepsilon = A \frac{u'^{2}}{\tau_{E,1}}$$  \[1.27\]

where the subscript 1 refers to a single directional component (for perfectly isotropic turbulence the value for $\varepsilon$ calculated using any of the three components should give the same value). The integral time scale can be measured experimentally from Laser Doppler Velocimetry (LDV) data by the integration of the velocity time autocorrelation function which is given by:

$$R_{E,1}(t) = \frac{u'_{1}(t') \cdot u'_{1}(t' + t)}{u'^{2}_{1}}$$  \[1.28\]

and the Eulerian integral time scale is:

$$\tau_{E,1} = \int_{0}^{\infty} R_{E,1}(t) dt$$  \[1.29\]

Typically, the integration is not carried out to infinity, but only up to the first zero crossing of the autocorrelation function. Thus, the spatial distribution of the integral time scale and fluctuating velocity can be used to estimate the spatial distribution of the turbulence dissipation rate at each point where LDV data are available. See Section 3.1.1 for details regarding the LDV technique.

It is also possible to estimate the dissipation rate experimentally from Particle Image Velocimetry (PIV) data (see Section 3.1.2 for details) using the so called Large Eddy PIV method (LE PIV). Because the spatial resolution of PIV is typically not fine enough to resolve the smallest scales at which dissipation occurs, this method employs a sub-grid scale model similar to the large eddy turbulence simulation (LES) in order to calculate the dissipation for unresolved scales. The LES turbulence simulation method will be described later in Section 2.2.
1.3.3 Mean Droplet Size

From the previous two sections, the role of turbulent energy dissipation in mixing was described. For estimation of extraction rates and ultimately the stage efficiency, it is necessary to next evaluate the surface area for mass transfer which is clearly related to the distribution of droplet sizes. Droplet sizes are typically referred to by the Sauter mean droplet diameter \( d_{32} \) which can be experimentally determined from the measured droplet distribution and is defined by:

\[
d_{32} = \frac{\sum f_i d_i^3}{\sum f_i d_i^2}
\]

[1.30]

where \( f_i \) is the experimentally determined fraction of droplets within a given diameter interval \( i \). The interfacial surface area per unit volume \( a \) of a two-phase mixture with a dispersed phase volume fraction \( \phi \) is related to the Sauter mean diameter by:

\[
a = \frac{6\phi}{d_{32}}
\]

[1.31]

The maximum stable droplet diameter has been found to be proportional to the Sauter mean diameter \( (d_{32} \propto d_{\text{max}}) \) and the constant of proportionality can range from 0.38 to 0.70.\(^{[90]} \) Haas\(^{[84]} \) and others\(^{[86]} \) have experimentally determined the approximate relation of the mean to max droplet diameters as \( d_{32} \approx 0.56d_{\text{max}} \) such that Equation 1.21 becomes:

\[
d_{32} = \frac{2}{3} \left( \frac{\sigma}{\rho_c} \right)^{3/5} \varepsilon^{-2/5}
\]

[1.32]

Zhou and Kresta\(^{[90]} \) provide a useful compilation of the many correlations for mean drop size that have been developed by various researchers. Most of these correlations are of the form:

\[
\frac{d_{32}}{D} = c_6 (1 + c_7 \phi)(W e_T)^{-0.6}
\]

[1.33]

where \( D \) is a characteristic length (typically the impeller diameter), \( \phi \) is the dispersed phase volume fraction and \( W e_T \) is the Weber number of the mixing tank given by:

\[
W e_T = \frac{\rho_c \Omega^2 D^3}{\sigma}
\]

[1.34]

for \( \Omega \) being the rotation rate \([s^{-1}]\) of the mixer. Using a long aspect ratio annular mixing device, Tison\(^{[70]} \) studied the characteristics of the mixing zone of a centrifugal contactor and developed a
correlation with general form of Equation 1.33 where the characteristic length is taken to be the annular gap width $\Delta r$.

$$\frac{d_{32}}{\Delta r} = 74.95 \times 10^{-3}(1 + 2.7\phi)(W e_T)^{-0.125} \quad [1.35]$$

The above correlation was fit from data for aqueous continuous operation with a dispersed organic phase volume fraction ranging from about 0.03 to 0.3. Note that droplet size correlation equations of this nature do not explicitly include the energy dissipation. Rather, their purpose is to provide a simple estimate of the overall mean droplet size directly from the overall operational parameters (mixer rotational speed, fluid properties, etc.).

Another method for modeling droplet sizes is via a population balance approach. For this method, models are assumed for the rates of breakup and coalescence which include local turbulence quantities. The local flow field and turbulence can be calculated via CFD providing the information for the population balance equations (PBE). The droplet size distribution (and consequently the interfacial area) can then be calculated throughout the mixing domain using an appropriate transport equation for droplet population. This method could be useful for analysis of the liquid–liquid mixing in the contactor as part of a future study; it has only recently found limited incorporation in commercial CFD software packages.

### 1.3.4 Approximating Stage Efficiency

If the Sauter mean diameter and turbulence dissipation rate can be determined and it is assumed the mass transfer coefficients can be approximated in some way (or gotten from experiment or MD simulation), it is then possible to calculate an approximate value for the stage efficiency (see Section 1.2.6). For calculation of the Murphree efficiency according to Equation 1.14, the unknown values are the mass transfer coefficient $K_D$ and the interfacial area per unit volume $a$. In the previous section it was shown that $a$ can be calculated according to Equation 1.31 from the Sauter mean diameter $d_{32}$ (which depends either explicitly or implicitly on the dissipation rate $\varepsilon$ ) and the dispersed phase volume fraction.
Determining an adequate approximation of the mass transfer coefficient is not a simple task. Mass transfer at the liquid–liquid interface involves complex phenomena which are not fully understood but which are the subject of ongoing research in a variety of fields using both experimental and computational techniques (e.g. Molecular Dynamics (MD) Simulation). Further, in the case of uranium extraction by tributyl phosphate (TBP), an interfacial solvation reaction take place as given by:

\[
UO_2^{2+} + 2NO_3^- + 2TBP \rightleftharpoons UO_2(NO_3)_2 \cdot 2TBP
\]  

The introduction of surface active agents such as TBP also results in interfacial turbulence as a result of the creation of surface tension gradients. This interfacial turbulence is referred to as Marangoni phenomena and can significantly increase the mass transfer rate.\cite{100} It has been shown that as this interfacial turbulence decays with time as does the overall mass transfer coefficient.\cite{101}

Despite these complexities, there are a wide variety of correlations for predicting the mass transfer coefficients for liquid dispersions.\cite{9, 79} The overall mass transfer coefficient is a combination of the coefficients for the dispersed and continuous phases, \( k_d \) and \( k_c \):

\[
\frac{1}{K_{OD}} = \frac{1}{k_d} + \frac{1}{D_i k_c}
\]  

where \( D_i \) is the distribution coefficient for the transferred species. Correlations for \( k_d \) and \( k_c \) are available for various limiting conditions which take into account the Sauter mean droplet size and the molecular diffusivities of the extracted species in each phase along with the necessary geometric and operational parameters.

Combining these ideas, a possible method for estimating the stage efficiency is as follows:

1. Calculate the average energy dissipation (\( \varepsilon \)) and liquid hold-up volume \( V \) using CFD model.
2. Given \( \sigma \) and \( \rho_c \), use \( \varepsilon \) to calculate the Sauter mean diameter \( d_{32} \) using Equation 1.32.
3. Use Equation 1.31 to calculate the interfacial area per unit volume \( a \) for a given volume fraction \( \phi \).
4. Calculate the overall mass transfer coefficient \( K_{OD} \) using appropriate correlation or measured value.
5. Use Equation 1.14 to calculate the Murphree stage efficiency.
Clearly this method involves several critical approximations and the accuracy of a value for stage efficiency obtained in this way is dubious at best. This method is outlined here merely to highlight the fact that it is possible to combine molecular level transport properties with local turbulence predictions from CFD and calculate a value for the overall stage efficiency of a centrifugal contactor. From a design perspective, however, one is primarily interested only in the relative mixing behavior of various configurations rather than an estimation of their absolute values. Therefore, in practice it is sufficient to look at the predicted turbulence dissipation rates and the total liquid volume within the mixing zone and make direct conclusions regarding the relative mixing behavior of various designs.
Chapter 2

Computational Methods

While the applicability of computational fluid dynamics to a wide variety of problems has been greatly aided by the steady increase in the capability of modern high-performance computing, there are still obstacles to rigorous treatment of a problem such as the centrifugal contactor. The flow in a centrifugal contactor is extremely turbulent, unsteady, and for solvent extraction operation consists of at least three phases (two liquid phases and air). To accurately model the details of this kind of flow, each of these issues must be considered. A general overview of turbulence and multi-phase modeling methods will be given here with specific emphasis on the methods to be employed as part of this research project.

The main goal of this research is to analyze the flow in a contactor through the application of computational fluid dynamics using existing methods rather than the development of new numerical methods. As such, the commercial CFD package FLUENT\(^{102}\) will be used for the simulations done in this study. FLUENT is a very widely used computational package which uses finite difference solution methods and incorporates current turbulence modeling techniques, advanced numerical algorithms, and is particularly well-developed for multi-phase modeling.

The following sections will give an overview of some of the important modeling techniques which are applicable to exploration of the centrifugal contactor using CFD. The author refers readers to the many extensive textbooks covering other aspects of computational fluid dynamics\(^{103}\) and to the FLUENT user’s guide\(^{102}\) for more details on the specific implementations and solution methods employed by FLUENT. Details regarding the actual model geometries and solution parameters used for the contactor mixing zone and separation zone models will be given in Chapters 4–6 and Chapter 7, respectively.
2.1 Turbulence Modeling

While not specific to the contactor problem, the issue of turbulence always requires careful consideration when approaching any complex flow problem. It is well beyond the scope of this study to review the entire field of turbulence modeling and the reader is referred to pertinent texts\cite{94} for more detail. While more complex turbulence simulation techniques such as the Large Eddy Simulation (LES) method have become much more feasible in recent years, basic Reynolds’s averaged Navier-Stoke’s (RANS) solution methods such as the $k–\varepsilon$ method are still widely used for practical engineering problems as they generally have lower computational requirements. Such turbulence modeling methods were used for certain portions of this research and will be described in this section. Section 2.2 gives an overview of the LES method which was used for the detailed mixing studies presented in Chapters 5 and 6.

2.1.1 The Momentum Equation

The transport of momentum in an incompressible ($\rho = \text{const}$) fluid continuum with constant viscosity is described by following set of equations referred to as the Navier-Stokes equations:

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} \tag{2.1}$$

$$\nabla \mathbf{u} = 0 \tag{2.2}$$

where $p$ is the dynamic pressure defined by:

$$p = P - \rho g x \tag{2.3}$$

or the total pressure $P$ minus the static pressure. Equation 2.2 is the continuity equation but is often included as part of the Navier-Stokes set of equations. Equations 2.1 and 2.2 combined represent four equations for which there are four unknowns $p$, $u_1$, $u_2$, and $u_3$. While this set of equations can be solved directly as is done for Direct Numerical Simulation (DNS), because of the enormous range of length and time scales required for adequate representation of turbulence in actual engineering problems such an approach is generally not feasible. For example, scales of interest for real problems may be for lengths on the order of a few centimeters and times of 10s of
seconds while the critical scales for turbulence are microns and microseconds. Thus, attempts to model rather than simulate turbulence are often practical.

2.1.2 Mean Flow Equations

Starting from the assumption that the individual components of instantaneous velocity $u_i$ can be subdivided into a mean value plus a fluctuating quantity according to:

$$u_i(t) = \overline{u_i} + u_i'$$  \[2.4\]

it is possible to substitute this formulation into Equation 2.1 and derive a transport equation for mean momentum. This mean momentum or Reynolds equation is given by:

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial}{\partial x_j} (\overline{u_i}u_j) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \overline{u_i}}{\partial x_i} - \overline{u'_i u'_j} \right)$$  \[2.5\]

where $\nu = \mu/\rho$ is the kinematic viscosity and the last term is referred to as the turbulent Reynolds stress tensor $\tau_{ij}^R$. A transport equation for the Reynolds stresses could be written, but it would contain nine equations and introduce more unknowns requiring addition equations for closure. This method of turbulence modeling is possible and is referred to as Reynolds Stress Models (RSM). The more common route is to model $\tau_{ij}^R$ according to the turbulent viscosity hypothesis which states that the Reynolds stresses are related to the mean gradients by:

$$\overline{u'_i u'_j} = \frac{2}{3} k \delta_{ij} - \nu_T \left( \frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right)$$  \[2.6\]

where $k$ is the turbulent kinetic energy defined by:

$$k = \frac{1}{2} \overline{u'_i u'_i}$$  \[2.7\]

For conditions where this hypothesis is valid, the solution of the mean momentum equation requires only that we know the form of the turbulent viscosity $\nu_T$. The turbulent viscosity is generally assumed to be equal to the product of a length scale and a velocity scale ($\nu_T = U^* L^*$). The $k-\varepsilon$ turbulence model used two differential equations (one each for $k$ and $\varepsilon$) to specify the velocity and length scales which combine to give the turbulent viscosity needed to solve the mean momentum equations.
2.1.3 General $k$–$\varepsilon$ Model

The $k$–$\varepsilon$ model uses two differential equations for the transport of turbulent kinetic energy (TKE) $k$ (Equation 2.7) and its dissipation $\varepsilon$ (Equation 1.24) to specify a length scale ($L^* = k^{3/2}/\varepsilon$) and a time scale ($\tau^* = k/\varepsilon$). These two scales can be combined to form the turbulent viscosity according to:

$$\nu_T \propto U^* L^* \propto (L^*/\tau^*) (L^*) = C'_{\mu} \frac{k^2}{\varepsilon}$$

where $C'_{\mu}$ is typically given the value of 0.09. This is the first of several empirical constants required by the model. The transport equation for $k$ is given by:

$$\left(\frac{\partial k}{\partial t} + \bar{u} \cdot \nabla k\right) = \nabla \cdot \left(\frac{\nu_T}{\sigma_k} \nabla k\right) + P - \varepsilon$$

where the production of turbulent kinetic energy $P$ is given by:

$$P = -u'_i u'_j \frac{\partial \pi}{\partial x_j}$$

and $\varepsilon$ is the dissipation of TKE. Again the assumption is that the production of turbulence is related to the mean velocity gradients. The transport equation for $\varepsilon$ is constructed according to:

$$\left(\frac{\partial \varepsilon}{\partial t} + \bar{u} \cdot \nabla \varepsilon\right) = \nabla \cdot \left(\frac{\nu_T}{\sigma_\varepsilon} \nabla \varepsilon\right) + C'_{\varepsilon 1} \frac{P \varepsilon}{k} - C'_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

The standard values for the five constants in the two equations are given in Table 2.1. It is important to keep in mind that these values have primarily been fit using data from turbulent boundary layers and other simple turbulent flows. The standard values for the model constants have been defined as such to provide the widest range of application with minimal or no adjustments.

2.1.4 Variations and Limitations

While the $k$–$\varepsilon$ model is easily the most widely applied turbulence modeling method and performs well for most simple shear flows, it can fail for more complex 3D flows. The poor performance is thought to be caused by the $\varepsilon$ equation and can be somewhat improved upon by altering $C'_{\varepsilon 1}$ or $C'_{\varepsilon 2}$ or by adding a correction term to the transport equation for $\varepsilon$. One such reformulation of the $k$–$\varepsilon$ model is the so-called Renormalization Group Theory (RNG) model by which the model
Table 2.1: Model constants for the standard $k-\varepsilon$ model and the RNG $k-\varepsilon$ model.\textsuperscript{[94]}

<table>
<thead>
<tr>
<th>Constant</th>
<th>Standard Value</th>
<th>RNG Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_\mu$</td>
<td>0.09</td>
<td>0.0845</td>
</tr>
<tr>
<td>$C_{\varepsilon 1}$</td>
<td>1.44</td>
<td>1.42</td>
</tr>
<tr>
<td>$C_{\varepsilon 2}$</td>
<td>1.92</td>
<td>1.68</td>
</tr>
<tr>
<td>$\sigma_k$</td>
<td>1.0</td>
<td>0.72</td>
</tr>
<tr>
<td>$\sigma_{\varepsilon}$</td>
<td>1.3</td>
<td>0.72</td>
</tr>
</tbody>
</table>

Constants are given new values and an extra term is added to the $\varepsilon$ equation. The values for the five RNG $k-\varepsilon$ model constants are given in Table 2.1 next to the standard model values.\textsuperscript{[94]} The additional term in the dissipation equation makes the RNG $k-\varepsilon$ model more accurate for highly strained and swirling flows.\textsuperscript{[102]}

While $k-\varepsilon$ type RANS turbulence models have been widely used for a variety of problems, it is recognized that they have several important limitations. Fundamentally, these models solve the mean flow equations (Equation 2.5) and so the solutions obtained from these models are ensemble-averaged. Some have argued that ensemble-averaging does not equal time-averaging and have shown that unsteady RANS solution methods are able to qualitatively and even quantitatively capture complex flows which are not statistically stationary (i.e. periodic vortex shedding) with greater accuracy as compared to steady RANS solutions.\textsuperscript{[104–106]} Even so, unsteady RANS are not, strictly speaking, a simulation of turbulence but only of the statistics of turbulence.\textsuperscript{[105]} For actual turbulence simulation on engineering scales, Large-Eddy Simulation (LES) and Very Large-Eddy Simulation (VLES) methods are required\textsuperscript{[107]} (see also Pope 2000,\textsuperscript{[94]} Chapter 13). RANS models of the $k-\varepsilon$ variety also make the assumption that turbulence is isotropic. This is an adequate assumption for simple shear flows such as boundary layers but becomes less accurate for true three-dimensional flows with large scale vortical structures.

Despite these limitations, RANS modeling is widely used today and has provided useful insight into many engineering-scale problems. The RNG $k-\varepsilon$ turbulence model was used for the simplified
models presented in Chapter 4. A partial justification for the original choice of the RNG $k-\varepsilon$ model as opposed to another RANS model is given in Section 4.1.4. A full evaluation of the accuracy of the various turbulence modeling methods as compared to experimental measurements of flow in the contactor was performed as part of this work and is presented in Chapter 5. From this, it was determined that turbulence simulation using the Large Eddy Simulation (LES) technique gave the most accurate predictions and LES was used for the mixing vane evaluations presented in Chapter 6.

2.2 Turbulence Simulation using Large Eddy Simulation (LES)

While RANS-type turbulence modeling methods have been widely and successfully applied to a variety of flows, the inherent assumptions outlined in the previous section inhibit their applicability to truly complex, three-dimensional turbulent flows. On the other hand, direct solution of the Navier-Stokes equations via Direct Numerical Simulation (DNS) is not possible for engineering problems of practical importance. However, it is possible to filter the Navier-Stokes equations such that only the velocity field larger than the filter width is resolved and that smaller than the filter is modeled. Ideally, one would like to have the filter width small enough to capture more than 80% of the energy containing eddies\textsuperscript{[94]} although simulations in which only larger eddies are resolved are also possible.\textsuperscript{[108]} An outline of the LES method with specific focus on the implementation used in FLUENT will be given here.

2.2.1 Filtered Navier-Stokes Equations

Analogous to the Reynolds decomposition used to generate the mean momentum equations presented in Section 2.1.2, the Navier-Stokes equations can be filtered according to:

$$ u(x, t) = \overline{u}(x, t) + u'(x, t) \tag{2.12} $$

where the overbar now represents the filtered velocity field and the prime is the residual field.\textsuperscript{[94]} The corresponding filtered Navier-Stokes equations (incompressible flow) are given as:

$$ \frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\overline{u}_i \overline{u}_j) = -\frac{1}{\rho} \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial \overline{u}_i}{\partial x_j} \right) \tag{2.13} $$
in which $\tau_{ij}$ is the stress tensor for the subgrid-scale:

$$\tau_{ij} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \quad [2.14]$$

In LES, it is only $\tau_{ij}$ that requires modeling. This will be discussed in the next section.

### 2.2.2 Subgrid Models

Similar to models for the turbulent viscosity in order to solve the mean flow equations, there are a variety of methods for modeling the sub-grid scale (SGS) stress tensor. The various alternatives are outlined elsewhere\cite{94, 102, 109} and only the specific implementation in FLUENT as used for this research project will be discussed in detail here. This follows the approach of Kim and Menon\cite{110} which uses a transport equation to model the dynamic SGS turbulent kinetic energy.

The SGS stress tensor needed to solve Equation 2.13 above is typically modeled as:

$$\tau_{ij} = -2C_{\tau} \Delta k_{sgs}^{1/2} \overline{S}_{ij} + \frac{2}{3} \delta_{ij} k_{sgs} \quad [2.15]$$

in which $\Delta$ is the filter width which is taken to be the cube root of the computational cell volume ($\Delta = V^{1/3}$) and $\overline{S}_{ij}$ is the resolved-scale strain-rate tensor with the form of:

$$\overline{S}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad [2.16]$$

The form of the transport equation which is solved for $k_{sgs}$ is very similar to the $k$ equation used in the $k-\varepsilon$ model (Equation 2.9) and includes terms for production, dissipation, and diffusion of $k_{sgs}$:

$$\frac{\partial k_{sgs}}{\partial t} + \overline{u_i} \frac{\partial k_{sgs}}{\partial x_i} = -\tau_{ij} \frac{\partial u_j}{\partial x_j} - \varepsilon_{sgs} + \frac{\partial}{\partial x_i} \left( \nu_T \frac{\partial k_{sgs}}{\partial x_i} \right) \quad [2.17]$$

As before, $\nu_T$ is the eddy viscosity except for now it is only for the sub-grid scale and is given by:

$$\nu_T = C_{\tau} \Delta k_{sgs}^{1/2} \quad [2.18]$$

Note that this same group appears in Equation 2.15. For this formulation, the SGS dissipation rate is modeled according to:

$$\varepsilon_{sgs} = C_{\varepsilon} k_{sgs}^{3/2} \overline{\Delta} \quad [2.19]$$
The coefficients $C_\tau$ in Equation 2.15 and $C_\varepsilon$ in Equation 2.19 are determined dynamically as described in the original paper\cite{110} or the corresponding paper outlining implementation of this model in FLUENT.\cite{109}

### 2.2.3 Limitations

Unlike RANS techniques which solve for the mean flow, LES solves for the instantaneous resolved flow field and therefore inherently requires a transient solution method and time averaging of results to get a mean field. This added computational cost coupled with the general need for more refined grids is perhaps the chief limitation of LES. However, if the problem of interest already requires a time-dependent simulation, the added computational cost of LES versus RANS may not be significant. Indeed, this is the case for simulation of free surface flow in the annular centrifugal contactor as will be described in Section 2.3.1.

For high $Re$ flows of practical interest, full nodalization for accurate resolution of the turbulent structures in the near-wall region is prohibitively expensive and therefore much effort has been put into developing methods for modeling the near-wall region.\cite{111,112} (see also Blazek\cite{103} Section 7.3.4 or Pope\cite{94} Section 13.6.5). Other methods for improving the performance of LES in the near-wall region have also been proposed.\cite{113} Complete resolution of the near wall region was not possible for models of the flow in the centrifugal contactor due to the already large number of computational cells required to resolve the liquid–air interface and the already high computational cost of this free surface modeling as described later in Section 2.3.1. FLUENT’s implementation of standard wall functions was chosen for the simulations performed in this study;\cite{102} comparison with experimental measurements as presented in Chapter 5 (see also Section 6.2) shows that this method gives good accuracy for the given problem.

### 2.3 Multi-phase Modeling

As has been described, the flow in an annular centrifugal contactor consists of multiple liquid phases and air. Even more difficult from a multi-phase modeling standpoint is that there are regions of the flow in which the two liquid phases are completely separate and others in which the two exist
as a near homogenous dispersion. While particulates should not be present in the contactor under normal conditions, understanding the flow of particulates in the contactor is also important and requires special modeling.

There are various methods for calculating the distribution of multiple phases within a computational domain.\textsuperscript{102,114,115} Some of the available methods and their applicability to the contactor problem are briefly described below. This overview was also published by the author as part of a preliminary contactor modeling study in 2006.\textsuperscript{116}

**VOF** The Volume of Fluid method was developed for tracking a liquid free surface such as a water/air interface. A single set of momentum equations is solved for the entire system and the volume fraction of each phase is tracked within each computational cell. The details of this model are given in Section 2.3.1. This method has been applied to modeling the flow of water in and the height of liquid in the annular (mixing) region as described in detail in Chapters 5 and 6.

**ASM** The Algebraic Slip Mixture model tracks the mean volume fraction of a dispersed phase in a continuous phase. As with the VOF method, a single set of momentum equations is solved for the entire system. The relative velocities of the dispersed and continuous phases are assigned via an algebraic slip velocity formulation. The dispersed phase droplet diameter must be specified and is typically assumed to be constant.

**Eulerian** For this method, separate sets of momentum and continuity equations are solved for each of the phases in the system. Coupling of the phases is done through exchange coefficients. This method, although more complex than the ASM model, is probably the more applicable to modeling of the liquid–liquid dispersion formed in the contactor and has been used by others for modeling liquid–liquid extraction.\textsuperscript{117} It is also possible to include the effects of interphase mass transfer using any of the above models. As mentioned in Section 1.3.3, this method can also be combined with the population balance method for tracking the evolution and distribution of droplets. However, it is not readily possible in commercial CFD applications to combine this model with explicit free surface tracking using the VOF model.
**Lagrangian**  This method tracks individual particles or droplets as they move through the continuous fluid in a Lagrangian reference frame. These particles can interact with the continuous phase and exchange mass, momentum, or energy. A key assumption of this method is that the dispersed phase occupies a small volume fraction such that particle–particle interactions can be ignored. It is therefore not applicable to the liquid–liquid mixture as in the contactor system, but could be used to track the flow of particulates or to calculate the residence time of a discrete fluid element within the contactor. Such calculations were performed as part of the preliminary modeling investigation mentioned previously\[^{116}\] and are described in Section 4.1.3.1.

A single technique which can accurately resolve every detail of the flow in all of the various regions of the contactor while maintaining computational feasibility does not seem to exist. As an example, Figure 2.1 gives a depiction of the various levels of multi-phase modeling which could be applied to the liquid flow in the mixing zone of a centrifugal contactor charted by their relative ability to capture the realistic aspects of the flow and their computational cost. A similar chart could be generated for flow in the separation zone with the various models being more or less applicable to the specific characteristics of that flow. While a single method cannot reasonably predict all the complexity of contactor flow, selective modeling of specific aspects of the flow can yield very useful information from the standpoint of unit operation and design. As described in previous sections, the flow of the air–liquid free surface and its effect on fluid–rotor contact is a critically important characteristic of the flow in the mixing zone and models which cannot account for this aspect lack physical realism. In general, understanding contactor ‘hydraulic’ operation with a single liquid phase (and air) would allow the evaluation of flow patterns and energy dissipation and provide a method for predicting mixing efficiency without the need for explicit modeling of the liquid–liquid mixing. Therefore, the main focus of this modeling effort has been to accurately model hydraulic operation within the various regions of the contactor.

With this focus on single-liquid free surface flow, the VOF method provides the best combination of realism and practical applicability. This method is able to capture the major aspects of the flow (droplet, rivulet flow from inlets, liquid contact with rotor, etc.) and allow the prediction of
Figure 2.1: Conceptualization of various levels of multi-phase modeling as applied to the liquid flow in the contactor mixing zone as a function realism and computational cost.

The liquid volume in the mixing zone and the annular liquid height. Further, the effects of geometric and operational parameters on the flow in the annulus could be observed. The next section will discuss the details of the VOF method as well as its limitations. In particular, the accuracy of the VOF method depends on its ability to resolve the interface location which is limited by computational grid resolution. For flow in the mixing zone of the contactor, the liquid–air interface is not confined to a single position but is rapidly moving throughout the annulus as droplets, rivulets, and entrained air bubbles; therefore, good grid resolution throughout the entire domain is required. As grid resolution is increased, the accuracy of the interface capture improves and it is possible to resolve smaller and smaller droplets and bubbles, but the computational cost increases significantly. Therefore, it was necessary to select an appropriate balance between computational cost and overall accuracy. The results of the simulations performed using this method show that good accuracy can be achieved as compared with actual experimental measurements (see Chapters 5 and 6). The VOF method is equally applicable to the hydraulic operation of the separation zone. However, in this region the modeling is simplified in that the free surface is confined to certain regions and is relatively stationary. Analysis of the flow in the separation zone is given in Chapter 7.
While the main purpose of this research effort is the useful application of existing modeling methods to the centrifugal contactor rather than the development of new methods, future developments in multi-phase modeling may provide possibilities for building on these hydraulic studies and ultimately simulating the flow of multiple liquid phases and air in the contactor. For example, Cerne et al.\cite{118} have suggested a potentially useful method of coupling the VOF interface tracking with the two-fluid mixture model to be able to model both regions where fluids are segregated and also where they are dispersed. At present, however, this coupling method has not been developed to the point of implementation in any production CFD codes such as FLUENT. As noted above in regards to the Euler-Euler two-fluid mixing models, that method is also applicable for such segregated/dispersed flows but limited in its capability of predicting the physics and evolution of the free surface which are critical to the problem at hand.\footnote{At the time of writing, the next version of FLUENT (6.4/12.0) was in beta testing and introduced limited capability for combining VOF surface tracking with Eulerian multiphase models. ANSYS CFX also has similar limited capability.}

### 2.3.1 Volume of Fluid Method

While there are numerous methods for performing numerical flow simulations which involve moving interfaces (see Shyy et al.\cite{119} and Caboussat\cite{120}) one that has found the widest application in modeling free surface flows is the Volume Of Fluid (VOF) method.\cite{122} Reviews of the various developments in VOF methods are given by Kothe and Rider\cite{122} and Tang et al.\cite{123,124}

With the VOF method, the dynamics of the interface are tracked by the evolution of the volume fraction in each cell. The volume fraction of the $q$th fluid is defined as:

$$\alpha_q = \begin{cases} 
0 & \text{cell is empty of } q\text{th fluid} \\
1 & \text{cell is full of } q\text{th fluid} \\
0 < \alpha_q < 1 & \text{cell contains interface between } q\text{th fluid and any other fluid}
\end{cases} \quad [2.20]$$

$$\sum_{q=1}^{n} \alpha_q = 1 \quad [2.21]$$
The volume fraction of the fluids in a given cell must sum to unity as shown in Equation 2.21. The evolution of the volume fraction $\alpha_q$ is governed by the transport equation:

$$\frac{1}{\rho_q} \left[ \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \mathbf{u}) \right] = S_{\alpha_q} + \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp})$$

[2.22]

where $S_{\alpha_q}$ is a mass source for phase $q$ and $\dot{m}_{pq}$ and $\dot{m}_{qp}$ are the mass transfer from phase $q$ to $p$ and $p$ to $q$ respectively. Equation 2.22 reduces to:

$$\frac{\partial \alpha_q}{\partial t} + \mathbf{u} \cdot \nabla \alpha_q = 0$$

[2.23]

assuming incompressibility ($\rho_q$ = constant), $S_{\alpha_q} = 0$, and no interphase mass transfer. The flow is governed by a single momentum equation for incompressible flow.

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{F}$$

[2.24]

This is the same as Equation 2.1 with the addition of a source term for explicit formulation of the body forces $\mathbf{F}$. The fluid properties in each cell are taken as the volume average according to Equations 2.25 and 2.26 for a two phase system.

$$\rho = \alpha_2 \rho_2 + (1 - \alpha_2) \rho_1$$

[2.25]

$$\mu = \alpha_2 \mu_2 + (1 - \alpha_2) \mu_1$$

[2.26]

The actual interface position in each cell is not explicitly tracked, rather, the volume fraction is tracked and the interface is reconstructed at each time step. The general algorithm for solution of the dynamics of the fluid–fluid interface according to the VOF method is:

1. $\alpha_q(t_n)$
2. Interface reconstruction
3. Interface advection
4. Calculate $\alpha_q(t_{n+1})$

While various interface reconstruction schemes have been developed, Piecewise Linear Interface Construction (PLIC)\cite{125} is the most common in modern VOF applications because of its ability to
accurately model the interface and better capture the physics of complex flows as compared to simpler methods.\textsuperscript{[122]} The PLIC VOF model requires a time-dependent solution and is computationally intensive. For interface reconstruction by the PLIC method the interface in a cell can be uniquely defined by the cell’s volume fraction and an interface normal vector. The interface normal vector is calculated from the gradient of the volume fraction according to Equation 2.27 and represents the key step in the interface reconstruction.

\[
\hat{n} = \frac{\nabla \alpha}{|\nabla \alpha|} \tag{2.27}
\]

Advection of the reconstructed interface is then possible by calculation of the interface motion due to the flow field and the resulting fluxes of volume fraction into and out of each cell. For a discussion of the implementation of various algorithms for interface reconstruction and advection see Kothe et al.\textsuperscript{[126,127]} A recent paper by López et al.\textsuperscript{[128]} provides a good comparison of the relative accuracy of various methods. Surface tension effects can also be included according to the Continuum Surface Force (CSF) modeling scheme.\textsuperscript{[129]} The effect of surface tension is modeled as a volume source term added to the body force \( F \) in the momentum equation (Equation 2.24).

\subsection{Limitations of the VOF Method}

The VOF method has several important limitations which stem primarily from its dependence on the computational mesh spacing. Numerical errors of the VOF interface tracking method are due to inaccuracies in the interface reconstruction and advection as well as an effect called ‘numerical dispersion’ or ‘numerical surface tension’.\textsuperscript{[126,130]} Numerical dispersion is the tendency of the simulation to break up a single fluid volume such as a long fluid strip or rivulet into many small pieces with sizes comparable to the grid size (see Figure 2.2). This can be reduced by increasing the grid resolution in the region of the interface; however, this also increases the computational cost.

While the PLIC method is considered the most advanced and accurate reconstruction method, it is still an approximation of the interface and results in errors. These errors are primarily due to the fact that the interface, which can be highly curved, is modeled as a straight line (or a plane in
Figure 2.2: A vertical stripe deformed by shear flow (a) before and (b) after numerical dispersion. Figure taken from Cerne et al. [130]

Figure 2.3: Sketch comparing the reconstructed interface (shown with normal vector) with the actual interface. Shaded areas represent extra mass (striped) and lost mass (solid).

3D). For example, Figure 2.3 shows a comparison of the piecewise linear reconstructed interface with the actual interface and the potential for mass loss (or mass gain) due to inaccuracies in reconstruction. Again, this error due to interface reconstruction can be minimized by decreasing the grid size. Clearly the grid size must be significantly smaller than the smallest droplet which is to be resolved. Some have recommended that the ratio of resolved droplet diameter to grid spacing
\( \frac{d_{\text{min}}}{\Delta x} \) need only be greater than about 6;\(^{130}\) however, others claim it should be as much as 32.\(^{124}\) Regardless, it is obvious as grid resolution is increased the accuracy of the interface capture improves and it is possible to resolve smaller and smaller droplets and bubbles, but again the cost is an increase in the computational time for the simulation.

Further compounding this grid dependence, a decrease in grid size for the VOF simulation also necessitates a decrease in time step \( \Delta t \). This is because the VOF method is limited by a Courant number (\( Cr \)) of approximately 0.25 where the Courant number is given by:

\[
Cr = \frac{\Delta t}{\Delta x/u} \approx 0.25
\]

and \( u \) is the velocity of the interface. Equation 2.28 essentially states that the time step should be such that it takes approximately four time steps for the interface to sweep through a given cell with spacing \( \Delta x \). Thus, if the grid spacing is decreased, the time step must also be decreased to maintain a local Courant number less than 0.25. Even if one were to refine the grid only in the region of the interface to minimize the total number computational cells, the overall time step for the simulation is still somewhat influenced by the smallest cells near the interface. FLUENT does employ a sub-time stepping scheme for calculation VOF equation such that the time step used for the VOF calculation is a fraction of the larger global time step to take into account this local Courant number limit. Another method of mitigating the computational cost of the VOF model is by using FLUENT’s Non-Iterative Time Advancement (NITA) solver.\(^{102}\) Rather than a succession of global iterations over all equations at once until convergence is achieved for a given time step, this method iterates over groups of equations individually (i.e. converge momentum first, then pressure, then scalars). Use of this NITA method was found to result in a speedup of more than a factor of 2 for the contactor simulations. For example, the average computation time per time step for a LES simulation of the mixing zone (4-vane) using NITA and running in parallel on 20, 3.2 GHz Xeon processors was only 5.54 s whereas the standard global iteration scheme took 12.17 s per time step for the same simulation (NITA cut time by 54.5\%). More details regarding computation time and parallel scaling of FLUENT are given in Appendix A.

Ultimately, it is clear that a balance between the accuracy of interface resolution and the overall computational cost is required. For typical computational fluid dynamics studies it is standard
practice to perform a full grid resolution study by simulating the desired problem on a succession of increasingly finer meshes until it is determined that the solution of the problem no longer depends on the mesh. Beyond a narrow range of different mesh sizes (Appendix B), this evaluation was not possible for the contactor problem as the overall computational time was observed to be the limiting factor. Consequently, an important item this research needed to demonstrate was whether VOF modeling with limited resolution can give accurate predictions of fluid behavior, namely, the fluid–rotor contact and annular liquid height in the case of the annular centrifugal contactor. Comparison to the experimental observations and detailed measurements outlined in Chapter 3 was critical to this process. As will be shown in the latter chapters of this work, it was indeed demonstrated that these simulations could both qualitatively and quantitatively predict the flow in the centrifugal contactor.

### 2.4 Fluid Residence Time

The residence time distribution for the fluid in the mixing zone is an important parameter affecting mixing. The average fluid residence time in a given domain is equal to the total domain volume $V$ divided by the total volumetric flow rate $\dot{q}$.

$$
t_{\text{res}} = \frac{V}{\dot{q}} \tag{2.29}
$$

Often it is desirable to know the spatial distribution of residence time in the volume (e.g. to determine how long the fluid spends in high shear regions) or the residence time distribution at the outlet as is commonly measured with experimental tracer techniques. Two methods are outlined here for calculating the spatial distribution of fluid residence time. Note, however, that both of these methods are only practical for steady-state (or pseudo steady-state) calculation of the residence time.

#### 2.4.1 From Discrete Particle Flow

It is possible to track the movement of individual particles or droplets in a Lagrangian manner as they move through a volume in response to the local flow field. This technique is useful for analyzing the flow of particles in a flow geometry and, if neutrally buoyant particles are used, it
also can give the residence time distribution of the fluid. In FLUENT, this method is implemented as the Discrete Phase Model (DPM). Particle trajectories are solved by stepwise integration in time over a specified number of path length increments. For this method, the particle diameter and density must be specified and it is typically assumed that the particles are in such small quantities that they do not affect the flow of the continuous phase although coupling with the flow field is possible. If desired, it is also possible to include calculation of the erosion and accretion effects of the particles in transient simulations. For steady simulations, turbulence can be accounted for stochastically by allowing for random fluctuation of the instantaneous velocity proportional to the local turbulence intensity for each point along the integration path. Once particle trajectories have been calculated, it is simple to estimate the particle residence time as the total flow time from the point of release until the particle exits the volume through the outlet. In this manner, a significant number of particles could be tracked throughout the volume to get adequate information about the average behavior of the particles (or fluid elements).

This method may also ultimately be a useful tool for exploring the flow and accumulation of particles in the contactor. Results using this method for simplified contactor models are given in Section 4.1.3.1. As mentioned previously, the accumulation of particulates is important to the operation of contactors as well as the limits on contactor size due to criticality concerns. However, accurate modeling of the continuous phase is first required and this is the primary focus of the full mixing zone analyses. Further, this method is impractical for transient simulations such as those using VOF interface tracking as it would be required to run the entire simulation for longer than one residence time (after steady-state is achieved)—long enough that each particle exits the volume. As we will see in later sections, this is on the order of 5 s for the mixing zone; typical solutions consisted of ~2 s of equilibration time and 1 s of averaging time. Thus, transient particle tracking would have required significant additional simulation time.

2.4.2 From Passive Scalar Transport

As mentioned in the previous section, an estimation of the residence time at the outlet can be made using the particle tracking method. A more general method for calculation of the fluid
residence time is through the use of an additional scalar transport equation similar to what would be used to solve for the behavior of a tracer species. The general form for the transport of a scalar $\phi$ is:

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho u_i \phi - \Gamma \frac{\partial \phi}{\partial x_i} \right) = S_\phi$$ [2.30]

If we assume that the diffusion coefficient is much less than one ($\Gamma \ll 1$), the density is constant, and the source term $S_\phi$ is equal to the density $\rho$, Equation 2.30 simplifies to:

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x_i} (u_i \phi) = 1$$ [2.31]

It is clear that the scalar $\phi$ would then have units of time. If the boundary conditions for $\phi$ are set to a fixed value of zero at the inlet and a zero flux at the walls and outlet, the scalar $\phi$ is then equal to the fluid residence time referenced to the inlet. As an example, for the simple case of steady-state, laminar flow in a pipe with radius $R$ and a mean velocity of $U$ the velocity profile is given by:

$$u_z(r) = 2U \left[ 1 - \left( \frac{r}{R} \right)^2 \right]$$ [2.32]

The corresponding solution for $\phi(r, z)$ is:

$$\phi(r, z) = \frac{z}{u_z(r)} = \frac{z}{2U} \left[ 1 - \left( \frac{r}{R} \right)^2 \right]^{-1}$$ [2.33]

Just as for the discrete particle method described above, to solve the passive scalar residence time equation in a fully transient manner, would require one to solve for a flow time in excess of the mean residence time—from the time the fluid enters at the inlet until a steady profile is reached. On the other hand, it is possible to calculate the pseudo-steady solution of the residence time equation for a snap-shot in time of the instantaneous velocity field solution. To do this, the velocity field is solved as normal in a transient manner (as is required for the PLIC VOF model) and using the velocity field at a given time, the pseudo-steady spatial distribution of the fluid residence time is then calculated. For this case, the solved profile is a spatially-averaged one rather than a time-averaged one.
2.5 CFD Application to Mixing Equipment

Computational fluid dynamics methods have been applied to many problems in a variety of industries. The majority of the liquid–liquid mixing research and dispersion characterization as described in Section 1.3.3 have been done using cylindrical stirred tank reactors (STR). Such mixing vessels are critical components throughout the chemical process industry and CFD has been readily applied to modeling the complex fluid dynamics of this flow. There has also been successful CFD modeling application to static mixers.\[131]\]

An important consideration regarding modeling flows in STR-type mixing vessels is the decision to model a fully three-dimensional geometry versus a two-dimensional axisymmetric model. Turbulence is inherently three dimensional and, in general, it has been determined that accurate predictions require three dimensional simulations. In the case of the contactor (or even a baffled STR), 2D-axisymmetric treatment is not possible as a result of the housing vanes (as well as the inlet positions). Also important for stirred vessels is the method by which to treat the periodic nature of the mixing blade passage. Accurate treatment requires multiple rotating reference frames or moving meshes which complicate the simulation. For the contactor, this difficulty does not exist as the mixing occurs by shear induced where the rotor contacts the fluid. However, if the contactor mixing zone and separation zone were to be modeled together, multiple reference frames would be required. The mixing zone would be modeled in a stationary reference frame with a rotational velocity applied to the wall boundary that is the rotor while the interior volume of the rotor would be solved as a rotating reference frame relative to stationary solid boundaries. The rotor inlet would be the interface between the two reference frames. Also, if a modified contactor with vanes on the rotor\[33]\ were to be modeled, the blade passage would have to be accounted for using multiple reference frames or moving mesh similar to the impeller of a STR.

As discussed in Section 2.1 and 2.2 above, the accuracy of turbulent flow predictions are highly dependent on the methods used to simulate (or model) turbulence. Thus, for mixing vessels in which the Reynolds number (and consequently the turbulence) can be quite high, accurate predictions of the turbulence is vital to quantitatively accurate predictions of the overall flow field and
mixing. Jenne and Reuss\textsuperscript{[132]} have compared various $k-\varepsilon$ models’ prediction of the flow in a stirred tank reactor with experimental measurements done by others. It was concluded that none of the existing models gave adequately accurate predictions without modification of the model constants. Even so, RANS type turbulence models are still commonly used (e.g. Kumaresan et al. 2005\textsuperscript{[133]}), though more and more studies are making use of LES turbulence simulation methods (e.g. Yeoh et al. 2005\textsuperscript{[134]}).

In regards to the multi-phase modeling, the first and key step in understanding the multi-phase behavior in a mixing vessel is understanding its behavior with a single liquid phase. As a result, the majority of numerical studies of mixing have calculated only the flow patterns for single-phase flow in mixing devices. As discussed in Section 1.3.1, one can infer the liquid–liquid mixing behavior from the single-phase turbulent energy dissipation rate. Further, many studies ignore the liquid free surface as it plays a very minor role for the more efficient mixing, open baffled stirred tank. For open unbaffled tanks the free surface is more important on account of vortex formation at high rotation speeds.

A good example of CFD application to a problem comparable to the centrifugal contactor in terms of the computational modeling difficulties is the hydrocyclone separator, which separates particulates into different liquid streams using the centrifugal force of the swirling flow in the device. A summary of the efforts which have been made to apply CFD to this issue is given by Nowakowski et al.\textsuperscript{[135]} As with the contactor, this piece of equipment also involves turbulent swirling flow of multiple phases and therefore provides a good comparison of computational techniques. The Lagrangian method of particle tracking mentioned above has been applied to the prediction of particle distribution and the simulation results were in agreement with experimental values.\textsuperscript{[136]} Interestingly, during operation of the hydrocyclone an “air core” develops in the center of the spinning fluid.\textsuperscript{[137]} Along the axis of the rotor within the separation zone of the annular centrifugal contactor there is also a core of rotating air (shown in Figure 1.1) which adds some complexity to the modeling of this region. Olsen and Van Ommen\textsuperscript{[138]} reported successful modeling of the hydrocyclone air core using the ASM multi-phase model. In the same study, they used
CFD modeling for hydrocyclone design optimization and found good agreement with experimental results. More recently, Brennen has reported on the modeling of the hydrocyclone with an air core comparing both the ASM and the VOF models.\textsuperscript{[139]}
Chapter 3

Experimental Methods

The primary goal of this project was the application of computational fluid dynamics modeling to the annular centrifugal contactor in order to analyze the flow and provide a framework for improving design and operation. That said, this project was not entirely computational. Rather, without the support of careful experimental measurements and observations, the validity of the computational models of the flow in the contactor cannot be fully established. This chapter sets forth the various experimental methods and measurements which were performed by the author as part of this research project forming a critical foundation to the computational simulations. Section 3.1 will briefly explain the theory behind the two different velocity measurement techniques which were used, namely, Laser Doppler Velocimetry (LDV) and Particle Image Velocimetry (PIV). Section 3.2 will give detailed information about the contactor apparatus used for the experiments as well as specifics regarding the equipment setup and conditions for the velocity measurements and other measurement techniques used in this research.

3.1 Velocity Measurement Techniques

It was clear from the initial formulation of this research project that experimental data for the actual flow velocity and turbulence in the centrifugal contactor would be absolutely vital to establishing the utility of the computational models. To the author’s knowledge, there were no such measurements for flow in the centrifugal contactor performed by any previous researchers and certainly none are presented in the open literature. A basic overview of two velocity measurement techniques, Laser Doppler Velocimetry (LDV) and Particle Image Velocimetry (PIV), used for this
project are given in this section. Both techniques rely on laser light scattering from tracer particles to measure the flow velocity; the ability of tracer particles to follow the flow will be addressed in Section 3.1.3.

3.1.1 Laser Doppler Velocimetry (LDV)

Laser Doppler Velocimetry (LDV), also called Laser Doppler Anemometry, is a single point measurement technique capable of measuring instantaneous velocities within a typical interrogation volume with dimensions on the order of a few hundred microns. Only an overview of the basic principles behind this technique will be given here—a full review of this measurement method is given by Buchave et al.\textsuperscript{[140]} The technique involves the measurement of Doppler shifted light scattered from particles (including droplets or bubbles) in the flow. The general set-up involves a laser which is split into two beams as shown in Figure 3.1. The measurement volume is the region where the coherent beams cross, generating a fringed interference pattern. The component of velocity \textit{in the plane of the beams} is determined by measuring the frequency of the scattered light from particles passing through the measurement volume. Thus, particle seeding density is important for
maintaining a high data acquisition rate as measurements are only taken when a particle passes through the measuring volume. As a result, measurements are not equally spaced in time which requires some additional considerations in data processing to acquire certain turbulence quantities. Addition of a second set of beams (of a different wavelength for signal differentiation) in the plane perpendicular to the first set allows coincident measurement of two components of velocity. In practice these two-components can be measured relatively easily using a fiber optic beam head that emits the four beams coaxially. It is also possible to measure the third component of velocity, although this requires a second laser off axis (at a known angle) relative to the first. Collection of scattered light can be done in forward-scatter mode or back-scatter mode. For forward-scatter mode, a separate receiver is placed in the forward direction slightly off-axis of the incident beams. While this set-up has better efficiency due to the directional dependence of light scattering, in practice it is often much simpler to measure the back-scattered light using a transceiver that both transmits the laser beams and collects the scattered light. This is the configuration used for the current experimental measurements.

With LDV it is possible to measure the instantaneous velocity at a point with a sampling frequency in the kHz range. From this data, one can obtain the mean and fluctuating velocities from which other important turbulence quantities can be calculated or estimated. Spatial resolution is limited by the size of the measuring volume as well as the precision of the equipment positioning system. A typical interrogation volume for an LDV setup using an argon-ion laser is approximately $34 \times 180 \ \mu\text{m}^2$ (135 mm focal length lens). It is possible to have spatial resolution in the tens of microns allowing measurement throughout the flow as well as in boundary layers.

Details regarding the LDV setup and conditions for experimental measurements will be given later in Section 3.2.3.

### 3.1.2 Particle Image Velocimetry (PIV)

This method is a multi-point measurement technique capable of measuring a two-dimensional velocity field in a plane defined by a laser sheet. As with LDV, this optical technique also relies on particles in the flow to scatter laser light. Velocity measurements are made by taking two images
in rapid succession of the particles illuminated on a laser sheet and cross-correlating the images to
determine the direction and distance traveled for each particle during the specified time between
the two snapshots. The time between the pair of images can be specified such that the particles
travel only \( \sim 10^{-15} \) pixels for optimum cross-correlation of the two images. It is critical to measure
the dimensional scaling at the laser sheet in order to convert particle displacements from pixels to
meters. Figure 3.2 shows a sample double frame image with a exposure delay of 73.6 \( \mu s \). The
white band at the bottom of each frame is the opaque base of the housing. The corresponding
velocity field obtained from cross-correlation of the two frames is shown in Figure 3.3. Image
scaling was done by measuring in pixels the known distance between the bottom of the housing
and the bottom of the rotor for a bright field image of the liquid filled annulus. It is also possible
to double expose the same image and correlate particles within the image (auto-correlation) in a
similar manner; however, this introduces directional ambiguity without prior knowledge of flow
directionality. Cross-correlation was used for the measurements in this study. A multi-block av-
eraging scheme was applied to obtain a spatially continuous vector field. For example, the vector
field shown in Figure 3.3 was generated by performing two passes of a 64\( \times \)64 window followed
by a third pass of a 32\( \times \)32 window including 50% window overlap for the initial passes (see PIV
software manual\[141\] for more details). This processing level was chosen as it gave a vector field
with a spatial resolution similar to the original particle (bubble) density and therefore maximized
the data use but did not introduce excessive interpolation.

In general, the spatial resolution of the PIV measured velocity field is dependent on the particle
density as well as on the resolution of the imaging system. Temporal resolution is limited by the
maximum speed at which the camera system can record and store the two images and is typically
less than 10 Hz for common imaging equipment. As a result of the relatively low sampling rate,
only relatively low frequency fluctuations in the velocity field are detectable with this technique
and it is therefore mainly useful for obtaining the mean velocity field.

Details regarding the PIV setup and conditions for experimental measurements will be given
later in Section 3.2.4.
Figure 3.2: PIV images (exposure inverted) in which top and bottom frames are separated by 73.6 $\mu$s (scale in mm).
3.1.3 Flow Fidelity of Tracer Particles

For velocimetry techniques such as LDV and PIV described above which use light scattering particles, it is important to consider how the finite size of the particles affects the measurements. In this section the term particle is used to refer to not only solid particles, but also fluid particles (i.e. droplets and bubbles). Small particles tend to follow the flow more closely, but larger particles scatter more light and improve the quality of the measurements; thus, typically some optimum size particle is chosen for the given application which has adequate light scattering but is still small enough to also adequately follow the flow. Metallic oxide particles (e.g. TiO$_2$ or Al$_2$O$_3$) are commonly used to seed the flow although polymer spheres, glass beads, liquid droplets, and small gas bubbles have also been used.$^{[142]}$ As described in Section 1.2.5.1 above, the violent free surface flow in the mixing zone results in the entrainment of many small air bubbles. For the experiments
performed in this study, no artificial seeding was added to the flow, rather these small entrained air bubbles were used as light scattering media.

A paper by Mei\textsuperscript{[143]} gives a detailed theoretical analysis of the fidelity of tracer particles in turbulent flows. It is shown that gas bubbles tend to over-respond to high frequency turbulent fluctuations. Equations are given to determine the response of seed particles to fluctuations in turbulent flow as a function of the continuous fluid and particle properties. For high frequency oscillations, Mei 1996\textsuperscript{[143]} gives an energy transfer function $H(St)$:

$$|H(St)|^2 = \frac{(1 + St)^2 + (St + \frac{2}{3}St^2)^2}{(1 + St)^2 + [St + \frac{2}{3}St^2 + \frac{4}{9}(\rho_p/\rho_f - 1)St^2]^2}$$  \[3.1\]

where the last term in the denominator includes the ratio of the particle density $\rho_p$ to the fluid density $\rho_d$ and the Stokes number $St$ is defined as a function of the specified frequency $\omega$, the particle diameter $d$, and the kinematic viscosity $\nu$ (of the continuous fluid) as:

$$St = \sqrt{\frac{\omega d^2}{2\nu}}$$  \[3.2\]

From Equation 3.1, it can be found that the particle size cut-off of an air bubble in water for 5% error in a 600 Hz frequency minimum for which solution of Equation 3.1 exists is just slightly larger than 100 microns.

A similar analysis included in a paper by Rashidi and Banerjee.\textsuperscript{[144]} This study used oxygen bubbles as flow tracers and determined that the error in velocity response by gas bubbles can be determined by the ratio of the maximum particle velocity to the flow velocity ($u_p/u_{max}$) according to:

$$\frac{u_p}{u_{max}} = \frac{1}{(1 + \omega^2\tau^2)}$$  \[3.3\]

where the time constant $\tau$ is:

$$\tau = \frac{d}{9\sqrt{2\nu\omega}}$$  \[3.4\]

From this, we can calculate that the maximum measurable frequency of motion which gives less than a 5% error for a 250 micron air bubble in water is $\sim 300$ Hz. While a detailed analysis of the size distribution of air bubbles was not performed, it appears from PIV images such as shown in Figure 3.2 that the average air bubble diameter is $\lesssim 0.25$ mm (250 microns) over most of the annular
region. Note that bubbles of this size range are slightly larger than the longest dimension of the LDV measuring volume (Section 3.1.1). It is not clear what effect this had on the measurements; it may be that only bubbles smaller than the measuring volume were detectable. Comparison between LDV and PIV measured values gives a method of checking the consistency of the measurements. The effect of the bubble size was also explored (see Section 5.4.3).

3.2 Experimental Setup

This section will present the details regarding the modified contactor apparatus as well as the specific equipment and setup used for the various measurements and observations which comprised the experimental portion of this work. While experiments were conducted for various vane geometries and operational conditions to provide useful information in and of themselves, the standard case which was chosen to provide the basis for comparison with computational models was the 4-vane geometry at 3600 RPM (377 rad/s) with a total inlet flow rate of 600 ml/min.

3.2.1 Modified CINC V-2 Centrifugal Contactor

The experiments were done using a centrifugal contactor manufactured by Costner Industries Nevada Corporation (CINC) which was originally purchased by Argonne National Laboratory with a non-standard, transparent acrylic contactor housing with tangential inlets as described by Leonard et al. 2002 \cite{22} (Figure 3.4). This contactor has a rotor radius $r_r$ of 2.54 cm and a housing radius $r_h$ of 3.17 cm resulting in an annular gap of 0.63 cm and a radius ratio $r_r/r_h$ of 0.8. The contactor rotor is slightly different than the general sketch represented in Figure 1.1. This can be seen in Figure 3.5 which shows a diagram of the rotor used in the V-2 as taken from the 2002 Sheldon et al. patent \cite{38} which was mentioned previously. The outer radius of the upper section (labeled 14) is greater than the main section (12); only this lower section extends into the mixing zone. Notice that the upper weir (18) is removable and not open on top as in Figure 1.1 but rather is held in place with a cap (20) that defines four discrete exit channels. The radial dimensions of these heavy phase exit channels is also slightly less than the light phase exit channels (34). An
upper weir with a radius of 1.143 cm (0.45”) was used for all experiments (and simulations) except as described in Chapter 7.

To make detailed optical measurements possible, this same contactor unit was further modified such that the lower portion of the housing was replaced with a polished quartz cylinder. A sketch of the modified contactor housing is shown in Figure 3.6. A small, triangular quartz window was also emplaced in the bottom vane plate to allow visualization/measurement of the flow beneath the rotor. The modified contactor is shown in Figure 3.7. The bottom portion of the rotor, the vane plate, and the bottom support plate have been painted with flat black enamel in order to reduce reflections. The 8-vane plate is shown in place in Figure 3.7 and the other two vane plates are shown in Figure 3.8. The 8-vane and 4-vane plates were constructed of polyvinylidene fluoride (PVDF) and both were modified with a triangular quartz window (the 4-vane plate is
Figure 3.5: Diagram of an exploded view of the rotor of a CINC V-2 centrifugal contactor. Figure taken from Sheldon et al. 2002 patent.[38]

Figure 3.6: Sketch of the modified contactor housing showing the quartz cylinder and bracket assembly.
Figure 3.7: Modified contactor housing with reflective parts painted black. The quartz cylinder shown here was a back-up one that had not been polished and shows visible striations from manufacturing. The actual cylinder was well polished and had very few imperfections.

shown in Figure 3.8(a)). The V-2 unit as manufactured by CINC comes standard with a stainless steel curved-vane plate. This plate was also painted and used for selected observations but did not have a window (Figure 3.8(b)). The paint on the interior surfaces had a slight effect on the surface wetting, however, it appeared that this effect was small. Appendix C explains the contact angle measurements that were performed to demonstrate this (the effect of contact angle on the flow in models of the mixing zone is also briefly addressed). The mixing models presented in Chapter 6 use a uniform contact angle of 75° on all surfaces as an average wetting angle for water on stainless steel. There is also a very slight increase in the rotor radius due to the thickness of the paint (probably <1 mm); this was also assumed to be negligible in the models and the rotor radius was taken to be 2.54 cm.
Figure 3.8: Snapshots of painted vane plates with (a) four straight vanes and (b) curved vanes. The eight straight vane plate is shown attached in Figure 3.7.

Figure 3.9: Flow diagram of the continuous recirculation setup that was used during all experimental measurements.

Since the contactor was used only for hydraulic operation with distilled water as the working fluid, the contactor was setup for continuous recirculation as shown in Figure 3.9. No attempt was made to actively de-gas the feed liquid; however, inlet flow tubes extended to the base of the feed/receiving container and outlet streams were run down the container wall to avoid splashing and air intake at the pumps. The pumps were positive displacement piston pumps manufactured
by Fluid Metering Incorporated (FMI). One pump had a 0.635 cm (0.25 in) piston and the other had a 0.3175 cm (0.125 in) piston. Calibration curves were generated for each of the pumps. In practice, however, the flow rate was physically measured by timed flow (from the heavy phase exit line) into a volumetric cylinder for each set of measurements. Inlet feed lines to the contactor were 0.25” ID fluoropolymer (FEP) and outlet lines were 0.5” ID polyethylene (PE).

### 3.2.2 High-speed Flow Imaging

High-speed imaging of the flow in the contactor was performed to provide qualitative observation of the dynamics of the flow in the contactor mixing zone as well as some quantitative observation of the annular liquid height. A Redlake MotionPro (model HS-3-M-4) camera was used for the high-speed imaging. This camera was capable of 8-bit mono imaging at a maximum rate of 1040 Hz at the full resolution of 1280×1024 pixels.

High-speed video was taken for flow rates of 360, 600, and 830 ml/min at imaging speeds of 100 Hz and 1000 Hz for each of the three vane configurations (4-vane, 8-vane, curved). The exposure time for each frame was 1000 µs for the 100 Hz videos and 500 µs for the 1000 Hz videos. Due to size considerations, only 250 frames were saved for each observation (i.e. 2.5 s of flow @ 100 Hz, 0.25 s of flow @ 1000 Hz) except for the 1000 Hz measurements at 600 ml/min in the 4-vane geometry for which one full second (1000 frames) of flow time was recorded. Separate videos of operation from the front (camera axis normal to inlets) and from the side were performed resulting in a total of 18 video observations.

Separate videos of the flow under the rotor through the window in the vane plate were made for the 4-vane geometry as well. These were done at the standard conditions (600 ml/min and 3600 RPM) and were used for general observation of the flow in this region to complement the PIV imaging outlined in Section 3.2.4.

### 3.2.3 Laser Doppler Velocimetry (LDV)

The details regarding the LDV system and measurements will be given in this section. Please refer to Section 3.1.1 for background on the LDV method.
The LDV apparatus used for these experiments was a 2D LDV system from TSI Incorporated consisting of a 83 mm diameter, two-component fiberoptic transceiver (model TR260) with a 2-channel signal analyzer (model FSA4000-2) and 2-channel photo detector module (PDM1000-2). An argon-ion laser (model Spectra-Physics Stabilite 2017) was used to generate the source beam (max power \(\approx 1.5\) W) which was fed into the FiberLight Multicolor Beam Generator (model FBL-2) to generate the four beams required for the 2D-LDV (514.5 nm shifted and unshifted, 488.0 nm shifted and unshifted). The LDV system was controlled using a high-speed firewire connection between the signal analyzer and a PC running the FlowSizer 1.1 software. A diagram of the LDV system is shown in Figure 3.10. The shape and pulse characteristics of the LDV signal from the signal analyzer was also monitored during operation using an HP Infinium oscilloscope.

Because of the contactor’s annular geometry, only backscatter measurements were possible and, therefore, the transceiver was used rather than an off-axis or forward scatter receiver. The scattering media for the LDV measurements were the entrained air bubbles. While bubbles are
generally not ideal flow tracers as described in Section 3.1.3, due to the configuration of the centrifugal contactor they are unavoidable. Much of the debate regarding the applicability of LDV for bubbly flows focuses on large (>4 mm) bubbles at low volume fraction.\textsuperscript{[145–147]} For such cases, one is often interested in distinguishing the bubbly velocity from the liquid velocity. Such is not the case for the contactor in which the bubbles tend to be small (100–1000 $\mu$m) and spherical. Further, the void fraction of bubbles in the flow can be quite large as seen in Figure 3.2. Without using advanced techniques such as laser induced florescence (LIF) for wavelength discrimination, the light scattered from these bubbles would drown out any seed particles. Therefore, no attempt at phase discrimination was made for this study and the LDV measurements were made without the addition of any seeding materials aside from the bubbles. It is assumed that the slip velocity is small and therefore the measured bubble velocity is representative of the bulk flow. However, to determine if there was a significant effect due to bubble size, the LDV measurements for the 4-vane geometry were repeated using water with 25 mg/l sodium dodecylsulphate (SDS). Addition of this surfactant in low concentrations has been shown by others to inhibit bubble coalescence and produce smaller more uniform air bubbles.\textsuperscript{[148, 149]} Initially 50 mg/l SDS was tested, but this resulted in some undesirable foam build-up in the collector ring and storage vessel and consequently the concentration was reduced to 25 mg/l.

The transceiver probe was mounted on a traversing plate that enabled accurate measurement of the relative axial and radial position of the probe. Smooth radial movement of the probe in very small increments was possible using a manual crank; axial positioning was possible only in larger increments by physically sliding the mounting plate up or down on poles attached to the optics table. Figure 3.11 shows an image of the transceiver mounted on the traversing mechanism. The axial position of the probe was measured relative to the rotor bottom by determining the axial micrometer reading at which the two beams could just barely be seen below the bottom edge of the rotor with the rotor stationary and the annulus full of water. Due to the change of refraction index between the air, quartz, and water the incremental radial motion of the probe was not equal to that of the measuring volume and a correction to the radial position of the measuring location had to be applied. Further, the curvature of the glass also had an effect for the positioning of the tangential
Figure 3.11: Snapshot showing the traversing mechanism along with the two micrometers for measuring the relative axial and radial position of the transceiver probe.
(horizontal) velocity measurements. A 135 mm focal length lens was used on the transceiver probe as this was the shortest focal length lens available and would minimize these beam refraction issues due to the curved window. The correction to the radial position of the measuring location was applied to the data based on the ratio of the LDV-measured and known width of the annular gap. The physical traversing increment of the probe $\Delta d$ is proportional to the actual measuring volume movement $\Delta r$ (that is, $\Delta r \propto \Delta d$). The relative radial position of the measuring volume could be determined directly from the LDV measurements by finding the location of the outer wall and the rotor. When the probe was positioned such that the outer quartz wall passed through the LDV measurement volume, a high data rate reflected signal with zero velocity was measured. Similarly, at the rotor wall a signal spike with a velocity equal to the rotor surface velocity was measured. The constant of proportionality could be determined by dividing the known gap width (0.63 cm) by the distance traversed by the probe. Due to the surface curvature of the housing quartz, different values were found for the tangential velocity $u$ and the axial velocity $v$ components.\(^1\)

\[
(\Delta r = 1.1274\Delta d)_u
\]

\[
(\Delta r = 1.3054\Delta d)_v
\]

The value for the $v$ velocity measurement volume, which is free of curvature effects and therefore acts like a flat window, is very comparable to values reported by others.\(^{150}\)

LDV measurements were focused on the 4-vane geometry as it was selected as the base geometry for comparison with computational models; however, with the experimental apparatus as shown in Figure 3.7 it was possible to take data for the other configurations. Measurements of tangential and axial velocities for the 4-vane geometry were taken for the standard flow conditions (3600 RPM, 600 ml/min) along the radial direction perpendicular to the rotor at four axial positions: at the rotor bottom ($z = 0.00$ cm), near the mid-vane height under the rotor ($z = -0.46$ cm), and at two axial heights above the rotor bottom, $z = 0.61$ cm ($\approx 1 \cdot \Delta r$) and $z = 1.32$ cm ($\approx 2 \cdot \Delta r$). Additionally, at the rotor bottom height ($z = 0.00$ cm) measurements were taken for rotor speeds of 3000 RPM (314 rad/s) and 4000 RPM (419 rad/s). Each of these measurement lines were in the

\(^1\)Incidentally, this also means that coincident measurement of the two velocity components was not possible.
plane which is perpendicular to the inlets and bisects the region between vanes. The total number of measurements at each position varied according to the data rate—where the data rate was high (\(\sim 200–1000\ Hz\)), such as near the outside wall, as many as \(\sim 16,000\) data points were recorded; closer to the rotor, where the data rate was relatively low (\(\sim 30–200\ Hz\)), the number of recorded points was always greater than 2000. Where the data acquisition rate was sufficient, the power spectrum was also computed using the FlowSizer software.

### 3.2.4 Particle Image Velocimetry (PIV)

Please refer to Section 3.1.2 for the background and principles of the PIV technique. The purpose of this section is to discuss only the specific apparatus used for the experimental measurements and the measurement conditions.

A LaVision particle image velocimetry system was used for 2D PIV measurements of the mean flow field both in the annulus of the contactor and underneath the rotor. A Flowsizer3 (model 3S3D) camera having a 16-bit CCD detector and a resolution of 1280\(\times\)1024 pixels was used. The LaVision DaVis 6.2 software\(^{[141]}\) was used for both image acquisition and image processing to obtain mean velocity field information. A double pulsing Nd:YAG laser (1064 nm wavelength, \(\sim 10\) ns pulse width) and the necessary optics were used to generate a thin laser sheet. Firing of the laser and triggering of the camera was done with a LabView program running on a separate computer from the DaVis software which was used to collect the images. A diagram of the PIV system configuration is shown in Figure 3.12. The physical time delay between the successive laser pulses (and consequently the PIV exposures) was measured using a photodiode hooked to an oscilloscope. For measurements of the flow in the annulus, the laser sheet was directed with a mirror below the contactor up through the window in the vane plate and into the annular gap such that the laser sheet was vertical and tangential to the rotor at a radial distance of 2.96 cm (0.42 cm from the rotor). At this position the laser sheet was approximately 2 cm wide within the annular region. Figure 3.13 shows a sketch depicting the orientation of the laser sheet within the annular region as viewed from above. The PIV measurements in the annulus were not corrected for the curvature of the housing cylinder and therefore only the data on the centerline (where curvature is
Figure 3.12: Diagram of setup for PIV measurements.

Figure 3.13: Sketch showing the orientation of the laser sheet for PIV measurements within the annular region.
not an issue) will be used for quantitative comparison with simulation. For observations of flow under the rotor, the laser sheet was positioned horizontally and directed through the quartz housing wall at a height near the middle of the vanes. Photopaper was used to estimate the width of the laser sheet and determine its relative position within the contactor. Typically, the width of the laser sheet was less than 1 mm.

The data acquisition rate for the PIV system was approximately 1 Hz (mainly restricted by the speed of the camera). Due to the low data rate this technique was primarily used for obtaining a spatial map of the mean flow although root mean square (RMS) velocity values are also reported. Data were obtained for flow in the annular region of the 4-vane geometry at flow rates of 300, 600, and 1000 ml/min. For each of the two higher flow rates, data were recorded for varying rotor speeds of 3000, 3600, and 4000 RPM. For most of the conditions 50 double-frame images (as in Figure 3.2) were recorded except for runs at 600 ml/min or 3600 RPM for which 75–100 images were recorded; regardless, it was observed that the average flow field was not substantially altered for averages of greater than 50 images. Images were processed by cross-correlation as described in Section 3.1.2 using the adaptive multi-grid averaging scheme. Two passes of a $64 \times 64$ pixel window (with 50% overlap) followed by one pass of a $32 \times 32$ pixel window were used. Portions of the image which did not represent flow area were masked out of the vector fields (to eliminate spurious vectors which were generated in black areas of the image due to noise).

For flow underneath the rotor on the horizontal laser sheet at the vane mid-height, images were taken at each combination of three flow rate settings (300 ml/min, 600 ml/min, 1000 ml/min) and three rotor speed settings (3000 RPM, 3600 RPM, 4000 RPM) for a total of nine different conditions. These measurements were performed for both of the vane plates with windows (4-vane and 8-vane). It was possible to perform PIV processing of these images; however, due to the large average bubble size in this region this was useful mainly to look at general flow patterns for the various conditions and PIV image processing was performed only for the base conditions (600 ml/min and 3600 RPM) to give a qualitative description of the flow under the rotor.
3.2.5 Pressure Measurements

As described previously, the centrifugal contactor consists of two main regions, the annular mixing region (including the vane region under the rotor) and the separation region within the rotor. From a modeling perspective, it was useful to thus subdivide the contactor into two separate models. However, it is critical to understand how the two regions communicate in the real system in order to select an accurate representation of the boundary conditions. This is particularly true for the exit of the mixing zone (rotor inlet) for which an accurate representation of the pressure must be specified to correctly predict the volume of liquid maintained in the mixing zone. For this purpose, measurements of the static pressure at the rotor inlet were performed.

A Siemans differential pressure transducer (model PN-32) with a range of 1–20 mbar and an accuracy of ±1 Pa was used for these measurements. One side of the transducer was open to atmosphere and the other side was connected to a 1.59 mm (1/16”) OD stainless steel tube which was inserted into the drain connection of the contactor located along the rotor axis as shown in Figure 3.14. The probe tube was filled with water—except for the single set of measurements presented below which were taken with the contactor and probe tube completely empty—and therefore it was necessary to determine the ‘zero’ relative pressure reading once the probe was
positioned. In order to minimize the static head in the tube (and maximize the measurement range), the transducer was elevated such that its position was only slightly lower than the top of the probe. The ‘zero’ pressure reading was determined by taking the average of multiple measurements of the static liquid height of water above the probe end. Typical standard deviations for these calibration measurements were approximately ±3 Pa; this is a measure of the absolute offset of a given set of measurements and can be taken as the overall accuracy of the pressure measurements although the relative error between different measurements at the same calibrated setting would only be ~1 Pa. At each set of conditions (flow rate and rotor speed) the pressure reading was manually recorded at a rate of ~1 Hz over a typical period of 30 s (N≈30). From these measurements a time average and standard deviation were obtained for each set of conditions.

Pressure measurements were made for each of the three vane configurations (4-vane, 8-vane, and curved) as a function of rotor speed at a constant flow rate (600 ml/min) and as a function of flow rate for a constant rotor speed (3600 RPM). The main purpose of these measurements was to aid in selection of an accurate approximation for the pressure at the rotor inlet boundary for input into the mixing zone models. As explained later, one method for approximating the pressure at this point is to assume it is simply equal to the pressure generated by the rotating air column within the separating zone and can be calculated according to the Bernoulli equation for rotating flow:

\[ P_1 - P_2 = \frac{\rho \Omega^2}{2} (r_1^2 - r_2^2) - \rho g (h_1 - h_2) \]  

[3.7]

in which \( \rho \) is the mass density of air, \( \Omega \) is the rotational speed of the rotor, and \( g \) is the acceleration due to gravity. As an initial check of the pressure measurement system, measurements were taken as a function of rotor speed for a completely empty contactor (4-vane) with no inlet flow. Figure 3.15 shows a comparison of this data versus Equation 3.7 where point 1 is the location of the probe (rotor inlet center point) and point 2 is either the organic (light phase) or aqueous (heavy phase) exit port. As noted above, for the CINC V-2 contactor the radius of the heavy phase exit port is actually slightly less than that of the light phase (2.90 cm versus 3.15 cm) and it seems that this shorter radius sets the pressure within the empty rotor.
Figure 3.15: Plot of pressure at the center point of the rotor inlet as a function of rotor speed as compared to that calculated using Equation 3.7.
Part II

Mixing Zone
This portion will report the results of the flow analysis within the contactor mixing zone using experiments and CFD simulations. The first chapter of this portion (Chapter 4) will present the results of simplified computational models of the contactor mixing zone. These give a useful introduction to the flow in the mixing zone and also due to their relative simplicity allow exploration of a range of model conditions and geometric configurations.

Chapter 5 gives a detailed look at the flow in the mixing zone of the annular centrifugal using experimental measurements and observations to support the demonstration of free surface models of the mixing zone under the standard conditions for the base simulation case of the 4-vane contactor geometry operating at 3600 RPM with an inlet flow rate of 600 ml/min. In particular, experimental measurements were used to support the selection of the LES method for turbulence simulation.

The final chapter (Chapter 6) gives a complete application of the flow simulation methodology supported by experimental observation for analysis of the effect of the mixing vane geometry on the flow and mixing in the contactor.
Chapter 4

Simplified Models

As has been described, the real flow in the mixing zone of the annular centrifugal contactor is quite complex and consists of multiple phases. Various simplifications were employed to enable the initial computational exploration of the contactor mixing zone. The first of these will be described in the next section and employed a three-dimensional model of the lower portion of the mixing zone assuming a liquid full geometry. Two-dimensional annular models were also used to explore the two-phase (air, water) and three-phase (air, water, kerosene) flow in the annulus.

4.1 3D, Single-Phase Partial Mixing Zone Model

This section, with the exception of portions of Section 4.1.3.3, was previously published separately as Wardle et al. 2006.\textsuperscript{116}\textsuperscript{1}

While the contactor mixing zone actually extends along the entire length of the annular region from the base of the contactor housing to the tangential fluid inlets (see Figure 1.1), in order to minimize the volume of the computational domain in these initial simplified models, the mixing zone was only modeled to a height of 3 cm above the rotor bottom. The modeled contactor geometry is given in Figure 4.1 and the significant geometric parameters are listed in Table 4.1. The radius ratio (ratio of rotor radius to housing radius $r_r/r_h$) is also listed rather than the absolute width of the annular gap, as it is an important parameter for scale up of contactors. The model geometry was based on the commercially available CINC V-2 contactor unit manufactured by Costner Industry Nevada Corporation. For simplicity in this initial model, the computational

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volume was assumed to be completely full of a single liquid phase (water) and the inlet to the annular region was assumed to be flat and perpendicular to the rotor surface. In reality, for nominal input water flow rates in the same size contactor at similar rotor speeds (3000 RPM), the liquid height in the mixing zone ranges from 1.5 to 2.0 cm above the rotor edge (see Figure 1.4) and there is a liquid–air free surface that does not appear to be flat. Despite these departures, the solution for these approximated conditions will provide a starting point for understanding the flow in the mixing zone and should provide a physically realistic solution for the flow underneath the rotor. Two-phase air/water calculations which model the free surface and include the full length of the mixing zone are discussed in Chapter 5.

A grid resolution study was conducted to determine the dependence of the solution on the grid spacing (see Appendix B). The mesh was refined primarily near the rotor as this is a high shear region with the largest velocity gradients. Along with properties such as the rotor shear stress, volume-averaged tangential velocity, and axial fluid velocity at the midpoint of the rotor inlet, the $y^+$ value at the rotor wall was also monitored for successively finer meshes. The parameter $y^+$ (Equation 4.1) is a measure of the near-wall mesh and is a function of the fluid density $\rho$ and
Table 4.1: Key geometric parameters of partial mixing zone model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotor Radius</td>
<td>$r_r$</td>
<td>2.54 cm</td>
</tr>
<tr>
<td>Housing Radius</td>
<td>$r_h$</td>
<td>3.17 cm</td>
</tr>
<tr>
<td>Radius Ratio</td>
<td>$r_r/r_h$</td>
<td>0.801</td>
</tr>
<tr>
<td>Rotor Inlet Radius</td>
<td>$r_i$</td>
<td>0.505 cm</td>
</tr>
<tr>
<td>Vane Height</td>
<td>$h_v$</td>
<td>0.617 cm</td>
</tr>
<tr>
<td>Vane-to-rotor Gap</td>
<td>$h_{gap}$</td>
<td>0.159 cm</td>
</tr>
<tr>
<td>Mixing Zone Height</td>
<td>$h_m$</td>
<td>3.776 cm</td>
</tr>
</tbody>
</table>

Viscosity $\mu$, the friction velocity $u_r$ and the distance from the wall $y$.

$$y^+ = \frac{\rho u_r y}{\mu}$$  \[4.1\]

The friction velocity $u_r$ is determined from the shear stress at the wall $\tau_w$ by

$$u_r = \left(\frac{\tau_w}{\rho}\right)^{1/2}$$  \[4.2\]

Standard wall functions, as were used in this portion of the study, are valid for $y^+ > 30$ and therefore it was desired that the final mesh have a value of $y^+ \approx 30$.\[^{102}\] The final meshing scheme that was used for all the geometries in this portion of the study employed a quadrilateral mesh on the rotor side with spacing of 0.04 cm and 0.125 cm tetrahedral meshing for the rest of the volume as shown in Figure 4.2(a). In this way, the fine mesh of the base geometry consisted of 588484 tetrahedral cells. All meshes were generated using Gambit 2.1.6. from Fluent Inc.

### 4.1.1 Modeling Conditions and General Solution Method

Calculations of the steady-state flow solution were done using the commercially available Fluent 6.1. For this initial group of calculations, turbulence was modeled using the RNG $k-\varepsilon$ turbulence model see Section 2.1.4 and standard wall functions (see Section 4.1.4 for a comparison...
Figure 4.2: Contactor model mesh for FLUENT calculations. (a) Fine mesh consisting of a 0.04 cm quadrilateral mesh on the rotor surface and 0.125 cm tetrahedral mesh elsewhere used for all final solutions. (b) Coarse tetrahedral mesh with 0.15 cm spacing used for initial calculations.

of several different turbulence models in this simplified geometry). FLUENT’s default under-relaxation factors, interpolation schemes, and pressure-velocity coupling were used. The inlet was defined by a constant mass flowrate of 0.01 kg/s (∼600 mL/min) of water and the outlet was defined at a constant zero pressure relative to the inlet. The rotor and housing walls both had no-slip conditions and the rotor wall was also given a fixed rotational velocity. A rotor speed of 3000 RPM was assigned as the base case, but solutions for 1000 and 2000 RPM are also presented to evaluate changes in the flow due to rotor speed.

The solution method applied to the various cases was the same. A coarse mesh, consisting of a uniform tetrahedral grid with a spacing of 0.15 cm (Figure 4.2(b)), was generated and the solution for this coarse mesh was first calculated. Due to the high shear at the rotor wall boundaries it was necessary to also incrementally increase the rotor speed up to the desired rotation rate to achieve a converged final solution. Typically, the coarse solution was initially calculated for 1000 RPM and the rotation rate was increased in increments of 1000 RPM. The solution was not taken completely to convergence at the intermediate steps except where results are presented. With a converged solution for the desired rotor speed on the coarse mesh, it was then possible to interpolate this
solution onto the final, fine mesh and calculate the solution. In this way, no changes in rotor speed were necessary on the final mesh, minimizing computational time.

### 4.1.2 General Flow

For these models, the base case geometry was taken to be the geometry given in Figure 4.1 (which has eight straight housing vanes) and Table 4.1 with a rotor speed of 3000 RPM. In general, the flow patterns observed in the CFD model were found to be comparable to those seen during actual contactor operation (as observed through the transparent housing) as described later in Chapters 5 and 6.

Velocity vectors on a horizontal (Figure 4.3) and vertical plane (Figure 4.4) for the solution of the base case show the direction and relative magnitude of the flow field. It is apparent from Figure 4.3 that there are swirling patterns within the area between each of the vanes beneath the rotor. From Figure 4.4 it is clear that as would be expected, the flow of the highest magnitude is located near the rotor with a maximum value approximately at the axial midpoint on the rotor side. This behavior can be seen more clearly in Figures 4.5 and 4.6 which show the radial and axial flow components, respectively.

From Figure 4.5 a separation point from the side of the rotor is evidenced by the region of positive radial velocity (yellow). Figure 4.6 shows that the fluid region above this point is moving downward near the rotor and upward near the housing wall while the region below this point is flowing in the opposite direction—upward near the rotor and down at the housing wall. This flow pattern is characteristic of Taylor-Couette flow as described in Section 1.2.5.1. While the stability of these Taylor vortices cannot be shown without a transient solution, by experimental observation they can be somewhat oscillatory.
Figure 4.3: Velocity vectors on horizontal plane midway between housing bottom and rotor bottom colored by velocity magnitude (m/s).

Figure 4.4: Velocity vectors colored by velocity magnitude (m/s) on a vertical cross-sectional plane which bisects the region between vanes. The plane is shown at an angle to emphasize the direction and relative magnitude of vectors near rotor.
Figure 4.5: Radial velocity contours (m/s) on a vertical cross-section of the contactor mixing zone (see Figure 4.4 for the relative orientation of the plane). Positive radial velocity is defined as flow out from the rotor axis.

Figure 4.6: Contours of axial velocity (m/s) in which positive axial velocity is defined as flow upward or in the positive z-direction. Refer to Figure 4.4 for the relative orientation of the plane.
4.1.3 Additional Considerations

4.1.3.1 Particle Tracking

Tracking particles released from a specified point can provide useful information regarding the disposition of particulates (or droplets) in the volume. Particle tracking was performed using FLU-ENT’s Discrete Phase Model (DPM) which applies a Lagrangian approach to tracking particles of specified diameter and density through the system. Particle trajectories are solved by stepwise integration in time over a specified number of path length increments. For this calculation, it was assumed that the particles were in such small quantities that they do not affect the flow of the continuous phase. Two thousand particles of a specified density and diameter were injected with a zero initial velocity at a radial point in the center of the annulus on the inlet surface. Particles were tracked sufficiently long such that greater than 95% of the particles exited the system. Turbulence was accounted for stochastically by allowing for random fluctuation of the instantaneous velocity proportional to the local turbulence intensity for each point along the integration path. Residence time was defined as the total flow time from the point of release until the particle exited the volume through the outlet.

It was observed that as the particle diameter (and consequently its mass) was increased, the average particle residence time increased (see Figure 4.7). For 10 g/cm$^3$ particles, such as would be found due to poorly dissolved fuel ($\rho_{\text{UO}_2} \approx 10$ g/cm$^3$), the longer residence time was a result of particles not being able to pass through the first Taylor vortex. Particles are spun out from the rotor to the outer wall where the fluid is actually rising and therefore they are less likely to get below the height of the separation point on the rotor side. The particles appear to spend most of the time in this upper vortex, but once they get below the separation line into the lower region they typically quickly pass out of the volume (into the rotor). Particles larger than a critical diameter of $\sim 20$ microns rarely if at all were able to pass below the separation line and became trapped in the upper vortex. As the particle diameter was increased further, the particles tended to stay progressively closer to the top of the annular region. These results were for relatively dense particles and it
Figure 4.7: Particle residence time distribution for four different particle diameters \((\rho = 10 \text{ g/cm}^3)\).

The distribution for the largest diameter particle \((d = 20 \mu\text{m})\) is approximately constant through \(\sim180\) s.

would seem that for lighter particles (still more dense than water), such as would be representative of insoluble nitrate salts, the critical particle size would be larger.

As for particles less dense than water \((\rho = 0.8 \text{ g/cm}^3)\), there were no general obstacles to flow through the volume except for very large particles \((d > 0.2–0.25 \text{ mm})\) which, in contrast to dense particles, appeared to migrate toward the region near the separation line at the side of the rotor. It is possible to consider particles of this density as organic fluid particles such as kerosene, however, it has been shown that for liquid–liquid dispersions under the given conditions the droplet diameter would be an order of magnitude smaller than these values.\textsuperscript{74}

Another important class of particles are those which are neutrally buoyant such as might be representative of Pu(IV) colloidal polymers which have been found to form in PUREX processes.\textsuperscript{45,46} The trajectories of 1 g/cm\(^3\) particles of various diameters were calculated using the same methods, but in general these particles did not exhibit any notable behavior (i.e. change in residence time) in the mixing zone and appeared to follow the flow as would be expected. It should be noted, however,
4.1.3.2 Effect of Parameter Change: Rotor Speed

The effect of the rotor speed on the flow was evaluated by comparing the converged solutions for rotor speeds of 3000 (base case), 2000, and 1000 RPM. In general, the flow field was similar with only relative changes in magnitude. This would be expected for the present system as the volume was assumed fully liquid; however, during actual operation of contactors changes in rotor speed result in changes in the annular liquid level. Figures 4.8 and 4.9 show the axial velocity along a horizontal line beneath the rotor and the radial velocity along a vertical line running along the center of the annulus. From Figure 4.8 it is clear that beneath the rotor, a decrease in rotor
Radial velocity (m/s) as a function of axial position (normalized by the mixing zone height) along a vertical line midway between the rotor and housing for the three rotor speeds. Speed only decreases the relative magnitude of the flow field without significantly affecting the radial location of the maxima and minima. In the annular region (Figure 4.9), the axial height of the separation point on the side of the rotor decreases with decreasing rotor speed.

4.1.3.3 Design Considerations: Vane Geometry

It has been well established experimentally that the housing vane geometry has a large impact on the annular liquid height, stage efficiency, and contactor throughput.\textsuperscript{[22,39,40]} Consequently, modification of the vane geometry may provide a simple method for optimization of an individual stage for specific process conditions. ANL designed contactors have traditionally used straight housing vanes for simplicity; eight vanes are typical, although four-vane housings are also used. The commercial contactor units from CINC (such as the V-2 unit used for the experiments in this project) are primarily marketed as separator/extractors and are sold with curved vanes which were designed to increase contactor throughput. It has been observed that overall extraction efficiency with the curved vanes is comparable to that of the straight vanes for moderate and high flow rates but somewhat less for low flow rates.\textsuperscript{[39,151]} A full experimental/numerical analysis of the mixing
behavior for the three standard vane configurations (4-vane, 8-vane, curved) will be given later in Chapter 6. This section will report the results of some partial mixing zone calculations for the four-vane and curved-vane geometries as well as one other sample vane geometry which will be described. This latter geometry is presented mainly as evidence of the utility of the CFD modeling for predicting the flow in untested geometries. The grid generation methods for the partial mixing zone geometries presented here were the same as described in Section 4.1.1.

The major geometric parameters for the models presented here are the same as those shown in Table 4.1 save that the vane geometry has been modified. It was found that the flow in the annular portion of the geometry was not substantially affected by the vane changes. As a result, only the flow underneath the rotor will be discussed.

**Four Straight Vanes**

Figure 4.10 shows the areas of rotation that were evident in the base case eight-vane geometry (see Fig 4.4) have been shifted toward the rotor axis resulting in a more significant area of swirl centered on the rotor axis. The result of this swirling region around the rotor axis is a decrease in the magnitude of positive axial flow near the rotor axis as shown in Figure 4.11. This plot also shows that the regions of positive axial flow that were near the outer edge of the rotor ($r \approx \pm 0.8$) for the base geometry have been pushed radially outward.

**Curved Vanes**

The curved-vane housing geometry is shown in Figure 4.12. Recall that a similar type of curved vanes (only four) were part of the original contactor development at Argonne. While the curved vanes seem a natural extension of the desire to more smoothly direct the flow toward the axis of the rotor, these vanes, as used in the commercial CINC design, also have some unique features with less obvious qualities. Specifically, the vanes’ height near the annular region is half of that for the main portion under the rotor. There is also a gap between the vane and the outer housing wall equal to half of the annular gap. The purpose of these features is apparent by analysis of the CFD predictions for the flow patterns under the rotor. Figures 4.13 and 4.14 show the velocity vectors on a horizontal plane at half the vane height for the CINC curved vanes and for curved vanes without the notched section or wall gap. Figure 4.14 shows very efficient direction of flow toward the axis
Figure 4.10: Vectors of velocity magnitude (m/s) on a horizontal plane midway between the rotor bottom and housing bottom.

Figure 4.11: Comparison of axial velocity (m/s) profiles along a horizontal line beneath the rotor bisecting the region between vanes for both the base geometry (eight vanes) and the modified four vane geometry.
Figure 4.12: CINC curved vane geometry.

Figure 4.13: Plot of velocity vectors for the curved vane geometry.
Figure 4.14: Plot of velocity vectors for curved vanes which are full height and have no gap at the outer housing wall.

of the rotor with little apparent axial flow. While simulations of the full contactor mixing zone have not been performed for this full curved-vane geometry, it is very likely that this system would exhibit cyclic behavior and overall poor operation. The flow forcing of the vanes would be such that any fluid in the contactor would be rapidly pumped from the mixing zone with the result that the fluid would lose contact with the bottom of the rotor until a sufficient volume of fluid builds up in the annulus to be again rapidly expelled. Thus, a cyclic operation with virtually no mixing and slug-flow throughput would be generated. From Figure 4.13 it appears that the notch in the vanes generates some upward flow in the annular region and the vane-to-wall gap allows some extra circulation beneath the rotor. Both of these effects likely contribute to the generation of sufficient liquid volume in the mixing zone at adequate flow rates as observed by Leonard et al.[22] Even so, it appears that the mixing beneath the rotor may still be less than for the straight vanes resulting in poorer overall mixing for low flow rates (low liquid hold-up in annulus). These observations are more fully explored later in Chapter 6.

Eight Vanes with Staggered Half-Baffles
The great advantage that accurate CFD modeling has over physical experimentation is the ability to test new geometries and conditions without the time and cost of building a prototype. As an example, a unique straight vane geometry was ‘constructed’ consisting of eight straight vanes extending to the rotor edge with eight staggered baffles half the width of the annular gap extending from the outer housing wall. The geometry and flow under the rotor are shown in Figure 4.15 This hypothetical vane configuration results in significant forcing of flow toward the center of the unit by the staggered baffles. The gap between the end of the vanes and the end of the baffles, which is equal to half the width of the annular gap (0.5\(\Delta r\)), was intended to allow some circular flow between vane and baffle. It does appear that a small fraction of the flow is able to travel between vane sections in a somewhat staggered path.

4.1.4 Comparison of Turbulence Models

This section was previously published in summary as part the Transactions of the American Nuclear Society as Wardle et al. 2006[152] and presents the results of a comparison of various turbulence models for modeling the flow in partial mixing zone geometry using FLUENT 6.2.
The results from these calculations can be compared with those presented above (Section 4.1.2) in which the RNG $k-\varepsilon$ turbulence model was used. For these additional calculations, two other turbulence models based on the Reynolds Averaged Navier-Stokes (RANS) equations (see Section 2.1) were used, namely, the standard $k-\varepsilon$ model and the Reynolds Stress Model (RSM). For these preliminary calculations, quantitative experimental data of the flow had not yet been taken and a time-dependent calculation using the Large Eddy Simulation (LES) method as implemented in FLUENT was used in lieu of data. A comparison between the simpler RANS models with this LES solution was made.

The same mesh as described in Section 4.1 was used for each of the RANS model calculations as well as the LES simulation. While it is known that LES solutions are quite dependent on the grid size as they employ spacial filtering to model the subgrid scale turbulence (see Section 2.2), the mesh was not optimized for LES. Rather, as this was an initial attempt at applying LES methods to the contactor problem the same mesh was used for each of the turbulence models.

All solutions were initialized from the base case solution using the RNG $k-\varepsilon$ model for a flow rate of 0.01 kg/s of water and the rotor speed was 3000 RPM. For the LES calculations, a 2nd order implicit unsteady solution method was applied and two simulations were done using two different subgrid scale models. The first used the standard Smagorinsky-Lilly model which is referred to as a zero-equation model as it models turbulence with a simple algebraic equation. In the second LES calculation the subgrid scale turbulence was modeled with a one-equation turbulent kinetic energy transport model as described previously in Section 2.2.2. A constant time step of 0.5 ms was used for both LES simulations. This is 40 times smaller than the time for a single rotation (3000 RPM) and gave consistent convergence. The LES calculation was initialized from the steady-state RNG $k-\varepsilon$ solution and then allowed to run for $\sim$1 s of flow time after which data was averaged over a 0.5 s period in order to make comparisons to the RANS results.

Figures 4.16 and 4.17 show the axial velocity profile along a horizontal line beneath the rotor and the radial velocity along a vertical line running along the center of the annulus. As the results for the two LES simulations were similar, only the turbulent kinetic energy subgrid model results (LES_tke) are presented. It is clear from Figure 4.16 that there is virtually no difference between
Figure 4.16: Axial velocity (m/s) as a function of radial position (normalized by the housing radius) along a horizontal line midway between the bottom of the housing and the rotor bottom for the standard $k$–$\varepsilon$, RNG $k$–$\varepsilon$, RSM, and time-averaged LES solutions. Refer to Figure 4.8 for relative location of rotor.

Figure 4.17: Radial velocity (m/s) as a function of axial position (normalized by the mixing zone height) along a vertical line midway between along the center of the annulus for the three RANS models and the time-averaged LES solution. Refer to Figure 4.9 for relative location of rotor.
the RANS models. The time-averaged LES solution, however, is somewhat different with the minimum at $r_{\text{norm}} = 0.0$ and the maxima at $r_{\text{norm}} = \pm 0.2$ being more extreme. There is also another region of positive axial velocity near the outer wall which none of the RANS models are able to capture. Uniformity between the RANS models can be seen for the radial velocity profiles in the annulus (Figure 4.17). All predict the separation point to be at approximately $z_{\text{norm}} = 0.6$ which is approximately halfway up the rotor side (refer to Figure 4.5) while the LES model’s prediction was slightly higher axially and larger in magnitude.

The turbulence intensity along a horizontal line beneath the rotor for the three RANS models and the time-averaged LES simulation is plotted in Figure 4.18. While the RANS models each predicted the same general trend with the region increased turbulence near the center of the swirling regions between vanes (see Figure 4.3) each gave different levels for the magnitude of turbulence with the standard $k-\varepsilon$ being the greatest and the RSM model being the least. As there was no experimental data with which to compare it was difficult at this point to say which model better predicts the actual turbulent behavior. If one assumes that the LES solution represents the best approximation of the actual turbulence quantities, comparison with the RANS models shows that the RNG $k-\varepsilon$ appears to have the best agreement. The choice of turbulence models for the full mixing
Figure 4.19: Root mean square (RMS) velocity fluctuation (m/s) as a function of axial position along the center of the annulus for data taken over a 0.46 s period.

zone geometry with free surface flow will be compared with experimental velocity measurements in Section 5.

4.1.5 LES Time-dependent Solution

From the previous section it was observed that the time average of the LES solution appeared to be significantly different from the solutions predicted by all of the RANS models.\textsuperscript{2} The instantaneous velocity fields from the LES solution are examined here in order to explain some of these differences as well as to provide an introduction to the role of turbulence within the mixing zone of the model contactor. It was noted previously that the Taylor-vortices in the annulus are expected to be oscillatory. Figure 4.17 above showed that the LES prediction for the separation point at the rotor side was significantly higher in both its axial position and radial velocity magnitude than the corresponding RANS predictions. As one estimate for the stability of this separation point, Figure 4.19 shows a plot of the RMS velocity magnitude along the center of the annulus. The velocity fluctuations are highest near the bottom edge of the rotor and also at the separation point at the side of the rotor with a magnitude of the same order as the mean velocity. This shows that the location of this separation point is relatively static in time but the magnitude of the flow at

\textsuperscript{2}Incidentally, unsteady RANS (U-RANS) modeling using the RNG-\textit{k–\varepsilon} model was also performed; however, there was no significant time variation of the flow within this simplified model.
Figure 4.20: Instantaneous velocity vectors (m/s) on a horizontal plane at the end of the LES calculation. Compare to Figure 4.3. Rotor rotation is counter clockwise.

This point has a relatively large fluctuating component. The absence of large fluctuations in the position of the separation point is not surprising, since the experimentally observed fluctuation in annular vortices is primarily caused by the oscillating liquid free surface which is not present in this simulation. Simulations including this additional critical characteristic of the flow—the liquid free surface—are presented in later sections.

A snapshot of the instantaneous velocity field at the end of the LES simulation is given in Figure 4.20. It is clear that the swirling regions between the vanes are not static in time as multiple eddies of varying sizes are evident in each of the inter-vane compartments. While there are some regions that appear to have eddies of similar length scales to the large eddies seen in the RANS solution (Figure 4.3) such as the two cells on the right, there are also ones with smaller vortices closer toward the axis such as in the cell on the top just left of vertical. A series of snapshots of the velocity vector field at 5 ms intervals over the duration of the simulation were also made in order to observe the dynamic nature of the system. From the resulting animation it appeared that
vortices are created in the corner region of each cell where the highest velocities are found and these vortices grow and are sporadically shed up the side of the vane toward the axis of the rotor. Figure 4.21(a)-(d) shows four successive velocity contour plots which are all equally spaced at 50 ms intervals. This flow field is very similar to that seen in photographs and videos of the flow underneath the rotor in which the swirling regions are not all uniform either in time or space. Circular regions of low velocity magnitude (blue), such as the one near the center, are the rotational axis of an in-plane vortex. This vortex near the axis of the rotor appears to precess as can be seen from the successive frames. The center of the vortex is moving in a counter clockwise manner at a rate of one complete rotation per 0.2 s or 300 RPM. Interestingly, this is exactly 1/10th the rotational speed of the rotor. This secondary swirling motion is evident in previous Argonne National
Laboratory videos of contactor operation and provides a good qualitative validation for the LES predictions of the flow underneath the rotor. During the simulation, the axial velocity at the point on the center of the rotor inlet was monitored and it was observed that axial flow was generally slightly negative but was characterized by large but brief jumps in which significant axial flow up an out of the mixing zone occurred. It would seem that this behavior could be related to the precession of this near axis vortex. While the behavior of this precessing vortex for increasing flowrate was not explored, it would seem that it should stabilize with increasing flowrate. Indeed, this is what is observed experimentally in the videos of contactor operation. The high-speed imaging that was performed as part of this project was not able to evaluate this secondary flow behavior as only the majority of one quadrant of the flow under the rotor was visible (see Figure 6.12).

4.2 2D, Multi-phase Annular Model

As described in Section 2.3.2, the Volume of Fluid (VOF) interface tracking method for modeling free surface and immiscible flows has a distinct limitation in that it is very much dependent on the computational grid resolution. Evaluating the grid dependence of the VOF solution methods used in these simulations is critical to understanding the results and making accurate comparison to experimental observations. As an introduction to the VOF model as well as an initial exploration of the mesh dependence of this model two-dimensional, axisymmetric simulations of the free surface flow in the annulus were performed. The following section will explain the results of 2-phase (air–water) simulations and the last section will present a set of simulations with three phases (air–water–kerosene).

4.2.1 2-Phase (Air–Water) Annular Model

Figure 4.22 shows a sketch of the annular model in relation to the contactor geometry. The width of the 2D model was equal to the size of the annular gap for the standard contactor geometry, 0.63 cm, and the height was 7 cm. The rotor wall had a 3000 RPM rotational velocity about the axis; the radius of the inner (rotor) wall was specified as 2.54 cm. The bottom boundary, which in the full geometry is the liquid surface at the level of the rotor bottom, was specified as a wall. As it
was found that the liquid had a tendency to lose all contact with the rotor for the case of a free-slip bottom boundary ($\tau_{wall} = 0$), the bottom was assumed to have no-slip ($v_{fluid} = v_{wall} = 0$) for these calculations. It would also be possible to specify a bottom boundary condition taken from the full 3D model; however, for the sake of simplicity this was not done. The top boundary was specified as a zero pressure boundary and while in theory it would be possible for liquid to be lost at this boundary (backflow liquid volume fraction set to zero), in practice the total liquid level was kept low enough that this did not occur. Turbulence was modeled using the RNG $k-\varepsilon$ RANS model described in Section 2.1.4. Two different uniform tetrahedral meshes were generated to observe the dependence of the VOF solution on grid size. The grid spacings were 0.5 mm and 0.25 mm, respectively. Both simulations were initiated with a liquid level extending 2.5 cm up from the bottom edge. The Non-iterative Time Advancement (NITA) scheme was used with a constant time step of 0.1 ms (100 $\mu$s). Surface tension was also included with a surface tension value of 0.072 N/m. The default contact angle of 90° was used for all surfaces.

The dynamics of the interface were compared visually during the first 1.0 s of operation. It was observed that the predicted interface for the two simulations was nearly identical for approximately the first 0.25 s of flow from start-up. Figure 4.23 shows the volume fraction contours for the two
simulations at the 0.25 s point. The interface shape is no longer identical, but is still roughly similar in shape. The difference in mesh density is also apparent in the definition of the interface as well as the size of air bubbles which are resolved; although both simulations predicted negligible air entrainment. After this point \( t \approx 0.25 \) s the two simulations diverged (in the directional sense) and appeared to be slightly out of phase with one another—an event would happen first in the coarse mesh and a similar event occur at a slightly later time in the fine mesh simulation.

Following the first second of start-up, the simulation data were averaged over another 1 s of flow time to see if the average results were comparable even though the instantaneous dynamics appeared to be slightly different. A comparison of the mean and RMS volume fractions is given in Figure 4.24(a) and 4.24(b), respectively. It is clear that while the general distribution of the mean volume fractions is similar, there are important differences. In particular, the annular liquid height predicted from the mean volume fractions of the two simulations is slightly different. It appears that the maximum excursion for the coarse grid was somewhat higher than for the fine grid. This can also be seen from the contours of RMS volume fraction in Figure 4.24(b). The region where the interface position experiences the most change is more confined in the fine mesh compared to the coarser one.

As was mentioned in Section 2.3.1, errors in interface reconstruction and advection for the VOF model can result in loss of mass. In order to observe this ‘mass loss’ and evaluate its grid dependence, the total water volume fraction was tracked in both simulations for flow times \( t = 2.0 \text{ s} \) to \( t = 3 \text{ s} \). The change in water volume as a function of time for both grids is plotted in Figure 4.25 along with the rotor contact area. Both grids had an initial volume-average fraction of water equal to 0.357. It can be seen from this figure that even though there is no liquid entering or exiting the volume, there is a small fluctuation in the total liquid volume \((< 1\%)\). While the overall variation about the mean as given by the standard deviation \( \sigma \) is comparable for both grids, the drift of the mean total volume with time (slope of the least-squares fit line) is much greater for the coarse grid. The variation and drift in liquid volume are both assumed to be due to errors in the VOF formulation, namely, the reconstruction and advection methods as described in Section 2.3.1.
Figure 4.23: Snapshot of water volume fraction (water is red) at 0.25 s after start-up for the coarse mesh (top) and fine mesh (bottom)
Figure 4.24: Contour plots of (a) mean volume fraction and (b) RMS volume fraction. In both (a) and (b) the results for the coarse are on top and the fine on bottom. The dotted lines in (a) denote the 0.9 volume fraction line on the outer wall for comparison. The scale is not shown for the RMS volume fractions, but ranges from 0.0 (blue) to 0.5 (red).
Figure 4.25: Plots of the water volume fraction (black, left axes) evolution with time and the rotor contact area (grey, right axes) for the coarse (top plot) and fine (bottom plot) meshes. At time $t = 0$ s both simulations had a water volume fraction of 0.357. The equations shown on each plot are for the least squares fit to the water volume fraction data and $\sigma$ is the standard deviation.
Figure 4.25 also shows that there are regular intervals at which there is a maximum in the rotor-fluid contact area separated by periods in which there is complete loss of contact between the fluid and rotor. The approximate period of oscillation is 0.2 s corresponding to a frequency of 5 Hz (or 300 min$^{-1}$). Curiously, this is exactly 1/10th of the rotor speed (3000 RPM) and is the same frequency observed for the precessing vortex described in Section 4.1.5. While these two simulations are observing different phenomena, it is interesting (and perhaps merely coincidental) that a similar time dependent behavior is obtained. The free surface oscillation observed in experiment and full 3D simulations will be discussed more later in Chapter 5.

In general, these observations using the 2D, axisymmetric simulation show that accurate predictions of the annular liquid height and underlying interface dynamics need to take into account grid dependence. It is not possible to determine whether the fine mesh solution is grid independent without further refinement. It is also important to note that the dynamics of the three-dimension contactor system as described in the Chapter 5 are somewhat different from those of the 2D, axisymmetric model described here. In the 3D model there appeared to be no complete loss of fluid–rotor contact and as a result the average oscillations in liquid level are somewhat smaller. This is largely a function of the volume of liquid in the annulus, which for these 2D simulations is fixed, but for the 3D simulations is allowed to vary according to the geometry and conditions. Even so, the 2D model provides a reasonable approximation of the conditions in the actual contactor and is useful for this initial evaluation of solution grid dependence. Similar simulations (using the fine mesh) were also performed to explore the effect of contact angle. These are included as part of Appendix C.

### 4.2.2 3-phase (Air–Water–Kerosene) Annular Model

Using the fine meshing scheme (uniform 0.25 mm tetrahedral) from the 2-phase models presented above, similar simulations were performed to provide an initial exploration of the liquid–liquid mixing behavior in the simplified annular geometry. The simulation was initiated from rest with a total fluid height of 2.5 cm as before; although in this case the lower 1.25 cm layer was water and above this was a 1.25 cm layer of kerosene. Originally, these simulations were attempted
with an initial total liquid height of 5 cm (2.5 cm water, 2.5 cm kerosene), but this resulted in a significant loss of fluid out the top surface of the annulus. The time step was allowed to vary according to the global Courant number limit and the average time step was on the order of 20 \( \mu \text{s} \). This substantially smaller time step than the 2-phase simulations is due to the greater difficulty of capturing the dynamics of the liquid–liquid interface between the water and kerosene phases. Surface tension between the phases was included as before with values of 0.072 N/m, 0.025 N/m, and 0.013 N/m for air–water, air–kerosene, and water–kerosene, respectively. The default contact angle of 90\(^\circ\) was used for all phases although it would be possible to specify unique values for the contact angle for each of the fluid combinations.

Very similar oscillatory liquid level behavior was observed for these 3-phase simulation; the combined liquid phases—in relation to the air—acted almost like a single fluid. As with the 2-phase simulations, there was virtually no air entrainment. It was observed that mixing between the two liquid phase occurred only when there was significant contact between the fluid and rotor and that during the period when the combined liquid phases were spun out from and lost contact with the rotor that there was actually visible recombination (‘settling’) of the two phases. This can be seen in Figure 4.26 which shows a snapshot of the phase distribution at the end of a maximum in fluid rotor contact (a) and later in time as the fluid is settling back down just before another maximum in fluid–rotor contact. From Figure 4.26(a) the mixing due to Taylor-Couette vortices is apparent; a lower vortex rotating counter-clockwise at the bottom (far left) and a larger one above this rotating in the opposite direction (clockwise) can be identified by the swirling fluid streams. Despite this mixing during contact with the rotor, the fluid phases tend to separate when contact is lost as apparent by the higher degree of phase separation in Figure 4.26(b) at a later time as the fluid is returning back to the lower (high fluid–rotor contact) state but has not yet again contacted the rotor.

While these 3-phase simulations are certainly a significant oversimplification of the complex 3D flows in the real contactor during solvent extraction operation, they lend some insight into mixing behavior. Specifically, it appears that the liquid phases act almost like a single fluid phase in relation the air and the fluid free surface. This is not a novel observation, but it does lend support
Figure 4.26: Snapshots of phase contours (water = blue, kerosene = red, air = cyan) at two times: (a) $t = 1.200\,\text{s}$, near a maximum in fluid–rotor contact and (b) $t = 1.356\,\text{s}$, as the fluid is falling back down for a maximum in liquid height. The geometry and orientation is the same as shown in Figure 4.23 but only the lower portion of the annular model is shown here.

to the common technique of inferring liquid–liquid mixing behavior from detailed simulations of a single liquid phase as is done for the mixing studies reported in Chapter 6.
Chapter 5

Base Case Flow Analysis and Free Surface Flow Model Validation

While the partial mixing zone model is simple and can give useful predictions of the steady-state mean flow underneath the rotor, the flow and mixing in the annular region is very much affected by the air/liquid free surface and the discontinuous contact between the fluid and the rotor. Under typical operating conditions the flow in the annulus is primarily a free surface flow with droplet or rivulet flow from the inlets down the housing wall and into the mixing zone. This section presents the results of multi-phase computational fluid dynamics (CFD) modeling using the volume-of-fluid (VOF) interface tracking method (see Section 2.3.1) to characterize the mixing zone in a model centrifugal contactor. Experimental measurements including Laser Doppler Velocimetry (LDV) of the actual flow velocities within the contactor as described in Section 3.2.3 were also performed and are presented here. As part of the model development, a variety of turbulence modeling schemes were employed to evaluate their relative accuracy with respect to the experimental data and flow observations. The main purpose for the work presented in this chapter was to demonstrate the quantitative accuracy and practical utility of the computational models of the centrifugal contactor through comparison with experimental data for the selected base conditions: 4-vane geometry, 600 ml/min total inlet flow rate (water), 3600 RPM rotor speed. Chapter 6 will given a further application of the simulation methods demonstrated here to the full analysis of the flow and mixing for several different housing vane geometries.

The work in this section, with the exception of Section 5.7, was previously published in the AICHE Journal as Wardle et al. 2008. Refer to Section 3.2 for details regarding the experimental setup and the various measurement techniques employed.

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5.1 CFD Model Details

The simulations presented in this section provide a more realistic analysis of the flow in the mixing zone than those for the simplified models presented in Chapter 4 by including the free surface flow of water (and air) in the entire mixing zone using the Volume of Fluid (VOF) interface tracking method with piecewise linear interface construction (PLIC). The VOF technique is widely used for modeling interfacial flows and is capable of capturing complex interface dynamics including interface breakage and reattachment.\cite{122,124} Details on this method are given in Section 2.3.1. The continuum surface force (CSF) model\cite{129} was also used to account for surface tension effects on the air–water interface. The CFD modeling was done with Fluent 6.3 in parallel on \(\sim 16\), 1.3 GHz nodes in a Linux cluster.

The flow in the contactor mixing zone is highly turbulent \((Re = 6 \times 10^4\) at \(377\) rad/s [3600 RPM] based on the annular gap), and separate transient simulations using three different turbulence modeling techniques were performed for comparison with the experimental measurements. From this, the most appropriate model was selected for use in later simulations. These were the RNG k-\(\varepsilon\) model, the Large Eddy Simulation (LES) method, and the Detached Eddy Simulation (DES) method. Only a brief description of each model will be given here; more detailed descriptions were given in Section 2.1. The RNG k-\(\varepsilon\) model is a Reynolds Averaged Navier-Stokes (RANS) modeling technique which solves only for the statistical mean flow. This model is particularly suited for swirling flows (a swirl factor of 0.07 was used here) and was determined in the previous simulations of single-phase flow under the rotor to be a good RANS-type model for the flow in the centrifugal contactor (see Section 4.1.4). The LES technique fully resolves (solves the full Navier-Stokes equations for the instantaneous velocity field) those turbulent structures which are larger than the grid size and models those which are on the subgrid scale (see Section 2.2). A turbulent kinetic energy transport subgrid model was used for the LES simulation.\cite{102} The DES technique can be viewed as a hybrid RANS/LES method and was originally developed for application to very high \(Re\) number aerodynamic flows where fully resolved LES is not feasible. The realizable k-\(\varepsilon\) RANS model was used for the DES simulations.\cite{102}
All three simulations were done on the same computational mesh. This mesh was generated using Gambit 2.2 from Fluent Inc. Due to the high computational cost of running transient simulations using the VOF model, the mesh density for these simulations was necessarily somewhat coarse. A quadrilateral mesh with spacing of 0.1 cm on the rotor surface and 0.15 cm tetrahedral mesh elsewhere was used to slightly enhance the mesh clustering near the rotor. The resulting mesh had a total number of 286K computational cells. The time step $\Delta t$ was allowed to vary such that a Courant number $Cr$ of 0.25 was maintained locally. The $Cr$ number is given by:

$$Cr = \frac{\Delta t}{\Delta x/u} \approx 0.25$$

where $u$ is the local interface velocity and $\Delta x$ is the local grid spacing. A $Cr$ number of 0.25 ensures that the time step is sufficiently small that the VOF-tracked fluid interface takes at least four sub-time steps to pass through a computational cell. For operation at 377 rad/s (3600 RPM), the resulting global time step was on the order of 30 $\mu$s. Calculations were performed using Fluent’s non-iterative time advancement (NITA) algorithm resulting in a significant speed-up in calculation time per time step. Pressure discretization used the Body Force Weighted method and pressure-velocity coupling was facilitated using the PISO algorithm. The Body Force Weighted scheme was chosen as it is recommended for most free surface flow problems and as it was observed to give better convergence results when using Fluent’s NITA solver. The typical solution time was about 100 hours per 1 second of flow time for all simulations. Because the VOF method requires a transient simulation regardless of the turbulence model and because the same grid was used for all simulations, the increased computational cost of LES as compared to RANS was not significant for the present study.

In regards to the grid density at the walls, the previous chapter introduced the parameter $y^+$ (Equation 4.1) as a dimensionless measure of the near-wall mesh. For multi-phase modeling, note that the $y^+$ value depends on which fluid (water or air) is in contact with the wall. The average $y^+$ values in liquid contact regions were approximately 30 on the housing wall and 40 on the rotor side. Thus standard wall functions (law of the wall), which are applied in Fluent for $y^+ > 30$, were used for all simulations. While the applicability of standard wall models to Large Eddy Simulations has been debated, the work presented in this chapter provides an evaluation of the accuracy of
Figure 5.1: Full mixing zone model for 4-vane geometry with selected dimensions labeled. Corresponding values are given in Table 5.1.

coarse grid LES with wall functions as compared with RANS and DES by direct comparison to actual experimental data for the annular centrifugal contactor problem.

Figure 5.1 shows the geometry for the mixing zone model. The top surface is defined as an atmospheric pressure boundary to enable the volume of air (incompressible) in the system to vary and allow the volume of liquid in the mixing zone to reach an equilibrium level depending on the operating conditions (i.e. inlet flow rate and rotor speed) and the mixing zone outlet pressure. The mixing zone outlet pressure for these simulations was calculated by assuming that the pressure at the center point of the outlet surface is simply equal to the pressure generated by the rotating air column within the separating zone (see Figure 5.2). The pressure difference at any two points (denoted by subscripts 1 and 2) in the rotating air column within the rotor can be calculated according to the Bernoulli equation for rotating flow:

\[ P_1 - P_2 = \frac{\rho \Omega^2}{2} (r_1^2 - r_2^2) - \rho g (h_1 - h_2) \]  

[5.2]
Table 5.1: Selected geometric parameters of 4-vane contactor mixing zone model as shown in Figure 5.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotor Radius</td>
<td>$r_r$</td>
<td>2.54 cm</td>
</tr>
<tr>
<td>Housing Radius</td>
<td>$r_h$</td>
<td>3.17 cm</td>
</tr>
<tr>
<td>Radius Ratio</td>
<td>$r_r/r_h$</td>
<td>0.801</td>
</tr>
<tr>
<td>Rotor Inlet Radius</td>
<td>$r_{r,in}$</td>
<td>0.505 cm</td>
</tr>
<tr>
<td>Vane Height</td>
<td>$h_v$</td>
<td>0.617 cm</td>
</tr>
<tr>
<td>Vane-to-rotor Gap</td>
<td>$h_{gap}$</td>
<td>0.159 cm</td>
</tr>
<tr>
<td>Mixing Zone Height</td>
<td>$h_m$</td>
<td>8.13 cm</td>
</tr>
<tr>
<td>Inlet Bottom Height</td>
<td>$h_{in}$</td>
<td>7.00 cm</td>
</tr>
<tr>
<td>Inlet Diameter</td>
<td>$d_{in}$</td>
<td>0.63 cm</td>
</tr>
</tbody>
</table>

Figure 5.2: Sketch of the annular centrifugal contactor with labeled points used for calculating the relative outlet pressure. Figure modified from Leonard et al. 2002.\textsuperscript{[22]}
in which $\rho$ is the mass density of air, $\Omega$ is the rotational speed of the rotor, and $g$ is the acceleration due to gravity. As noted on Figure 5.2, if we choose point 1 to be the less-dense phase rotor outlet (which is assumed to be always open to the atmosphere for single liquid operation below the zero-point flow rate), it is possible to calculate the pressure at the center point on the rotor inlet (point 2). For a rotation rate of 377 rad/s (3600 RPM) the relative pressure at the rotor inlet is found to be slightly negative ($>-100$ Pa). For this set of simulations, the outlet pressure was set equal to a spatially constant value of $-53.6$ Pa. This is the value obtained for point 1 having a radius equal to the rotor radius (2.54 cm). As was noted in Section 3.2.1 the actual radius for the light phase outlet port for the CINC V-2 contactor is larger than the radius of the lower section of the rotor; consequently, the pressure setting was corrected to account for this in the subsequent simulations presented in the next chapter. Actual measurements of the pressure at the center point of the rotor inlet have also been performed and are presented in Section 6.3.1. It was found that this method gives a reasonably accurate value for the pressure at the rotor inlet center point for the 4-vane geometry.

The simulations were initiated from rest with a stationary water level approximately 1.5 cm above the rotor bottom and were allowed to run for several seconds of flow time until the liquid volume reached a steady-state level (the equilibration procedure is described in Appendix D). Time averaging over 0.5 s of flow time was performed for all three turbulence methods. All simulations were done for the same conditions as the experimental measurements to which they will be compared, that is, a total mass flow rate of 0.01 kg/s (0.005 kg/s at each inlet $\approx 600$ ml/min) and a rotor speed of 377 rad/s (3600 RPM).

5.2 Mean Flow Field from CFD

The time-averaged flow field obtained from the LES simulations will be described first as it helps lend a visual picture to the quantitative data that will be presented in the next section. Figure 5.3 shows the time-averaged velocity vectors within a vertical cross-sectional plane—that is, only the radial and axial mean velocity components are included. This highlights the presence of a stable Taylor-Couette cell just above the rotor bottom in which the fluid is moving upward at
Figure 5.3: In-plane time-averaged velocity vectors on a vertical cross-sectional plane. Vectors are colored by mean axial velocity. Only the flow in the lower portion of the model at one side of the rotor is shown.

the rotor and downward at the housing wall. This is consistent with the flow patterns observed in previous single-phase contactor simulations[116] (Section 4.1). Above this height at the upper edge of the Taylor-Couette cell where the flow is directed radially outward, the free surface appears to dominate the flow and prevent the formation of any other stable Taylor-Couette vortices in the liquid phase.

Figure 5.4 shows that below the rotor there are large swirling vortices within each section between vanes in which each vortex is swirling in the direction of rotor rotation (counter-clockwise). Some slight asymmetry is apparent between the regions directly adjacent to the inlets and the other two regions. For the two opposing sections nearest the inlets, the center of each vortex appears slightly shifted towards the forward rotational direction and the vortex is somewhat less compact and circular as compared to the two regions not adjacent to the inlets. The velocity magnitude at the outside wall is also slightly higher for the regions adjacent to the inlets. This results in an eye-shaped crossing flow pattern at the axis of the rotor with flow exiting each vortex in a direction parallel to the forward vane and joining the flow within the adjacent region.
Figure 5.4: Time-averaged velocity vectors within a horizontal plane under the rotor at the mid-vane height. Vectors are colored by mean velocity magnitude. Note that the tangential flow inlets are not in the same plane as the vectors (see Figure 5.1), but are shown to give their position relative to the vanes.

5.3 Fluid–rotor Contact and Annular Liquid Height (ALH)

Figure 5.5(a) shows a snapshot of the instantaneous water volume fraction $\phi$ (fraction of the given cell that is water) on the rotor side and a vertical cross-section. The air–water interface is also shown ($\phi = 0.5$, green) providing a visualization of the free surface flow in the mixing zone. It is evident that the fluid rotor contact (areas on the rotor side that are red) is not continuous. This is also clear from Figure 5.5(b) which shows the time-averaged water volume fractions. There is continuous contact between the liquid and rotor for only a height of about $1 \cdot \Delta r$ above the rotor bottom. Beyond this point contact is intermittent in both space and time although there appear to be some circumferential bands where contact can be as high as 25%.

It was also observed that the liquid height in the annulus varies in time; in fact, it was found that the ALH actually oscillates at near constant frequency and magnitude. The ALH of Figure 5.5(a) is at an intermediate value for a time where the ALH is increasing from the minimum. This oscillating flow behavior will be discussed in a later section as the frequency and magnitude of oscillation provide valuable points of quantitative comparison between experiment and simulation.
Figure 5.5: Instantaneous (a) and time-averaged (b) contour plots of water volume fraction $\phi$ for the four-vane mixing zone geometry. In (a) the air–water interface is also shown ($\phi = 0.5$, green).

5.4 LDV/CFD Comparison

This section will present a comparison of the mean and root-mean-squared (RMS) tangential and axial velocity profiles as measured by LDV with those calculated from the CFD simulations using the three different turbulence modeling schemes.

5.4.1 Mean Velocity

The mean tangential and axial velocity components are plotted in Figure 5.6 where (a)–(d) are plots of the mean tangential velocity at the four different axial positions (with their relative position shown in the insets) and (e)–(h) are the corresponding mean axial velocity plots. The time-averaged results from the CFD simulations are also plotted. As one indicator of the relative consistency
of the experimental measurements, intersecting points from a data set of separate particle image velocimetry (PIV) measurements on a vertical plane (perpendicular to the LDV measurement lines) are also shown. The complete PIV data will be presented later in Section 5.7.1 and compared with simulations in the following chapter. As expected, the tangential velocities are an order of magnitude larger than the axial velocities except for in the vane region. The formation of a stable Taylor-Couette cell (as seen previously in Figure 5.3) can be seen in Figure 5.6(f) in which the flow is upward near the rotor and downward near the housing wall. The CFD models seem to slightly overpredict the height of this rotational cell, however, in that the predicted flow (at least for the LES and DES models) still has a positive axial component near the rotor for the \( z = 0.61 \) cm position (Figure 5.6(g)) whereas the data show a slightly negative axial velocity near the rotor evidencing the start of what would be an upper Taylor-Couette vortex which rotates opposite this lower one. This discrepancy was related to the error in the radius of the light phase outlet used for specification of the outlet pressure as noted above which resulted in a slightly too large equilibrium volume of liquid in the mixing zone (and a higher ALH); this was corrected in the simulations presented in the following chapter.

Aside from the \( z = 0.61 \) cm height, all of the computational models capture to some degree the main flow characteristics for both velocity components at axial heights above the rotor bottom. However, the LES calculations appear to capture the measured values with greater accuracy. This is particularly evident for the mid-vane height \( (z = -0.46 \text{ cm}) \) measurements. The LES model is able to capture the magnitude of the downward flow near the outer wall (Figure 5.6(e)) as well as predict a maximum tangential velocity at the same point which is much closer to the measured value than either the RNG or the DES models.

### 5.4.2 RMS Velocity

The superiority of the LES method is further evident from the corresponding plots of the RMS tangential (Figure 5.7(a)–(d)) and axial (Figure 5.7(e)–(h)) velocity data and simulation results. Note that for both experiment and simulation, the RMS quantities include both the bulk variations in flow velocities caused by the free surface motion as well as the turbulence induced fluctuating
Figure 5.6: Data plots of the LDV measurements at the four different axial positions as compared to the CFD model predictions for the mean tangential velocities [(a)–(d)] and the mean axial velocities [(e)–(h)]. The radial position is relative to the rotor side and has been normalized by the gap width $\Delta r$. 
component of velocity. Again, none of the models gave very good predictions for the RMS velocity profile at the \( z = 0.61 \) cm height due to the overprediction of the height of region of continuous liquid–rotor contact and the resulting Taylor-Couette cell. At the other axial heights, the agreement between the LES prediction and measured values is significantly better than the other two turbulence modeling schemes. Interestingly, the DES model tends to severely overpredict the tangential RMS velocity component while at the same time giving results similar to LES for the axial RMS velocity. In virtually all cases, the RANS model underpredicts the actual RMS velocities.

The deviation of the LES model from the experimental values near the rotor is not surprising due to the relatively coarse nature of the computational grid (as compared to traditional LES) and the use of wall functions. It will be shown later (see Figure 6.2) that improvement in the predicted mean velocities near the rotor was obtained using a finer computational mesh (and modified outlet boundary condition) facilitated by an increase in the available computational resources. Moreover, experimental measurements near the rotor were also difficult due to the complex interactions of the free surface in this region. As set forth in Section 1.3.1, it is well known that the mixing behavior of liquid–liquid dispersions is characterized by the maximum rate of turbulent energy dissipation \( \varepsilon_{\text{max}} \).\textsuperscript{[81, 85, 90]} Unfortunately, it was not possible to experimentally measure the dissipation rate near the rotor where the area of maximum dissipations occurs due to the relatively low LDV data rate and spatial resolution in this region. However, useful estimation of the mixing behavior in the contactor can be obtained directly from the CFD simulations. For comparison with the dissipation rates of other liquid–liquid mixing systems, approximate values predicted by LES simulation are given here. These simulations of the 4-vane geometry predict a maximum subgrid dissipation rate (scaled by liquid phase volume fraction to get liquid phase contribution only) of 900 W/kg on the rotor side with an area-weighted average value of 90 W/kg over the surface of the rotor. The value averaged over the entire mixing zone volume (both phases) was 12 W/kg. Note that these are instantaneous values taken at the same flow time as Figure 5.5(a). A more complete analysis of the turbulence dissipation rate in the liquid phase and the energy imparted to the fluid by the rotor is given in the next chapter.
Figure 5.7: Data plots of the LDV measurements at the four different axial positions as compared to the CFD model predictions for the RMS tangential velocities [(a)–(d)] and the RMS axial velocities [(e)–(h)].
Figure 5.8: Plot of mean gate chord for the LDV measurements at the rotor bottom height ($z = 0.0 \text{ cm}$) comparing the LDV measurements with only water with those repeated using 25 mg/L SDS.

### 5.4.3 LDV measurements with SDS

The LDV measurements presented in the previous section were taken using entrained air bubbles as the scattering media. To explore the effect of bubble size on the consistency of the measurements, some repeat LDV measurements were made using water with 25 mg/L SDS. As a measure of the change in bubble size, Figure 5.8 gives a comparison of the average “gate chord” measured at the rotor bottom height ($z = 0.0 \text{ cm}$) for the LDV with pure water and that with the added surfactant. The “gate chord” has been defined as the product of the average fluid velocity [m/s] and the average Doppler signal time (or gate time) [$\mu$s] at a given point yielding a quantity of length with units of $\mu$m. The change in fluid particle size is clearly evident between the two measurements and shows a decrease of nearly a factor of three close to the rotor. Thus, it appears that the addition of the surfactant causes a measurable decrease in the characteristic length of the air bubbles passing through the LDV measuring volume.

Despite this substantial change in the measured length scale, the measured velocities were not altered significantly. Figure 5.9 shows the measured mean tangential velocities with both pure water and water with the surfactant as measured at the rotor bottom height. Only a slight change in
Figure 5.9: Plot of the mean tangential velocity LDV measurements along the rotor bottom comparing the LDV measurements with only water (same as Figure 5.6(b)) with those repeated using 25 mg/L SDS. The magnitude of the measured mean tangential velocity profile is evident. This gives an indication that the LDV measurements in this study may not be strongly dependent on the air bubble size.

5.5 Annular Liquid Height (ALH) Oscillations

It was observed both experimentally and through the CFD simulations that the liquid height in the annular mixing zone oscillates at steady frequency and magnitude. Experimentally, this was seen through the use of high-speed video imaging as well as with the LDV measurements. Figure 5.10 shows two snapshots separated by 0.11 s which show a minimum (a) and successive maximum (b) in ALH. The liquid height at the minimum position is easily distinguishable and appears relatively flat in the circumferential direction. The maximum is difficult to identify from the image as it extends beyond the optical quartz section. From physical observation the average magnitude of the oscillation was observed to be 1.8 ± 0.4 cm. It is also apparent in Figure 5.10(a) that there may be a second turbulent Taylor-Couette vortex that forms above the lower one during the time when the liquid is at its minimum height; however, this upper vortex breaks down as the fluid loses contact with the rotor (Figure 5.10(b)). The CFD model predicts similar behavior.
Figure 5.10: Snapshots of flow in the mixing zone of the 4-vane geometry showing a minimum [(a), $t = t_0$] and maximum [(b), $t = t_0 + 0.11$ s] of the liquid height oscillations. For reference, the rotor bottom is at $\sim1.3$ cm on the ruler. The exposure time was 500 $\mu$s as evidenced by a band of high time-averaged fluid rotor contact above the region of continuous contact (see Figure 5.5(b)).

It was possible to determine the frequency of the oscillation as observed by a spike in the power spectrum plots generated by taking a fast Fourier transform (FFT) of the time auto-correlation of the LDV data for measuring points near the outer wall where the data rate was sufficiently high. A representative power spectrum plot is shown in Figure 5.11 in which the frequency spike from the free surface oscillation is denoted and shows up at 4.85 Hz. Averaging over 24 separate frequency observations, it was determined that the mean frequency of the liquid surface oscillation for the given conditions was $4.75 \pm 0.16$ Hz.

Similarly, the magnitude and frequency of the ALH oscillation can be predicted by the CFD simulations. The predicted annular liquid height and rotor-side liquid contact area over an arbitrary 1 s period of flow time from an LES simulation of the contactor (4-vane) is given in Figure 5.12. The ALH in Figure 5.12 was determined by integrating the area of liquid contact on the
housing wall, dividing by the circumference $2\pi r_h$, and subtracting the height of the rotor bottom (0.776 cm); thus it is the circumferentially averaged liquid height above the rotor bottom. The steady oscillation of the liquid height is quite apparent. It can also be seen that the liquid height minima correspond to maximum values in the rotor contact area. In fact, the maximum contact area occurs at the instant just after the liquid height reaches its minimum. This predicted behavior was also verified by the high speed videos in which the fluid contacting the rotor is spun off the rotor.
Table 5.2: Comparison of predicted and measured values for the frequency and magnitude of liquid height oscillation.

<table>
<thead>
<tr>
<th></th>
<th>Exp</th>
<th>CFD (LES)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency [Hz]</td>
<td>4.75 ± 0.16</td>
<td>4.07 ± 0.18</td>
</tr>
<tr>
<td>Magnitude [cm]</td>
<td>1.8 ± 0.4</td>
<td>2.19 ± 0.23</td>
</tr>
</tbody>
</table>

and can be seen impinging on the outer wall just after the liquid height falls to the minimum value. For reference, the integrated fluid rotor contact area for the image in Figure 5.5(a) is 26.5 cm².

From the LES simulations, the average magnitude of the oscillations for an 8 cycle period was found to be 2.19 ± 0.23 cm which is within the range of the experimental value. As for the frequency, taking an average of the trough-to-trough time increment over the same 8 cycles we find an average predicted oscillation frequency of 4.07 ± 0.18 Hz which is somewhat lower than the measured value. This error appears to simply have been a result of the limited grid resolution for this set of simulations as it can be seen in the work of the next chapter using more refined meshing that a very accurate prediction of the oscillation frequency can be obtained. A summary comparison of experimental and simulation values for the annular fluid height oscillation are shown in Table 5.2.

While this dynamic behavior may not be surprising—the fluid contacts the rotor, is spun off, and falls back down—it is important to note that it is only observed for the four-vane housing configuration. For the eight-vane housing at the same flow conditions, the liquid height is significantly lower (< 50%) and does not exhibit the oscillations seen here. The curved-vane geometry also does not produce these liquid height oscillations though the liquid height is somewhat higher than for the eight-vane contactor. A comparison of the flow for these different vane geometries will be explored in greater detail in the following chapter.
5.6 Conclusions From Mixing Zone Model Evaluation

This portion of the overall study has presented a comparison of experimental measurements and computational modeling of the free surface flow in the mixing zone of an annular centrifugal contactor. It was found that CFD modeling using the LES turbulence simulation method even for a relatively coarse computational grid was able to qualitatively and quantitatively predict the actual dynamics of the flow in the contactor mixing zone. Comparison with LDV data showed that the mean and RMS velocities were captured with much better accuracy by LES modeling than for either RANS or DES on the same mesh. Thus, for transient modeling of the flow in the contactor using the VOF interface tracking method, it appears that greater accuracy can be obtained from LES without a significant increase in computational cost. As one purpose of the overall research study is to develop a detailed modeling scheme for use in exploring design and operational optimizations, the trade-off between computational cost and predictive accuracy is critical.

More importantly, this portion of the study has demonstrated that the velocity predictions and free surface dynamics from CFD modeling of the centrifugal contactor are experimentally verifiable. Thus, these CFD tools can be used with greater confidence to explore and explain the flow in the centrifugal contactor and provide insights into how operation might be improved. Chapter 6 presents detailed simulations based on the modeling scheme presented using VOF free surface tracking combined with LES turbulence simulation for analyzing the flow in the mixing zone for a range of different vane geometries.

5.7 Additional Experimental Observations

This section presents several additional sets of experimental data that are helpful to the general understanding of the flow in the centrifugal contactor. Simulations for comparison with experimental measurements were done primarily for the base case operating conditions as presented above; however, additional LDV and PIV data were also obtained for other conditions. This data may be useful for further validation of contactor simulations at different flow conditions.
5.7.1 Particle Image Velocimetry (PIV) Data

The flow field on the vertical laser sheet as measured in the 4-vane contactor geometry using Particle Image Velocimetry (PIV) will be discussed here. Refer to Section 3.2.4 for details regarding the experimental setup used for the PIV measurements. As noted in that section, no correction was applied to account for the curvature of the housing and consequently only the data along the vertical centerline (rotor axis) are quantitatively valid for direct comparison with simulation. Such comparison between the PIV results and simulation predictions for the standard conditions will be given in the following chapter.

The time averaged velocity field obtained from PIV analysis of the flow in the annular region is shown (as streamlines) in Figure 5.13. The position of the origin was set axially at the bottom edge of the rotor and horizontally at the axis of the rotor as delineated on the figure. The corresponding RMS velocity field is given in Figure 5.14. The trailing flow behind one of the housing vanes can be seen in the lower part of Figure 5.13. It is also evident from this figure that there is a distinct average axial height (~7–8 mm above rotor bottom) below which the flow has a clear downward component and above which the flow has a very slight but noticeable upward component; this upward flow is likely diminished by the steady oscillations of the free surface.\(^2\) This is consistent with the vector fields shown in Figure 5.3. From the velocity fluctuations (Figure 5.14), the trailing vortices behind the vane are again evident. The highest measured velocity fluctuations occur near the bottom of the rotor in the region of the plane near the rotor axis—the point where the plane is closest to the rotor. Recall, however, that the laser sheet is somewhat removed from the surface of the rotor and the velocity fluctuations at this distance are significantly less than the levels very near the rotor. Even so, this view does support the type of fluid–rotor contact predicted by the simulation and shown in Figure 5.5(b) where there is a band of continuous contact near the bottom of the rotor.

\(^2\)The consistency of these PIV measurements was also checked by repeating the measurements with the camera viewing area shifted upward; the axial height of this separation line relative to the rotor bottom was found to be consistent between the two sets of measurements.
Figure 5.13: Plot of streamlines for the time-averaged velocity field from PIV of flow in the annular region of the 4-vane contactor at 600 ml/min and 3600 RPM. For reference, the rotor bottom and axis are delineated.
Figure 5.14: Plot of RMS velocity magnitude from PIV measurements in the annular region of the 4-vane geometry.
Figure 5.15: PIV data of the mean tangential velocity (a) and mean axial velocity (b) along a vertical line even with the rotor axis for rotor speeds of 3000 RPM, 3600 RPM, and 4000 RPM. The rotor bottom is noted by the horizontal dashed line.

Quantitative PIV of the flow underneath the rotor was not performed due to the large bubble distribution and bubble–bubble interaction in this region. The general flow patterns observed experimentally in this region will be discussed in the following chapter (see Section 6.3.3).

5.7.2 PIV as a Function of Rotor Speed and Flow Rate

PIV data similar to that presented in the previous section for the base case conditions were also obtained for other flow rates and rotor speed settings as described in Section 3.2.4. All this data is from the 4-vane geometry. Only the data along the vertical line within the measurement plane that is even with the axis of the rotor are given here (vertical dot-dash line in Figure 5.13).

The PIV-measured average velocity profiles for three rotor speeds (3000 RPM, 3600 RPM, 4000 RPM) are shown in Figure 5.15. The corresponding RMS velocity profiles are shown in Figure 5.16. It is apparent from the plots of the mean velocity profiles that with increasing rotor speed the velocity magnitude increases but the overall shape of the profile (i.e. axial location of maximum tangential and axial velocities) does not change significantly. As for the velocity
Figure 5.16: PIV data of the RMS tangential velocity (a) and RMS axial velocity (b) for different rotor speeds.

fluctuations, in general a similar sort of behavior is evident although the magnitude of the change appears small though there is a clear elevation of fluctuations for the higher rotor speed.

On the other hand, changes in inlet flow rate result in slightly more complex behavior. The PIV-measured average velocity profiles for various total inlet flow rate settings (300 ml/min, 600 ml/min, 1000 ml/min) are shown in Figure 5.17. The corresponding RMS velocity profiles are shown in Figure 5.18. Two profiles are shown for the 300 ml/min flow rate setting; one is for 300 ml/min in the front inlet only (same side as PIV plane) and the other the back inlet only. No measurement was taken with an evenly distributed inlet flow (i.e. 150 ml/min in each inlet) as was the case for both the 600 ml/min and 1000 ml/min settings. Note that there is an increase in the average annular liquid height (ALH) and ALH oscillation magnitude with increasing flow rate (see Section 6.3.2). For a total inlet flow rate of 300 ml/min the annular liquid height (above the rotor bottom) was observed to be approximately 3 cm with little oscillations; for flow rates above ~300 ml/min, the ALH oscillation magnitude increases steadily. For 600 ml/min, the minimum ALH is around 3.5 cm and the max 5.3 cm. For 1000 ml/min, the minimum and maximum ALH are approximately 4.8 cm and 9 cm. The increase in the minimum ALH is directly related to an
Figure 5.17: PIV data of the mean tangential velocity (a) and mean axial velocity (b) along a vertical line even with the rotor axis for total inlet flow rates of 300 ml/min, 600 ml/min, and 1000 ml/min.

Figure 5.18: PIV data of the RMS tangential velocity (a) and RMS axial velocity (b) for various total inlet flow rates.
increase in the liquid hold-up in the mixing zone. This effect may partly explain the difference in
the tangential velocity profiles for the different flow rates. However, it does not seem to explain the
axial velocity profiles. There, the lower flow rate setting actually was found to have higher axial
velocity magnitudes.

As was seen with the rotor speed changes, the changes in the RMS velocities (Figure 5.18)
are less dramatic, although there does appear to be a general trend towards increasing velocity
fluctuation with increasing flow rate. This is in general agreement with the change in annular
liquid height. Greater liquid height results in greater fluid–rotor contact and greater turbulence in
the liquid phase.

In general, these data could be better explained by additional CFD simulations to look at the
overall flow patterns and complex fluid–rotor interactions as inlet flow rate and rotor speed are var-
ied. Understanding these effects may ultimately aid in the optimization of operational parameters.

5.7.3 LDV as a Function of Rotor Speed

Additional LDV data for the 4-vane geometry were taken for rotor speeds of 3000 RPM and
4000 RPM along with the base case value of 3600 RPM that was already plotted previously. This
additional data was taken only along the radial line at the axial height even with the rotor bottom
($z = 0.0$ cm as in Figure 5.6(b) and (f)). The mean tangential and axial velocity profiles are
given in Figures 5.19(a) and (b), respectively. The RMS velocities are given in Figure 5.20. As
was observed with the PIV measurements, increasing the rotor speed resulted in an increase in
the magnitude of the flow velocities without substantially altering the shape of the profiles. This
is particularly evident for the tangential velocity near the rotor for the 4000 RPM case. Notice
that there also seems to be a very slight enhancement of both the upward and downward flow of
the Taylor-Couette cell near the rotor bottom as rotor speed is increased (Figure 5.19 (b)) The
differences in RMS velocity profiles are not substantial except for a somewhat higher tangential
velocity fluctuation near rotor for the 4000 RPM rotor speed.
Figure 5.19: LDV data for the mean tangential velocity (a) and mean axial velocity (b) along a radial line even with the rotor bottom (as in Figure 5.6(b) and (f)) for rotor speeds of 3000 RPM, 3600 RPM, and 4000 RPM.

Figure 5.20: LDV data for the RMS tangential velocity (a) and RMS axial velocity (b) along a radial line even with the rotor bottom (as in Figure 5.6(b) and (f)) for rotor speeds of 3000 RPM, 3600 RPM, and 4000 RPM.
Table 5.3: Frequency of liquid height oscillation in 4-vane geometry as a function of flow rate (constant rotor speed of 3600 RPM) as estimated from the high-speed video images. ALH maxima and minima were approximated by direct external observation (see Figure 6.9).

<table>
<thead>
<tr>
<th>Inlet Flow Rate, ml/min</th>
<th>Frequency, Hz</th>
<th>Minimum ALH, cm</th>
<th>Maximum ALH, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>360</td>
<td>5.41 ± 0.26</td>
<td>3.0</td>
<td>3.3</td>
</tr>
<tr>
<td>600</td>
<td>4.88 ± 0.29</td>
<td>3.5</td>
<td>5.3</td>
</tr>
<tr>
<td>830</td>
<td>4.47 ± 0.17</td>
<td>4.0</td>
<td>7.3</td>
</tr>
</tbody>
</table>

Table 5.4: Frequency of liquid height oscillation in 4-vane geometry as a function of rotor speed (constant flow rate of 600 ml/min) as measured with LDV. ALH maxima and minima are average values approximated from direct external observation.

<table>
<thead>
<tr>
<th>Rotor Speed, RPM</th>
<th>Frequency, Hz</th>
<th>Minimum ALH, cm</th>
<th>Maximum ALH, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000</td>
<td>5.21 ± 0.07</td>
<td>3.1</td>
<td>4.4</td>
</tr>
<tr>
<td>3600</td>
<td>4.75 ± 0.16</td>
<td>3.5</td>
<td>5.3</td>
</tr>
<tr>
<td>4000</td>
<td>4.55 ± 0.05</td>
<td>3.8</td>
<td>7.0</td>
</tr>
</tbody>
</table>

5.7.4 ALH Oscillation (4-vane) as a Function of Rotor Speed and Flow Rate

The frequency of the liquid height oscillation was also observed as a function of rotor speed (from LDV) and inlet flow rate (from high-speed video imaging). In general, it was observed that the oscillation frequency was inversely related to the rotor speed and flow rate—that is, increasing the rotor speed results in a decrease in the oscillation frequency as too does increasing the inlet flow rate. The observed values are shown in Tables 5.3 and 5.4. In general, it appears that the change in oscillation frequency can be explained by the relationship between the mixing zone liquid volume (as observed by the minimum ALH) and the maximum fluid–rotor contact—which decreases as liquid volume decreases. For example, this effect seems to explain how the observed oscillation...
frequency changes with flow rate (Table 5.3); a lower flow rate results in lower liquid volume, less fluid-rotor contact, and consequently less momentum imparted by the rotor on the fluid resulting in a lower oscillation magnitude but a higher frequency.

For the effect of varying rotor speed (Table 5.4), the liquid volume (minimum ALH) was also seen to increase slightly with higher speed for this geometry. While one might reasonably postulate that for a given liquid height a higher rotor speed would have less fluid–rotor contact, it appears that this is more than compensated for by the greater surface velocity of the rotor resulting in a larger amount of momentum imparted on the fluid. This momentum of the fluid is translated into potential energy as the fluid is spun out and up the housing wall and then back into kinetic energy as the fluid collapses back down where it contacts the rotor again. This greater magnitude of oscillation seems to result in a lower oscillation frequency.

CFD simulations for a range of flow conditions would lend greater quantitative evidence for these proposed explanations; this would be a useful contribution of future studies based on the simulation framework that has been demonstrated here. For this current research effort, however, it was chosen to employ this simulation scheme to analysis of the effects of housing geometry changes for a given set of operational parameters. This is the focus of the following chapter.
Chapter 6

Mixing Vane Study

The previous chapter presented the results of simulations of free surface flow in the mixing zone of a model centrifugal contactor and a comparison with experimental measurements of velocity and turbulence. From this, it was shown that the modeling scheme using the Large Eddy Simulation (LES) technique for turbulence simulation gives quantitatively accurate predictions of the flow in the contactor. Based on this demonstration, additional simulations were performed to take advantage of the detailed spatial and temporal flow information generated from the CFD modeling to explore the effect of the housing vane configuration on the flow and mixing in the contactor. While it is well known that the shape and orientation of the housing vanes have a significant effect on the flow in the mixing zone and the operation of the contactor, to the author’s knowledge there have not been any detailed comparative studies of the merits of different vane configurations. Straight housing vanes have typically been used for solvent extraction operation; however, commercial centrifugal separator units manufactured by CINC employ curved housing vanes. It is vital to understand how this design modification affects the operation of the contactor, especially as these commercial ‘separator’ units are being evaluated for use in a variety of solvent extraction applications. At least one such research effort has noted that the curved vanes seem to result in poorer overall stage efficiency at low flow rates as compared to standard straight vanes.

A detailed analysis of the flow in each of three standard vane geometries—four straight vanes, eight straight vanes, and eight curved vanes—is presented here. Additionally, a similar computational analysis for a couple of variations on the 8-vane geometry are presented in Section 6.6. It is assumed that the simulation scheme—which was shown in the previous chapter to be valid for the
4-vane geometry—is equally valid for these other vane configurations. Where possible, com¬
parison with additional experimental observations were made to provide support for this assumption.
Other experimental observations of the flow in the mixing zone are also presented to support the
simulation results as well as provide valuable insight into the general characteristics of the flow for
the different vane geometries at different flow rates and rotor speeds.

6.1 CFD Model Setup

The general modeling scheme for these simulations was based on the VOF/LES simulations
presented in the previous chapter. However, a few key changes that were made to the CFD model
setup are explained in this section.

The CFD simulations were performed using Fluent 6.3. All simulations employed the Volume
of Fluid (VOF) model with piecewise linear interface construction (PLIC) and the Large Eddy
Simulation (LES) technique for simulation of turbulence. The combination of these two models
as implemented in Fluent uses first-order time discretization. The boundary conditions and set
up of the CFD simulations were the same as those used previously (600 ml/min water inlet flow,
3600 RPM rotor speed) except for a few changes. Firstly, the contact angle of the liquid on the
solid surfaces of the model was changed to 75° to better account for the actual contact angle of
water on steel (the typical material of construction for contactor units); this change had a very
minor effect on the overall predictions of the simulations as described in Appendix C. A second
important change in the model configuration, namely, the specification of the pressure distribution
on the mixing zone outlet (rotor inlet) is discussed in Section 6.1.2.

6.1.1 Geometries and Meshing

The flow in the mixing zone was analyzed for the three experimentally available vane geomet-
ries (4-vane, 8-vane, and curved vane). Additional variations to the standard eight straight vane
gallery are presented in Section 6.6. Regardless of the vane geometry, the vane height $h_v$ for
each configuration was 0.515 cm. This was corrected from the previous models to match the experimental setup. Note also that each vane type had a vane thickness of 0.159 cm (1/16”), consistent with the experimental geometry.

The 4-vane geometry used here is identical to that in Figure 5.1 and Table 5.1 (with the exception of $h_v$). The 8-vane housing geometry is similar to the four (i.e. same vane dimensions, etc.) save that there are eight housing vanes instead of four. The vane orientation relative to the inlets for the full mixing zone model of the 8-vane housing is similar to that of the simplified 8-vane geometry which was shown previously in Figure 4.1.

The curved vane geometry is shown in Figure 6.1 and the corresponding geometric quantities are listed in Table 6.1. Some of the general characteristics of this configuration were described previously in Section 4.1.3.3; these features are described in more detail here. It can be seen in Figure 6.1(a) that the vanes have a two-tiered construction. There is a section of full height ($h_1$), equivalent to the vane height for either the 4- or 8-vane geometries, that extends out to a radius $r_1$ of 2.1 cm (recall that the rotor radius $r_r$ is 2.54 cm). Beyond this radial distance, the height of the vanes is decreased by about half. Further, the vanes—of which there are eight—do not
Table 6.1: Selected geometric parameters of curved vane contactor mixing zone model as shown in Figure 6.1. Values not listed are the same as the 4-vane geometry as given in Table 5.1. The vane thickness is 0.159 cm (1/16”).

<table>
<thead>
<tr>
<th>Vane Parameter</th>
<th>Symbol</th>
<th>Value, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Height</td>
<td>$h_1$</td>
<td>0.515</td>
</tr>
<tr>
<td>Stepped Height</td>
<td>$h_2$</td>
<td>0.248</td>
</tr>
<tr>
<td>Radius of Curvature</td>
<td>$r_{\text{curve}}$</td>
<td>2.855</td>
</tr>
<tr>
<td>Radius (full height)</td>
<td>$r_1$</td>
<td>2.100</td>
</tr>
<tr>
<td>Radius (total)</td>
<td>$r_2$</td>
<td>2.855</td>
</tr>
</tbody>
</table>

extend all the way to the housing wall but end at the midpoint of the annular gap. It was shown in the simplified models of this geometry (Section 4.1.3.3) that these features allow for a band of steady tangential flow around the outer edge of the bottom of the housing and the stepped feature also generates some degree of upward flow. Specifics regarding the additional modifications to the basic eight vane geometry that were also explored are discussed later in Section 6.6.

Access to additional computational resources through a National Science Foundation TeraGrid grant (TG-ECS070009) enabled these simulations to be conducted at a higher level of grid refinement than those in the previous chapter. Specifically, it was possible to incorporate an increase in node density of a factor of nearly 3 compared to the simulations presented in the last chapter that were performed on a local Linux cluster; all the meshes used for the various geometries presented here had ~800 K tetrahedral computational cells. The grid points were refined within critical regions of the flow (i.e. the lower portion of the side of the rotor, the bottom of the rotor, and the narrow gap between the vanes and the rotor bottom); for each case, the smallest cells had dimensions of 0.05 cm and the largest 0.1 cm. Appendix E gives further details regarding the meshing schemes applied for the various geometries. Table 6.2 lists the total number of computational cells for the various models. As before, the time step was allowed to vary to maintain a
Table 6.2: Number of computational cells for the models of the various mixing vane geometries.

<table>
<thead>
<tr>
<th>Vane Geometry</th>
<th>N Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-Vane</td>
<td>797 K</td>
</tr>
<tr>
<td>8-Vane</td>
<td>829 K</td>
</tr>
<tr>
<td>Curved</td>
<td>776 K</td>
</tr>
<tr>
<td>8-Vane, vane–wall gap</td>
<td>858 K</td>
</tr>
<tr>
<td>8-Vane, ( \eta = 0.9 )</td>
<td>829 K</td>
</tr>
</tbody>
</table>

global \( Cr \) flow number of 2.0 (see Section 5.1); for these simulations the typical time step was approximately 15 \( \mu s \). The 4-vane and curved vane simulations were performed in parallel on 40 processors (3.2 MHz) and the 8-vane simulations were done on 44 processors. In general, it was found that a distribution of approximately 20,000–25,000 cells per processor was near the speed-up threshold. Similar to the previous simulations, the required computation time was approximately 80–100 hours per 1 second of flow time. More details regarding the computational scaling of Fluent on parallel systems as observed during this research project are given in Appendix A. Sample scripts that were used for batch job submission and post-processing are given in Appendix F.

6.1.2 Modification of Outlet Boundary Condition

The simulations presented in Chapter 5 applied a spatially (and temporally) constant pressure boundary condition of \(-53.6\) Pa on the mixing zone outlet. As was noted previously, this was the value computed using the Bernoulli equation for rotating flow (Equation 5.2) with the radius of the light phase outlet being equal to the rotor radius (2.54 cm). The actual radius of the light phase outlet (\( r_{org} \)) for the rotor of the CINC V-2 contactor which was used for the experiments is 3.15 cm. Using this value, the calculated pressure from Equation 5.2 (for a rotation rate of 3600 RPM) is \(-83.3\) Pa. As is shown later in Section 6.3.1, this is indeed an accurate value for the actual measured pressure at the center point of the rotor inlet for the 4-vane geometry. Initially, simulation of the 4-vane geometry (using the refined meshing outlined in the previous
section) was performed using a radially uniform $-80.0$ Pa outlet pressure. While it was found that the predicted average minimum annular liquid height decreased from the $-53.6$ Pa outlet case by about 2 mm, this was still approximately 12 mm higher than the experimentally observed value. Based simply on a hydrostatic balance of liquid heights, a 12 mm difference in liquid height (of water) corresponds to a decrease of approximately 120 Pa; thus, it was determined that the average pressure of the rotor inlet boundary must actually be $-200$ Pa in order for the simulation to match experiment.

Since it was established from experimental measurement that the pressure at the center point of this surface is $-80$ Pa (see Section 6.3.1), it was assumed that there could be a pressure profile across the inlet surface such that the pressure is indeed $-80$ Pa at the center but decreases radially such that the average pressure of the surface equals $-200$ Pa. Further, a profile of this nature has a reasonable physical explanation. It was observed from mixing zone simulations that the majority of the flow enters the rotor near the outer edge of the rotor inlet surface. This flow tendency is also likely enhanced in reality because the rotor inlet acts as a weir such that fluid entering the rotor is quickly spun out toward the outer wall of the hollow rotor. This is true of a ‘fully-pumping’ rotor in which the liquid/air free surface within the rotor has a radial position greater than the radius of the rotor inlet (by design) in order to help pump fluid into the rotor. It has been observed experimentally that increasing the radius of the rotor inlet increases the height of liquid in the annular region.\[39] This likely occurs due to a decrease in the magnitude of negative pressure at the rotor inlet and a flattening of the radial pressure profile.

For the simulations presented here, a parabolic pressure profile $P(r)$ of the form:

$$P(r) = C_0 + C_1 \cdot r^2$$

$$C_0 = -80 \text{ Pa}$$

$$C_1 = -1.44 \times 10^7 \text{ Pa/m}^2$$

was applied to the mixing zone outlet pressure boundary. A parabolic profile was chosen as this is the form for static pressure head in ‘rigid’ rotation. The coefficients $C_0$ and $C_1$ were determined such that the pressure at the center point ($r = 0$) is $-80$ Pa and the average pressure obtained by integrating over the entire surface is $-200$ Pa. For this profile, the minimum pressure of $-448$ Pa
occurs just at the outer edge of the rotor inlet \((r = 0.505 \text{ cm})\). It was chosen to use this same outlet boundary pressure profile for each of the simulations of the different vane geometries performed in this work. This was based on the assumption that the negative pressure generated at the rotor inlet is governed primarily by the flow within the rotor and is not a strong function of the mixing vane geometry. The limitations of this assumption are discussed more in the presentation of the actual pressure measurements (Section 6.3.1). The code for this boundary profile is given in Appendix F along with a few sample scripts that were used for Fluent batch job submission and post-processing of data files.

### 6.2 Additional Comparison with Velocity Data

The main purpose of the simulations in the previous chapter were to demonstrate the validity of the computational modeling scheme and aid in the selection of the most appropriate turbulence modeling method through direct comparison with experimental data. In order to demonstrate the improved accuracy of these more refined-grid simulations, comparison with the laser Doppler velocimetry (LDV) measurements and the previous simulations (LES) are shown here. Additionally, quantitative comparison with experimentally measured velocity profiles from particle image velocimetry (PIV) are also given. Again, the standard operating conditions of 600 ml/min and 3600 RPM are used. Averaging of the equilibrated simulations was done over 1 s of flow time.

#### 6.2.1 Comparison with LDV Data and Previous Simulation

Figure 6.2 and Figure 6.3 give plots of the average and RMS velocity profiles in the annular region as obtained from the current simulations compared with experimental data from LDV. This LDV data is the same as was shown previously in Figure 5.6 and Figure 5.7. The profiles obtained from the LES simulations of the 4-vane geometry presented in the previous chapter are also included for comparison. It is evident that there is an improvement in the accuracy of the current CFD simulations with more refined meshing. Ideally, one would like to refine the mesh as much as necessary to achieve a grid independent solution; however, as noted in the discussion of the VOF model (Section 2.3.1) this is not feasible for the given computational problem due to the violent
Figure 6.2: Plots of the LDV measured mean velocities for the 4-vane geometry at the four different axial positions (relative location noted by inset images) as compared to the current CFD simulation predictions (N=797 K) and those from Chapter 5 (N=286 K, see Figure 5.6). The radial position has been normalized by the annular gap width $\Delta r$. 
Figure 6.3: LDV-measured and CFD-computed RMS velocity profiles for the 4-vane geometry at the four different axial positions (location noted on inset images). The RMS values from CFD include both the calculated time variation and the contribution from the sub-grid turbulent kinetic energy $k$. 
free surface motion and bubbly flow within the mixing zone of the contactor. Consequently, the improved accuracy shown here is not unexpected. In particular, the slope of the tangential velocities near the rotor are more accurately captured with the current simulations. Also, it can be seen that there is improvement in the predictions of the flow at the $z = 0.61$ cm height, particularly for the axial velocity. This improvement is primarily due to more accurate prediction of the absolute magnitude of the annular liquid height due to the modified outlet pressure profile. In Figure 6.2(g) it can be seen that the height of the lower Taylor-Couette cell (denoted by upward flow near rotor in Figure 6.2(f)) is better predicted and there is downward flow near the rotor in the simulation at the $z = 0.61$ cm height.

The annular liquid height predictions for the various geometries are compared later (see Table 6.3). For the 4-vane geometry, a significant improvement in the predicted liquid height oscillation frequency was also observed with the current simulations. An average oscillation frequency of $4.74 \pm 0.9$ Hz was predicted from these simulations which is very consistent with the value of $4.75 \pm 0.16$ Hz obtained from LDV measurements (see Table 5.2).

### 6.2.2 Comparison with PIV Data

Subsequent to the simulations presented in the previous chapter, full analysis of the particle image velocimetry (PIV) data was performed. All the data covering a range of rotor speeds and inlet flow rates was given in the last part of Chapter 5. This data provides another method of evaluating the quantitative accuracy of these CFD simulations of the free surface flow in the contactor mixing zone.

Figure 6.4 shows a comparison of the simulation results (solid line) and the PIV-measured mean tangential velocity along the horizontal line at the rotor bottom for the acquired velocity field shown previously in Figure 5.13. This figure is included here simply to demonstrate the window curvature effect that was mentioned in Section 5.7.1 which causes an artificial outward deflection of measured PIV data away from the rotor axis.\(^1\) As was pointed out previously, due

\(^1\)Theoretically, it should be possible to correct the data such that the points collapse inward (and onto the simulation predicted values); however, this was not possible due to a lack of the necessary details regarding the orientation and setup of the camera (i.e. effective lens focal length, distance between camera plane and measurement plane, etc.)
Figure 6.4: Comparison of PIV data and CFD simulation for the mean tangential velocity along a horizontal line even with the rotor bottom showing the outward deflection of the experimental data away from the rotor axis (vertical dot-dash line) due to housing curvature effects.

to these curvature effects, only the experimental data along the axis of the rotor (vertical dot-dash line) are used for quantitative comparison between experiment and simulation.

A comparison of the mean tangential and axial velocity profiles along this vertical line are shown in Figures 6.5(a) and (b), respectively. The agreement between the experimental data and simulation predictions for the tangential velocity is remarkably good (Figure 6.5(a)). The maximum tangential velocity has a very comparable magnitude though it occurs at a slightly lower axial height. Such is also the case for the axial velocities (Figure 6.5(b))—the magnitude of the maximum value is comparable but occurs at a somewhat lower height than the measured profile. The experiment evidenced a maximum downward flow velocity at approximately 0.25 cm above the rotor bottom whereas the CFD-predicted value occurs at 0.25 cm below the rotor bottom. In general, the comparison is good and provides further support for the accuracy of these CFD simulations of the free surface flow using LES turbulence simulation.
6.3 Experimental Observations

6.3.1 Pressure Measurements

It was recognized at a very early stage in the overall design of this research effort that it would be useful to divide the contactor model into two separate models for the two regions of the contactor. Accurate specification of the boundary between the two regions, particularly the outlet of the mixing zone model, has been a continual point of consideration. In general, it had been previously assumed that the pressure at the rotor inlet is primarily governed by the flow in the rotor—that is, the flow is \textit{pulled} into the rotor by a negative pressure rather than \textit{pushed} in by the force of the flow on the vanes. As simulations proceeded, the validity of this assumption became somewhat unclear and therefore physical measurements of the pressure at the rotor inlet were conducted to provide some insight into the characteristics of this region and aid in the boundary value specification. Details regarding the experimental setup for these measurements is given in Section 3.2.5. Measurements were conducted over a wide range of flow rates (for a constant rotor speed of 3600 RPM) and rotor speeds (for a constant flow rate of 600 ml/min) for each of the three available vane plates.
The measured pressure as a function of rotor speed is shown in Figure 6.6 along with the Bernoulli equation (Equation 5.2). For the 4-vane geometry, there is good general agreement with the Bernoulli equation and thus it appears that the flow is indeed predominately ‘pulled’ into the rotor by the negative pressure of the rotating column of air in the rotor. For the other vane configurations, however, there are varying degrees of positive deviation from the pressure predicted by Equation 5.2. Consequently, it appears that there is also some degree of forcing of the flow into the rotor by the vanes which elevates the pressure relative to that predicted by the Bernoulli equation. Moreover, it was observed that abrupt changes in the annular liquid height were accompanied by changes in the measured pressure. This can be seen in the sudden change in pressure for the curved vanes at approximately 3400 RPM. Below this speed, there was a sharp decrease in the liquid height as the flow switched abruptly from an ‘expanded’, large void flow to a ‘collapsed’, bubbly flow. Incidentally, there is also a visibly noticeable transition as a function rotor speed for the 8-vane geometry which was observed to occur at approximately 4000 RPM although there did not appear to be an obvious effect of this in the pressure data.

Similar behavior can be observed as a function of flow rate (Figure 6.7). Again, the 4-vane
Figure 6.7: Measured rotor inlet pressure as a function of flow rate for the three different vane geometries. Rotor speed is 3600 RPM.

The 4-vane geometry is ‘well-behaved’ relative to the value given by the Equation 5.2 (−83.3 Pa). Note also that over the entire range of flow rates for the 4-vane geometry there is a continuous rise in the ALH (and ALH oscillation), but no change in the overall flow pattern (this is described more later, see Figure 6.9). Such is not the case for either the 8-vane or the curved vane geometries. Both experience a dramatic flow transition as the flow rate goes from high to low (or visa-versa). This transition occurs at ∼750 ml/min for the curved vanes as can be seen in pressure measurements shown in Figure 6.7. The 8-vane geometry also experiences a similar transition, although the transition point was observed to vary over a relatively wide band of possible flow rates (∼350–600 ml/min). Note that the apparent transition for the 8-vane geometry in Figure 6.7 that occurs at ∼600–650 ml/min was not accompanied by an observable flow structure change. For this case, the transition to expanded flow did not occur until about 350 ml/min. The discontinuity observed in the pressure data for this case may have been the result of a change in flow structure under the rotor that was not visually observed but occurs at a higher flow rate than, and is perhaps a precursor to the overall transition to expanded flow.
In general, for the ‘low’ end of the flow rate range (i.e. below the transition point) the flow in both geometries is an open type flow characterized by a higher ALH but with large voids within the flow and a distinct ‘separation line’ approximately 0.5 cm above the bottom of the rotor. Above the transition point, the flow collapses down to a more compact flow characterized by a dense bubbly appearance. These ‘expanded’ and ‘collapsed’ flow patterns can be seen for the curved geometry at the 600 ml/min and 830 ml/min settings as shown later in Figure 6.8. It was also observed, particularly for the 8-vane geometry, that there is a region of operation where the flow pattern becomes unstable and at times even experiences a steady alternation (at ∼1 Hz) between the two flow types for certain flow conditions. It was not possible to determine if there is a liquid volume change between the two flow types; however, it is thought that there is not a change in volume only in overall void distribution. This open (or ‘expanded’) flow structure is described more in the following section.

It is clear that there are effects due to the vane geometry which impact the pressure at the rotor inlet. As intuition might imply, the pressure in this region is indeed somewhat affected by both the flow downstream (in the rotor) and the flow upstream in the vane region under the rotor; it seems reality is not as free of complexities as one might hope. Even so, it does appear that the 4-vane case corresponds quite well to the previous assumptions of downstream dominated pressure. These effects for the other vane configurations are not fully understood and more exploration in this area in the future could aid in the development of a rigorous method for specifying the pressure at this boundary for a given rotor speed, flow rate, and geometry. Ultimately, it may be that division of the contactor flow area at this point is not advised for some configurations due to the strong coupling between the inner and outer regions and a combined modeling approach is needed. Initial attempts at a combined model have not yielded a valid approach. However, for the 4-vane geometry this does not appear to be a significant issue as it follows the prediction of the Bernoulli equation quite well and exhibits little flow rate dependence.

Lacking a better, more generalizable method for specifying this boundary condition across a variety of vane geometries, it was chosen to apply the same rotor inlet boundary pressure profile given in Equation 6.1 to the simulations of each of the various vane geometries. Comparison of
the results of these simulations with experimental observations for the 8-vane and curved vane configurations will help in understanding the impact of this approximation for these cases. Note, however, that it was seen previously from a 4-vane case in which the radially uniform pressure setting was changed from \(-53.6\) Pa to \(-80.0\) Pa—a difference approximately equal to the difference between the measured pressure of the 4-vane and the curved vane geometries for the given conditions—that the effect on the overall annular liquid height was minimal (\(\sim 2\) mm decrease in average ALH) although there was a noticeable decrease in liquid hold-up volume (\(\sim 15\%\)). As will be shown by the results of the simulations, the differences in mixing behavior for the various vane configurations are much more than 15% and therefore the observed trends are considered valid despite this potential uncertainty due to the outlet pressure specification. Using the accompanying experimental observations to take these limitations into account and aid in interpretation the simulation results, it is possible to use the detailed information from these CFD simulations to provide a valid and valuable means of comparative analysis for the flow and mixing in the various housing vane configurations as a guide to contactor design.

### 6.3.2 Flow in Annular Region

A comparison of the flow in the annular region for each of the three standard vane cases is given here. High-speed imaging of the flow in this region was very useful in observing the differences in flow resulting from the different vane designs. Figure 6.8 shows a composite of snapshots taken from high-speed video imaging of the flow in the mixing zone at several flow rates for each of the three standard geometries. Snapshots were taken at the ALH minimum (maximum contact area) for the 4-vane and curved vane geometries which both have liquid height oscillations (the curved vane much less so). There are very noticeable differences in annular flow characteristics for the three different vane configurations.

The 4-vane geometry tends to have a significantly higher liquid level than the others and it was observed that the minimum ALH (as is shown in the figure) for this configuration increases with flow rate. Additional observations of the annular liquid height for this geometry were made over a wide range of flow rates and are plotted in Figure 6.9. From this figure it is apparent that not only
Figure 6.8: Snapshots from high speed imaging (1000 Hz, 500 µs exposure) of the flow in the annular region. The rotor speed was 3600 RPM. The rotor bottom is at approximately \( \sim 1.3 \) cm on the ruler.
Figure 6.9: Annular liquid height observations as a function of flow rate for the 4-vane geometry. All flow rates were equally distributed between the two inlets. Error bars denote the standard deviation of a number of repeat observations. The horizontal dashed lines show the position of the bottom of the inlets (7 cm) and the extreme top of the mixing zone (~9.25 cm).

does the minimum ALH increase with increasing flowrate as can be seen in Figure 6.8, but the ALH oscillation magnitude also increases. The frequency of this oscillation was discussed previously in Section 5.7.4 and it was seen from the additional data presented there that changes in frequency were inversely proportional to changes in magnitude (i.e higher frequency for lower magnitude oscillation). Both of these in turn seem to be directly driven by the change in the overall liquid level; an increase in liquid level leads to an increase in oscillation magnitude and a corresponding decrease in frequency.

The 8-vane geometry has a relatively low liquid level that does not vary significantly with flow rate. This is consistent with observations made previously by others.\textsuperscript{[22]} As noted above in the context of the pressure measurements, this geometry also experiences a flow ‘expansion’ at low flow rates. This transition was found to be somewhat variable, occurring at slightly different flow rate settings on different days. It may have been a function of how warm the contactor
unit was since it was observed that the expanded flow type (virtually identical in appearance to the flow structure in the curved vane image at 300 ml/min in Figure 6.8) was steady for flow rates up to \(\sim 600\) ml/min just after the unit was started up but occurred only for low flow rates \(\leq 400\) ml/min after the unit was warm. As seen in Figure 6.8, the collapsed flow type was stable down to 360 ml/min during the high-speed imaging of this geometry. This collapsed flow structure had a very low liquid height (\(\sim 1\) cm above the rotor bottom) with substantial entrainment of air and a bubbly appearance.

Quite similar to the 8-vane geometry, the curved vane housing also evidences a flow pattern transition which occurs above \(\sim 750\) ml/min as was mentioned previously. This transition is indeed apparent for the range of flow rates shown in Figure 6.8. For the highest flow rate setting (830 ml/min), the flow is similar to the collapsed structure in the 8-vane geometry save that the liquid level is somewhat higher within the curved vane housing. For the two lower flow rate settings, the flow is ‘expanded’ with a relatively stable separation line (evidenced by the cloudy horizontal band) at \(\sim 1\) cm above the bottom of the rotor. It appears that this band marks the region of highest fluid–rotor contact where the fluid is spun out from the rotor and impinges on the housing wall. Above this band there is a continuous free surface with little contact with the rotor. Below this band there seems to be very intermittent fluid–rotor contact and large voids.

This flow behavior was explored in more detail experimentally with a very limited set of observations of the identical ‘expanded’ flow structure in the 8-vane geometry using a vertically oriented laser sheet. These observations were for settings of 600 ml/min and 3600 RPM and during a period when the expanded flow type was stable for these conditions. A snapshot of the annular flow illuminated by the laser sheet is given in Figure 6.10. The inset shows the orientation of the laser sheet. The bright field in the upper left is generated by light scattering from the high concentration of small bubbles in a ring near the housing wall marking the ‘separation line’ as was seen previously for the curved vane images in Figure 6.8. As described above, this image indeed shows a region on the side of the rotor where the liquid appears to be in consistent contact with the rotor surface. This author has chosen to refer to this band as the ‘separation line’ as it appears to demarcate the location of high fluid-rotor contact and high radial flow somewhat analogous to that
Figure 6.10: 10 $\mu$s exposed image of the flow in the annular region illuminated by a laser sheet (see inset). The approximate location of the rotor and one visible vane are outlined. Flow is from right to left.
Figure 6.11: Simplified sketch of the ‘expanded’ flow structure seen in the 8-vane geometry. Similar structure was seen in the curved vane geometry as well.

seen in the simplified contactor models (e.g. Figure 4.5). Above this band, a liquid/air free surface was consistently present for all the laser sheet images taken (~50) demonstrating the lack of fluid–rotor contact in this region. Below this horizontal band of contact, there were large air voids generated from the intermittent fluid–rotor contact. A cross-section sketch of what this expanded flow structure seems to look like is shown in Figure 6.11. While this detailed exploration was for the ‘expanded’ flow structure in the 8-vane geometry it is likely to be the same for the ‘expanded’ flow structure of the curved vane geometry as seen in the lower two flow rate settings in Figure 6.8.

6.3.3 Flow Under the Rotor

For the 4-vane and 8-vane housing geometries, a window was placed in the vane plate to observe the flow in the region between vanes underneath the rotor. The same set-up used for particle image velocimetry (PIV) as described in Section 3.2.4 was used for imaging of the flow in this region. Due to the relatively large bubble sizes, these were not used for quantitative information, but rather simply to observe the general flow patterns. Some PIV-processed flow fields at the standard conditions in the 4-vane and 8-vane geometry are given later in Section 6.4.2. Composite images of the flow under the rotor for each of these geometries at the nine different combinations of three
flow rates and three rotor speeds are shown in Figures 6.12 and 6.13 for the 4-vane and the 8-vane geometries, respectively. The snapshots shown in the figures were chosen from among the 50–100 images obtained at each setting and are representative of the flow at the given conditions. For both geometries, there is flow rotation in the clockwise direction (see Figure 6.17 below for processed vector fields of the standard conditions).

For the 4-vane geometry (Figure 6.12), it appears that the effect of flow rate is much more significant than rotor speed for the ranges explored here as can be seen by the general decrease in bubble size with increasing flow rate. Recall from Figure 6.9 that the liquid level increases with increasing flow rate. For the lowest flow rate setting, the bubble size distribution is much larger and there is a relatively stable large bubble that is maintained at the center of a large vortex region (clockwise rotation). It also appeared that the size of this central bubble increased slightly with rotor speed as the rotational speed of this vortex also increased, stabilizing the void. As flow rate is increased, the corresponding increase in liquid level was accompanied by an increase in rotor contact resulting in higher turbulence as evidenced by the shrinking bubble size. The large bubble under the rotor, which was relatively stable for the lowest flow rate, became unstable at higher flow rates and was observed to be sporadically generated, undergo distortion, and then become broken into several smaller bubbles. For the highest flow rate tested (1000 ml/min), the average bubble size appeared to be quite small (< 250 µm); however, in general it appeared that the higher rotor speed was accompanied by larger air pockets near the rotor surface (the underlying ‘ripples’ in these images). Assuming that the air bubble size is directly related to the degree of mixing and turbulence near the rotor, it appears that these images support the general conclusion made previously that there is better mixing for higher liquid levels.

For the 8-vane geometry (Figure 6.13), the combined effect of the rotor speed and flow rate is more complex. In general, it appeared that the type of annular flow structure (expanded or collapsed) which was stable for the given combination of flow rate and rotor speed had the biggest effect on the characteristics of the flow observed under the rotor. For example, the collapsed flow

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2Only a narrow range of rotor speeds (3000–4000 RPM) was explored because in general the rotor speed is determined by the high degree of phase separation needed within the rotor and therefore low rotor speeds are typically not used.
Figure 6.12: Flow under the rotor for the 4-vane geometry as a function of flow rate (columns) and rotor speed (rows).
Figure 6.13: Flow under the rotor for the 8-vane geometry as a function of flow rate (columns) and rotor speed (rows).
structure was stable for each flow rate condition at the lowest rotor speed setting and the flow is similarly very bubbly for all flow rates with perhaps a slight decrease in average bubble size for the highest flow rate. At the middle rotor speed, the expanded flow structure became stable at the lowest flow rate and the effect on the entrained air bubble size is stark. The same structure was stable for both the low and middle flow rate settings at 4000 RPM. It was not specifically recorded what type of flow structure was present for the other conditions (mid and high at 3600 RPM and high at 4000 RPM), but judging from the appearance of the flow it may have been some unstable combination of the two types.

### 6.4 Comparison with Simulations for the Base Conditions

The previous section presented experimental observations over a range of rotor speeds and flow rates. This section looks only at the results from the base case settings (600 ml/min, 3600 RPM) for which detailed simulations were conducted for each of the geometries.

#### 6.4.1 Flow in the Annular Region

Figure 6.14 shows time-averaged images of the flow at 600 ml/min (300 ml/min in each inlet) and 3600 RPM as viewed from the side for each of the three cases (flow is from right to left). These are the same conditions for the middle row of Figure 6.8. For these time-averaged images (averaged over 2.5 s) it is easier to get a good overall picture of the flow in the annular region. Again, the differences in annular liquid height between the three vane types are very apparent.

The computational simulations for each of the three standard vane configurations were able to accurately capture the same trends in annular liquid height as seen from the time-averaged liquid volume fractions on the housing wall shown in Figure 6.15. The specific values for the CFD-predicted and experimentally observed annular liquid levels are given in Table 6.3. The ALH was extracted from the simulations in the same manner as outlined in the previous chapter—taking an integral of the water volume fraction over the housing wall area, dividing by the circumference of the housing (\(2\pi r_h\)) and subtracting off the height of the rotor bottom—however, in this case the resulting ALH values were then also corrected to eliminate the spurious ‘liquid height’ added by the
Figure 6.14: Time-averaged images for the flow in the annular region for the 4-vane (a), 8-vane (b), and curved vane (c) geometries. Each image is an average of those taken at 100 Hz over 2.5 s of flow time (250 images). The rotor bottom is at ~1.3 cm on the ruler.
Figure 6.15: Time-averaged water volume fractions in the annular region from CFD for the 4-vane (a), 8-vane (b), and curved vane (c) geometries.

Table 6.3: Comparison of experimentally observed and simulation predicted annular liquid heights above rotor bottom (at 3600 RPM and 600 ml/min).

<table>
<thead>
<tr>
<th>Vane Type</th>
<th>Experiment</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ALH min, cm</td>
<td>ALH max, cm</td>
</tr>
<tr>
<td>4-Vane</td>
<td>3.50 ± 0.34</td>
<td>5.28 ± 0.26</td>
</tr>
<tr>
<td>8-Vane</td>
<td>1.1</td>
<td>–</td>
</tr>
<tr>
<td>Curved</td>
<td>2.4</td>
<td>3.4</td>
</tr>
</tbody>
</table>

integrated area of the inlet rivulet running down the housing wall (which for the 8-vane geometry in particular is a significant fraction of the real liquid height) in order to provide a more consistent comparison with experiment. The experimental ALH measurements given in Table 6.3 are a visual approximation from direct observations during experimentation as well as post-experimental analysis of high-speed video images. For the 4-vane geometry in particular, a greater number of observations were made as part of several different experimental runs and therefore an average value and standard deviation are reported (same as in Figure 6.9). The 8-vane and curved vane ALH
values from experiment are only estimates of the averages as observed from high-speed imaging and a few recorded observations. In general there is good comparison between the experiments and values predicted from simulation. The liquid height prediction for the curved vane geometry is somewhat lower than the actual value; it appears that the flow structure predicted from the simulation is more consistent with the ‘collapsed’ flow type that occurs experimentally at slightly higher flow rates (see Figure 6.8). This may be due to the outlet boundary pressure specification being slightly too negative.

The real power of the computational models is in providing a means for complete visualization of the interior of the flow enabling a comparison of the fluid–rotor contact for the various vanes. Figure 6.16 shows plots of the time-averaged water volume fractions on the rotor side and a vertical cross-sectional plane (instantaneous snapshots are shown later in Figure 6.20). It is clear that the amount of fluid–rotor contact is significantly higher for the 4-vane case than either of the other two. There is a region near the bottom of the rotor where the contact is consistently high and above this there are bands where there is contact as much as 30% of the time. This is consistent with the previous results shown in Figure 5.5(b). For the 8-vane geometry (Figure 6.16(b)), there is very little contact between the fluid and the side of the rotor. Further, the volume of liquid in the mixing zone is significantly less and there are large air voids near the lower outer edge of the rotor as well as air being pulled under the rotor. Similar but less dramatic features are visible for the flow in the curved vane geometry (Figure 6.16(c)). Here also, the average fluid contact on the side of the rotor is quite low.

Another critical characteristic of the flow for evaluating operation is the steady-state liquid hold-up volume in the mixing zone. It is clear from the experimental images in Figure 6.14 that there is a significant difference in liquid volume for the three different cases. This difference is discussed further in the context of the mixing evaluation presented in Section 6.5.

### 6.4.2 Flow Under the Rotor

The flow underneath the rotor for the base case conditions will be discussed here. Experimentally, the flow under the rotor was observed using high-speed and PIV imaging as discussed
Figure 6.16: Time-averaged water volume fractions on the rotor side and a vertical annular cross-section from CFD for the 4-vane (a), 8-vane (b), and curved vane (c) geometries.
Figure 6.17: PIV processed vector fields of the flow underneath the rotor at 600 ml/min and 3600 RPM for the 4-vane (a) and 8-vane (b) geometries. The approximate location of the outer edge of the rotor is marked on the bisecting line (dashed line).

previously in Section 6.3.3 for both the 4-vane and 8-vane geometries. While the large bubble sizes in this region precluded quantitative use of PIV processed vector fields, this data is still quite informative for providing a qualitative description of the flow field under the rotor. The vector field (and corresponding streamlines) for the 4-vane and 8-vane PIV measurements are shown in Figure 6.17. For the 4-vane geometry there is a large central vortex rotating in the clockwise direction (same as rotor rotation) that is shifted slightly off-center in the forward flow direction. The center of this vortex corresponds with the location of the large voids described in Figure 6.12. For the 8-vane geometry, there is only a very weak general rotation and the majority of the flow appears to go straight up the forward vane wall towards the axis of the rotor.

The same vector fields predicted by CFD simulation are shown in Figure 6.18(a)-(c) for the 4-vane, 8-vane, and curved vane geometries, respectively. Note that the simulation geometry is a mirror image of the experiment. The predicted flow field in the 4-vane geometry is very consistent with that seen from the PIV imaging as shown in Figure 6.17(a). Again, there is flow in each of the vane regions that is rotating in the direction of rotor rotation (counter-clockwise in the model). The highest magnitudes are in the area of the forward corner of the vane region and flowing radially
Figure 6.18: Mean velocity vectors for the flow under the rotor on a horizontal plane located at the mid-vane height from simulations of the 4-vane (a), 8-vane (b), and curved (c) housing geometries.

Figure 6.19: Snapshot of the formation of a large air bubble under the rotor as viewed from below for the 4-vane simulation. The images are separated by 42 $\mu$s.

inward up the forward vane. The results from this current simulation are very consistent with those from the previous chapter (compare to Figure 5.4). The simulations were also able to capture large air bubbles underneath the rotor. These large bubbles appeared to be generated by detachment from the main free surface at the side of the rotor as shown in Figure 6.19(a) and (b). In general, large bubbles such as this were unstable in the simulations and broke up into many smaller ones soon after their formation; this is consistent with the experimental observations noted above in respect to the same conditions in Figure 6.12.
For the 8-vane geometry (Figure 6.18(b)), the overall flow magnitudes in this region are somewhat less than for the 4-vane case. Consistent with Figure 6.17(b), the highest flow magnitudes are at the outer wall and flowing radially inward on the forward vane. Note, however, that the orientation of the vanes relative to the inlet is shifted by $22.5^\circ$ as compared to the orientation in the experiment. This may have had a slight effect on the predicted flow field as compared to experiment since it is apparent that there is a small degree of asymmetry between the various vane sections with those away from the inlets having slightly higher mean velocities.

The flow under the rotor in the curved vane geometry, for which experimental observation was not possible, is shown in Figure 6.18(c). Consistent with the previous simplified models (see Figure 4.13), there is a significant amount of continuous tangential flow near the housing wall due to the gap between the vanes and the wall. There is also a peak in mean velocity just behind the outer edge of the vanes where there is some slight generation of additional turbulence. It appears that the length of the full-height section would likely have an effect on the inward radial flow of the fluid. A longer full-height section would probably result in greater radial pumping; simplified modeling of a similar geometry was done previously which also demonstrated this (see Figure 4.14). While such a full curved vane geometry was not simulated with the current modeling methods, it is likely that this system would exhibit very low liquid volumes and poor mixing.

### 6.5 Mixing Analysis: 4-Vane, 8-Vane, Curved

A great advantage of these CFD simulations of the flow in the mixing zone of the contactor is their potential for aiding in the evaluation of the mixing behavior for various alternative configurations. While in these simulations the only ‘mixing’ is that between air and water, as was explained previously it is also useful to explore the characteristics of the flow of the liquid phase and infer from this the probable liquid–liquid mixing behavior. This was discussed at length in the latter part of Chapter 1 (see Section 1.3). As outlined there, the turbulent energy dissipation rate $\varepsilon$ is a key metric for understanding and evaluating liquid–liquid mixing.
The turbulence dissipation rate is highest at the rotor side where the velocity (and its gradients) are largest. Further, for mixing within the liquid phase, the total area over which this high dissipation rate occurs (the fluid-rotor contact area) also has a substantial impact on how much energy is imparted to the fluid. Also directly related to mixing is the mean fluid residence time which can be estimated as the mean liquid volume divided by the volumetric flow rate (refer to Section 2.4). Each of these factors can be predicted from the mixing zone simulations and are discussed here.

As described previously in the context of the time-averaged plots (Figures 6.15 and 6.16) of these simulations, there are stark differences between the fluid–rotor contact and overall liquid volume for the three different vane cases. Instantaneous snapshots of the characteristic free surface flow and fluid–rotor contact from the CFD simulations of the three standard vane geometries are shown in Figure 6.20. The images shown here are from times of maximum fluid–rotor contact (minimum ALH—recall Figure 5.12). The fluid contact area on the side of the rotor over the 1 second of flow time following equilibration and during averaging for each vane system is plotted in Figure 6.21. Time zero on the plot is not the initial starting time of the simulations, but the starting time of the averaging period. The contact area plot shown here for the 4-vane geometry is generally the same as that seen previously in Figure 5.12 except that the oscillation frequency and magnitude have been improved in the current simulations as noted above. The simulation of the curved vane geometry also evidences a periodic fluctuation in contact area; however, in this case the magnitude of the oscillation is somewhat lower than the 4-vane case and the maximum amount of contact area is roughly equal to the minimum contact area for the 4-vane geometry. There is a relatively constant low value of contact area between the fluid and the rotor side for the 8-vane geometry. The average contact area for this configuration is more than a factor of \( \sim 3 \) less than the minimum area in the 4-vane system.

In order to generate a useful metric for comparison of the mixing between the different systems, it is necessary to take into account not only the magnitude of the turbulence dissipation rate \( \varepsilon \) on the rotor side, but also the area and duration of contact between the fluid and the rotor. One method for doing this is to define a mixing metric \( M_{\text{mix}} \) equal to the time average of the product of the
Figure 6.20: Snapshots of characteristic maximum fluid–rotor contact for the 4-vane (a), 8-vane (b), and curved vane (c) geometries. The upper image is a view from above showing the contact between the fluid and the bottom of the rotor.
Figure 6.21: Plot of the fluid contact area on the side of the rotor for the three vane configurations. Plots are for 1 s time period of flow averaging during steady-state operation.

Spatially-averaged sub-grid scale dissipation rate on the rotor $\varepsilon(t)$ (averaging over the liquid phase contact area only) and the contact area $A(t)$ according to the integral:

$$M_{mix,rs} = \rho \int_{t_0}^{t_1} \varepsilon_{rs}(t) \cdot A_{rs}(t) \cdot \delta \cdot dt$$

for the rotor side (subscripted as $rs$). Multiplying by the fluid (water) density $\rho$ and a characteristic length $\delta$ allows this mixing metric to have units of power [W]. For a constant time step, Equation 6.2 becomes a simple average rather than an integral.

$$M_{mix,rs} = \rho \cdot \delta \cdot \left( \varepsilon_{rs}(t) \cdot A_{rs}(t) \right)$$

While a variable time step was used in these simulations, the variation in the time step was quite small and it was found that there was <1% difference between the integral and the simple average. The simple average (and standard deviation) are used here.

A constant value of 1 mm was chosen for $\delta$ as the dissipation rate was seen to decrease nearly linearly outward from the rotor surface within this region such that the actual energy dissipation

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3In Fluent, values of the dissipation rate on a boundary surface such as this are interpolated from the nearest cell-center values.
rate within this 1 mm liquid layer on the rotor side $P_{mix}$ is proportional to $M_{mix}$.

$$P_{mix} \approx \beta \cdot M_{mix} \quad \text{[6.4]}$$

For the metric to be equivalent to the actual power dissipated in the thin liquid volume within 1 mm of the rotor surface (i.e. $\beta = 1$), an average value for the dissipation rate within this 1 mm liquid layer would be needed rather than simply taking the value at the rotor surface as was done. This is more complicated and time-consuming to do during the simulation run and therefore the mixing metric $M_{mix}$ is useful because it employs surface-averaged quantities that are more readily calculated.

In order to determine the relationship between $M_{mix}$ and $P_{mix}$ and provide a direct comparison between these two quantities, as well as to verify that this metric of comparison did not affect the trends seen for the various vane systems, the actual power dissipated in the 1 mm liquid layer (i.e. liquid contacted areas of the rotor only) out from the rotor (both on the side and bottom) was calculated for the cases where complete data sets were saved regularly during the 1 s averaging period; this was done for all of the ‘standard’ cases (4-vane, 8-vane, and curved). The calculation of the average power dissipated in the 1 mm liquid layer for each of these simulations was done via postprocessing of about 15 of the $\sim 300$ data sets spanning the entire 1 s of the averaging period for each geometry taking care to include extreme maximums, minimums, and mid-range values of rotor contact area. The instantaneous volumetric average of the sub-grid scale dissipation rate within the computational cells inside this 1 mm liquid layer was calculated for the each of the selected data sets. For the 4-vane and curved vane geometries, it was found that the actual power dissipated in the 1 mm liquid layer was 29.9 ± 1.6% of the mixing metric $M_{mix}$—that is, the constant of proportionality in Equation 6.4 was found to be $\beta_{4\text{-vane}} = \beta_{\text{curved}} = 0.30$. For the 8-vane geometry, the actual power dissipation $P_{mix}$ in the 1 mm layer was a slightly smaller fraction of $M_{mix}$ at 24.6 ± 1.9% ($\beta_{8\text{-vane}} = 0.25$). Note that these fractions were evaluated at various points over the 1 s averaging period and were found to be quite consistent over the entire range and were not themselves a function of the rotor contact area.\(^4\)

\(^4\)These percentages are valid for the given rotor speed (3600 RPM) and there may be an affect on this factor of changing rotor speed. Since these percentage values essentially depend on the radial gradient of the dissipation rate
Using these values for $\beta$, the mixing metric $M_{mix}$ is quite useful as it provides a simpler method for evaluation of the dissipation rate near the rotor during actual simulation and can be directly related to the actual power dissipation $P_{mix}$ predicted by the simulation. The values reported throughout this section are for the actual dissipation rate $P_{mix}$ as predicted from the mixing metric using Equation 6.4 and the values reported above for $\beta$ of each vane type. Sampling for the rotor side contact area and dissipation rate was done at every 20 time steps for each simulation except for the 4-vane simulation in which the dissipation rate on the rotor was not saved during simulation but was extracted from the saved data files after the simulation was complete and therefore was only sampled for every 200 time steps. In order to determine the turbulence dissipation rate for just the liquid phase contacted areas of the rotor, only the areas on the rotor surface with volume fraction $\phi$ greater than 0.5 were included in the surface average at each sampled time (this is also the initial step in the method that was used to find the cells in the 1 mm liquid layer near the rotor for determination of $\beta$). This was the process for the rotor side. For the rotor bottom, the dissipation rate was also similarly sampled during the duration of the simulation, however, the liquid contact area was not. There is minimal time variation of the contact area on the rotor bottom (subscripted as $rb$) and therefore a single time-averaged value was used such that Equation 6.3 becomes:

$$M_{mix,rb} = \rho \cdot \delta \cdot \varepsilon_{rb}(t) \cdot A_{rb}$$ [6.5]

Figure 6.22 shows a comparison of the predicted energy dissipation rate $P_{mix}$ in W as calculated via the mixing metric $M_{mix}$ using Equation 6.4. As expected from the trends in contact area observed in Figure 6.16 and 6.21, the energy dissipation in the 4-vane geometry is significantly greater than the 8-vane or curved vane. It was observed that the average (temporal and spatial) specific turbulence dissipation rate for the total liquid-contacted area of the rotor was similar for each of the various vane systems ($\sim$600 W/kg). The average dissipation rate for the rotor bottom surface only was also similar for all systems ($\sim$500 W/kg). Values for the rate on the side of the within the 1 mm layer, which would steepen with rotor speed, there would likely be a decrease in this ratio for a higher rotor speed. Incidentally, this may have been the reason for the smaller $\beta$ value for the 8-vane geometry since it tended to have slightly higher dissipation rates very near the rotor.
rotor ranged somewhat from $\sim 800 \, \text{W/kg}$ for the 4-vane to $\sim 1400 \, \text{W/kg}$ and $\sim 1200 \, \text{W/kg}$ for the 8-vane and curved vane geometries, respectively. While this difference in turbulence on the rotor side may seem dramatic and counter to the trends in Figure 6.22, the magnitude of the dissipation rate is only part of the mixing story for the free surface flow studied here—the greater the surface area over which this dissipation rate acts on the fluid, the greater the total energy imparted to the fluid, and consequently the greater the mixing. As such, the greatest difference in the energy dissipation rate as compared in Figure 6.22 was for the rotor side (where there is the greatest difference in contact area). Interestingly, the energy dissipated on the bottom of the rotor comprised the largest fraction of the overall dissipation for all but the 4-vane geometry. For the 8-vane geometry, where the contact area on the rotor bottom tended to be less, the overall dissipation rate in the bottom surface was lower. This data is summarized in Table 6.4. The mixing data from these simulations support the explanation that has been set forth throughout this study that the fluid-rotor contact, specifically on the side of the rotor, has the largest affect on enhancing the overall operation of the mixing zone. In quantitative terms, for the given operational parameters (3600 RPM, 600 ml/min) the mixing efficiency of the 4-vane geometry (as described by the energy dissipation rate near the
Table 6.4: Summary of the predicted average energy dissipation in the 1 mm liquid layer near the rotor for the 4, 8 and curved vanes.

<table>
<thead>
<tr>
<th>Vane Type</th>
<th>Rotor Side, W</th>
<th>Rotor Bottom, W</th>
<th>Total, W</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-Vane</td>
<td>0.279 ± 0.126</td>
<td>0.322 ± 0.004</td>
<td>0.602 ± 0.126</td>
</tr>
<tr>
<td>8-Vane</td>
<td>0.062 ± 0.021</td>
<td>0.209 ± 0.011</td>
<td>0.271 ± 0.023</td>
</tr>
<tr>
<td>Curved</td>
<td>0.135 ± 0.073</td>
<td>0.270 ± 0.007</td>
<td>0.405 ± 0.073</td>
</tr>
</tbody>
</table>

Table 6.5: Steady-state liquid volume, fluid residence time and air-entrainment rate for the three standard vane cases.

<table>
<thead>
<tr>
<th>Vane Type</th>
<th>Liquid Volume, ml</th>
<th>Residence Time, s</th>
<th>Entrained Air Flow Rate, ml/min (% of total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-Vane</td>
<td>52.69 ± 0.70</td>
<td>5.27 ± 0.07</td>
<td>2.11 (0.35%)</td>
</tr>
<tr>
<td>8-Vane</td>
<td>20.59 ± 0.21</td>
<td>2.06 ± 0.02</td>
<td>17.89 (2.98%)</td>
</tr>
<tr>
<td>Curved</td>
<td>35.55 ± 0.39</td>
<td>3.55 ± 0.04</td>
<td>15.64 (2.61%)</td>
</tr>
</tbody>
</table>

rotor) is approximately twice that of the 8-vane geometry and approximately 50% more than the curved vane geometry. Thus, it can be concluded that efforts at increasing the fluid rotor contact—which generally can be achieved through increasing the annular liquid height—will be the most effective at increasing the mixing efficiency of the contactor mixing zone.

As noted previously, the other critical piece to the evaluation of mixing and overall efficiency is the equilibrium mixing zone liquid volume and the corresponding mean fluid residence time. The results from the CFD simulations are shown in Table 6.5. Obviously, the increased liquid volume identified for the 4-vane geometry is directly correlated with the observation of greater liquid height and greater fluid–rotor contact. Even so, this greater liquid volume has a further compounding effect on the overall efficiency of operation; for liquid–liquid operation, not only would the fluids be more thoroughly mixed due to greater fluid–rotor contact, but the time that the
two fluids are in contact is also longer—by more than a factor of 2.5 compared to the 8-vane and 1.5 compared to curved vane.

Another indicator of the potential operational behavior of the various contactor housing geometries is the amount of air entrainment. It was noted previously in Section 1.2.3 that various researchers identify air entrainment as having a detrimental effect on extraction efficiency. Due to the poor fluid–rotor contact and relatively strong forcing of the fluid into the rotor for the 8-vane and curved vane geometries there is significant bubble entrainment in these configurations as observed by the pumping of air into the rotor (last column of Table 6.5). In general, all of these indicators point toward a ranking of the relative mixing zone operational efficiency for the three different vane types at the given operational settings examined here according to: 4-vane > curved vane > 8-vane.

6.6 Modifications to the 8-Vane Geometry

A couple of additional housing geometry variations based on the standard 8-vane geometry were explored using the CFD simulation methods described above.

The first alternative configuration was that of an 8-vane geometry with a vane–wall gap equal to half of the annular gap $\Delta r$. A similar 8-vane geometry with a full $\Delta r$ vane–wall gap (i.e. vanes only extended to the outer edge of the rotor) was also tried but it was found that this configuration would have extremely poor operating characteristics due to the formation of a stable vortex in the annulus. The liquid height at the outside edge of the vortex at the time it was decided to stop the simulation extended virtually to the very top of the mixing zone model despite the fact that there was essentially no fluid contact with the rotor side. This appears to have been the result of insufficient forcing of flow towards the rotor inlet and the allowance of too much residual tangential flow.

The second 8-vane variation employed a modified housing in which in the width of the annular gap was decreased such that a radius ratio $r_r/r_h = \eta = 0.9$ was achieved. For the same rotor radius of 2.54 cm the corresponding housing radius was $r_h = 2.82$ cm for an absolute annular gap width of 2.8 mm. It was noted previously in Section 1.2.3 that the CINC V-2 unit was designed
to receive an annular sleeve to actually reduce mixing and enhance throughput for operation as a dedicated liquid–liquid separator. As such, the basic CINC V-2 contactor has a relatively wide annular gap ($\eta = 0.8$). A radius ratio of 0.9 was chosen here as a representative value for more typical extraction units.

The meshing scheme for both of these geometries was similar to that for the other geometries; details are given in Appendix E. As has been the case for the simulations throughout this work, the total inlet flow rate was set to 600 ml/min and the rotor speed was 3600 RPM. The same outlet boundary pressure profile used for the simulations presented earlier in this chapter (Equation 6.1) was employed here as well. The simulation setup and solution procedure was the same as for the simulations of the other vane geometries.

### 6.6.1 Flow in the Annular Region

As with the standard 8-vane configuration, there were no significant liquid height oscillations for either of these additional cases. The time averaged water volume fractions for the standard 8-vane case as compared to these two additional variations are shown in Figure 6.23 (instantaneous snapshots are shown later in Figure 6.25). Note that the geometries have been rotated 22.5° in the clockwise direction to show the flow on the vertical plane that bisects the inter-vane regions and therefore the outside position of the vane relative to the wall is misleading (instead see Figure 6.24 in the following section). It can be seen that the addition of the vane–wall gap results in a slightly higher average annular liquid height (Figure 6.23(b)). The general characteristics of the flow are not significantly altered, though there does appear to be smaller void generation under the rotor and slightly enhanced fluid-rotor contact. For the narrow gap simulation (Figure 6.23(c)), the voids under the rotor are similar to the standard geometry. Thus it appears that this feature is primarily related to the fluid pumping ability of the vanes which is slightly scaled back by the introduction of the vane–wall gap. For the narrow gap, there are bands of contact between the fluid and the side of the rotor which indicate increased mixing for this configuration. There is also additional fluid–rotor contact where the fluid from the inlets impinges onto the rotor surface just after entering
Figure 6.23: Time-averaged water volume fractions on the rotor side and a vertical annular cross-section from simulations of the 8-vane (a), 8-vane, vane–wall gap (b), and 8-vane, $\eta = 0.9$ (c) geometries.
Figure 6.24: Vectors of mean velocity for flow underneath the rotor for the standard 8-vane case (a), 8-vanes with a vane–wall gap (b) and 8-vanes with a radius ratio of 0.9.

6.6.2 Flow Under the Rotor

Mean velocity vector fields depicting the general flow underneath the rotor in each of the 8-vane geometries are shown in Figure 6.24. Similar to what was observed with the curved vane geometry, there is a ring of high tangential velocity fluid just outside the edge of the vanes for the geometry with the addition of a vane–wall gap (Figure 6.24(b)). Also consistent with the curved vanes is a maximum in velocity magnitude at the outer edge of the vane. The narrower gap was seen to generate a velocity field under the rotor similar to the standard case but with somewhat higher velocity magnitudes and an even more prominent counter-rotating vortex along the axis of the rotor. This feature was mentioned previously in the context of simplified 8-vane geometry simulations of single-phase flow under the rotor using the LES turbulence simulation technique (see Section 4.1.5).
6.6.3 Mixing Analysis

The effects of these different geometric variations on mixing were also explored using a similar analysis as performed above for the three ‘standard’ vane geometries to calculate the energy dissipation rate near the rotor. Figure 6.25 shows characteristic snapshots of the instantaneous water volume fractions and air–water interface location within the annular region for each geometry. As with the snapshots in Figure 6.20, instances of maximum fluid–rotor contact were chosen. The increase in water volume in the mixing zone for the added vane–wall gap is apparent. The enhancement of the fluid–rotor contact, particularly on the bottom of the rotor can also be seen. For the narrow gap simulation (Figure 6.25(c)), the annular flow from the inlets has transitioned to droplet flow as opposed to the rivulet flow previously seen for all of the ‘wide’ gap cases. Though the liquid height is somewhat higher, the liquid volume is much less (see Table 6.7 below) because of the decreased flow area within the narrow annular gap. Also, the fluid contact with the rotor bottom is more like the standard 8-vane case in which there is a significant amount of air that is drawn down under the rotor.

As set forth previously, the energy dissipation near the rotor side was calculated and compared for these two additional cases via the mixing metric $M_{\text{mix}}$ and Equation 6.4 using the value of $\beta = 0.25$ obtained from the 8-vane simulation. This data is plotted in Figure 6.26 along with the original 8-vane case. It can be seen that the average energy dissipation on both the rotor side and the rotor bottom were both slightly increased with the addition of the vane–wall gap. The total average energy dissipation for this modification was over 20% greater than the standard 8-vane case. The narrow gap simulation also displayed enhanced overall energy dissipation near the rotor relative to the standard case. In this case, however, there actually was a decrease in the dissipation on the rotor bottom which was more than made up for by the enhanced contact between the fluid and the side of the rotor. This mixing data for these two 8-vane variations along with the data for the standard case are compared in Table 6.6.

The impact of these two geometry variations can also be evaluated in the context of the mixing zone liquid volume and mean fluid residence time. This data is given in Table 6.7. As with mixing, there was also an enhancement in the equilibrium mixing zone liquid volume and consequently the
Figure 6.25: Snapshots of the water volume fraction distribution (red is water, blue is air) and the air–water interface location (green) for the three 8-vane variations (standard 8-vane (a), with vane–wall gap (b), narrow annular gap (c)).
Figure 6.26: Comparison of the average (spatial and temporal) energy dissipation rate on the rotor side and bottom for the standard 8-vane geometries and the two variations. Notice that the scale is half that of Figure 6.22.

Table 6.6: Summary of energy dissipation in the 1 mm liquid layer near the rotor for the 8-vane variations.

<table>
<thead>
<tr>
<th>Vane Type</th>
<th>Rotor Side, W</th>
<th>Rotor Bottom, W</th>
<th>Total, W</th>
</tr>
</thead>
<tbody>
<tr>
<td>8-Vane</td>
<td>0.062 ± 0.021</td>
<td>0.209 ± 0.011</td>
<td>0.271 ± 0.023</td>
</tr>
<tr>
<td>8-Vane, vane–wall gap</td>
<td>0.096 ± 0.053</td>
<td>0.236 ± 0.008</td>
<td>0.332 ± 0.054</td>
</tr>
<tr>
<td>8-Vane, η = 0.9</td>
<td>0.158 ± 0.037</td>
<td>0.188 ± 0.010</td>
<td>0.346 ± 0.039</td>
</tr>
</tbody>
</table>
Table 6.7: Equilibrium mixing zone liquid volume and the corresponding mean fluid residence time for the 8-vane variations.

<table>
<thead>
<tr>
<th>Vane Type</th>
<th>Liquid Volume, ml</th>
<th>Residence Time, s</th>
</tr>
</thead>
<tbody>
<tr>
<td>8-Vane</td>
<td>20.59 ± 0.21</td>
<td>2.06 ± 0.02</td>
</tr>
<tr>
<td>8-Vane, vane–wall gap</td>
<td>31.80 ± 0.09</td>
<td>3.18 ± 0.01</td>
</tr>
<tr>
<td>8-Vane, η = 0.9</td>
<td>19.64 ± 0.24</td>
<td>1.96 ± 0.02</td>
</tr>
</tbody>
</table>

Fluid residence time for the addition of the vane–wall gap. The simulation predicts that an increase of more than 50% can be achieved for these quantities relative to the base case. This 50% increase in residence time coupled with the 20% increase in mixing observed for this case combine to result in what would likely be a significant increase in operational efficiency for this minor modification. On the other hand, the increase in liquid height for the narrow gap case is counteracted by the decrease in the annular flow area resulting in an equilibrium liquid volume slightly less than the standard case.

In general, this set of simulations has demonstrated the effect that a couple of minor variations to the standard 8-vane geometry can have on the flow in the mixing zone. An increase in mixing for the same overall liquid volume was observed for the narrow annular gap geometry. Perhaps more importantly, it was demonstrated that a very simple modification to the standard 8-vane geometry—the addition of a vane–wall gap—could result in a 22% increase in mixing efficiency and a 54% increase in fluid residence time relative to the standard 8-vane case. While this was not explored, the ‘trade-off’ for increased mixing through the addition of the vane–wall gap would likely be a decrease in the maximum throughput of the mixing zone. However, contactors are generally

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5Though it was not explored here, the vane–wall gap may also have the additional benefit in that it removes a potential area of accumulation for particulates (i.e the region where the vane meets the wall).
designed such that the maximum throughput is limited by the amount of phase separation that can be achieved for the given separation height\textsuperscript{[43]} so this decrease may not be an issue.

6.7 Conclusions from Mixing Vane Analysis

The research presented in this chapter has applied a range of experimental measurements and observations to the analysis of the flow in the mixing zone of the annular centrifugal contactor. The computational methodology that was demonstrated in the previous chapter has been further validated and applied to perform a detailed analysis and comparison of the flow and mixing for several possible housing vane configurations. In general, it has been seen that the housing vane geometry has a significant impact on the overall flow patterns, liquid height and liquid volume, fluid–rotor contact, and energy dissipation rate in the rotor region.

In terms of mixing effectiveness, two main effects were compared here, namely, the dissipation rate and the fluid residence time—which translate into greater mass transfer area and greater mass transfer time, respectively. Without the addition of detailed coupled chemical and extraction kinetics to the modeling, it is not possible to evaluate the optimum balance of surface area, contact time, and throughput. Certainly, the optimum balance would depend on the characteristics of the specific process being employed within the contactor units. Further development of the modeling scheme to include these factors would be a useful subsequent stage in the centrifugal contactor simulation effort (this and other suggestions for future direction are discussed in Section 8.4). Even so, this present comparison has shown both qualitatively and quantitatively that the mixing vane geometry has a clear impact on the overall effectiveness of the mixing zone. The conclusions obtained from the simulations were compared with a variety of experimental observations and found to have generally good predictive accuracy for the flow of water in the mixing zone. From this, it is anticipated that the experimental analysis and modeling scheme set forth here can aid in the proper selection of contactor geometry as well as lend insight into ways to improve the design of existing contactor units with minimal modification.

In particular, from this comparison it can be concluded that among the given configurations, one might select the 4-vane geometry for better low flow rate operation as it maintains a predictable
liquid volume with greater fluid–rotor contact; however, at high flow rates ($\gtrsim 1000$ ml/min) the liquid level is such that nearly the entire mixing zone is filled and there is the risk of overflow into the lower phase collector ring and phase contamination. This marks a practical upper limit for this geometry. While high flow rates were not simulated, it has generally been observed that adequate operation can be achieved with either the curved vanes or 8-vanes at high flow rates. For some processes and phase pairs, there may be issues with overmixing and emulsification. In such cases, this type of analysis could certainly aid in selecting an appropriate geometry and targeting experiments for improving operation for the flow conditions specified by the process. It has also been demonstrated that a noticeable improvement, both in terms of mixing and residence time, can be achieved through the simple addition to the standard 8-vane geometry of a vane–wall gap with a width equal to half the annular gap ($0.5\Delta r$).
Part III

Separation Zone
Chapter 7

Separation Zone Models

The research presented in the previous three chapters comprising Part II of this work focused on the analysis of the flow in the annular mixing zone. Those models had as their outlet the inlet to the rotor. This chapter analyzes the flow within the separation zone of the centrifugal contactor—that is, once the flow leaves the mixing zone and enters the rotor.

Heretofore CFD modeling techniques have not been applied to rotor design. However, a useful analytical method has been demonstrated for determining the proper dimensions of the weirs based primarily on experimental correlations and hydrostatic balance arguments. While this method has been generally quite successful for rotor sizing of contactors with an open upper weir (and the obsolete air-controlled upper weir), some experiments with closed upper weir systems such as in the CINC V-2 contactor unit have produced behavior which cannot fully be explained by the existing theoretical models. One such unexplained behavior is the elevated throughput (as compared to theory) that has been observed for large upper weir sizes in these units. This same behavior has also been observed in larger units of the same design. As has been stated previously, one of the main goals of this overall research effort is to enable better general understanding of the flow in the various regions of the contactor to not only aid in the design of future contactor units, but also provide an invaluable method for critical evaluation of current designs and support deployment of these contactors. As with the mixing zone models, the basis for the separation zone geometry simulated here is the CINC V-2 contactor unit; this product line is currently the only commercially available annular-type centrifugal contactor. Units of this design were used for various research and development efforts related to the CSSX process for cesium extraction.
and will presently be used in actual plant implementation of this process; analysis of the flow in this specific design is therefore particularly relevant.

To the author’s knowledge, there is only one other published study which attempts to apply CFD to the separation zone of an annular centrifugal contactor. That study by Padial-Collins et al. of Los Alamos National Laboratory[47] was primarily a code capability demonstration looking at the separation of the liquid mixture; their simulations employed a substantially simplified rotor geometry and did not consider the flow of air or the liquid/air interface within the rotor. Better understanding of the flow within the rotor and specifically the flow over the weirs requires full simulation of the complex rotor and weir geometries and analysis of the liquid free surface flow as done in the work presented here. Further, such hydraulic simulations can calculate important flow quantities which characterize the rotor and weirs such as the zero-point flow rate.[22,75]

While the geometry of the mixing zone is quite amenable to external observation via the housing modifications that were made to the existing contactor apparatus (see Section 3.2.1), similar detailed experimental observations such as velocity measurements for the flow within the rotor were not possible. As such, this chapter will rely primarily on the results of computational analyses with the support of certain experimental observations made within the context of the current work as well as some made by others.

7.1 Flow Within the Rotor

Unlike the mixing zone, there has been no direct observation of the flow within the contactor rotor. Consequently, the simulations presented here have utility simply as a tool for visualizing the flow in this region. Beyond this simple qualitative application, these simulations can provide a means for improving understanding of the flow in this region.

As described in Chapter 1, the role of the centrifugal contactor for use in liquid–liquid extraction is to thoroughly and efficiently mix the two process fluids and then in an equally thorough and efficient manner separate them completely. The separation occurs as the dispersion of the two liquid phases enters the hollow rotor through the inlet at the bottom. The centrifugal action of the spinning rotor forces the fluids outward and the phases separate due to their density differences
as they steadily flow upward. In principle, it is possible to think of the flow in the rotor as being analogous to that in a two-phase gravity settling trough as shown in Figure 7.1 In the case of the centrifugal contactor, however, the orientation is vertical and at typical operating speeds (around 3600 RPM for a 5 cm rotor) the outward force at the outer wall is caused by an acceleration a few hundred times that of gravity. Thus, the orientation relative to gravity becomes negligible at high speeds and the flow (relative to the axis of the rotor) appears similar in principle to the settling trough. Of course, just within the rotor inlet as well as just above the weirs, the tangential velocity of the fluid relative to the rotor rotation is significant and the simple comparison to the horizontal trough breaks down.

For liquid–liquid separation, as the flow rate is increased the width of the dispersion band (the region of unseparated fluid mixture) at the top of the active separating height (the underside of the light phase weir) increases. Depending on the organic-to-aqueous flow ratio (O/A) and the weir radii, there is a maximum flow rate at which the width of the dispersion band is equal to the radial difference between the light phase weir and the heavy phase underflow slot. Increasing the flow rate of either phase results in phase carryover and contamination of the other stream. As mentioned above, theoretical models developed at Argonne National Laboratory have employed analytical techniques coupled with experimental correlation to predict this behavior and select the optimum weir sizes for a given throughput and O/A ratio (or visa-versa).[22,75]

For single liquid phase flow in the contactor rotor, as is the focus of this current study, an important characterizing parameter is the flow rate at which the separation zone becomes filled—that is, the point at which the single-phase flow rate entering the rotor is such that the liquid
volume maintained in the rotor increases to the point where flow begins to come out the light phase exit port. The Argonne model is capable of accurately predicting this point given that the pressure above the aqueous weir is known. For an open upper weir such as is shown in the general contactor sketch in Figure 7.2, the pressure is equal to the atmospheric pressure (the splash plate is not air tight on the rotor shaft). Similarly for an air-controlled aqueous weir the air pressure is the known specified value. Along with analyzing the general single-liquid flow characteristic in the separation zone, another useful purpose of this current modeling effort is to examine the behavior of the closed upper weir of the CINC rotor.\footnote{The purpose of this upper weir cap which effectively closes the upper weir is to hold the removable weir plate in place. For a permanent upper weir plate, the weir cap should be unnecessary.}

7.2 CFD Models

Computational modeling of the 3D, two-phase (air/water) flow within the rotor was done using the commercial CFD package Fluent 6.3. As with the simulations of the flow in the mixing zone as
presented in Chapters 5 and 6, the Volume of Fluid (VOF) method with piecewise linear interface construction (PLIC) was used to track the volume fraction and simulate the physics of the air/water free surface. As with the previous free surface simulations, surface tension was included using the Continuum Surface Force method\textsuperscript{[129]} with a value of 73 dynes/cm (air/water interfacial tension) and the water contact angle on all surfaces was set 75\degree to simulate the contact of water on steel in air. It was assumed that the flow in this region of the contactor is laminar. All simulations were time-dependent using Fluent’s non-iterative time advancement (NITA) solver\textsuperscript{[102]} and most\textsuperscript{2} were performed in parallel using 10–20 processors. Some were done using a local Linux cluster and others were executed on the Tungsten Xeon Linux Cluster at the National Center for Supercomputing Applications (NCSA).

### 7.2.1 Geometry and Mesh

The geometry used for the separation zone model was based on the rotor of the commercially available CINC V-2 contactor (see Figure 7.3). As no official drawings of this contactor rotor were available, the various dimensions were directly measured by micrometer and a computer model was thus directly constructed from the physical dimensions of the rotor. In order to minimize the computational cost by taking advantage of symmetry, only a one-quarter section was modeled with 90\degree rotationally periodic boundary conditions. Figure 7.4 shows several views of the model rotor geometry. As this geometry is quite complex, a complete list of dimensions will not be included here; several important dimensions of the model rotor geometry are given in Table 7.1. Two different aqueous weir dimensions are listed in the table; the larger 1.15 cm weir radius was used for all of the simulations (this is also the same as used for all of the experiments from previous chapters). The zero-point simulations as described in Section 7.4 were also repeated using a smaller, 1.08 cm radius to compare with an experimental measurement of the zero-point. The separation height $h_{sep}$ is the height from the interior bottom of the rotor to the underside of the light phase weir. In this chapter ‘light phase’ and ‘organic phase’ will be used interchangeably as

\textsuperscript{2}One zero-point simulation was done using a dual-core Linux machine. These took much longer but enabled efficient use of the limited number of software licenses.
Figure 7.3: Diagram of an exploded view of the rotor of a CINC V-2 centrifugal contactor. Figure taken from Sheldon et al. 2002 patent.\cite{38}

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner Radius</td>
<td>( r_{in} )</td>
<td>2.38</td>
</tr>
<tr>
<td>Separation Height</td>
<td>( h_{sep} )</td>
<td>10.60</td>
</tr>
<tr>
<td>Aqueous Underflow Height</td>
<td>( h_{aq} )</td>
<td>1.66</td>
</tr>
<tr>
<td>Organic Weir Radius</td>
<td>( r_{w,org} )</td>
<td>1.037</td>
</tr>
<tr>
<td>Organic Exit Radius</td>
<td>( r_{org} )</td>
<td>3.15</td>
</tr>
<tr>
<td>Aqueous Weir Radius</td>
<td>( r_{w,aq} )</td>
<td>1.15 (0.45”)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.08 (0.425”) (zero-pt only)</td>
</tr>
<tr>
<td>Aqueous Exit Radius</td>
<td>( r_{aq} )</td>
<td>2.90</td>
</tr>
<tr>
<td>Flow Height Above Upper Weir</td>
<td>( h_{aq,up} )</td>
<td>0.30</td>
</tr>
</tbody>
</table>
Figure 7.4: Separation zone model with pressure outlets colored yellow, the mass flow inlet blue, and all periodic boundaries green. (a) Full model including periodic images of the modeled quadrant. (b) Side view of upper section of model quadrant showing ‘tiered’ aqueous underflow. (c) Angled view of upper section of the model quadrant showing weirs. (d) Close view of bottom section (with periodic images) showing inlet, diverter disk, and divider vanes with a notched flow passage at the bottom outer edge.
will ‘heavy phase’ and ‘aqueous phase’. In practice, the heavy phase is usually, though not always, the aqueous phase. The aqueous (heavy) phase underflow height listed in Table 7.3 is the vertical distance between the underside of the organic weir and the underside of the aqueous weir plate.

The upper weir plate (labeled 18 in Figure 7.3) is held in place by a weir cap (20) that forms the upper flow section and the four square heavy phase outlet channels shown in the model (see Figure 7.4(a)). The height of the flow area above the weir $h_{aq,up}$ is only 3 mm. As will be shown with the results of these simulations, this restricted flow area has an impact on the high flow rate operation of the rotor. Notice also that the heavy phase outlet and light phase outlet are staggered at 45° relative to one another. While care was taken to include each detail of the actual rotor geometry, one subtle but perhaps important difference between the real rotor and the model rotor is that the weirs in the model both have a perfectly sharp edge. This is a good representation of the actual features of the experimental apparatus when it comes to the light phase weir, however, the heavy phase weir in the CINC V-2 unit has a slightly beveled edge. For certain quantities of interest such as the zero-point flow rate, this difference may impact the ability for direct quantitative comparison with experiment.

While not very apparent from the views in Figure 7.4, the thin flow volume of the rotor inlet as it extends through the bottom ‘shell’ of the rotor (1.59 mm thick) was modeled in BOTH the mixing zone and the separation zone models. That is, the exit of the mixing zone model as presented in the previous two chapters is even with the inside surface of the rotor whereas the inlet to the separation zone model as presented in this chapter is positioned at the outer surface of the rotor. This thin volume of the inlet passing through the rotor wall can be seen better in Figure 7.6 given later.

The mesh was created using Gambit 2.4 and consisted of all unstructured, tetrahedral cells with nodes clustered near the inlet and bottom surfaces as well as in the upper region of the rotor around the weirs and the surface of the upper weir to achieve better resolution of the gas–liquid interface at these critical sections. As before, the necessity of transient simulations made it such that the overall mesh density was primarily limited by computational cost and a full grid resolution study was not feasible. Two different levels of meshing were used for the simulations presented here. For simulations of the general flow for which a detailed solution at a given flow rate was desired,
Table 7.2: Number of computational cells for the various separation zone meshes.

<table>
<thead>
<tr>
<th>Weir Cap Type</th>
<th>Upper Weir Radius, cm</th>
<th>N Cells</th>
<th>Simulation Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>1.15</td>
<td>311 K</td>
<td>General Flow</td>
</tr>
<tr>
<td>Standard</td>
<td>1.15</td>
<td>146 K</td>
<td>Zero-point</td>
</tr>
<tr>
<td>Vented</td>
<td>1.15</td>
<td>178 K</td>
<td>Zero-point</td>
</tr>
<tr>
<td>Standard</td>
<td>1.08</td>
<td>159 K</td>
<td>Zero-point</td>
</tr>
<tr>
<td>Vented</td>
<td>1.08</td>
<td>165 K</td>
<td>Zero-point</td>
</tr>
</tbody>
</table>

a finer mesh was applied. For simulations aimed at determining the zero-point flow rate, which required simulations over relatively long times for varying inlet flow rates, a more manageable mesh was used. As will be described later, simulations (and selected experiments) with a modified ‘vented’ upper weir cap were also performed. The number of computational cells for each of the various models and meshes used are listed in Table 7.2. More details regarding the meshing schemes applied to generate the computational grids for these models is given in Appendix E.

7.2.2 Model Setup

The setup of the CFD models for simulation of the flow in the separation zone are discussed here. In particular, the various boundary conditions applied as well as the method for incorporating the rotation of the rotor are presented.

As with the flow inlets for the mixing zone, the inlet to the separation zone was treated as a spatially and temporally constant mass flow rate boundary. While it certainly was possible to apply a mass flow rate profile across this boundary (even taking it directly from the average profile at the exit of the mixing zone model for the case where the total flow rate simulated was the same), it was found that this did not have a noticeable effect on the predicted flow field and therefore a constant value boundary condition was applied. The inlet boundary also did not have a specified tangential velocity; recall, however, that the inlet to the separation zone model is flush with the outer bottom surface of the rotor and therefore this is an acceptable boundary condition since there
is little rotation of the flow here and it is only once the flow enters the rotor inlet that it begins to be significantly re-accelerated. Separate simulations looking at the general flow in the rotor were performed at two different inlet flow rate settings: 600 ml/min and 1600 ml/min. For the simulations used to predict the zero-point flow rate, the inlet flow rate was not fixed, but was varied using a function coupling it to the overall mass balance and the position of the air/water interface relative to the organic weir. This was done using a piece of add-on code referred to as a User-Defined Function (UDF) in Fluent and is discussed more in Section 7.4.

Each of the phase outlets (light phase and heavy phase) was specified as a pressure outlet with the boundary pressure set equal to atmospheric pressure. The backflow condition was specified with a water volume fraction equal to zero—that is, if there was reverse flow (which indeed there was at the light phase exit) it would be air, consistent with the real case.

For the case of the flow inside the rotor, the entire domain is rotating and thus the solution can be determined relative to a single frame of reference. A rotational speed of 3600 RPM was applied to the entire fluid domain and the velocity field was solved for within this rotating frame of reference. While this method is valid for the current case where the flow inside the rotor is modeled completely separate from that in the annular mixing zone, if the separation zone and mixing zone were combined into a single model it would be necessary to define two separate reference frames (one for the rotating domain inside the rotor and one for the stationary domain outside the rotor). Initial attempts at exploring such a multiple reference frame combined zone model were restricted by the long computational times due to the size of the mesh required for the combined model geometry and were thus not included as part of this current project. Additionally, there appeared to be some difficulties with accurate coupling and communication of the flow at the interface between the two reference frames. A combined model could also be done with more fidelity using a sliding mesh in which the rotating flow domain within the rotor is actually in motion relative to the stationary one. This latter method would be substantially more computationally intensive.

As before with the mixing zone models, these simulations were time-dependent and employed a variable time step according to the Courant flow number (Equation 5.1). The typical time step for the finer mesh simulations was approximately 16 µs while that for the zero-point simulation
meshes was 20–30 µs. Typical simulation times were about 70 hours per 1 s of flow for the general flow simulations (on 20 processors) and 40–50 hours per 1 s for the smaller zero-point simulations (on 10 processors). Because of the relatively long flow times (several seconds at least) that were required for the zero-point flow rate simulations, the global $Cr$ number that determined the overall time step was increased as much as possible while still maintaining adequate convergence and good stability at each time step; for these simulations, the global $Cr$ number was as much as 5.0 (it was 2.0 for all of the previous simulations). Even so, the local $Cr$ number limit of 0.25 necessary for the VOF model is still maintained within Fluent by applying sub-time stepping for the volume fraction calculation.

As with the simulations of the mixing zone, the initial simulation of the separation zone was started from rest with a fixed liquid height and all subsequent simulations were initiated with a patched-in velocity field for the flow already in motion to avoid this start-up time. The liquid volume in the model was allowed to equilibrate before any steady-state flow observations such as those described here were made. The characteristic equilibration time was much slower for the separation zone than for the mixing zone. Whereas it was observed that the flow in the mixing zone achieved liquid hold-up volume equilibration following a moderate change in flow conditions within about 1 s of flow time, equilibration for the separation zone took several seconds of flow ($\sim 3–5$ s) for similar changes. This difference is simply related to the large difference in the liquid volume maintained in each region. The nominal liquid volume in the separation zone is approximately 160 ml. This is several times that of the mixing zone (see Table 6.5) and translates into a mean fluid residence time within the rotor several times larger than that in the annular region. Incidentally, the difference in the overall response time scales of the two regions has implications for understanding how process upsets effect the performance of the equipment.

7.3 General Flow

Simulations of the flow in the separation zone using the more refined mesh were performed at two different flow rates, the standard 600 ml/min and a much higher 1600 ml/min. Both of these were for the larger (1.15 cm) aqueous weir. Note that 1600 ml/min is very near the experimentally
Figure 7.5: Cross-section plots of the water volume fraction distribution in the separation zone at 600 ml/min (a) and 1600 ml/min (b). The vertical cross-section shown here bisects the regions between rotor vanes.

observed zero-point flow rate of 1592 ml/min which was measured previously by others for flow in this very same contactor unit.\cite{22} The general flow behavior for these two flow rate settings will be discussed here.

7.3.1 Air Core

Figure 7.5 shows a cross-section view of the flow of water (red) and air (blue) in the separation zone of the contactor for the two inlet flow rate settings. The more diffuse appearance of the air/water interface in the central portion of the separating region above the diverter disk and below the lower weir is simply an artifact of the larger computational cells used in this region. From this cross-sectional view, there are only subtle differences between the two flow rate settings. As will
be described in more detail in the following two sections, these differences occur primarily near the inlet and above the upper weir. The distinctive feature of the flow in the main separation region of the rotor is the essentially vertical air/water free surface. As both simulations were for flow at the same rotor speed (3600 RPM) it is not surprising that the general position and shape of the free surface is consistent between the two. It was observed for some initial scoping simulations of the separation zone that were performed early on that the free-surface becomes more parabolic at lower rotor speeds (∼1500 RPM).

It was also observed that there was radially recirculating flow of air in the organic exit channels as these were empty of water and open to the atmosphere for both settings. This allowed for a balance in the volume of air in the rotor as the volume of water increased to the equilibrium level from the initial starting volume. For the higher flow rate setting there was not as yet any flow out of the light phase exit port as would be expected if the zero-point had been exceeded. In fact, as will be discussed later the features of the flow above the aqueous weir lead to a significant elevation in the predicted zero-point flow rate.

7.3.2 Flow Near Inlet

As was shown previously in Figure 7.4(d), there are vanes within the rotor that divide the interior of the rotor into four separate regions. For most of the height, these vanes seem to have little effect (i.e. there is very little azimuthal variation in the flow); however, they are very important near the inlet as they force the fluid entering the rotor to quickly accelerate up to the speed of the rotor. In practical terms, the separate regions also helps to maintain balance of the spinning, fluid-filled rotor. Near the inlet, these vanes actually do not extend all the way to the axis of the rotor and there is an open section below the diverter disk (which also has a hole in it). The flow simulations predict that near the inlet there is a stable column of liquid that is maintained below the diverter disk in this empty region near the axis where the vanes do not extend.

The sweeping of the rotor vanes pumps the fluid from the edge of this water column radially outward into the rotor. This behavior can be observed in Figure 7.6 which shows the flow of water on the rotor vanes (as well as a cross-section of the inlet water column). This image is at 45°
Figure 7.6: Cross-section of water volume fractions near the inlet and on the rotor vane walls for flow rates of 600 ml/min (a) and 1600 ml/min (b).

relative to the one shown in Figure 7.5 in order to show the flow on the surface of the vanes (rather than between them as in that previous figure). At the lower flow rate (Figure 7.6(a)), it appears that the flow is by droplets or very thin ‘filmlets’ on the backside vane. There is also some flow traveling up through the hole in the diverter disk and then being propelled outward. For the higher flow rate setting (Figure 7.6(b)), there is a continuous layer of water on the backside vane. Notice that the force of this water layer as it flows radially outward also results in the entrainment of air which collects within the small channels which pass through the vanes at the outer bottom corner (to allow redistribution of fluid between the regions).

These same effects can be further observed in the differences in the velocity field on the bottom surface of the interior of the rotor as shown in Figure 7.7. In this figure the velocity field (for both phases) relative to the rotor rotation is shown; thus, the magnitude of the tangential velocity is highest near the inlet where the water entering the rotor has a rotational speed less than that of the rotor but is being accelerated. Conversely, the magnitude of the difference between the rotor velocity and the fluid velocity is small near the outer wall and therefore the vectors are small. From Figure 7.7(a) it is clear that there is little radial transference of momentum across the air gap between the inlet water column and the outer main fluid volume for the lower flow rate setting. On the other hand, there is significant radial momentum transported within the continuous water film propelled outward by the vane for the 1600 ml/min case (Figure 7.7(b)). For this case, there is flow that extends all the way to the inter-vane channel and then sweeps back down the rotor vane towards the free surface at the edge of the air core. Recall that it was assumed that the flow is
Figure 7.7: Velocity vectors showing flow relative to the rotor rotation on the bottom interior surface of the rotor for flow rates of 600 ml/min (a) and 1600 ml/min (b). The dashed circles denote the general locations of the inlet water column (inner circle) and the outer free surface at the inner edge of the main fluid region (outer circle) [see Figure 7.5]. An outline of the lower portion of the rotor geometry is also visible.

Laminar in the separation zone. While this is likely an adequate approximation, in reality there is certainly decaying turbulence and perhaps even some turbulence generation near the bottom of the separation zone where large velocity gradients exist while the fluid is being accelerated (such as depicted in Figure 7.7(b)).

### 7.3.3 Flow Above Heavy Phase (Upper) Weir

Unlike most contactors, the CINC centrifugal contactor has a removable upper weir that is held in place by a cap that effectively carves out a narrow flow area above the upper weir as described in previous sections. From the simulations of the two different inlet flow rates, this feature was found to have a very dramatic effect on the overall flow behavior.

The flow over the upper weir at 600 ml/min had the general characteristics of what one might expect the flow over a completely open upper weir to have—that is, it consisted primarily of
Figure 7.8: Plot of instantaneous (a) and mean (b) water volume fractions on the top surface of the aqueous weir and water contacted areas of the upper weir cap at 600 ml/min and 3600 RPM. Rotation is in the counter-clockwise direction. Periodic images of the modeled quarter-section are shown for continuity.

droplet/rivulet flow from the inner weir edge outward along the surface of the weir. An instantaneous snapshot of the flow above the upper weir as predicted by simulation is shown in Figure 7.8(a) and to give a better view of the flow paths of the individual droplets, a time average of the water volume fractions is shown in Figure 7.8(b). The flow over the weir is primarily as discrete droplets which curve outward in characteristic demonstration of the Coriolis effect. Note that droplets which impinge on the outer surface of the weir cap tend to ‘climb’ up the wall and link up with droplets below them. The droplets then accumulate as a film on the backside of the outlet channel where they exit the rotor model (and are spun out into the collector rings).

A dramatic difference for flow in the same region at the higher flow rate (1600 ml/min) can be seen in Figure 7.9. Only an instantaneous snapshot is shown as there was very little time
Figure 7.9: Plot of the instantaneous water volume fractions above the aqueous weir at 1600 ml/min (3600 RPM).

variation of the flow for this case. The simulation shows that the air space above the upper weir no longer has open communication with the outside (atmospheric) pressure and has been completely sealed by a ring of water. The radial thickness of this water ring is $\sim 2$ mm. Previous hydrostatic balance-based models of the rotor\cite{22,75} assume that the pressure above the aqueous weir is equal to atmospheric pressure. For the case shown in Figure 7.9 it is obvious that such an assumption may be invalid for the current configuration. The pressure above the aqueous weir as predicted by this simulation is approximately $-1900$ Pa for this flow rate as compared to only $-30$ Pa for the 600 ml/min case. The behavior of the flow in this ‘water-sealed’ case is somewhat analogous to that of a siphon; there is a large negative pressure which helps draw the fluid up and the overall flow rate through the rotor is enhanced relative to what could normally be achieved. In fact, because of this siphoning, the total liquid volume in the rotor for this high flow rate case is actually slightly less than for the 600 ml/min case.

While this behavior has not been directly observed experimentally (i.e. with a transparent upper weir cap), its effects certainly have been. It was noted by Leonard et al.\cite{22} that there were unexplained effects that caused an elevation in the zero-point flow rate for large upper weir radii for which the zero-point flow rate was in excess of 2000 ml/min. Other researchers have also noted unpredictably high flow rate behavior including a variable zero-point accompanied by oscillatory

\footnote{Because the free surface position does not vary significantly in the rotor for most cases, it was originally attempted to perform steady-state calculations. These were found to be insoluble likely due to the interface discontinuities above the upper weir and therefore were abandoned. It may be possible to obtain a converged time-invariant solution for high flow rates such shown in Figure 7.9 although this was not attempted.}
outlet flow.\textsuperscript{[155]} This oscillatory behavior is not unexpected based on the simulation predictions outlined here. While the ‘water ring’ predicted here was apparently stable, it could be imagined that the corresponding seal ring that forms in the real system could easily be disrupted by surface imperfections and/or could exhibit a cyclic formation–growth–breakdown type behavior over certain flow rate ranges. In general, this behavior of the flow above the aqueous weir and the corresponding elevation of the zero-point can be considered deleterious as it restricts one’s ability to select appropriate weir dimensions that have predictable and consistent operation over the entire range of desired flow rates.

In regards to the creation of this water ring, the droplet linking that was seen for the 600 ml/min flow rate case may lend some insight into the general formation mechanism. Several potential methods for ameliorating this behavior (by design) are also readily apparent. A couple ideas are shown in Figure 7.10. For example, one might give the outlet channels a slight reversed slant in order to increase ‘pumping’ of liquid out of this region (Figure 7.10\textsuperscript{c}). Similarly, modifying the weir cap and outlet channel such that the water ring is disrupted because the outer edge is no longer a continuous circle could be done as shown in Figure 7.10\textsuperscript{c}). Beyond this, other more substantial changes could also be envisioned such as adding vanes in this upper section to help propel the fluid out of this region. The effectiveness of any of these potential modifications could easily be explored through similar CFD simulations.
7.4 Prediction of Zero Point Flow Rate

As mentioned previously, the single phase flow rate at which the separation zone fills and all of the flow can no longer go over the upper weir is called the ‘zero-point’ flow rate; this is a useful quantity for rotor flow characterization. For example, the zero-point flow rate is used in practice for verification of the consistency of fabrication of rotors with the same specifications such as might be used in a multi-stage bank of contactors.

Based primarily on hydrostatic arguments and flow correlations using analogy to the gravity separation trough as sketched in Figure 7.1, it is possible to obtain an accurate prediction of the zero-point flow rate for given rotor geometry. However, as was shown in the previous section there are regions of flow where the assumptions required for general theoretical analysis of this type are not valid. Flow simulations of the type outlined here are a useful secondary tool for determining the zero-point flow rate and explaining ‘off-normal’ experimental observations.

Experimentally, the zero-point is identified by the flow rate at which flow begins to come out of the light phase exit. This condition is difficult one on which to converge either with the hydrostatic rotor models or with the present simulations. For the hydrostatic models, convergence to a non-zero value of flow from the light phase exit requires tedious manual iteration. Similarly, for CFD simulations the pre-defined endpoint of a set discrete level of outlet flow is difficult to determine.

Thus, it was chosen for the CFD simulation-based prediction method developed here to define the ‘zero-point’ of the simulation as the flow rate at which the air/water interface is positioned right at the edge of the organic weir (i.e. $r_{interface} = r_{w,org}$). While this introduces some ambiguity in direct comparison with experiment, it also eliminates the effects of surface adhesion and surface tension on the weir edge which, though physically included in the modeling, would make identification and definite demarcation of the zero-point difficult. That is not to say that such is not possible, it certainly is. However, the primary purpose of these simulations for prediction of the zero-point were to understand the effects of the weir cap and ‘water seal’ that were described above and therefore the ambiguity relative to experiment was deemed acceptable. Consequently, the zero-point flow rate measured experimentally would be somewhat higher than the effective
zero-point determined here by simulation. This is further compounded by the sharp versus beveled weir effect that was noted previously which would also likely tend to increase the predicted zero-point flow rate by increasing the effective pressure drop of the flow over the sharp-edged weir relative to the beveled one.

As noted earlier, different meshing was employed for the zero-point flow rate simulations in order to decrease the total number of cells and speed up the overall calculation. The zero-point flow rate was calculated for two different upper weir radii, 1.15 cm and 1.08 cm. Simulations were performed for each of these weir radii for a geometry employing the standard weir cap and one with a modified ‘vented’ weir cap which will be described later.

7.4.1 Calculation Method

Prediction of the zero-point flow rate was done through a code module written by the author and linked to the CFD simulations to couple the inlet flow rate with the overall mass balance and the position of the interface (air/water) relative to the organic weir. The actual code for this module is included in Appendix G. A general description of the methodology employed will be outlined here.

The general scheme for determining the zero-point flow rate is as follows:

1. For the current flow rate setting, perform a specified number of time steps (iterations).
2. Calculate overall mass balance \( \sum \dot{m}_{\text{out}} - \sum \dot{m}_{\text{in}} \) and determine if system is at steady-state.
3. If system is at steady-state, change inlet flow rate proportional to the deviation of the current average position of the air/water interface \( \bar{r}_{\text{int}} \) from the setpoint \( \bar{r}_{\text{w,org}} \). Return to step 1.
4. If system is not yet at steady-state for the current flow rate setting, do not change flow rate. Return to step 1.
5. Stop the simulation when the setpoint is reached \( \bar{r}_{\text{int}} - r_{\text{w,org}} \approx 0 \).

Steady-state in step 2 above was defined as a deviation of less than 2.5% in the overall mass balance averaged over 250 time steps (approximately 75 ms). It was found that this was a sufficient number of time steps to achieve a steady value in the overall mass balance. Once it was determined that
steady-state was achieved at the current flow rate setting, the flow rate was changed proportional to the setpoint of the defined ‘zero-point’ (the gas–liquid interface position, $r_{\text{int}}$, at the organic weir radius, $r_{w,\text{org}}$) according to:

$$\dot{m}_{\text{in, new}} = \alpha \cdot \dot{m}_{\text{in, old}} \left(1.0 + \frac{r_{\text{int}} - r_{w,\text{org}}}{r_{w,\text{org}}} \right)$$ \[7.1\]

where $\dot{m}_{\text{in}}$ is the inlet mass flow rate and $\alpha$ is an under-relaxation factor that was set to 0.25 to ensure smooth convergence to the zero-point and avoid overshoot. The air/water interface position $r_{\text{int}}$ was defined as the average radial position of the interface (time- and spatially-averaged over the same 250 time steps) in the region beginning at the top of the light phase weir and extending 5 mm below the weir. As has been done throughout this work, the interface is defined as the surface of constant water volume fraction $\phi = 0.5$. As an example, from Equation 7.1 we see that if the radial position of the air/water interface $r_{\text{int}}$ is greater than the organic weir radius $r_{w,\text{org}}$ the flow rate is increased correspondingly resulting in an increase in the fluid volume in the rotor and a shift in the interface position moving it closer to the light phase weir radius (i.e. a decrease in $r_{\text{int}}$).

Because of the slow approach to steady-state after each inlet flow rate change, relatively long overall simulation times were required to converge to the ultimate zero-point flow rate. It was possible to minimize the computation time by providing an initial starting flow rate that was near the measured zero-point based on previous measurements for this configuration.\[22\] Though there are certainly modifications that could be made to improve the overall speed of this prediction method (e.g. optimization of the parameter $\alpha$ in Equation 7.1 or changing the tolerance level for determination of steady-state), time and effort was not invested in doing so at this point as the method was deemed sufficient for the present demonstrative purpose.

7.4.2 Upper Weir Cap Modification

While several potential weir cap modifications were presented in Figure 7.10, it was chosen to make a simple modification to the weir cap that did not significantly alter the general flow behavior but still allowed for communication of pressure between the air space above the weir and the outside pressure. This was facilitated by introducing a small hole, or vent, in the weir cap.
near the rotor shaft. While the limitation of pumping capacity for the existing experimental setup (≲ 1000 ml/min for equally distributed flow, see Section 3.2.1) precluded extensive experimental measurements, a modified weir cap was constructed and is showed in Figure 7.11. Since the simulation geometry was in fact a quarter section, it actually had four of these semi-circular vents. The modified model geometry can be seen in the image of the flow for the vented geometry given in the following section (Figure 7.13).

7.4.3 Zero-Point Predictions

Simulations were performed to determined the zero-point flow rate for each of the four cases outlined above. The resulting predictions are presented in Table 7.3 along with some experimentally observed values for comparison; recall that it was anticipated that there would be a difference between the predictions and experiments because of the difference in the definition of the zero-point between the two. Due to pumping deficiencies in the current setup, it was only possible to obtain experimental values with the vented cap for the smaller weir radius for which the magnitude of the zero-point flow rate is within the capacity of the pumps.

For the smaller weir ($r_{w,aq} = 1.08$ cm), there was no difference in the predicted zero-point value from the simulations. Interestingly, there was a slight elevation (~15%) in the experimentally measured zero-point for the standard cap relative to the vented one. For these experiments, the inlet flow rate was gradually increased and the zero-point flow rate was defined as the average value of the first total flow rate setting at which flow from the light phase exit was observed and
Table 7.3: Zero-point flow rate values predicted from CFD simulation. For general comparison of the trends, values observed experimentally for the same contactor unit are also shown.

<table>
<thead>
<tr>
<th>Weir Cap</th>
<th>Aq. Weir Radius, cm</th>
<th>Zero-point Flow Rates, ml/min</th>
<th>Simulation</th>
<th>Current Experiment</th>
<th>Leonard et al.\textsuperscript{[22]}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard</td>
<td>1.15</td>
<td>2230</td>
<td>–</td>
<td>1592</td>
<td></td>
</tr>
<tr>
<td>Vented</td>
<td>1.15</td>
<td>1451</td>
<td>–</td>
<td>n/a</td>
<td></td>
</tr>
<tr>
<td>Standard</td>
<td>1.08</td>
<td>287</td>
<td>431</td>
<td>467</td>
<td></td>
</tr>
<tr>
<td>Vented</td>
<td>1.08</td>
<td>290</td>
<td>375</td>
<td>n/a</td>
<td></td>
</tr>
</tbody>
</table>

the last setting at which no flow was observed. Plots of the measured flow rate out of the light phase exit versus the total inlet flow rate for the two weir caps are given in Figure 7.12. It is not absolutely certain that the observed difference is significant. As can be seen between the value for the standard cap measured in this current work and the one reported previously by Leonard et al.,\textsuperscript{[22]} there is some variability in measurement of the zero-point. On the other hand, the simulations did in fact predict a slight difference in the pressure above the aqueous weir for the two cases. The pressure above the aqueous weir was approximately $-40$ Pa for the standard case and $-20$ Pa for the vented case; this slight excess negative pressure in the standard cap case may be the source of the measured zero-point elevation that was seen even for this relatively low flow rate where the exit ports remain fully ‘open’.

For the larger weir size ($r_{w,aq} = 1.15$ cm), there is a significant increase in the zero-point flow rate caused by the siphon effect of the ‘water seal’ maintained in the standard closed upper weir cap; the zero-point predicted for the standard weir cap was 54% higher than for the vented cap. It was verified that for this flow rate ($2230$ ml/min) the standard cap had a sealing ring of water similar to that shown previously in Figure 7.9 for 1600 ml/min. The thickness of the water ring did not appear to have changed significantly and was still $\sim 2$ mm thick. With the introduction of the vent in the upper cap into the simulated rotor geometry, the sealing water ring was observed to immediately break down and the flow above the upper weir quickly returned to a general pattern
Figure 7.12: Plot of zero-point flow rate measurements for the 1.08 cm aqueous weir using the standard (closed symbols) and vented (open symbols) weir caps.

Figure 7.13: Instantaneous flow of water above the aqueous weir at the predicted zero-point (1451 ml/min) for the vented cap and the 1.15 cm aqueous weir.

of droplet flow as shown in Figure 7.13. While some droplet linking flow can be seen around the outer edge of the weir cap, the liquid in this region is still discontinuous and the exit ports remain open. While the general flow pattern seen here is similar to that shown in Figure 7.8, the pressure above the aqueous weir was found to be 0 Pa in this case as compared to approximately $-30$ Pa.
for the flow with the standard cap at 600 ml/min. Also, the film thickness at the backside of the exit channels is understandably somewhat greater than seen at the lower flow rate.

It is clear from these simulations using the vented weir cap that the restricted flow space above the aqueous weir due to the closed weir cap has a significant effect on the zero-point flow rate. These simulations help to explain the zero-point elevation that was observed previously for high flow rates in the CINC V-2 contactor. The author of that study had also previously postulated that the air-tightness of the upper weir cap around the rotor shaft may have had some effect on these off-normal zero-point effects; indeed, such is the behavior predicted by these simulations. In that study, however, this effect was only observed for weirs greater than 1.15 cm (with zero-points \( \gtrsim \) 2500 ml/min). These current simulations have predicted this behavior at flow rates as low as 1600 ml/min although an incremental range of flow rates was not explored in order to determine the specific flow rate at which this behavior first arises. The effect of liquid surface contact and perhaps even surface roughness in the region above the upper weir would likely have an effect on the specific conditions at which this water siphon forms as well as on its overall stability.

7.5 Conclusions From Separation Zone Simulations

The flow in the separation zone of the annular centrifugal contactor has been explored through the application of detailed computational flow simulations of the actual geometry of a model rotor of a CINC V-2 centrifugal contactor. It was found that there is indeed a vertical column of air that develops along the axis of the spinning rotor. For moderate flow rates the heavy phase exit ports above the upper weir remain open and there is droplet flow over the weir. At high flow rates, the flow area above the upper weir becomes sealed with water and forms a siphon which tends to disproportionately increase the amount of flow that can pass over the aqueous weir. This was observed quantitatively through prediction of the zero-point flow rate for the standard sealed upper weir cap and one with venting. This research effort has viewed the contactor from the perspective of solvent extraction and has therefore deemed the zero-point elevation an undesirable quality; for operation of the contactor primarily as a dedicated separation device, it might be argued
that a higher aqueous throughput is advantageous. Even so, it can generally be concluded that a \textit{predictable} throughput is preferable in all cases regardless of the operational focus of the unit.

To the author’s knowledge, these simulations have provided the first detailed view of the flow structures within the rotor of the centrifugal contactor. In particular, specific details of the flow above the upper weir have helped to explain previously observed behaviors for this design of contactor rotors. As mentioned elsewhere in the presentation of this overall project, this commercial contactor design has been, in general, favorably evaluated for solvent extraction use by a number of studies.\textsuperscript{[22,39–41]} The research presented here provides a tool for critical evaluation of this design as well as a method for enabling greater general understanding of the flow and hydraulic operation of the separation zone of the contactor.
Part IV

Conclusions and End Matter
Chapter 8

Conclusions and Recommendations

This final chapter provides a summary of the main conclusions and recommendations that are made from this computational and experimental analysis of the flow in the annular centrifugal contactor. Additionally, suggestions for future applications of the demonstrated modeling framework will also be outlined. Finally, potential improvements and suggestions for future work to expand the capability of these modeling schemes to further enable not only the understanding of general flow and equipment design as have been explored with the present hydraulic simulations, but actual liquid–liquid mixing analysis and simulation of complete solvent extraction processes.

8.1 Summary of Major Conclusions

8.1.1 Conclusions Based on Mixing Zone Flow Analysis

The flow in the annular mixing zone is characterized by violent free surface motion and discontinuous fluid–rotor contact. This work has demonstrated that the combination of the Volume of Fluid (VOF) volume tracking method for modeling the air/water free surface with Large Eddy Simulation (LES) of turbulence provides an accurate simulation method for the hydraulic operation of the centrifugal contactor annular mixing zone. It was shown in Chapter 5 that even for a relatively coarse computational mesh better accuracy as compared to the actual velocities measured by laser Doppler velocimetry (LDV) was achieved using the LES method than for other turbulence modeling methods. Further, the simulations presented in Chapter 6 using this same combination of models with more refined meshing were found to have even greater accuracy.
From the computational and experimental analysis of the flow and mixing in the annular mixing zone it is clear that the fluid–rotor contact has the most significant effect on energy transfer to, and mixing in the fluid. Further, it is evident from both experimental observations and detailed simulations presented in Chapter 6 that the geometry of the mixing vanes has a substantial effect on the amount of fluid–rotor contact. Additionally, it is clear that modeling of the liquid free-surface is essential to accurately capturing the fluid–rotor contact. Any modeling effort which attempts to ultimately explore complete solvent extraction processes in the centrifugal contactor will need to adequately capture the free surface characteristics and complex fluid–rotor interaction.

Experimental observations of the flow in the annular mixing zone for a range of flow rates and rotor speeds using three different mixing vane geometries have highlighted the differences in annular flow for the three systems. In particular, the 8-vane and curved vane geometries have sudden flow structure changes which likely affect the mixing and fluid–contact. On the other hand, the 4-vane geometry may not be able to operate to as high a flow rate as the other two due to flooding of the mixing zone above \( \sim 1000 \text{ ml/min} \) (for the 5 cm contactor at 3600 RPM), but it also has a higher liquid height with more predictable variation over different flow rates and rotor speeds. Even at very low flow rates, the 4-vane geometry maintains an adequate liquid height. The results of the detailed mixing analysis from the simulations presented in Chapter 6 (at 600 ml/min and 3600 RPM) indicate that the 4-vane contactor geometry appears to have better mixing characteristics for low to moderate flow rates in the given contactor geometry \((r_r = 2.54 \text{ and } r_r/r_h = 0.8)\).

### 8.1.2 Conclusions Based on Separation Zone Modeling

The modeling scheme applied in Chapter 7 was found to provide a useful description of the flow in the separation zone of the annular centrifugal contactor. It was shown that at operating rotational speeds (3600 RPM in the 5 cm contactor) the air/water free surface is completely vertical and there is indeed a stable column of air along the rotor axis within the separation zone.

From the work presented in Chapter 7 it can be further concluded that the flow above the aqueous weir has a significant effect on the overall operation of the rotor as characterized by the
zero-point flow rate. Specifically, the rotor design upon which the computational model geometry was based (CINC V-2) has a restricted flow area above the upper weir that becomes sealed with water at high flow rates ($\gtrsim 1600$ ml/min). This reduces the pressure above the aqueous weir and results in an siphoning effect which elevates the observed zero-point flow rate. This effect, investigated and explained for the first time by these CFD simulations of the flow in a detailed model rotor geometry, is consistent with and provides explanation for previous experimental observations.\cite{22} Consequently, it is concluded that predictable operation of contactor rotors with a closed upper weir cap (such as the CINC V-2 simulated here) over a wider range of total inlet flow rates may require that modification of the upper weir cap be made to avoid this water siphon formation in the narrow space above the aqueous weir. While it could not directly be determined from these 5 cm contactor simulations whether this same siphon formation would be observed in larger contactor units, other researchers have confirmed that larger units of the same design exhibit similar elevated throughput behavior.\cite{155} In general, the characteristics of this siphon effect in large contactor units with an upper weir cap would depend on what scaling rules are used for the upper weir flow area. Such scaling issues were not studied here but would be a useful future project (see Section 8.2.3).

### 8.1.3 Potential Impacts of This Work

Beyond the valuable contribution of this work toward improving the general understanding of the flow in the annular centrifugal contactor, this work has provided a critical evaluation of a specific contactor design which is at present particularly relevant. The CINC V-2 centrifugal contactor is a commercial unit that has been studied by researchers over the past several years and is being implemented for actual solvent extraction processes. The simulations presented here have provided an analysis of the flow in a model geometry based on this contactor design and enabled the identification of design characteristics of this ‘separator’ which may affect its successful operation as an ‘extractor’.

While in general it appears that the CINC unit studied here can successfully operate as an extractor over a reasonable range of flow rates, concerns arise at low flow rates (due to a decrease in annular liquid volume and poor mixing for the curved vanes) and at high flow rates (due to the
siphoning effect above the upper weir). These simulations not only helped identify and quantify these effects, but it is hoped that they provide a basis for further study of the issues to support the industrial implementation of these process units.

Moreover, it is anticipated that the simulation framework demonstrated here will form a foundation for additional efforts at improving the design and operation of centrifugal contactors and provide a starting point for progress towards simulation of solvent extraction processes. Some suggestions for how these simulations might be extended, expanded upon, and equipped with further functionality in order to explore and quantify liquid–liquid mixing and extraction are discussed later in Section 8.4.

8.2 Suggestions for Additional Applications

The simulation methodology demonstrated in this work provides a very useful tool for exploring a wide variety of parameters and inputs (both operational and geometric) in order to get a broader understanding of how each affects overall operation. Due to the necessarily well-defined and finite scope of this research project, it was chosen to use the simulation scheme demonstrated and validated in Chapter 5 to explore the effect of various mixing vane geometries for a given flow rate (Chapter 6). There are a multitude of other issues beyond this which could be explored through additional simulations based on the work done here. Some suggestions for application of this simulation methodology will be outlined here. While the ideas presented here could in general be undertaken based solely on the simulation schemes used for this current work, they could also clearly benefit from the additional model refinements discussed in Section 8.3. Suggestions which are primarily directed at each of the main contactor zones and those which are more generally applicable are presented separately; this is merely for simplicity in presentation and the divisions are not so distinct. Where applicable, ideas for additional experiments using the same methods employed in this work are also included. A summary list of the ideas outlined here is given at the end of Section 8.2.3 (Table 8.1).
8.2.1 Mixing Zone

Perhaps one of the most relevant issues that could be explored is the operation of the contactor at low flow rates ($\lesssim 200$ ml/min for the current size unit). It has been identified by many researchers that typical centrifugal contactors, perhaps especially the CINC contactor with curved vanes, exhibit poor operational efficiency at low flow rates. While some experiments were performed for other flow rates and rotor speeds as presented in Section 5.7 and parts of Chapter 6, the simulations presented in Chapter 6 were all done at a moderate flow level (600 ml/min). It would be a useful additional application of the existing simulation methods to look also at very low flow rate operation in each of the various mixing vane geometries providing analysis similar to that presented in Section 6.5. Such a mixing analysis could also be done for varying rotor speed in order to understand the relationship between rotor speed, liquid height, and mixing for each of the vane systems.

Important geometric parameters could also be explored. While full exploration of parameter optimization may be better facilitated by future simulations capable of modeling actual liquid–liquid mixing, an initial exploration to identify important parameters and trends using the hydraulic flow simulations demonstrated here would be quite useful. As an example, a geometry with a more narrow annular gap was simulated as part of the work presented in Section 6.6. It was shown there that the increase in fluid–rotor contact and mixing due to the narrower gap is to some degree counteracted by the decrease in liquid volume and fluid residence time. A few possibilities for other geometric parameters to explore include: the vane height, vane-to-rotor gap, rotor bottom shape (recall the taper from certain patents mentioned in Section 1.2.3), and the relative height of the inlets. Further, a number of other mixing vane geometries beyond the few explored in Section 6.5 and Section 6.6 could also be imagined.

This work studied only the hydraulic operation of the contactor using water as the working fluid for both simulations and experiments. For solvent extraction operation, there are two liquid phases (plus air) flowing in the contactor. Ideas for extending the capability of these models for treating liquid–liquid mixing are discussed in Section 8.4, but there is also very useful information that could be obtained from direct application of the existing schemes. As a first step, simulations could
be done using the organic phase as the only liquid phase. An additional step beyond this would be
to simulate the flow of a pseudo-fluid with constant properties (viscosity and density) which mimic
the average properties of the liquid–liquid dispersion (for a given O/A flow ratio) to explore how
the flow of the liquid–liquid dispersion compares to the flow of only water (or only organic) in the
model centrifugal contactor. For example, is there a similar liquid height oscillation for the flow of
the liquid–liquid dispersion in the 4-vane geometry? If so, how do the oscillation characteristics
compare to the water only case? It would also be possible to perform numerical experiments to
explore phase inversion of the pseudo-fluid by implementing an artificially forced transient change
in fluid properties starting from those characteristic of one phase being the continuous phase and
transitioning over a specified time period to fluid properties of the other phase being continuous.
Such an ‘experiment’ would help understand the changes in overall flow characteristics that occur
at phase inversion.

8.2.2 Separation Zone

There are also various areas that could be explored through additional simulations of the flow
in the separation zone. Several design issues that could be researched include: the height of the
dispersion disk, the geometry of the dispersion disk (e.g. radius and hole size), the geometry of the
aqueous riser section (flow channel below the aqueous weir), the effect of a rotor bottom interior
that slopes upward from the rotor inlet, the radius of the rotor inlet, and the effect of outward
sloping rotor sidewalls (i.e. slightly conical shaped rotor interior). This last was determined by
Padial-Collins et al.\cite{47} to have a beneficial effect on phase separation in their simulations of a
simplified rotor geometry.

As was noted in the previous chapter (Chapter 7), the models for the separation zone geometry
had perfectly sharp edges for the two weirs as well as the rotor inlet. Additional simulations to
look at the effect on the predicted zero-point of including a beveled aqueous weir (as is the case
for the actual weir used in the experiments) would be helpful in allowing a more direct comparison
between the zero-point flow rate predicted by simulations and the actual value measured by experiments. The relative effect on the flow of beveling on the light phase weir and even the rotor inlet could also be evaluated.

It would be beneficial to perform additional experimental measurement of the zero-point flow rate for the 1.15 cm aqueous weir using the modified, ‘vented’ upper weir cap. This will require different pumps capable of total flow rates up to \( \sim 3 \text{ L/min} \) to study larger weir sizes where siphoning effect was observed experimentally by others. This is not a difficult pumping requirement; however, time constraints and equipment availability did not allow for such measurements as part of this current project. Combined with a better general understanding of the beveled weir issue, these additional measurements may enable a more direct comparison of the zero-point flow rate from experiment and simulation and provide a quantitative measure for assigning greater confidence in the accuracy of the separation zone simulations.

The simulated flow above the upper weir using the standard closed weir cap was characterized by the formation of a water seal and siphon as described in Chapter 7. Simulations were performed only for a few discrete flow rate settings and additional simulations over a range of flow rates might enable better understanding of the formation mechanism for this flow feature. Further, the stability of the water seal could be explored both experimentally and numerically to understand the relative importance of surface tension, the contact angle, and surface roughness. Several potential weir cap design changes aimed at avoiding this siphon formation were suggested in Figure 7.10; these could also be evaluated through additional simulations using the same methodology employed here.

### 8.2.3 General

It was mentioned previously that the flow and accumulation of particulates in the contactor is an issue of critical importance. This was only briefly explored with the simplified mixing zone models presented in Section 4.1. Some preliminary attempts showed that the techniques used there may require additional modifications in order to be compatible with the VOF models used for the free surface flow. It was decided for this project to first lay the foundation for understanding the
hydraulic operation in the contactor and consequently particle flow was not revisited for the simulations in Chapters 5 through 7. Even so, better understanding of particle flow in both the annular region and the rotor region can provide useful insight into the issue of particle accumulation and nuclear criticality in the contactor and could be a valuable contribution of an additional simulation effort. The information obtained from simulations of particle flow could also provide input for a separate detailed computational study that could be performed to explore neutron transport and criticality in the centrifugal contactor. Such a study could evaluate the utility of design-level incorporation of criticality mitigation through inclusion of design modifications such as proposed by Ogino and Washiya \cite{34} (see Section 1.2.3) or through incorporation into the existing design and materials of construction (e.g. use of borated material for rotor vanes or general surface-level materials modifications via ion implantation onto base material).

Another general issue for facilitating wider application of centrifugal contactors and supporting plant-level implementations is equipment scaling. The simulations and experiments conducted as part of this work were all based on the 5 cm centrifugal contactor. Exploration of scaling issues may be somewhat difficult from a computational intensity standpoint because a larger size contactor geometry will clearly require a larger number of computational cells to get the same mesh spacing. While this bigger mesh would simply require a corresponding increase in the required number of processors (and software licenses if Fluent is used) for the parallel computation, due to communication losses between process nodes the overall time required for each second of simulated flow would invariably be greater. Further, the larger fluid volume and residence time in the model geometry will require that solutions be performed for much longer flow times to reach steady-state. Consequently, it would likely be necessary to reevaluate the acceptable balance between mesh density and accuracy based on the resource limitations (both in hardware availability and software licenses) for this to be a feasible future project.

Above all, an important next stage for this overall simulation effort is to evaluate alternative simulation codes. Specifically, it should be determined whether an open-source computational fluid dynamics resource is available that can meet (or surpass) the performance and accuracy of
the current software (Fluent) and at the same time eliminate the onerous licensing restrictions\(^1\) and provide the flexibility required for the advanced developments needed for capability expansion to explore liquid–liquid mixing (including a free surface) and eventually complete solvent extraction processes. One such candidate code that appears to have the necessary features is an open-source CFD package collection called openFOAM.\(^2\) OpenFOAM is a CFD ‘toolkit’ that contains modules for modeling all aspects of complex flows as well as a well-developed framework for implementing new models and methods as will be required for the development of capability for simulation of solvent extraction processes. In particular, openFOAM has an available CFD solver capable of combining the VOF model for free surface flow with LES for turbulence similar to that used for the free surface simulations performed within this work.\(^3\)

The suggestions outlined here for additional applications of these simulations are summarized in Table 8.1. Those that the author feels are of particularly high priority and can have a high near-term benefit are listed in bold.

### 8.3 Potential Model Refinements

Suggestions for future applications of the general simulation methodology used for this work were outlined above. In addition to those items, there are various refinements that could be made to the modeling scheme to enable more consistent, robust, and efficient simulation of the liquid flow in the contactor. For the most part, these specific limitations were mentioned previously in the text and are laid out in more detail here.

#### 8.3.1 Mixing Zone Model

A significant limitation of the mixing zone model for general application to a variety of geometries and flow conditions is the difficulty in specification of the outlet pressure boundary condition.

\(^1\)Fluent licenses its software on per processor basis—that is, a 40 processor job requires 40 licenses. While there are dedicated parallel licenses that can be purchased at somewhat reduced cost, it is the opinion of this author that the per processor licensing structure is excessively and unreasonably restrictive.

\(^2\)www.opencfd.co.uk

\(^3\)In fact, this solver is capable of second-order time discretization—Fluent only uses first-order for this combination of models.
Table 8.1: Summary of suggestions for additional applications of the simulation schemes used in this project. High priority items are listed in bold.

<table>
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<th><strong>• Mixing Zone</strong></th>
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| – Operational     | * **Low flow rate operation for different vanes**  
|                   | * Varying rotor speed (for each vane type)  |
| – Geometric/Design| * Varying vane height, vane-to-rotor gap, rotor bottom shape, inlet height, etc.  
|                   | * Additional mixing vane geometries  |
| – Fluid Properties| * **Organic phase only (plus air)**  
|                   | * **Pseudo-fluid with dispersion properties** ($\mu_{eff}$ and $\rho_{eff}$)  
|                   | * Artificial phase inversion ‘experiment’  |

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<th><strong>• Separation Zone</strong></th>
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| – Geometric/Design    | * Varying dispersion disk geometry (height, radius, etc.), geometry of aqueous riser section, rotor bottom (interior) shape, rotor inlet radius and shape, outward sloping rotor wall  
|                       | * **Weir edge shape (sharp vs. beveled)**  
|                       | * Upper weir cap modifications to eliminate siphon formation  |
| – Other               | * Zero-point experiments with 1.15 cm aqueous weir and vented cap  
|                       | * Upper weir ‘water seal’ formation mechanism and stability  |

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<th><strong>• General</strong></th>
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<td>– Particulate flow</td>
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<td>– Unit scaling issues</td>
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<td>– <strong>Open-source software evaluation</strong></td>
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As noted in the text, a general method for specifying the outlet (rotor inlet) boundary pressure profile taking into account the complex coupling between the mixing region and the flow inside the rotor has not been developed. While actual experimental measurements of the pressure were performed, these were only done at the center point of the rotor inlet. As described in Section 6.1.2, in order to achieve a simulation result (for the 4-vane geometry) that was consistent with both the measured pressure at the rotor inlet center point and the observed overall annular liquid height, it was determined that the average pressure across the rotor inlet surface must actually be less than the measured value at the center point and from this an adequate pressure profile was assumed. However, a more generalizable method for specifying this boundary condition is desirable such that one would be able to specify the correct condition as a function of rotor speed and to some extent mixing vane configuration without any prior knowledge of the annular liquid height. As noted in Chapter 6 it was chosen to use the same outlet boundary profile for all the simulations of different vane geometries performed in this work; however, it may be possible to devise some useful correction to the pressure profile to account for differences due to vane geometry based on the pressure measurements presented in Section 6.3.1 both as a function of rotor speed and flow rate. Further, it is not explicitly clear how to incorporate the rotor inlet diameter in the specification of the outlet boundary of the mixing zone model. It is well known that increasing the rotor inlet diameter leads to an increase in the annular liquid height.\textsuperscript{[39]} This type of behavior was not explored with the simulations to this point. A general method for specification of this boundary condition should be developed which takes all these factors into account. The additional PIV and LDV data presented in Section 5.7 would provide one means of validating this improved outlet boundary specification scheme (along with the overall annular liquid height). A useful initial test case would be to explore the interaction of liquid volume, liquid height oscillations, and fluid–rotor contact in the context of the measurements given in Section 5.7.4.

Another area for which a valuable refinement to the model can be made is to develop a subroutine to calculate the actual energy dissipation in the fluid near the rotor and in the bulk during the simulation run rather than through post processing of data (see Section 6.5). This would be a useful diagnostic tool for future liquid–liquid mixing simulations and be generally applicable to
other flow conditions whereas the method used in Section 6.5 requires calculation of the values for $\beta$ in Equation 6.4. ‘In situ’ calculation of the energy dissipation could be done in a relatively straightforward manner with a user-defined function (UDF) for Fluent and should also be possible should another code such as openFOAM be employed as the basis of future simulations.

### 8.3.2 Separation Zone Model

In terms of the overall methodology of the separation zone models, a major limitation is the long calculation times required to predict the zero point flow rate. While it would be possible to gain some incremental efficiency benefits through implementing a creative way to decrease the number of flow rate changes required to reach the zero-point, a very significant benefit could be achieved if a steady-state calculation method for zero-point were possible. In theory, the free surface position within the separation zone at steady-state should not depend on the initial condition. Further, at steady-state the interface position does not vary significantly over most of the volume of the rotor. Unfortunately, it was found in attempts to employ the available steady-state free surface flow solution methods in Fluent that the simulation would not converge—even when the initial condition for the time-invariant simulation was the actual steady-state solution from the transient case. It is thought that the interface discontinuities for the flow above the upper weir caused this divergence. Perhaps the geometry could be simplified so as to eliminate this region from the model. However, as was demonstrated in Chapter 7, this region has a significant impact on the overall zero-point prediction and likely cannot be neglected for cases where siphon formation is possible or the pressure above the aqueous weir is much less than atmospheric. Even so, successful efforts to develop a steady-state solution method would make prediction of the zero-point flow rate from CFD simulation a more practical option.

### 8.3.3 Potential for Coupling Mixing and Separation Zone Models

The complex coupling between the annular region and the flow inside the rotor may make it less accurate in certain geometries to subdivide the entire flow domain into two separate models. Combination of the two regions into a single contactor flow model is more complex, but may
be a necessary alternative in these cases. Initial attempts at a combined model were severely re-
stricted by the unwieldy size of the resulting computational model. The rotational symmetry of the 
separation zone by itself allows a reduction in the model geometry to a one-quarter section, thus 
minimizing the number of computational cells required and consequently significantly reducing 
the computation time. It is not an existing option in the standard framework of Fluent to couple 
the mixing zone and separation zone models while solving only a quarter of the separation zone. 
However, it would seem like a method could be developed for mapping the full mixing zone out-
let onto a quarter-section inlet of the separation zone and visa-versa to enable efficient coupling 
between a full mixing zone model and a one-quarter separation zone model. If the entire $360^\circ$ 
geometry of the separation zone is modeled, combination of the two zones more than doubles the 
total number of computational cells of the total geometry for a grid resolution similar to the flow 
models in Chapter 6 and 7. Even so, further study on a combination of the two zones into a single 
model in the future may be necessary to understand the interplay of the two contactor zones and 
identify the dominant effects which define the flow near the rotor inlet. This could perhaps also aid 
in the development of a more general boundary condition between the two distinct zone models.

### 8.4 Simulation of Solvent Extraction

The research effort that comprises this computational and experimental flow analysis has looked 
only at the flow of water in the centrifugal contactor—that is, the hydraulic operation only. This 
was a critical first step and has provided a demonstration of the application of CFD techniques to 
modeling the general liquid flow in the centrifugal contactor as well as the exploration of some ma-
jor design considerations. Ultimately, the goal is to simulate complete solvent extraction processes 
including mass transfer between phases in order to be able to predict an accurate overall stage 
efficiency for a given set of process conditions and enable true optimization of design. Reaching 
this point will require accurate predictions of liquid–liquid interfacial area generation, chemical 
extraction kinetics, and complex liquid phase mixing (and separation) behavior. Presently, there is 
not an existing CFD package that is readily capable of accurately including all of these complex 
factors. However, it is anticipated that existing methods such as employed in this work will provide
a foundation into which additional models based on proven techniques can be implemented where applicable and new methods can be developed and employed where available methods are found to be inadequate. Progress towards this goal can be thought of in a stage-wise process in which successively complex simulations are conducted, identifying deficiencies and necessary improvements at each stage along the way.

Section 1.3.4 outlined a method for approximation of the overall stage efficiency based on various correlations for connecting calculation of the local flow field with the mean droplet size, interfacial area, and mass transfer coefficients. A more rigorous method avoiding empiricism needs to be developed through accurate simulations of the interfacial area generation and chemical extraction rates to provide useful inputs for plant-level and systems modeling.

### 8.4.1 Liquid–liquid Mixing Models

One complex issue required for accurate prediction of the overall mass transfer between phases is the interfacial area between the two liquids. This requires detailed understanding of liquid–liquid mixing and droplet formation as related to local flow characteristics (see Section 1.3). As concluded above, regardless of the ultimate method for treatment of mixing in the liquid phases it will be vital to accurately account for the flow of the free surface and the discontinuous fluid–rotor contact. As such, the simulations performed in this work provide a useful starting point. Presented here are a few preliminary ideas pointing towards potential methods that might have useful application for solvent extraction modeling.

As outlined above in Section 8.2.1, a useful first step towards understanding the general liquid–liquid dispersion flow can be investigated through direct application of the modeling methods used here to look at the flow of a single liquid phase with properties representing the effective fluid properties of a homogeneous liquid–liquid dispersion. This assumption of homogeneity may be an adequate approximation for cases such as the flow in the 4-vane geometry where the fluid volume is greater and the mixing is more intense (see Section 6.5). It would also be possible to define the fluid properties as a function of the local flow characteristics in order to capture some spatial
inhomogeneities (e.g. dispersion viscosity varying with effective dispersed phase droplet size as estimated by correlation to the local turbulence).

Simulation of multiple liquid phases could be built into the general framework used here by applying the VOF method for tracking the volume fraction and interface between the combined liquid phases and air (in order to capture the fluid–rotor contact) while using a separate modeling method to account for the mixing between the two liquid phases. The mixing between the two liquid phases could be implemented by various methods; a couple of potentially useful methods are described here.

A simple method for modeling the mixing of the liquid phases would be to treat them as a single fluid continuum (represented by a single set of momentum equations) and solve an additional volume fraction equation for the distribution of the two liquid phases (as well as the property variations linked with the momentum equation). This is a logical next step to a homogeneous model. This method typically requires specification of the droplet size for determining a velocity difference between the dispersed phase and the continuous phase (referred to as the slip velocity). However, it might also be possible to develop and implement a liquid–liquid analogue of a method which has recently been developed for two-phase gas–liquid flows that uses a transport equation (or equations) for modeling interfacial area concentration. An evaluation of existing data for droplet break-up and coalescence in liquid–liquid systems could provide some information for the development of such a model.

Another possible method would be to model each of the liquid phases separately as individual interpenetrating continua (typically referred to as the Euler–Euler method). This is essentially the method employed by Padial-Collins et al. for their simulation of phase separation. In that study, however, a constant dispersed phase droplet size was used based on correlation with an experimentally measured phase separation time. Alternatively, the droplet size distribution (and consequently the interfacial area) could be modeled according to a more complex population balance approach. For this method, models for rates of droplet coalescence and breakup are included and the size distribution and spatial distribution of droplets can be calculated. The interfacial area
transport equation mentioned above was originally developed from manipulation of these population balance equations.\textsuperscript{156}

It may be that none of the existing methods for modeling liquid–liquid interfacial area generation are adequate and that new methods need to be developed. Before such a conclusion can be made, the applicability of the existing methods should be fully evaluated and it should be determined whether they can be modified for application to the current problem for modeling liquid–liquid mixing and interfacial area in the centrifugal contactor.

\textbf{8.4.2 Interfacial Extraction Chemistry and Potential Multi-Scale Linkage with Molecular-Level Simulations}

Once an accurate method for interfacial area generation can be formulated, it would then be possible to implement models for chemical extraction kinetics into the CFD simulations and subsequently determined the overall stage efficiency. From a ‘black box’ or block diagram perspective, for a given set of conditions a centrifugal contactor stage has some definable extraction rate which determines the overall extraction efficiency for a specific chemical species. But the real drivers for chemical extraction are the complex physical interactions between solvent molecules, extractants, and ions near the liquid–liquid interface. Consequently, understanding the mechanisms of extraction through detailed molecular-level investigation of liquid–liquid interfacial processes provides a potential pathway for prediction of species mass transfer coefficients. Molecular simulation tools such as Molecular Dynamics (MD) are an increasingly valuable tool for detailed study of such processes.

In MD simulations, the interaction forces between molecules are used to solve the equations of motion over very short time scales.\textsuperscript{158} Time averaging of the molecular motions and distributions can be performed to predict useful fluid properties such as the fluid density and viscosity as well as interfacial tension. More importantly, the molecular interactions and transport mechanisms for movement of ions across the liquid–liquid interface can be investigated through these numerical experiments.\textsuperscript{159, 160} In regards to simulations of solvent extraction relevant systems, some work has been done in the last decade to model tri-butyl phosphate and other spent fuel relevant extractants.
(see Baaden et al. 2001[161] for example). From such simulations, it is potentially possible to
determine the rates of extraction (i.e. mass transfer coefficients) of various species for input into the
chemical kinetics models within the CFD simulations facilitating a calculation of the overall mass
transfer and a prediction of the stage efficiency. Moreover, MD and other molecular simulations
can also provide a tool for design of advanced extractants with desired functionality or which are
targeted to the extraction of a specific species.

A significant limitation of MD for simulation of relatively infrequent (on a molecular time-
scale) events such as extraction is the short times which can typically be simulated—several nano-
seconds for modest sized simulations up to perhaps micro-seconds for very long simulations. Thus
there is yet much work to be done in facilitating a full connection between the multiple scales of
interaction that are required for simulation of solvent extraction processes.
Appendix A: Fluent Parallel Scaling

All of the Fluent CFD simulations in this study except for the simplified models of Chapter 4 were run in parallel on two different Linux clusters. The first resource was a small local cluster which originally had \(~60\), 1.8 GHz processors (only one processor per node) and later added \(~32\), 3.2 GHz processors (two processors per node). This system has two available node-to-node connections: a standard fast ethernet connection (\(~100\) MB/s) and a gigabit ethernet connection (\(~1\) GB/s). The gigabit connection was used for the parallel simulations. This system was used for the simulations presented in Chapter 5 as well as most of those presented in Chapter 7. Parallel scaling information on this system is not presented here.

The second computational resource was the Tungsten Linux cluster at the National Center for Supercomputing Applications (NCSA) which was used for all of the simulations presented in Chapter 6. This cluster has 2560, 3.2 GHz processors (two processors per node). This system also has two available interconnects: a gigabit ethernet connection, and a Myrinet connection (\(~2\) GB/s). All of the scaling information presented in this appendix is for simulations run on the Tungsten cluster. Some of these data are from actual ‘production’ simulations while other are from short runs (typically only 10–100 time steps) which were performed simply to evaluate the parallel scaling. The actual time required per iteration\(^3\) was evaluated using Fluent’s built in parallel timer utility.

Figure A.1 shows the scaling observed using the gigabit ethernet connection on the Tungsten cluster for an 8-vane mixing zone model (similar meshing scheme to that used for the simulations in Chapter 5) using the RNG \(k-\varepsilon\) model for turbulence along with the scaling for a separation zone simulation (\(N\) is the number of computational cells). In both cases, it is clear that at some point the communication losses overtake the increased processing power of adding more processors. For the smaller simulation (in terms of the number of computational cells), the communication

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\(^1\)See www.ncsa.uiuc.edu for a full technical summary of the Tungsten cluster.

\(^2\)Myrinet connectivity use was first introduced into Fluent with version 6.3.

\(^3\)Recall that all of the transient simulations in this study employed Fluent’s non-iterative time advancement (NITA) scheme. For this scheme, there is only one global iteration per time step and therefore the terms ‘iteration’ and ‘time step’ are used interchangeably.
losses continue until eventually the overall speed of the calculation actually begins to decrease with extra processors. For this case, there is a maximum possible speedup for the given model, mesh size (number of cells), and parallel node-to-node communicator. As a general rule of thumb, the speedup ‘threshold’ for jobs using a gigabit ethernet connection was found to generally occur at a distribution level of $\sim 20,000–25,000$ computational cells per processor.

For larger simulations, such as those presented in Chapter 6, the potential speedup through parallel processing is much more significant. Figure A.2 shows a comparison of the parallel performance for the 4-vane simulation from Chapter 6 using the two different node-to-node connections available on Tungsten (gigabit ethernet, and Myrinet). The impact of the data transfer speed for node-to-node communications is very apparent. As with the observations shown in Figure A.1, the simulation on the gigabit ethernet was found to reach a plateau in speedup at a distribution level of $\sim 20,000–25,000$ computational cells per processor. On the other hand, the Myrinet connection was found to have much better parallel performance with near ideal scaling behavior ($<5\%$ deviation) up to about 32 processors (for the given size problem). Primarily due to limitations in

Figure A.1: Comparison of Fluent parallel scaling for an 8-vane mixing zone model and a separation zone model on Tungsten using the gigabit ethernet connection. Time per iteration (in seconds) is shown on the left axis and speedup relative to a single processor is shown on the right axis. The ideal speedup behavior (no communication losses) is shown by the dotted line.
Figure A.2: Comparison of the parallel scaling on Tungsten for the same simulation using the two available node-to-node connections: the gigabit ethernet and the Myrinet. The ideal speedup is shown by the dotted line.

Since the number of available Fluent software licenses, it was chosen to use \( \sim 40 \) processors (Myrinet connection) for the simulations done for the mixing vane study (Chapter 6).

Some additional data of the computation time per iteration for various size simulations (all using the Myrinet connection on Tungsten) are given in Figure A.3. While the data presented here are somewhat sparse they can give some further indication of how the Fluent software scales for different size problems. These simulations are all (except one) for the 4-vane mixing zone model using VOF and LES (the different size meshes are the same as presented in Section B.2 for the exploration of grid resolution effects). The simulation identifier in parentheses next to the total number of cells (\( N \)) identifies the geometry, grid spacing on the rotor side, and grid spacing in the rest of the volume (e.g. ‘4v_10_125’ is the 4-vane geometry with a grid spacing of 1.0 mm on the rotor side and 1.25 mm in the rest of the volume.) The simulation labeled ‘Combined3’ was actually a combined mixing zone (RNG \( k-\epsilon \)) and separation zone model using the multiple reference frame approach (as briefly mentioned in Section 8.3.3). It is interesting to note that it was observed that each simulation appears to asymptotically approach \( \sim 2-3 \) s/iteration. Based on the average value of the time step for a given simulation it is possible to use this ‘limit’ to estimate
Figure A.3: Parallel performance of various size simulations on Tungsten using the Myrinet connection. All except the one labeled ‘Combined3’ are for the 4-vane mixing zone model using VOF and LES.

the minimum total computation time (in terms of hours of real time per second of simulated time) that could be achieved through parallel processing of a given simulation.
Appendix B: Grid Resolution

B.1 Simplified Mixing Zone Model

As noted in the text, a grid resolution study was performed for the steady-state simulations of the simplified mixing zone that were presented in Chapter 4. Several quantities were monitored as a function of increasing mesh density to determine the level of mesh at which the simulation results no longer varied significantly with increasing mesh density. Since the largest gradients in the flow were near the spinning rotor, key quantities in this region were observed. Figure B.1 shows plots of the average shear stress (left axis) and the y+ value (right axis, see Equation 4.1 for definition of the y+ parameter) on the rotor side. A y+ value of ~30 on the rotor side was recommended for valid application of wall functions\textsuperscript{[102]} and therefore a mesh with approximately 600,000 cells was used for the simulations.

B.2 Full Mixing Zone Model with VOF

Subsequent to the mixing zone simulations presented in Chapter 5, additional simulations of the 4-vane geometry with decreasing mesh density were performed to explore the grid dependence

Figure B.1: Plot of average shear stress on the rotor side (left axis) and average y+ value on the rotor side for a range of mesh sizes in the simplified mixing zone model (8-vane).
Table B.1: Number of computational cells (tetrahedral) for the 4-vane mixing zone models used for exploration of grid dependence.

<table>
<thead>
<tr>
<th>Grid Spacing, cm</th>
<th>On Rotor Side</th>
<th>In Volume</th>
<th>N Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.15</td>
<td>276 K</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>0.125</td>
<td>327 K</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>0.1</td>
<td>468 K</td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>0.1</td>
<td>1.12 M</td>
<td></td>
</tr>
</tbody>
</table>

of the models. The time-averaged results of each simulation were compiled and compared with the experimental LDV data (same as shown in Figure 5.6). These simulations had a radially uniform outlet pressure boundary of \(-80\) Pa. The mesh spacing on the rotor side and in the bulk that were used to generate the different grids (unstructured tetrahedra) for this comparison are listed in Table B.1. The final mesh that was generated for the 4-vane simulation presented in Chapter 6 was similar to the most dense grid listed in Table B.1 in that it had a minimum spacing of 0.05 cm on the rotor side and a maximum spacing of 0.1 cm in the rest of the volume. However, as is described in Appendix E, a more complex meshing scheme using smoothly varying sizing functions was employed and as such the resulting number of cells for the production mesh was less than the similar mesh listed in the table. For reference, the simulation using the 1.12 million cell grid was done using 60 processors.

Figure B.2, shows the mean tangential and axial velocities for the different simulations as compared to the LDV data at the four axial heights (compare to Figure 5.6). Each of these simulations used VOF and LES although a separate one using the RNG \(k-\varepsilon\) turbulence model is shown for comparison. In general, some improvement in accuracy relative to the experimental data can be seen for the more dense grids. As it was observed that the grid with the 0.05 cm meshing on the rotor side seemed to result in better prediction of the high tangential flow velocities near the rotor, this level of meshing in this region was employed for the mesh generation scheme used for the
Figure B.2: Comparison of the mean tangential and axial velocity from LDV at the four axial heights (shown by the inset images) with simulations using the various computational grids listed in Table B.1. All simulations were done using LES for turbulence except the one labeled RNG $k-\varepsilon$. 
production simulations of the various vane geometries as described in Appendix E and given in Table 6.2.
Appendix C: Wall Contact Angle

C.1 Measurements

The rudimentary contact angle measurements that were performed to estimate the different wetting angles on the various surfaces of the experimental apparatus will be explained here.

The general procedure for these measurements was as follows. A small water droplet was produced from a syringe and dropped from a height of a few inches above the dry surface to be tested. Side-view images of the droplet on the surface were taken using a Nikon D40, 6.1 megapixel digital camera with a 105 mm lens (some images also used an additional 100 mm extender tube). This was repeated $\sim 10$ times for each surface type. The droplet images were analyzed within Adobe Photoshop 7.0 using the angle measure utility to measure the contact angle relative to the surface for each side of the droplet. Figure C.1 gives a sample image. The angles measured for all the images on a given surface type were combined to give a single average value for that surface. The average values for the various surfaces are reported in Table C.1. An attempt was also made to determine the effect on wetting angle of a droplet on a previously wetted surface. To do this, an area on the flat rotor bottom surface was wetted with many droplets which were lightly wiped off and the droplet test was immediately performed while the surface was still wet. This was found to have a substantial effect on the droplet wetting angle as seen in Table C.1 and also produced

![Sample image that was used for measurement of the contact angle of a water droplet on the stainless steel surface of the rotor side.](image)

Figure C.1: Sample image that was used for measurement of the contact angle of a water droplet on the stainless steel surface of the rotor side.
Table C.1: Average values and standard deviations for the measured contact angle of water drops on the various contactor surfaces.

<table>
<thead>
<tr>
<th>Surface</th>
<th>Average Angle (Std Dev), deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-vane plate, painted</td>
<td>62.4 (7.1)</td>
</tr>
<tr>
<td>4-vane plate quartz window</td>
<td>33.4 (6.7)</td>
</tr>
<tr>
<td>Quartz cylinder (inner, angle from tangent)</td>
<td>32.9 (8.0)</td>
</tr>
<tr>
<td>Rotor side, steel</td>
<td>59.4 (7.8)</td>
</tr>
<tr>
<td>Rotor side, painted</td>
<td>63.8 (5.1)</td>
</tr>
<tr>
<td>Rotor bottom, painted</td>
<td>71.6 (5.3)</td>
</tr>
<tr>
<td>Rotor bottom, painted (wetted)</td>
<td>29.2 (8.5)</td>
</tr>
<tr>
<td>Acrylic housing (inside)</td>
<td>37.7 (4.3)</td>
</tr>
<tr>
<td>Water on Teflon (for reference)</td>
<td>99.6 (5.3)</td>
</tr>
<tr>
<td>Rotor bottom, painted (25 ppm SDS)</td>
<td>65.1 (2.9)</td>
</tr>
<tr>
<td>Quartz cylinder (25 ppm SDS)</td>
<td>40.7 (6.0)</td>
</tr>
</tbody>
</table>

some irregular droplet shapes. In general, there was quite a lot of variability between the different surfaces.

It was difficult to find measured values in the literature for even very simple contact angles such as water on quartz or steel. Since the contact angle is dependent on the surface characteristics and even the surface history, most researchers measure their own contact angle (at least those who do not simply neglect such surface effects altogether).\[162\] From estimates that were obtained through a general search of various documents posted on the internet, it appears that these measured values reported here are reasonable. Sklowdowska et al.\[163\] report a contact angle for water on quartz of 32.79°. For water on steel an average value of 75.7° is reported elsewhere.\[164\] It was chosen to use a value of 75° for the contact angle on all surfaces in the mixing simulations presented in Chapter 6. The measured value reported in Table C.1 was somewhat lower than this but was taken
on the curved surface of the rotor and it is not clear what effect this may have had on the accuracy of the measurement.

C.2 2D, Annular Flow Simulations

Simulations similar to those presented in Section 4.2 using a two-dimensional annular model to simulate free surface flow in the mixing zone annulus were done to explore the effect of the contact angle specification on the oscillation characteristics of the liquid surface. These simulations employed a uniform 0.25 mm tetrahedral mesh and the rotor speed was 3600 RPM. Figure C.2 shows plots of the liquid height on the outer surface over many seconds of flow time. Times at which changes to the contact angle specification were made are denoted by a dotted line. From \( t = 7 \) s to \( t = 10 \) s the contact angle on all surfaces was set to 30° to simulate a wetting environment. At \( t = 10 \) s, the contact angle on the rotor boundary was changed to 120° (hydrophobic). At \( t = 13 \) s, the rotor boundary was decreased to 65° to simulate the slightly wetting nature of the painted surface. At \( t = 19 \) s, all surfaces were set back to 30°. In general, it seems that changing the contact angles for the rotor and housing surface introduces a secondary fluctuation which appeared to be due to different folding over behavior of the liquid surface when it falls back down from being spun out from the rotor. This is particularly apparent for the period between 10 s and 13 s where there is a significant difference between the specified contact angles of the inner and outer surface (120° and 30°, respectively).

As the three-dimensional results in the following section demonstrate, this predicted behavior in the simulation shown in Figure C.2 is perhaps somewhat magnified when compared to reality by the 2D, axisymmetric annular approximation.

C.3 Full Mixing Zone Model

While the variation of contact angle on the different surfaces appeared to have a significant effect in the 2D models, from 3D simulations that were performed it did not seem that there was as large an effect on the overall behavior of the main flow. A simulation of the full mixing zone
Figure C.2: Plot of liquid height on the outer wall. See text for a description of the contact angle specifications at different time periods.
Figure C.3: Plot of the circumferentially-averaged annular liquid height above the rotor bottom for a simulation with different contact angles. See text for a description of the contact angle changes.

similar to that for the results presented in Chapter 5 (although with a constant outlet pressure of -80 Pa) was performed in which the contact angles on the walls were changed at times during the simulation. The predicted annular liquid height as a function of the simulated flow time is shown in Figure C.3. For times $t = 0$ to 1 s all contact angles were at 90° (the default value). At time $t = 1$ s, the angle on the housing wall was set to 30° to model the quartz cylinder. At $t = 2$ s, the contact angle on the rotor was also modified and was set to 60° to model the painted surface. At $t = 3$ s, the contact angles for all surfaces were set to be 30° to model the measured wetted angles.

While it was not possible to explore these effects over more than a few seconds, in general the changes in contact angle did not have a substantial effect on the overall time-averaged behavior but did seem to perhaps introduce a secondary fluctuation in time with a period $>1$ s. Even so, the simulations with constant contact angle on all surfaces such as are described in Chapters 5 and 6 compared very well with the experimental data (LDV, PIV, High-speed imaging) from the real system (painted rotor, quartz housing, etc.) as presented in the text. Moreover, for general applicability of the model results—specifically those for the mixing vane study (Chapter 6)—it
was desirable to choose a single contact angle to represent complete stainless steel construction as would be found in a typical contactor unit for a spent fuel recycling application; therefore, the value of 75° was chosen as noted earlier in this appendix.
Appendix D: Model Equilibration

A key feature of the main computational models performed within this project was the ability to predict the volume of liquid maintained within the mixing zone (and similarly in the separation zone). The procedure for ‘start-up’ and equilibration of the various simulations of the free surface flow in the contactor mixing zone will be described here. A similar procedure was used for start-up and equilibration of the separation zone simulations.

The very first 3D mixing zone simulation was initiated from rest with a stationary water level approximately 1.5 cm above the rotor bottom. For all subsequent simulations, the flow solution was never started from rest; rather, a flow field already in motion was patched in as the starting condition in order to avoid the time necessary to get the fluid moving. For the very first simulation (8-vane geometry) a constant outlet (rotor inlet) pressure of 0 Pa was initially specified. Figure D.1 shows the change in outlet mass flow rate and corresponding change in total water volume fraction (normalized by the total mixing zone volume) for an outlet pressure of 0.0 Pa as the system approaches the equilibrium liquid volume following start-up from rest. The total volume fraction appears to reach a steady, equilibrium value at approximately 2.31 s after start-up. The overall mass balance also reaches equilibrium as noted by the outlet mass flow rate settling to an average value around $-0.01 \text{ kg/s}$ ($600 \text{ ml/min}$) which is equal to the total inlet flow rate.

For most simulations in this work, time averaging of the flow field was performed to determine the mean and RMS (root mean squared) velocity and volume fraction distributions and provide a more useful comparison to experimental observations (e.g. the annular liquid height (ALH) is typically measured experimentally by taking the average height of the liquid as observed on the housing wall). In each case, the liquid volume was allowed to equilibrate before averaging was performed. For many of the simulations, such as those presented in Section 5, 0.5 s of averaging was performed. For the mixing vane studies described in Section 6 averaging was done over 1 s of flow. This longer time was used for these LES simulations to ensure that constant average quantities were obtained. For example, it was thought to be particularly important to average over a sufficient number of liquid height oscillations for the flow in the 4-vane geometry such that the
Figure D.1: Time evolution from start-up ($t = 0$ s) of the total water volume fraction (black, left axis) and the outlet mass flow rate (grey, right axis). The vertical dashed line represents the approximate time that steady-state liquid hold-up is achieved.

Flow averages no longer strongly depended on the point in the free surface oscillation cycle at which averaging was started or stopped.

As a demonstration of liquid hold-up volume re-equilibration after a parameter change, at time $t = 3.0$ s of the simulation shown in Figure D.1, the outlet pressure was changed from 0 Pa to $-50.0$ Pa. It would be expected that if the outlet pressure is decreased, the liquid level in the mixing zone should correspondingly decrease. Figure D.2 shows that this indeed was the case. The outlet mass flow rate increased abruptly to just over twice its original value (negative value denotes flow out of the system) and then settled back to the steady state value ($-0.01$ kg/s) after approximately 2 s of flow time.
Figure D.2: Plot of water volume fraction (left axis) and outlet mass flow rate (right axis) versus flow time. The shaded area is the 0.5 s time period over which data were averaged.
Appendix E: Meshing Scheme

The meshing of the geometries for the CFD models was done using Gambit 2.4 from Fluent Inc. For the simulations presented in Chapter 5 the meshing consisted of a uniform quadrilateral grid on the rotor side with spacing of 0.1 cm and 0.15 cm tetrahedral meshing elsewhere for a total of 286 K computational cells as described in the text. For the simulations in Chapter 6 and 7, the meshing was more complex and employed sizing functions within Gambit to refine the grid points within critical regions such as the lower portion of the side of the rotor, the bottom of the rotor, and the narrow gap between the top of the vanes and the rotor bottom for the mixing zone; for the separation zone model, it was critical to have good mesh resolution near the bottom of the rotor around the inlet and rotor vanes as well as in the narrow upper sections such as the aqueous underflow slots and above the aqueous weir. These smoothly varying size functions are specified within Gambit by a starting value, a growth rate, and a maximum value.

E.1 Mixing Zone Mesh Parameters

Table E.1 shows the values used for the various size functions applied to generate the meshes for the different mixing zone geometries used for the mixing vane study (Chapter 6). Note that in each case, the vane tops were meshed first with a uniform tetrahedral mesh of 0.05 cm spacing. In the case of the 8-vane narrow gap geometry, the side of the rotor was also meshed before the volume in order to employ the meshed-face–volume size function. In all cases save the narrow gap simulation, the size functions were ‘attached’ to faces rather than to the volume. In the case of the narrow gap simulation, the rotor side mesh size function was ‘attached’ to the volume, resulting in a smaller and more smoothly varying mesh spacing across the more narrow annular gap.

E.2 Separation Zone Mesh Parameters

Table E.2 and E.3 show the size function parameters used for the meshing of the separation zone models for the refined mesh used for the general simulations and the more coarse mesh used for the zero-point simulations, respectively. For the separation zone, the keys areas for grid refinement
Table E.1: Mesh size functions applied to the various mixing zone geometries. Those listed in the lower half of the table were used in addition to those in the top half for the specific geometries listed.

<table>
<thead>
<tr>
<th>Desc./Attach Point</th>
<th>Type</th>
<th>Start Size (cm)</th>
<th>Growth Rate</th>
<th>Max Size (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotor Bottom,</td>
<td>rotor bottom edge</td>
<td>edge–face</td>
<td>0.05</td>
<td>1.05</td>
</tr>
<tr>
<td>Rotor Side,</td>
<td>rotor bottom edge</td>
<td>edge–face</td>
<td>0.05</td>
<td>1.01</td>
</tr>
<tr>
<td>Vane Top/Rotor Bottom</td>
<td>face–face</td>
<td>0.05</td>
<td>1.05</td>
<td>0.1</td>
</tr>
<tr>
<td>Vane Outer Edge</td>
<td>8-Vane vane–wall gap</td>
<td>edge–face</td>
<td>0.05</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>Curved</td>
<td>edge–face</td>
<td>0.075</td>
<td>1.25</td>
</tr>
<tr>
<td>Meshed Rotor Side</td>
<td>8-Vane, $\eta=0.9$</td>
<td>face–volume</td>
<td>–</td>
<td>1.1</td>
</tr>
</tbody>
</table>

were those in which the air/water interface influences the overall flow characteristics and good resolution of the interface is necessary. This is primarily near the rotor inlet, in the region above the aqueous weir, and near the weir edges. In the main section of the separating region (above the diverter disk and below the light phase weir), where the water/air interface is relatively stationary and smoothly varying, the largest mesh spacing was used. This is also mentioned in the context of Figure 7.5 in which it can be seen that the interface appears less sharp in this region.
Table E.2: Size function parameters for the refined meshing of the separation zone model used for the single flow rate simulations.

<table>
<thead>
<tr>
<th>Desc./Attach Point</th>
<th>Type</th>
<th>Start Size (cm)</th>
<th>Growth Rate</th>
<th>Max Size (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous Weir, weir upper face</td>
<td>face–vol</td>
<td>0.05</td>
<td>1.1</td>
<td>0.2</td>
</tr>
<tr>
<td>Phase Outlet Backsides</td>
<td>face–vol</td>
<td>0.05</td>
<td>1.1</td>
<td>0.2</td>
</tr>
<tr>
<td>Heavy Phase Slot (inside faces)</td>
<td>face–vol</td>
<td>0.05</td>
<td>1.1</td>
<td>0.2</td>
</tr>
<tr>
<td>Lower Edges, all edges below disk</td>
<td>edge–vol</td>
<td>0.05</td>
<td>1.1</td>
<td>0.2</td>
</tr>
<tr>
<td>Lower Vane Edges, edges below</td>
<td>edge–vol</td>
<td>0.05</td>
<td>1.05</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table E.3: Size function parameters for the mesh of the separation zone model used for the zero-point flow rate simulations.

<table>
<thead>
<tr>
<th>Desc./Attach Point</th>
<th>Type</th>
<th>Start Size (cm)</th>
<th>Growth Rate</th>
<th>Max Size (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aqueous Weir, weir upper face</td>
<td>face–vol</td>
<td>0.05</td>
<td>1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>Phase Outlet Backsides</td>
<td>face–vol</td>
<td>0.075</td>
<td>1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>Heavy Phase Slot (inside faces)</td>
<td>face–vol</td>
<td>0.05</td>
<td>1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>Lower Edges, all edges below disk</td>
<td>edge–vol</td>
<td>0.075</td>
<td>1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>Lower Vane Edges, edges below</td>
<td>edge–vol</td>
<td>0.05</td>
<td>1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>Weirs, top inner edge</td>
<td>edge–face</td>
<td>0.05</td>
<td>1.2</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Appendix F: Sample Fluent Scripts

Examples of the various scripts that were used for running the Fluent simulations and processing results are given in this appendix. The scripts will not be explained in line-by-line detail—only a general outline of the purpose of each will be given. This is because for the most part these scripts and commands are unique to Fluent and will likely only be of interest to someone already familiar with Fluent. They are included here to serve as a useful future reference and not as a tutorial on running Fluent (which can be found elsewhere).

F.1 Pressure Boundary Profile

Below is the Fluent user-defined function (UDF) used for the outlet boundary pressure profile as given in Equation 6.1.

```c
/******************************************
udf pressure profile for rotor inlet parabolic profile such that
p_avg = -200 and the p(0) = -80 (on axis position)
******************************************/
#include "udf.h"

#define c0 -80
#define c1 -1.44163e7

DEFINE_PROFILE(MP_p200prof,tf,position)
{
  real x[ND_ND];
  real r2;
  face_t f;

  begin_f_loop(f,tf)
  {
    F_CENTROID(x,f,tf);
    r2=(x[0]*x[0]+x[1]*x[1]);
    F_PROFILE(f,tf,position) = c1*r2+c0;
  }
  end_f_loop(f,tf)
}
```
F.2 LSF Batch Job Submit Script

A sample batch job submission script for the LSF scheduler as used on the Tungsten Linux cluster (NCSA) is given below. This specific script was for starting a job from within the home directory, copying all the necessary files for the job to the scratch disk space, and then following the run, copying all of the output files to the Unitree mass storage at NCSA.

```
#~/bin/csh #
# batch script for submitting parallel fluent jobs on Tungsten
# must be saved as Fluent.Script and submit using
# the command: bsub < Fluent.Script
#
# use "bjobs" command to check status
#

#BSUB -n 40 #specify number of processors
#BSUB -W 100:00 #specify wall time limit (HH:mm)

#BSUB -o error.%J.o #store output and error in file
   fluentjob.jobID.o (optional)

#BSUB -J 4v_05sfv-3dat #specify job name (optional)
#BSUB -B #BSUB -N #send e-mail at end
#BSUB -w "done(1108603)" #don’t run job until this one has finished
# End of embedded BSUB options

# Copy input files to batch $SCR directory

cp 4v_05sfv.* $SCR/
cp *sfv.out $SCR/
cp 4v3-dat.in $SCR/4v3-dat.in

cd $SCR

/usr/apps/cfd/Fluent-6.3.26/Fluent.Inc/bin/fluent 3d -gu -driver
   null -t40 -pmyrinet -ssh -cnf=${LSB_NODEFILE} -i 4v3-dat.in >&
   4v05sfv-40_3avg.out

# Copy all output files from $SCR to Unitree msscmd cd 4v_05sfv,
   mkdir run1, cd run1, mput *.out, mkdir data200, cd data200, mput *.gz
```
In the script above, the file named ‘4v3-dat.in’ is the input journal file (identified by the ‘-i’ flag) with the commands to be executed within Fluent. The text of this file is shown below (text following a semi-colon (;) are comments).

```
rcd 4v_05sfv.cas.gz ;read in case a data files
so set var , , , 3 , , , , ;change end time to 3s
so set data yes 10 , , ;turn on time-averaging
file auto cas 0 ;output frequency for case file
file auto data 200 ;output frequency for data file
file auto over no ;no overwrite of output files
so du 100000 yes yes yes yes yes yes ;iterate, append output files
wcd 4v_05sfv-3.cas.gz ;write case and data upon completion
yes ;confirm overwrite
parallel timer usage ;report stats on parallel performance
exit
```

This sample job submit script was used for a single job (total wall time of 100 hours) starting from case and data files for the 4-vane mixing zone at time $t = 2$ s with an equilibrated liquid volume that would be set to run continuously for the entire 1 s of flow time during which flow data was averaged and complete data sets were outputted at regular intervals (every 200 time steps). This was the method used for generating the data sets that could be used for post-processing to create flow animations, etc. (a sample script and the procedure for post-processing is given later).

For a simulation that was still in the equilibration phase, jobs were typically submitted with short wall times (∼10 hours) to decrease queue wait times. Multiple jobs were submitted consecutively and each successive job was flagged to wait until the previous job had finished (using the “-w/done(jobID)” LSF flag). The submit script for an equilibrating case would be similar to the one shown above except that the wall time limit would be “-W 10:00” and since these jobs were run and the output saved directly to the home directory, no copying of files to scratch was necessary. A sample Fluent input command file for such a case is shown below.

```
rcd 4v_05sfv.cas.gz
so du 9000 yes yes yes yes yes
wcd 4v_05sfv.cas.gz
yes
parallel timer usage
exit
```
F.3 Postprocessing Scripts

During the actual simulation run various quantities were monitored and output to file at regular intervals (≈20 time steps) including: the total water volume, the outlet mass flow rate, the overall mass balance, the mass flow rate through the top surface of the annulus, the integral water volume fraction on the housing wall (from which the ALH was calculated), and the total liquid contact area with the rotor side. This data was recorded for all times during the simulation run (i.e. during both equilibration and averaging). The mass balance and water volume integral were used to identify when equilibration was reached. Additionally, for some simulations the turbulence dissipation rate for the liquid contacted area on the rotor side, on the rotor bottom, and averaged over the entire rotor (liquid contacted areas only) was also monitored.

Using the batch job submit scripts shown above, complete data files for post-processing were also recorded for the 4-vane, 8-vane, and curved vane simulations at regular intervals (every 200 time steps) during the 1 s averaging period totaling about 325 data files for each of the three simulations. The average file size (compressed as .gz) for each data file was approximately 125 MB. Consequently, over the 1 s of flow time during the averaging period a total of approximately 40 GB of data was accumulated for each of the three vane types. Despite the memory storage requirements, from these complete files it was possible to use batch processing scripts to analyze additional data and output images for creation of flow animations and videos. Incidentally, Fluent does have the capability to directly output images for videos during a simulation run but the process is tedious for more than a single view (and also uses up valuable computation time).

Below is an example of a shell script that was used to generate a complete Fluent journal file to process each file in the data set based on a template file of commands.¹

```bash
    echo "making animation journal file based on elem-avgs-file.jou"
    more elem-avgs-file.jou
    for i in { `ls data200/4v_05sfv_p200prof-*.dat.gz` }
      do
        j=`echo $i | awk -F- '{print $2}' | awk -F.d '{print $1}'`
        echo $i | awk -F- '{print $2}' | awk -F.d '{print $1}' |
        awk -F. '{print $1}'
        ## echo $j
```

¹These scripts were modified from examples posted on the Fluent Technical Support Portal archives under solution number 229, “Notes on various methods to create animations from FLUENT results.”
sed s/zzz/$j/ elem-file.jou >> complete-file.jou
done
echo "finished"

Here is a sample journal template file (elem-file.jou) as would be processed using the preceding shell script for outputting images of contour plots of the water volume fractions (the purpose of the last line will be described later).

```
rd 4v_05sfv_p200prof-zzz.dat.gz
di co phase-1 vof 0 1 ;plot volume fractions for phase-1 (water)
di co phase-1 vof 0 1
di vi res side ;set view to side
(set-annotate) ;annotate image
di ha ../anim_vect/4v-p200prof-vect-zzz.tif ;output tif file
di clo 0
(write-g-file pt1 "average" 'sgs-dissipation-rate
(list 'vof05-rot 'vof05-rotside 'vof05-rotbot))
```

Prior to reading the resulting complete journal file created by running the shell script above, a contour plot on the desired surfaces was first generated within Fluent such that as successive data files were read in using the complete journal file of commands, the plots created would be on the same list of surfaces last registered in Fluent’s ‘memory’. The command “(set-annotate)” in the elementary (template) file causes the current simulation flow time to be annotated onto the image output using the following Fluent scheme file:

```
;;setup graphics window
;(ti-menu-load-string "dis set wind text vis no")
;(ti-menu-load-string "dis set wind scale vis no")
;(ti-menu-load-string "dis set wind main left -1")
;(ti-menu-load-string "dis set wind main bottom -1")
;(ti-menu-load-string "dis set ha x-res 900")
;(ti-menu-load-string "dis set ha y-res 900")

;;; Below taken from Fluent Tech Support Solution 1291
(define set-annotate
(lambda ()
(with-output-to-file "junk"
(lambda ()
```
; ADD POSTPROCESSING COMMANDS

(define a (rpgetvar 'flow-time))
(ti-menu-load-string "dis c-ann")
(cx-use-window 0)
(cxsetvar 'annotate/font/size "30")
(cxsetvar 'annotate/font/wt "Medium")
(cxsetvar 'annotate/font/slant "Regular")
(cxsetvar 'annotate/color "foreground")
(cxsetvar 'annotate/font/name "helvetica")
(cx-annotate '() '(-0.035 0.0375 0) "V<"
  (format #f "Velocity, m/s Time = ~d sec" a))
;(cx-annotate '() '(-0.035 -0.045 0) "V<"
  (format #f " Time = ~d sec" a));side
;(cx-annotate '() '(-0.02 0.0365 0) "V<"
  (format #f " Time = ~d sec" a));under
;(cx-changed 'scene-list)

; SAVE HARDCOPY
))
)
)

This annotation is useful for creating flow animations showing the running flow time. The last line
in the template file shown above outputs various surface averages to file (similar to those which
could otherwise be done during the simulation run) using the Fluent scheme function below.

;;;; From Fluent Tech Support Solution 477
;;;; This Scheme function is computing
;;;; the averaged / mass-averaged value
;;;; of any quantity on a list of
;;;; zones identified through their names
;;;; and saves the values in spreadsheet format
;;;; in files named as defined by the user
;;;;
;;;; Usage

;;;; 1) After reading the case and data file, type the
;;;; TUI command
;;;;
;;;; (define pt1 (open-output-file "av1-export.xls"))
;; (define pt2 (open-output-file "av2-export.xls"))
;; ... and so on.
;;
;; These commands will open the files for output
;; under ports pt1, pt2, ..
;;
;; 2) File>Read>Scheme .. this file (wgen-file.scm)

;; 3) Set a monitor command in GUI
;; Solve>Monitor>Command
;; with the following content
;;
;; (write-g-file used-port average-type quantity list-of-zone-names)
;;
;; A correct syntax for the list-of-zone-names looks like
;;
;; (list 'inlet-1 'outlet-2 'outlet-3)
;; so for this example the content of the Command Monitor is:
;;
;; (write-g-file pt1 "mass-average" 'total-temperature
(  list 'inlet-1 'outlet-2 'outlet-3))

;; or
;;
;; (write-g-file pt2 "average" 'temperature (list 'inlet-1))
;;
;; the type "average" corresponds to area averaging
;; the type "mass-average" corresponds to mass averaging

;; the symbol 'temperature stands for static temperature
;; the symbol 'total-temperature stands for total temperature
;; other symbols maybe used after asking for support

;; the variable pt1 or pt2 indicates in which file should the
;; averages be recorded

;; 4) Set the frequency of executions - Every "n" Time steps

;; 5) Run the transient analysis

;; 6) Once you want to close these file you must type the TUI command
;;; (close-output-port pt1)
;;; (close-output-port pt2)

;;; Do not change below this line without calling for support
;;; ===============================================================
(define (write-g-file uport gtype gquantity list-surface-names)
  (let ((tim)(ll)(g-surface-average))
    (set! g-surface-average
      (lambda (type quantity list-of-surf-names)
        (let ((g-surface)(list->strip))
          ;;
          (set! list->strip
            (lambda (inputlist)
              (let ((stri "")
                (ll (length inputlist)))
                (let loop ((i 0))
                  (if (< i ll)
                    (begin
                      (set! stri (string-append stri " 
                        (number->string (list-ref inputlist i))))
                      (loop (+ i 1)))
                    stri ))))
          ;;
          (set! g-surface
            (lambda (typx surfx cell-onlyx?)
              (if (equal? typx "average")
                (surface-average surfx cell-onlyx?)
                (surface-mass-average surfx cell-onlyx?))))
          ;;;
          (let* ((surf-list (map surface-name->id list-of-surf-names))
            (input-strip (list->strip surf-list))
            (ti-menu-load-string
              (string-append "(cxisetvar 'xy/surfaces \"\") ()")
            (ti-menu-load-string
              (string-append "(cxisetvar 'xy/surfaces \"\") " input-strip ",")
            (let ((of quantity))
              (if of

              ;; the next line changed from (cell-only? (cx-cell-only-field? of))
              ;; to (cell-only? (cx-cell-only-field? "mixture" of))
              ;; to cope with F6.3 format. mlo}
(let ((cell-only? (cx-cell-only-field? "mixture" of))
  (surfaces (cxgetvar 'xy/surfaces)))
  (client-set-node-values #f)
  (client-fill-node-values of)
  (cx-fill-face-zone-values surfaces of)
  (g-surface type surfaces cell-only?)))
)
(set! tim (rpgetvar 'flow-time))
(format uport " ~a " tim)
(set! ll (length list-surface-names))
(let loop ((i 0))
  (if (< i ll)
    (begin
      (format uport " \	 ~a" (g-surface-average gtype gquantity
          (list (list-ref list-surface-names i))))
      (loop (+ i 1)))
    (newline uport)
  ))
)

Additional coding was used to perform time-averaging of flow variables that are not by default averaged within Fluent (e.g. the turbulent kinetic energy and dissipation rate). This was done by adding a line such as “de ud eod avg::libudf” to the template file above. This calls and executes another add-on function (this one referred to as an ‘execute-on-demand’ UDF) the text of which is given below.

/***********************************************
KWardle 1/2008
averaging scheme modified from
Fluent Technical Support Solution 1272
changed to use user-defined memory rather than UDM and
to write out final average to this UDM rather than overwrite existing data
NOTE: you must define UDMs first *AND* then patch
in zero initial values for each one before running avg_init
***********************************************/
#include "udf.h"

#define nf 327 /*the total number of data files to be averaged*/
DEFINE_ON_DEMAND(avg_init)
{
    Domain *d,*d2;
    Thread *t;
    cell_t c;
    FILE *fp1, *fp2;
    real a0, a1, a2, a3, a4, a5, a6, a7, a8;
    d = Get_Domain(1); /*mixture level domain thread*/
    d2 = Get_Domain(2); /*primary phase domain thread*/

    /*set up UDMs*/
    Set_User_Memory_Name(0,"AVG_XVEL");
    Set_User_Memory_Name(1,"AVG_YVEL");
    Set_User_Memory_Name(2,"AVG_ZVEL");
    Set_User_Memory_Name(3,"AVG_TKE");
    Set_User_Memory_Name(4,"AVG_EPS");
    Set_User_Memory_Name(5,"RMS_TKE");
    Set_User_Memory_Name(6,"RMS_EPS");
    Set_User_Memory_Name(7,"AVG_VOF");
    Set_User_Memory_Name(8,"RMS_VOF");

    /*enum
    {
        AVG_XVEL,
        AVG_YVEL,
        AVG_ZVEL,
        AVG_TKE,
        AVG_EPS,
        RMS_TKE,
        RMS_EPS,
        AVG_VOF,
        RMS_VOF
    }*/

    fp1 = fopen("temp_data","w+");

    thread_loop_c(t,d)
    {
        if (FLUID_THREAD_P(t))
            begin_c_loop(c,t)
            {
                C_UDMI(c,t,0) = 0.0;
            }
    }
C_UDMI(c,t,1) = 0.0;
C_UDMI(c,t,2) = 0.0;
C_UDMI(c,t,3) = 0.0;
C_UDMI(c,t,4) = 0.0;
C_UDMI(c,t,5) = 0.0;
C_UDMI(c,t,6) = 0.0;
a0 = 0.0;
a1 = 0.0;
a2 = 0.0;
a3 = 0.0;
a4 = 0.0;
a5 = 0.0;
a6 = 0.0;
fprintf(fp1, "%f %f %f %f %f %f\n", a0, a1, a2, a3, a4, a5, a6);
end_c_loop(c,t)
}
close(fp1);

fp2 = fopen("temp_data2","w+");
thread_loop_c(t,d2)
{
if (FLUID_THREAD_P(t))
begin_c_loop(c,t)
{
    C_UDMI(c,t,7) = 0.0;
    C_UDMI(c,t,8) = 0.0;
a7 = 0.0;
a8 = 0.0;
    fprintf(fp2, "%f %f\n ", a7, a8);
}
end_c_loop(c,t)
}
close(fp2);
}
/**********end avg-init**********/

DEFINE_ON_DEMAND(avg)
{
    Domain *d, *d2;
Thread *t;
cell_t c;
FILE *fp1,*fp2;
real a0, a1, a2, a3, a4, a5, a6, a7, a8;
real l, subdiss;
d = Get_Domain(1);
d2 = Get_Domain(2);

fp1 = fopen("temp_data","r");

thread_loop_c(t,d)
{
if (FLUID_THREAD_P(t))
begin_c_loop(c,t)
{
    fscanf(fp1, "%f %f %f %f %f %f %f
",&a0, &a1, &a2, &a3, &a4, &a5, &a6);
    C_UDMI(c,t,0) = a0;
    C_UDMI(c,t,1) = a1;
    C_UDMI(c,t,2) = a2;
    C_UDMI(c,t,3) = a3;
    C_UDMI(c,t,4) = a4;
    C_UDMI(c,t,5) = a5;
    C_UDMI(c,t,6) = a6;
}
end_c_loop(c,t)
}
fclose(fp1);

fp2 = fopen("temp_data2","r");

thread_loop_c(t,d2)
{
if (FLUID_THREAD_P(t))
begin_c_loop(c,t)
{
    fscanf(fp2, "%f %f
",&a7, &a8);
    C_UDMI(c,t,7) = a7;
    C_UDMI(c,t,8) = a8;
}
end_c_loop(c,t)
}
fclose(fp2);
fp1 = fopen("temp_data","w");
thread_loop_c(t,d)
{
    if (FLUID_THREAD_P(t))
        begin_c_loop(c,t)
        {
            /***collect sums***/
            C_UDMI(c,t,0) = C_UDMI(c,t,0) + C_U(c,t); /*x-velocity*/
            C_UDMI(c,t,1) = C_UDMI(c,t,1) + C_V(c,t); /*y-velocity*/
            C_UDMI(c,t,2) = C_UDMI(c,t,2) + C_W(c,t); /*z-velocity*/
            /**SGS turb kinetic energy**/
            C_UDMI(c,t,3) = C_UDMI(c,t,3) + C_K(c,t);
            /**calculate sgs dissipation rate**/
            l = pow(C_VOLUME(c,t),1./3);
            subdiss=C_STORAGE_R(c,t,SV_LES_C_EPSILON)*C_K(c,t)*sqrt(C_K(c,t))/l;
            C_UDMI(c,t,4) = C_UDMI(c,t,4) + subdiss; /*SGS turb dissip. rate*/
            /* sums of squared vals for RMS*/
            /*SGS turb kinetic energy - squared*/
            C_UDMI(c,t,5) = C_UDMI(c,t,5) + SQR(C_K(c,t));
            /*SGS turb dissip. rate - squared*/
            C_UDMI(c,t,6) = C_UDMI(c,t,6) + SQR(subdiss);
            /**write sums to temp file**/
            fprintf(fp1, "%g %g %g %g %g %g\n",C_UDMI(c,t,0),_
                    C_UDMI(c,t,1),C_UDMI(c,t,2), C_UDMI(c,t,3),C_UDMI(c,t,4),_
                    C_UDMI(c,t,5),C_UDMI(c,t,6));
            /**compute averages***/
            C_UDMI(c,t,0) = C_UDMI(c,t,0)/nf;
            C_UDMI(c,t,1) = C_UDMI(c,t,1)/nf;
            C_UDMI(c,t,2) = C_UDMI(c,t,2)/nf;
            C_UDMI(c,t,3) = C_UDMI(c,t,3)/nf;
            C_UDMI(c,t,4) = C_UDMI(c,t,4)/nf;
            C_UDMI(c,t,5) = sqrt(fabs(fabs(C_UDMI(c,t,5)/nf -_
                        SQR(C_UDMI(c,t,3))/SQR(nf))));
            C_UDMI(c,t,6) = sqrt(fabs(fabs(C_UDMI(c,t,6)/nf -_
                        SQR(C_UDMI(c,t,4))/SQR(nf))));
        }
        end_c_loop(c,t)
    }
fclose(fp1);

fp2 = fopen("temp_data2","w");
thread_loop_c(t,d2)
if (FLUID_THREAD_P(t))
    begin_c_loop(c,t)
    {
        /****collect sums***/
        C_UDMI(c,t,7) = C_UDMI(c,t,7) + C_VOF(c,t); /*vof*/
        C_UDMI(c,t,8) = C_UDMI(c,t,8) + SQR(C_VOF(c,t)); /*squared vof*/
        /**write to temp file***/
        fprintf(fp2, "%g %g\n", C_UDMI(c,t,7), C_UDMI(c,t,8));
        /****compute average and RMS***/
        C_UDMI(c,t,7) = C_UDMI(c,t,7)/nf;
        C_UDMI(c,t,8) = sqrt(fabs(C_UDMI(c,t,8)/nf - 
            SQR(C_UDMI(c,t,7))/SQR(nf)));
    }
    end_c_loop(c,t)
}
fclose(fp2);
}
Appendix G: Fluent Function for Zero-Point Evaluation

The following is the code that was attached to Fluent as a user-defined function (UDF) in order to couple the inlet flow rate with the overall mass balance and air/water interface position near the organic weir for evaluation of the zero-point flow rate.

/*================================================================---------*
* ** UDF Name: MP_zero_pt **
* This UDF solves for the zero point flow rate -- that is, the flow rate at which flow just begins to overflow the organic weir
* MUST BE HOOKED AS A MASS FLUX PROFILE (fluent 6.3)
* - The original framework of this UDF was based on soln 718 from the fluent tech support portal -
* - For 2D and 3D problem --> Factor to 1.0
* - For 2D-Axisymmetric --> Factor = 2.0*Pi
* - For 3d periodic quarter-section model --> Factor = 4.0
* NOTE: It appears that the RP_HOST process is NOT called within DEFINE_PROFILE
*-------------------------------------------------------------------------*/

#include "udf.h"
/**include "para.h"*/
#include "surf.h"

#define Pi 3.14159265359
#define Factor 4.0 /*2.0*Pi*/
#define primary_phase_ID 2
#define volconv 6.011e4 /*convert from kg/s to ml/min FOR WATER rho=998.s*/
#define aqoutID 14 /*Set ID for aqueous outlet surface*/
#define orgoutID 13 /*Set ID for organic outlet surface*/
#define vofsurfID 14 /*ID for vof = 0.5 CLIPPED iso-surface (z = top of oweir .. 5mm below) */
#define r_orgweir 0.01037 /*organic weir radius **IN METERS** */
#define pflag 1 /* 0 = no output, 1 = output to file zp.out, 2 = output to Message0 Console*/
#define ssmax 250 /*number of steps for steady-state averaging (100)*/
#define orgoutflag 0 /*1 increment inlet until flow out org exit,
0 zp defined as interface at orgweir*/
static int iflag = 0; /*static global vars for change flag */
static int icount = 0;
static real curr_time;
static int sscount=0; /*static vars for Steady-state counters*/
static real ss_sum=0.0, ss_avg=0.0, Z_avg=0.0, Z_sum=0.0;
FILE *fp1;

static int istart=1; /*flag to show parallel node intros on start-up*/

static real area_in,mfr,mfr_in,mfr_aq,mfr_org;
static int surfNP;
static real mflux_new,sumarea,sumMFR;
static real radsum = 0.0;
static real mfr_new,mflux, SS, Z;
static real r_avg, delmflux, delr;

/***********Define function for calculating new flow rate setpoint*******/
real dFCompute(real mfrO_target, real alpha,int zoneID)
{
  /*BEGIN FUNCTION*/
  int i;
  cell_t cell;
  CX_Cell_Id c;
  face_t f;
  real A[ND_ND],xc[ND_ND], rad;
  Domain * d = Get_Domain(primary_phase_ID);
  /*this is domain for water phase */
  Surface surf = SurfaceList[vofsurfID];

  /*find face threads*/
  tf = Lookup_Thread(d,zoneID);
  tf_aq = Lookup_Thread(d,aqoutID);
  tf_org = Lookup_Thread(d,orgoutID);

  if (istart==1) /*do only once at initial start-up*/
  {
    Message("*** Hello, I am node %i **** \n",myid);
    istart=0;
    if (pflag==1) Message0("Writing output to file zp.out \n");
  

if (pflag==2) Message0("Writing output to console \\
");
}

/***** loop over vof-05-clip surface to get interface
    position near org weir ******/
/** looping method borrowed from soln 1056
   on fluent tech support portal **/
radsum=0.0;
for(i=0;i<surf.np;i++)
{
c=surf.points[i].cell;
cell=RP_CELL(&c);
cell_thread=RP_THREAD(&c);
C_CENTROID(xc,cell,cell_thread);
rad=sqrt(pow(xc[0],2.0) + pow(xc[1],2.0));
/*rad=xc[1];*/
radsum += rad;
}

/*collect sums from compute nodes*/
radsum=PRF_GRSUM1(radsum);
surfNP=PRF_GRSUM1(surf.np);

r_avg=radsum/surfNP; /*this is a spatial average
              NOT a time average*/
/* test messages
Message0("*** surfNP = %i, radsum = %f, r_avg = %f",surfNP,radsum,r_avg);
*/

/------ loop over faces on the inlet --------*/
/*zero out sums*/
sumarea = 0.0;
sumMFR = 0.0;
area_in = 0.0;
mfr=0.0;
mfr_in=0.0;
mfr_aq=0.0;
mfr_org=0.0;

begin_f_loop(f,tf)
{
if (PRINCIPAL_FACE_P(f,tf))
F_AREA(A,f,tf);
area_in = Factor*NV_MAG(A); /*get face area*/

/* assume pressure-based solver (seg) */
mfr = F_FLUX(f,tf);
mfr = Factor*mfr*(-1.0); /*by default flux is NEGATIVE for flow into domain
(don’t ask me why...)*/

sumarea += area_in;
sumMFR += mfr;
}
end_f_loop(f,tf)

/*collect sums from compute nodes*/
sumarea=PRF_GRSUM1(sumarea);
sumMFR=PRF_GRSUM1(sumMFR);

area_in=sumarea;
mfr_in=sumMFR;
mflux = mfr_in/area_in;

/******* loop over faces on the aq outlet(s) *******
sumMFR = 0.0;

begin_f_loop(f,tf_aq)
if (PRINCIPAL_FACE_P(f,tf_aq))
{
/* assume pressure-based solver (seg) */
mfr = F_FLUX(f,tf_aq);
mfr = Factor*mfr*(-1.0);

sumMFR += mfr;
}
end_f_loop(f,tf_aq)

/*collect sums from compute nodes*/
sumMFR=PRF_GRSUM1(sumMFR);

mfr_aq=sumMFR;

/******* loop over faces on the aq outlet(s) *******
sumMFR = 0.0;
begin_f_loop(f,tf_org)
if (PRINCIPAL_FACE_P(f,tf_org))
{
    /* assume pressure-based solver (seg) */
    mfr = F_FLUX(f,tf_org);
    mfr = Factor*mfr*(-1.0);

    sumMFR += mfr;
}
end_f_loop(f,tf_org)

/*collect sums from compute nodes*/
sumMFR=PRF_GRSUM1(sumMFR);

mfr_org=sumMFR;

/*calculate mass balance*/
SS=(mfr_aq + mfr_org + mfr_in)/mfr_in;
    /* signs should be: outlets (-), inlet (+)*/
/*Message0("****** SS= %f ******",SS);*/
/* mass balance averaging to check for steady-state */
sscount++;
ss_sum += SS; /*sum SS to take average*/
ss_avg = ss_sum / sscount;
Z = mfr_org/mfr_in;
Z_sum += Z;
Z_avg = Z_sum / sscount;
if (fmod(sscount,25)==0.0)
{
    if ((pflag==1)&&(myid==0))
    {
        if ((fp1 = fopen("zp.out","a"))==NULL)
            Message0("\n\n  **Error opening file zp.out (S1)** \n\n");
        fprintf(fp1,"%2.5f -- Mass Balance for %i calls.\n",curr_time,sscount);
        fprintf(fp1," SS = %+2.2f %%, SS_avg = %+2.3f %% \n", _
            SS*100,ss_avg*100);
        fprintf(fp1," r_avg - r_orgweir = %+1.3f cm, AVG Org Outflow = _
            %+2.3f %% \n",(r_avg-r_orgweir)*100, Z_avg*100);
        fprintf(fp1," Current Inlet Mass Flow Rate = %4.2f \n", _
            mfr_in*volconv);
    }fclose(fp1);
if (pflag==2)
{
Message0("%2.5f -- Mass Balance for %i calls.\n",curr_time,sscount);
Message0(" SS = %+2.2f %%, SS_avg = %+2.3f %% \n",SS*100,ss_avg*100);
Message0(" r_avg - r_orgweir = %+1.3f cm, AVG Org Outflow = %+2.3f _%
(r_avg-r_orgweir)*100, Z_avg*100);
Message0(" Current Inlet Mass Flow Rate = %4.2f \n", mfr_in*volconv);
}
/*if (sscount<ssmax)
{
if ((pflag==1)&&(myid==0) fclose(fp1);
}*/
}
if ((sscount>=ssmax)&&(fabs(ss_avg) <= 0.025))
/*steady-state avg for ssmax calls < 2.5% */
{
    sscount=0; /*reset counter*/
    ss_sum = 0.0; /*reset sum*/
    Z_sum = 0.0;
if (Z_avg < mfr0_target)
{
    delr = r_avg - r_orgweir;
if ((delr*100 <= 0.05)&&(orgoutflag==1))
{
    mfr_new = mfr_in + 5.0/volconv; /*if very close to zero-pt,
    increment mfr by 5 ml/min*/
if ((fp1 = fopen("zp.out","a"))==NULL) _
        Message0("\n\n **Error opening file zp.out (S1b)** \n\n");
printf(fp1," ** Close to Zero-pt, incrementing mfr by 5 ml/min ** \n");
fclose(fp1);
} else
{
    delmflux = alpha*(delr)/r_orgweir;
    mfr_new = mfr_in*(1.0 + delmflux);
} mflux_new=mfr_new/area_in;

if ((pflag==1)&&(myid==0))
{
if ((fp1 = fopen("zp.out","a"))==NULL) _
Message0("\n\n **Error opening file zp.out (S2)** \n\n");
fprintf(fp1,"\%2.5f -- STEADY-STATE at Mass Flow Rate =\%f ml/min \n", curr_time,mfr_in*volconv);
fprintf(fp1," CHANGED VALUE, New Mass Flow =\%f ml/min ** \n", mfr_new*volconv);

/* fprintf(fp1,"\%2.5f -- STEADY-STATE at Mass Flux =\%f kg/m2*s \n", curr_time,mflux);
fprintf(fp1," CHANGED VALUE, new Mass Flux =\%f kg/m2*s ** \n", mflux_new);*/
fprintf(fp1," Percent Change = \%2.2f \% \n", delmflux*100);
fprintf(fp1," Skipping profile call 100 times to allow flow to _
 respond. \n");
fclose(fp1);
}
if (pflag==2)
{
Message0("\%2.5f -- STEADY-STATE at Mass Flow Rate =\%f ml/min \n", curr_time,mfr_in*volconv);
Message0(" CHANGED VALUE, New Mass Flow =\%f ml/min ** \n", mfr_new*volconv);
/* Message0("\%2.5f -- STEADY-STATE at Mass Flux =\%f kg/m2*s \n", curr_time,mflux);
Message0(" CHANGED VALUE, new Mass Flux =\%f kg/m2*s ** \n", mflux_new);*/
Message0(" Percent Change = \%2.2f \% \n", delmflux*100);
Message0(" Skipping profile call 100 times to allow flow to _
 respond. \n");
}
iflag = 1; /*set flag to show change was made*/
return mflux_new;
}
else /*steady state with organic outflow*/
{
if (((pflag==1)&&(myid==0))
{
if ((fp1 = fopen("zp.out","a"))==NULL) _
Message0("\n\n **Error opening file zp.out (Z1)** \n\n");
fprintf(fp1,"\%2.5f -- Org outflow greater than \%1.1f percent detected ** _
\n", curr_time,mfr0_target*100);
fprintf(fp1," AVG Org outflow = \%+2.2f \% \n", Z_avg*100.0);
fprintf(fp1," Zero-Point Flow Rate = %4.3f ml/min \n",mfr_in*volconv);
fprintf(fp1,"******STOPPING SIMULATION****** \n ");
fclose(fp1);
}
if (pflag==2)
{
Message0("%2.5f -- Org outflow greater than %1.1f percent detected ** \
", curr_time,mfrO_target*100);
Message0(" AVG Org outflow = %+2.2f % \n", Z_avg*100.0);
Message0(" Zero-Point Flow Rate = %4.3f ml/min \n",mfr_in*volconv);
Message0("******STOPPING SIMULATION****** \n ");
}
RP_Set_Boolean("stop",1); /*for automatically stopping iterations, 
 requires scheme function zp-iter.scm*/
mflux_new=mflux; /*don't change mflux*/
return mflux_new;
} /* IF1 end*/

/*SS counter less than 10 OR counter = 10 but ss_avg is > 0.02*/
if (sscount >= ssmax) /*if we got here because ss_avg was > 0.02 
then reset*/
{
    sscount = 0;
    ss_sum = 0.0;
    Z_sum = 0.0;
    if ((pflag==1)&&(myid==0))
    {
        if ((fp1 = fopen("zp.out","a"))==NULL) 
            Message0("\n\n **Error opening file zp.out (S3)** \n\n");
        fprintf(fp1,"NOT AT STEADY-STATE \n");
        fprintf(fp1,"
");
        fclose(fp1);
    }
    if (pflag==2)
    {
        Message0("NOT AT STEADY-STATE \n");
        Message0("\n");
    }
}
mflux_new=mflux; /*no change to mflux*/
return mflux_new;

} /*END FUNCTION*/

/***************************************************************************/

DEFINE_PROFILE(MP_zero_pt,tf,position)
{
  face_t f;
  int zoneID;
  real mfrO_target,alpha,mflux_new;

#ifdef RP_NODE
  Message("Profile Call Initiated. I am node %i \n ",myid);
#endif

  curr_time = CURRENT_TIME;

/*if ((pflag==1)&&(myid==0))
{
  if ((fp1 = fopen("zp.out","a"))==NULL)
  {
    Message0("Error opening file zp.out\n");
    return 0;
  }
}
}*/

if (iflag == 1) /*skip function if change was made within last 100 calls*/
{
  icount++; /*increment counter on host only*/
  if (icount >= 100)
  {
    icount = 0;
    iflag = 0;
    if ((pflag==1)&&(myid==0))
      {
        if ((fp1 = fopen("zp.out","a"))==NULL) _
          Message0("\n\n **Error opening file zp.out (DEF)** \n\n");
        fprintf(fp1,"%.5f -- %i steps reached. \n",curr_time, icount);
        fclose(fp1);
      }
}
if (pflag==2) Message0("%2.5f -- %i steps reached. \n", curr_time, icount);
}
/*else
{
if ((pflag==1)&&(myid==0)) fclose(fp1);
}*/
}

else
{
  mfrO_target = 0.01; /* Target Organic outflow of 1% */
  alpha = 0.25; /* Relaxation factor */

  zoneID = THREAD_ID(tf);

  mflux_new = dFCompute(mfrO_target, alpha, zoneID);
  /*function returns MASS FLUX*/
  /*Message0("******* mflux_new = %f ********", mflux_new);*/
  /* send value to nodes */

  /*#if RP_NODE */
  Message("Profile Called. I am node %i \n ", myid);
  #endif*/

  /*------ distribute new mass FLUX ------*/

  begin_f_loop(f,tf)
  if (PRINCIPAL_FACE_P(f,tf))
  {
    F_PROFILE(f,tf,position) = mflux_new;
  }
  end_f_loop(f,tf)

  } /* end else */

} /* end DEFINE_PROFLILE*/
LIST OF REFERENCES


