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CHARACTERIZING LIQUID FILM THICKNESS IN SPINNING DISC REACTORS

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ABSTRACT

Hydrodynamic behaviour of the liquid film in a spinning disc reactor was investigated using computational fluid dynamics. Flow characteristics of the liquid film were studied over a range of operating conditions. Both 2D and 3D simulations were carried out using the volume of fluid method and compared with experimental data and empirical correlations published in literature. While the film thickness predicted by 3D simulations was in good agreement with experimental data, the high computational time required rendered the simulations too costly. The 2D simulations reported closer agreement with available empirical correlations, however, the film thickness was much lower compared to the experimental values. The results obtained here provide insight into the hydrodynamics and would be useful in accessing performance of the spinning disc reactor for multiphase reactions.

Keywords: Spinning disc, Liquid film flow, CFD and VOF.

NOMENCLATURE

D	Disc diameter, m.
F	Force, N.
g	Gravitational acceleration, m s^{-2}.
h	Film thickness, m.
K	empirical constant.
L	Liquid.
m	mass flow rate, kg s^{-1}.
P	Pressure, Pa.
r	radius, m.
s	Source term.
t	Time, s.
u, v, w	Velocity components in x, y and z direction, m s^{-1}.
V	Velocity, m s^{-1}.
Q	Volumetric flow rate, $m^3 s^{-1}$
Greek Letters:	
α	Volume fraction.
μ	Dynamic viscosity, kg $m^{-1} s^{-1}$.
ν	Kinematic viscosity, $m^2 s^{-1}$
σ	Surface tension, N m^{-1}.
ρ	Density, kg m^{-3}.
ω	Rotational speed, rad sec^{-1}.
ε	Void fraction.
Subscripts:	
f	Fluid.
i,j,p,q	Phases.
r	Radial component.
n	Nusselt component.

INTRODUCTION

Spinning disc reactors (SDRs) are gaining popularity in carrying out fast multiphase reactions since they offer large interfacial area, and short residence times (Aoune and Ramshaw, 1999), In the SDR, liquid is fed into the centre of a reactor chamber consisting of a rotating disc. The rotational speed is usually high (upto 3000 rpm) which generates thin, unstable and wavy liquid film over the disc. The liquid travels in plug flow in the film from center to the periphery. Due to the thin film created, these reactors offer high heat transfer coefficients between the disc and the liquid and high mass transfer coefficients between the liquid and the gas above the liquid. This is of particular advantage when performing fast liquid-liquid reactions such as nitration, sulphonation and polymerization (Stankiewicz and Moulijn, 2004). These reactors have also shown potential benefits in unit operations such as absorbers, humidifiers, dust collectors, dryers, evaporators etc (Leshev and Peev, 2003). Owing to these advantages SDRs have also found various applications manufacturing of fine chemicals and pharmaceuticals (Aoune and Ramshaw, 1999).

The performance of the SDR depends on the underlying hydrodynamics of the film which is governed primarily by the rotational speed and volumetric flow rate of the fluid along with the physical properties of the fluid and the disc. A Considerable number of empirical and experimental investigations have been performed to correlate these governing parameters with the hydrodynamics of the film flow. Some of these are listed in table 1.

Espig and Hoyle (1965) in their experiments observed three different flow regimes over the spinning disc. Near the inlet region, the flow is a waveless laminar flow this is followed by the flow characterized by axisymmetric wave formation, this is followed by a turbulent region which shows three dimentional surface waves that are a combination of axisymmetric and helical waves. Charwat et al. (1972) identified that the turbulent waves decay towards the end of the spinning disc giving rise to a second laminar-wave region. Similar decay in the amplitude of the waves was also observed in experiments by Butuzov and Puhovoi (1976).

Wood and Watts (1973) performed an experimental study to characterize the heat and mass transfer on rotating discs. They showed existence of several wavy regimes in concentric zones across the radius of the disc. Nature of these waves is strongly dependent on the operating conditions (flow rate, rotational speed), liquid properties

Name	Equation	Comments
Charwat et al. (1972)	$$h=2h_n\left(\frac{Q_v}{r^5\omega^2}\right)^{1/15} \quad (1)$$	Correlation was developed based on experimental values. Film thickness was measured using optical absorption. About 50% variance from experimental value and 30-70% variance from Nusselt theory.
Wood and Watts (1973)	$$h_n=\left(\frac{3Qv}{2\pi r^2\omega^2}\right)^{1/3} \quad (2)$$ $$u\frac{\partial u}{\partial r}-\frac{v^2}{r}=\frac{12\pi^2r^2K_1v}{Q^2}u^3 \quad (3)$$ $$u\frac{\partial v}{\partial r}+\frac{uv}{r}=-\frac{12\pi^2r^2K_2v}{Q^2}(r\omega-v)u^2 \quad (4)$$	Two dimensional models. Nusselt film thickness as described by Wood and Watts. Assumes fully developed laminar flow over the disc. Also known as Pigford model.
Lepehin and Riabchuk (1975)	$$h=0.886Q^{0.348}v^{0.328}\omega^{-0.676}r^{-0.70} \quad (5)$$ $$u_r=\frac{\omega^2rh^2\left[1-\left(1-z/h\right)^2\right]}{2v} \quad (6)$$ $$h=0.782Q^{0.333}v^{0.333}\omega^{-0.667}r^{-0.67} \quad (7)$$	Three dimensional models. Assumes laminar axis-symmetrical flow. Inertial forces have negligible effect over centrifugal and coriolis forces. These two equations for h were compared by Leshev and Peev (2003) experimentally using micrometric watch needle

Table 1: Various models for characterisation of film flow

and the size of the disc. Later, Woods (1995) photographed the behaviour of a fully wetting dilute film of ink as it travelled over a spinning glass disc. He investigated the flow of the steady-state film, and the waves which occur on it. His theoretical model was investigated in its steady-state form (no waves present) using both asymptotic and numerical techniques. His experimental investigation employed a light absorption technique to obtain accurate film thickness measurements across individual three dimensional wave profiles. In his experiments, the dependence of the wave characteristics on the system parameters was carefully measured. Woods observed a constant inner film that eventually broke into an array of spiral ripples. Some chaotic waves were also formed at higher disc speeds.

Despite of these experimental works, the factors affecting the flow structure in the film still remain unclear. Burns et al (2003) compared these factors in detail experimentally and also proposed theoretical model. They also compared their model with the Nusselt theory but found that that the Nusselt model for the flow could not be used accurately for the inertial flow conditions, characterised by low Ekman numbers. The use of a more complex two-dimensional Pigford model of Wood and Watts was recommended. These experimental data also puts qualitative and quantitative insight into various zones existing on the thin liquid films.

Modelling of the hydrodynamics of the liquid films was first performed in 1916 when Nusselt modeled the downward flow of a condensing liquid film. He assumed that the liquid film falling under the gravity was stable and no shear exists at the gas-liquid interface. But this is not true in case of liquid films forming over the spinning discs. Hence, it is vital to make some modifications into his theory to predict film flow under the influence of the centrifugal force. Espig and Hoyle (1965) studied the effect of the Nusselt component in their theoretical model and compared their results with the experimental data. They found that found that the theoretically predicted film thickness were around 40% less than the experimental values. According to them this discrepancy was due to the omission from Nusselt's theory of the factors causing wave motion. After this study there have been various correlations developed to describe the stationary waveless flows and their linear stability (Dorfman, 1967, Rauscher et al., 1973, Shkadov, 1973, Lepekhin et al., 1981, Sisoev et al., 1986, Shvets et al., 1992) by various researchers based on the asymptotic analysis. Some of these correlations are summarized in Table 1.

Leneweit et al. (1999) studied the steady flow of a liquid jet from a nozzle onto the centre of a spinning disc with a streak line method and determined the superficial velocity of the spreading liquid film. Their model was based on the kinematic principle of wave generation with the source of perturbation being point like and stationary in laboratory frame of reference. It is rather unlikely that the perturbations are stationary and the inlet condition will not have any effect on the wave modulation thus, it is significant to examine the inertia effect on the wave modulation. Later, Matar and co workers (Matar and Lawrence, 2005, Matar et al, 2008) examined inertial effects alongwith the effect of disc topography and time modulation of the liquid flow rate at the inlet on the dynamics of a thin film flowing over a spinning disc. They used a combination of boundary-layer theory and the

Kármán–Polhausen approximation to derive coupled equations for the film thickness, and radial and azimuthal flow rates. They studied the effect on the dynamics of topographies of different shapes, square and saw-tooth patterns. Their numerical results indicate that, for a constant flow rate, square-shaped patterns appear to be more effective than saw-tooth ones in giving rise to a larger degree of interfacial waviness, which exceeds that associated with the smooth disc case.

COMPUTATION OF FILM THICKNESS

The hydrodynamic behaviour of the film directly influences the heat and mass transfer performance of the spinning disc reactors (Burns et al., 2003). The performance of liquid films can be closely related to the falling film theory, and a considerable amount of theoretical and experimental work has been done to evaluate the falling films (Matar and Lawrence, 2005). But there is still very little understanding on the behaviour of the films under the influence of the centrifugal force. The flow over the rotating disc is characterized by very thin liquid film over the rotating boundary surface with a sharp gas liquid interface that changes continuously in shape. It is essential to reliably predict the film thickness as most of the hydrodynamic properties like radial velocity, heat and mass transfer coefficients directly depend on the film thickness. In this study, a computational fluid dynamics (CFD) is used to model the SDR.

Computational Model

Various methods are available for the dynamic characterization of free surfaces such as the front tracking, level set, marker particle, shock capturing, smooth particle hydrodynamics, lattice Boltzmann and the volume of fluid (VOF) (Gopala and Wachem, 2008). In this study, the VOF formulation was used due to its particular advantages in interface tracking over other approaches. It is also relatively simple and accurate to apply to the boundary fitted grids and accommodates breaking and forming of interfaces. In the VOF approach, a single set of momentum equations is shared by the fluids. The volume fraction of each fluid, in each computational cell, is tracked throughout the domain (Fluent, 2007). The governing equations of the VOF formulation for multiphase flows are listed in Table 2. The flow was assumed to be incompressible laminar, dominated by the centrifugal forces.

The spinning disc used in this study, consists of a 30 cm diameter disc. Centre of the disc consists of a recess with 40mm diameter and 2mm height. Liquid (water) was fed to the centre of the disc into the recess through a jet inlet. The jet is situated 10mm above the recess and 8 mm above disc with the diameter of 5mm. A schematic of the geometry modeled is shown in Figure 1. The geometry and mesh were created using GAMBIT 2.4 (of Fluent Inc.).

Grid size is critical in properly resolving distinct interfaces involving small dimensions. In the VOF model at any given instance, a cell in the computational domain has either of three conditions; completely filled, completely empty or interface. Hence an initial estimate of the expected minimum film thickness must be made to decide the grid size. In the experimental investigation by Burns et al. (2003), smallest film thickness observed was around 100 μm. In order to resolve such a small film thickness, a uniform grid of size 50 μm was used in both 2D and 3D. In 2D, the map scheme was used, where unit aspect ratio was maintained, whereas in 3D the Hex-cooper scheme was used where unit aspect ratio was maintained near the disc but gradually increased in the Z direction. Increased aspect ratio in Z direction will not have any significant effect on the results since the physics of the system suggest that the liquid phase only occupies a small height over the disc. The computational domain selected for 3D geometry was 35mm in diameter and 10mm in height. The resulting grid size was 360000. For the 2D case, an axisymmetric domain of 100mm in diameter and 10mm in height was selected. This configuration was used to study the effect of rotational speed and volumetric flow rate on the film thickness.

Transient simulations were carried out using FLUENT 6.3 (of Fluent Inc.) for the operating conditions as described in Table 3. A velocity inlet condition for the inlet and a pressure outlet boundary condition for the outlet was used with gauge pressure equal to zero (in equilibrium with atmosphere). The PRESTO (pressure staggering option) scheme was used for pressure interpolation. The pressure-velocity coupling was done using the SIMPLE scheme. A second order upwind discretization was applied for the momentum equation. Liquid Wall contact angle was specified at wall-disc, Interface Interpolation was performed using geometric reconstruction. Finally, for 2D model moving reference frame and for 3D model wall boundary was given rotational effect.

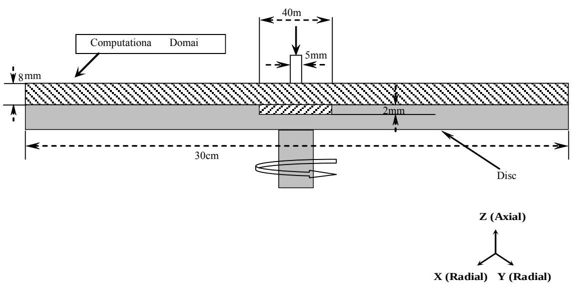


Figure 1: Schematic of the computed domain for model validation.

No.	Parameter	Value
1	Volumetric flow rate	10-18 ml sec^{-1}
2	Rotational speed	0-84 rad sec^{-1}
3	Liquid	Water
4	Disc orientation	Horizontal
5	Liquid wall contact angle	30°

Table 2: Operating conditions for computing liquid film thickness.

For interpolating the gas-liquid interface geometric reconstruction scheme was used. Adequate time step (usually 1×10^{-5} s) was used to limit global courant number to 0.25. The results were considered to attain steady state and converged when global mass fluxes were balanced and all the residuals were maintained below 1×10^{-3}. After the steady state was achieved, the time averaged film thickness was calculated for a quantitative analysis. A second order upwind method was used for discretization of momentum equation whereas QUICK scheme was used for volume fraction equation. A double precision solver was used to minimize truncation errors.

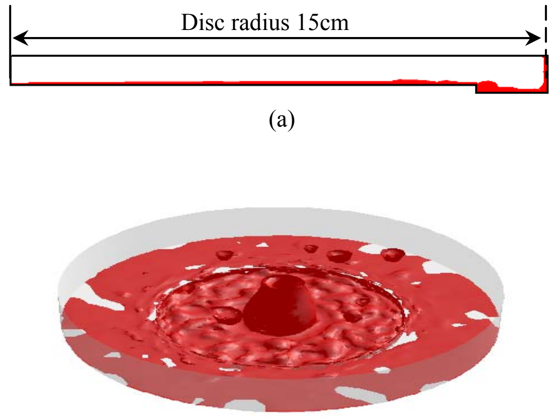
RESULTS AND DISCUSSION

The flow over a spinning disc exhibits a combination of flow regimes a waveless laminar regime in the initial section followed by axisymmetric wave formation, turbulent region and a second laminar-wave region near the outer perimeter. The wave formation and wave structures are not symmetric and therefore a 3D model is necessary to accurately capture the flow structure. The film thickness (~ 100 mm) is very small compared to the disc diameter (~ 15 cm). In order to capture such a small feature, very fine grid is required. This increases the demand on computations immensely making practical 3D computations impossible. Therefore, in this work a small domain was selected for carrying out 3D simulations. The full disc was simulated using a 2D axisymmetric model to reduce the computational requirements. The results from the 2D simulations were compared with emperical correlations of Lepehin and Riabchuk (Lepekhin and Riabchuk, 1975, Lepekhin et al., 1981) as these are closest to the 2D axixymmetrical approach. The next section compares the 2D and 3D results. The effect of various operating parameters is then examined using a 2D axisymmetric model.

Comparison of 2D and 3D model

A section of the geometry with a radial distance of 3.5 cm from the centre was simulated in 3D. The average film thickness was computed at given radial position. The film thickness was also calculated using a 2D axisymmetric model spanning over the entire diameter of the disc. The calculated film thicknesses were compared with experimentally measured film thickness by Burns et al (2003).

It was found that 3D model predicted unstable liquid films. Whereas, 2D model qualitatively showed a constant linear film with reducing film thickness in radial direction as shown in Figure 2. For the 3D domain simulated, the computed film thickness was in close agreement with the experimental data of Burns et al (2003). The film thickness computed using the 2D axisymmetric approximation were much lower than the thickness computed by 3D simulations and the data of Burns et al. (2003). However, the results from 2D simulations were in good agreement with available imperical correlations (eq. 5 and 7). One reason for this disagreement can be the inability of the 2D model to capture the the asymmetric nature and wave formation phenomena. The empirical correlations developed in literature often neglect these two aspects to arrive at a solution, therefore, the 2D simulations showed much closer agreement with the empirical correlations. For further investigations, 2D simulations were conducted. The results obtained from these simulations were compared with the empirical correlations available.



(a)

(b)

Figure 2: Computed volume fraction of water for 2D (a) and 3D (b) model. Q = 18 ml $s^{-1}$$\omega$ = 21 Rad sec^{-1}, 2D radius 15 cm, 3D radius 3.5 cm.

Method	Film thickness in mm
Equation 5	0.232
Equation 7	0.255
Burns et al (Experimental)	0.33
2D model	0.2
3D model	0.36

Table 3: Measured and calculated film thickness in mm.

Effect of rotational speed

Figure 3 demonstrates the effect of the rotational speed on the calculated dimensionless mean liquid film thickness for various rotational speeds. The profiles indicate that the liquid film thickness is largest near the entrance of the disc and reduces along the radius of the disc. With an increase in the rotational speed, the liquid film thickness reduces. It can be seen from Figure 3 that at 84 rad/sec the liquid film becomes unstable. At higher rotational speeds a constant liquid film collapses as the liquid moves away from the centre.

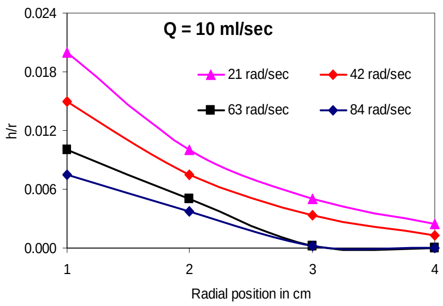


Figure 3: Effect of rotational speed on the non dimensional liquid film thickness Q = 10 ml s^{-1}, Disc diameter = 10 cm

This is due to the fact that larger centrifugal forces overcome the surface inertial and viscous forces. The resulting film thickness can be incorporated in the Wood and Watts model (Wood and Watts, 1973) to compute the radial velocity component within the liquid film (Burns et al., 2003). As shown in Figure 4 and Figure 5, simulations with higher liquid flow rates gave qualitatively similar result, albeit with relatively larger film thickness.

Effect of volumetric flow rate

It is evident from equations 5 and 7 that the volumetric flow rate at which the liquid enters at the centre of the disc plays an important role in determining the hydrodynamics of the liquid film. To study the effect of volumetric flow rate on the non-dimensional mean liquid film thicknesses, simulations were carried out at constant rotational speed for uniform disc with a diameter 10cm without the liquid recess. Computed film thickness are compared with the analytically calculated and experimental obtained film thickness by Burns et al (2003) and shown if Figure 6. It can be seen from Figure 6 that the results of the CFD are in good agreement with analytical solutions and experimentally measured film thickness. It is evident that equation 5 over predicts and equation 7 under predicts the film thickness. This is because the empirical constants in analytical equations are approximates. But it will appear that the CFD results are more or less close to average values of those obtained with the two equations. In the experimental work by Burns et al. (2003) it has been shown that the liquid film thickness reduces with the increase in flow rate. Such phenomenon was not observed in our model. There are various reasons for such phenomenon to occur. One of them could be the presence of liquid recess minimizes the inertial effect at the inlet. Secondly, Burns et al. (2003) calculated the film thickness indirectly from the reported average radial velocity.

Figure 7 shows the film thickness as a function of radial position without the presence of recess and it is clear that calculated film thicknesses are similar to those with recess (Figure 2). Hence, subsequent simulations were performed on a 10cm diameter disc without the liquid recess at constant rotational speed of 21 rad/sec and varying volumetric the flow rates (Figure 7).

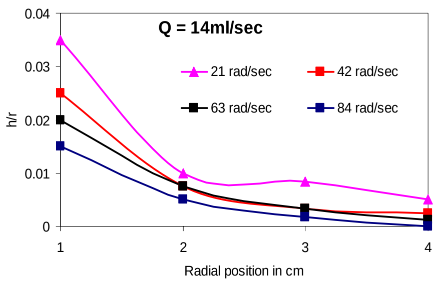


Figure 4: Effect of rotational speed on the non dimensional liquid film thickness Q = 14 ml s^{-1}, Disc diameter = 10 cm.

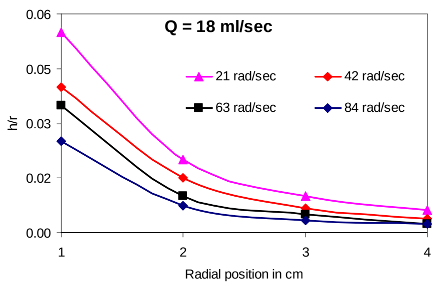


Figure 5: Effect of rotational speed on the non dimensional liquid film thickness Q = 18 ml $\mathbf{s^{-1}}$, Disc diameter = 10 cm.

Equation name	Equation
Equation of Continuity	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$
Momentum Equation	$\frac{\partial(\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \left[\mu\left(\nabla \vec{v} + \nabla \vec{v}^{t}\right)\right] + \rho \vec{g} + \vec{F}$
Volume Fraction Equation; If for qth fluids volume fraction is α_q then; For $\varepsilon_q = 0$; cell is empty (for qth fluid) For $\varepsilon_q = 1$; cell is full (for qth fluid) For $0 < \varepsilon_q < 1$; cell contains interface between qth fluid and other fluids.	$\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}\left(\varepsilon_q \rho_q\right) + \nabla \cdot \varepsilon\left(\alpha_q \rho_q \vec{v}_q\right) = s_{\varepsilon_q} + \sum_{q=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right]$ $\sum_{q=1}^{n} \varepsilon_q = 1$ $\frac{\varepsilon_q^{n+1} \rho_q^{n+1} - \varepsilon_q^{n} \rho_q^{n}}{\Delta t} V + \sum_f \left(\rho_q^{n+1} u_f^{n+1} \varepsilon_{q,f}^{n+1}\right) = \left[\sum_{p=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right] V$
Continuum surface force (CSF) Model; Surface Tension	$F_{vol} = \sigma_{ij} \frac{\rho K_s \nabla \varepsilon_i}{\frac{1}{2}(\rho_i + \rho_j)}$
Courant number	$Co = \frac{\Delta t}{\Delta x_{cell} / v_{fluid}}$

Table 4: Governing equations of VOF model.

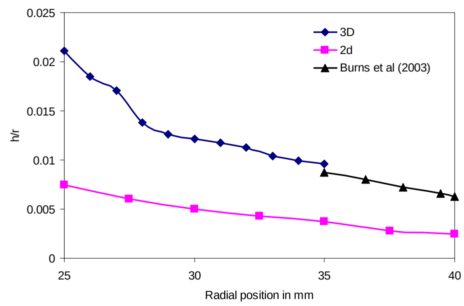
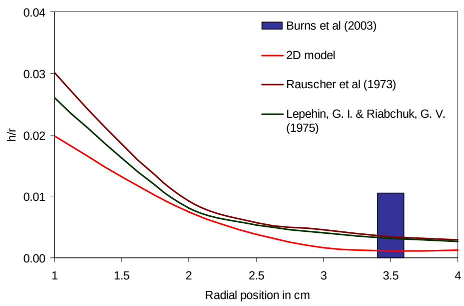
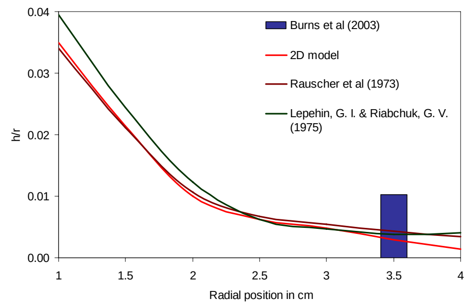


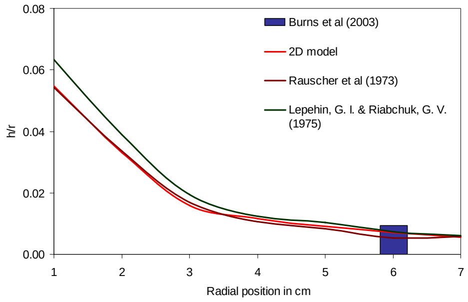
Figure 6: Effect of volumetric flow rate on measured and calculated non dimensional film thickness**.** Q = 10 ml s^{-1}ω = 21 Rad sec^{-1}, 2D radius 15 cm, 3D radius 3.5 cm.



a)



b)



c)

Figure 7: Non dimensional film thickness on a 10cm diameter disc for varying volumetric flow rate.

CONCLUSION

The volume of fluid model was used to study the film hydrodynamics of a spinning disc reactor. The effect of various operating parameters on the film thickness was studied. 2D axisymmetric and 3D computations were performed to calculate the film thickness. The 2D CFD simulations predicted the liquid film thicknesses that were in good agreement with empirical correlations, however, the thickness reported was much lower than the thickness observed experimentally. The 3D model was able to predict the film thickness reasonably well, however, the computational costs limited the application of the 3D model. It was also observed that the physical and operating parameters predominantly controlled the nature of the liquid film. Owing to the volume of fluids formulation, both the 2D and 3D models were unable to capture the flow and turbulence inside the liquid film. Due to this, phenomena like wave formation/ breakup and relaminarization were not captured in the present model. The liquid film flow model will be the subject for future developments. The study is a useful step in this direction.

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