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Study of Flow Behavior of Aqueous Solution of Rhodamine B in Annular Reactor Using Computational Fluid Dynamics

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***Abstract*—**The present study deals with the modeling and simulation of flow through an annular reactor at different hydrodynamic conditions using computational fluid dynamics (CFD) to investigate the flow behavior. CFD modeling was utilized to predict velocity distribution and average velocity in the annular geometry. The results of CFD simulations were compared with the mathematically derived equations and already developed correlations for validation purposes. CFD modeling was found suitable for predicting the flow characteristics in annular geometry under laminar flow conditions. It was observed that CFD also provides local values of the parameters of interest in addition to the average values for the simulated geometry.

***Keywords*—**Annular reactor, computational fluid dynamics (CFD), hydrodynamics, Rhodamine B

I. Introduction

ANNULAR reactors have been extensively studied in literature because of advantageous basic features of this geometry. Some of the studies on annular geometry include investigation on role of a Pt/Al_2O_3 catalyst in the oxidative dehydrogenation of propane [1], kinetics of carbon monoxide oxidation at high temperature [2], partial oxidation of methane [3], treatment of dye manufacturing plant effluent using UV/H_2O_2 and multi –UV lamps [4], photocatalytic degradation of some of VOCs in the gas phase [5], role of gas-phase chemistry in the rich combustion of H_2 and CO over a Rh/Al_2O_3 catalyst [6], simulation of degradation of perchloroethylene in air [7], influence of fins on photocatalytic removal of formaldehyde [8], photocatalytic degradation of gaseous 1-propanol: kinetic modeling and pathways [9], modeling of annular flow [10] and direct conversion of methane to formaldehyde under high temperature and short residence time [11].

The hydrodynamics of the flow is one of the most important issues in the annular reactors depending upon the kinetics, operating conditions, and geometrical properties of the system. Hence modeling, design and scale-up of these reactors require an accurate prediction of hydrodynamics. The traditional methods of predicting fluid flow in annular reactors depends heavily on theoretical modeling and empirical correlations. These theoretically developed equations are suitable only to specific reactor configurations and not take into account the local effects [12].

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A new method to estimate the hydrodynamics is required which should also be able to predict the velocity profiles and concentration fields in the annular reactor for better design and scale-up applications. A very effective approach to tackle this challenge is computational fluid dynamics (CFD). Computational fluid dynamics (CFD) is a well established technique for the analysis of systems involving fluid flow, mass transfer, heat transfer, reaction and associated phenomena. There are several advantages of using CFD such as ability to study hazardous system in a safe environment and reduction in the time and cost of analysis [13]. The recent CFD studies on annular reactors include simulation of a pilot-scale annular bubble column photocatalytic reactor [14], analysis of photocatalytic gas phase vinyl chloride oxidation [15], simulation of trichloroethylene (TCE) oxidation at various pollutant concentrations, flow rates, and reactor lengths [16] and study of annular photoreactor hydrodynamics [17]. More recently, Duran et al. [12] applied CFD to investigate single-phase flow mass transfer prediction in annular reactor for laminar, transitional and turbulent flow condition. It was found that laminar model predicted mass transfer successfully under laminar conditions. For turbulent conditions, AKN (Abe, Kondoh and Nagano) model, and RSM (Reynolds Stress Model) performed well. Santoro et al. [18] studied the oxidation of tributyl phosphate (TBP) and tri(2-chloroethyl) phosphate (TCEP) in parallel and cross-flow annular photoreactor. CFD simulations enabled the spatial visualization of hydrogen peroxide and hydroxyl radical distributions in the reactor. Queffeulou et al. [19] investigated the removal of acetaldehyde in annular photocatalytic reactor with a thin film of TiO_2 coated on stainless steel plate. Modeling of fluid dynamics and reaction was realized with a CFD approach. In terms of conversion yield, model predictions and experimental results were found in good agreement. Vincent et al. [20] studied the hydrodynamics and degradation of acetone in annular reactor. It was observed that CFD modeling estimate the kinetic parameters of the degradation of acetone very close to the experimental results.

The aim of the present work was to carry out CFD modeling of the annular geometry to predict the fluid flow of aqueous solution of a dye at various hydrodynamic conditions. The aqueous solution of dye was used to explore the application of annular reactor for dye degradation in future. The results of the CFD model were compared with theoretical modeling for validation of the model. Rhodamine B was used as model dye. It is organic in nature and most important xanthene dye [21].

II. CFD Modelling

A. Governing Eequations

In present study, it is assumed that the fluid is Newtonian, incompressible, isothermal and non-reactive with constant physical properties. The hydrodynamics of Rhodamine B solution was modeled by solving mass and momentum equations using commercial CFD code Fluent 6.3.26 (Fluent Inc., USA). The general forms of the governing equations for modeling the system are as follows:

Mass conservation equation:

$$\nabla.(\rho\,\vec{v}) = 0 \quad (1)$$

Momentum conservation equation:

$$\nabla.(\rho\vec{v}\vec{v}) = -\nabla P + \nabla.(\bar{\bar{\tau}}) + \rho g \quad (2)$$

In (1) - (2), ρ is density, $\vec{v}$ is velocity vector, P is pressure, $\bar{\bar{\tau}}$ is stress tensor, g is gravitational force. Detailed description of the conservation equations along with the associated correlations and parameters are provided in the Fluent Manual [22].

B. Hydrodynamic Model

The simulation of the present system was performed with a three dimensional, steady state laminar flow model. The laminar flow model has been successfully used for CFD simulations of annular photocatalytic reactors for air treatment [15], experimental and CFD analysis of photocatalytic gas phase vinyl chloride oxidation [19], CFD modeling of mass transfer in annular reactors [12] and Three-dimensional CFD modeling of a flat plate photocatalytic reactor [23]. This model utilizes (1) and (2) combined with Newton's law of viscosity for computation of velocity field within the reactor domain. Further information and examples of laminar flow model can be found in Bird et al. [24]. The same model has been used in the present work to evaluate CFD modeling of hydrodynamics at flow velocities of 1.8, 3.6, 5.5, 7.3 and 9.1 mm/s. These flow velocities correspond to Reynolds numbers (Re) of 20, 40, 60, 80 and 100 respectively through the annular section.

C. Geometrical Model

The annular reactor geometry studied in the present research is shown in Fig. 1. The geometry was created in commercial software Gambit. The reactor consists of 39 mm outer tube diameter, 27 mm inner tube diameter and 500mm total length with 12 mm diameter inlet and outlet tubes.

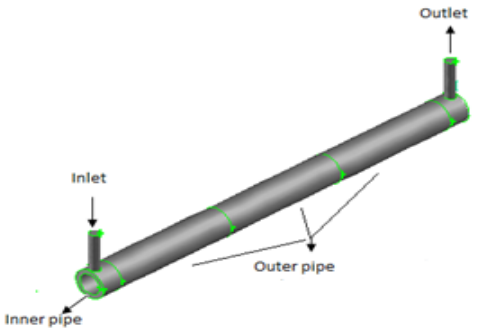

Fig. 1 Schematic diagram of annular geometry

The inlet and outlet tubes were placed 1 mm from each respective end to form a U-shape annular reactor. The length of both the inlet and outlet tubes were chosen 50 mm to ensure fully developed flow at the entrance of the reactor.

D. Mesh Design

The commercial mesh generator Gambit was used to create the grid. The hexahedral cells were used to discretize the reactor domain where the flow behaviour was to be studied (middle annular region of length 450nm). The utilized grid for the reactor had approximately 1.2 million elements and they were verified to give mesh independent results

E. Boundary Conditions

The boundary conditions for the CFD model were defined as follows. At the inlet, velocity of the fluid was specified. The direction of the flow was defined normal to the boundary. At the outlet, boundary condition pressure-outlet was specified with a value of 1 atm. At all the walls, a no-slip boundary condition was imposed. Also, zero diffusive flux of species was specified at the walls.

F. Physical Properties

The physiochemical process studied in this investigation is the isothermal flow of aqueous solution of Rhodamine B at 300K. At this temperature the saturation concentration of of Rhodamine B in water is very low so the physical properties of water can be assumed for the system. The density and viscosity of water considered are 998.2 kg/m^3 and 10.03×10^{-4} Pa.s respectively.

G. CFD Solution

Commercial CFD code Fluent 6.3.26 was used to perform simulations. The governing equations were solved using pressure based three dimensional solver. Second order upwind discretization scheme was employed except for pressure. PRESTO was selected as discretization scheme for pressure. The SIMPLE algorithm was chosen for the pressure-velocity coupling. The already mentioned under-relaxation factors were considered. Convergence of numerical solution was ensured by monitoring the scaled residuals to a criterion of 10^{-4} for the continuity and momentum variables. The solution of the model was utilized to find out the velocity vector field, velocity profile and average velocity.

III. Mathematical Modelling

The mathematical modeling of velocity distribution and average velocity was also done for the reactor. The results of CFD modeling were compared with the outcome of mathematical modeling for evaluation purpose. The expression for velocity distribution and average velocity for the reactor geometry was obtained by applying momentum balance on a cylindrical shell of infinitesimally small thickness within the reactor domain. The assumptions of laminar flow, constant density and no end effects were also considered. Equations (3) and (4) represent the derived expressions for velocity distribution and average velocity respectively.

$$v_z = \frac{(P_0 - P_l) r_0^2}{4\mu l}\left[1 - \left(\frac{r}{r_0}\right)^2 + \left(\frac{1-\kappa^2}{\ln(1/\kappa)}\right)\ln\left(\frac{r}{r_0}\right)\right] \quad (3)$$

$$< v_z > = \frac{(P_0 - P_l) R^2}{8\mu l}\left[\left(\frac{1-\kappa^4}{1-\kappa^2}\right) - \left(\frac{1-\kappa^2}{\ln(1/\kappa)}\right)\right] \quad (4)$$

Where r_0, r_i, μ, l are the inner radius of outer cylinder, outer radius of inner cylinder, viscosity of fluid and length of reactor respectively. P_0 and P_l are the pressures at inlet and outlet of the annulus respectively. κ is a dimensionless ratio (r_i/r_o). Further details of derivations of such expressions may be seen in Bird et al. (2002).

IV. Results And Discussion

The hydrodynamics of an annular reactor is characteristic of its overall performance and it helps to evaluate the nature of flow patterns in the reactor. In the present research, hydrodynamics have been characterized in terms of axial velocity profile, average velocity and velocity contours to assess the flow structures within the reactor. CFD simulations of the annular reactor operating at flow velocities of 1.8, 3.6, 5.5, 7.3 and 9.1 mm/s were performed. Fig. 2 depicts the CFD modeled variation in axial velocity with respect to radial distance within the annular region at various Reynolds number.

The results correspond to a line between the inner and outer cylinder at the exit of the annular section under study.

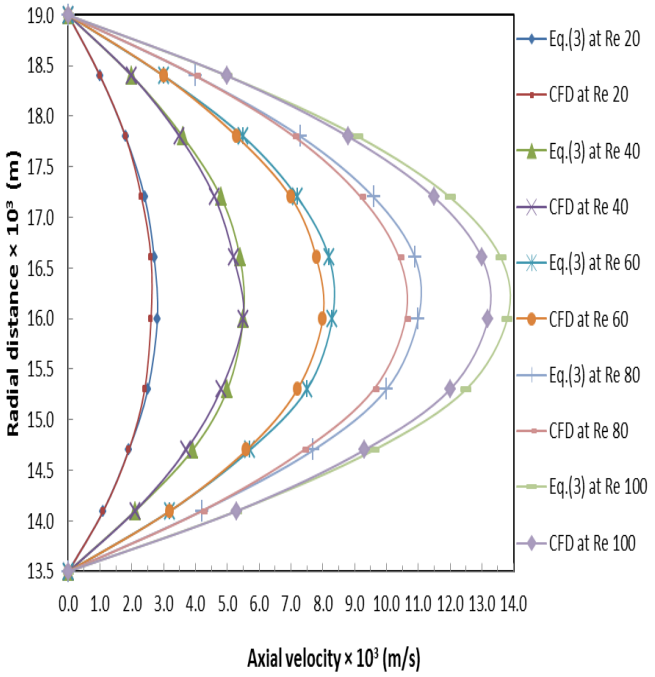

Fig. 2 Axial velocity within the annular region of reactor

The velocity distribution depicted by CFD simulations along the annular space is parabolic which is the characteristic of laminar flow in agreement with Bird et al. [24]. Fig. 2 also represents a comparison between mathematically developed (3) and CFD modeling at various Reynolds numbers. CFD simulations also show that the velocity is minimum at the walls and maximum near the middle of annular region which is in accordance with (3). CFD modeling closely maps the velocity profiles calculated by mathematically developed (3) as obvious from Fig. 2. The average relative error in prediction of axial velocity by CFD modeling is around 2.1% which is acceptable from industrial point of view. Fig. 3 represents the average velocities predicted by CFD modeling. It also shows a comparison of CFD modeling with mathematically developed (4) in determination of average velocity. It is obvious that the outcome of CFD modeling is in agreement with (4) with a little deviation. The average relative error in prediction of average velocity is 5.8%.

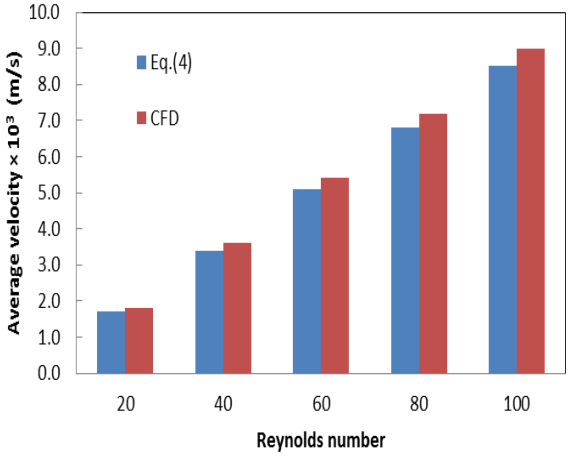

Fig. 3 Average velocity through the annular region of the reactor

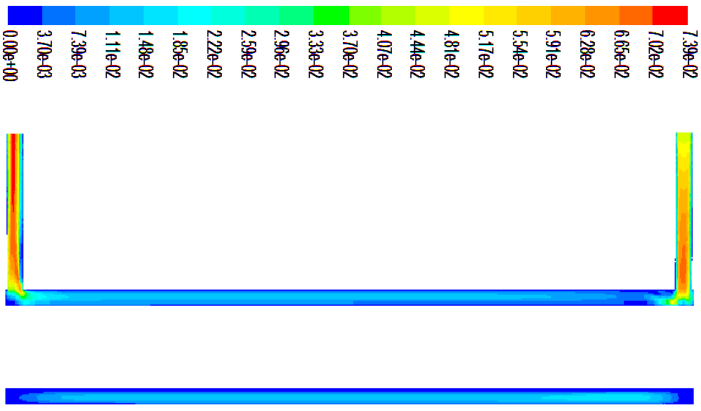

Fig. 4 Velocity magnitude (m/s) contours within the reactor for flow velocity of 9.1 mm/s

Fig. 4 shows the contours of velocity magnitude (m/s) for the annular geometry for a flow velocity of 9.1 mm/s through the annulus. The results correspond to longitudinal center plane of the reactor. Similar velocity magnitude contours (different in magnitude) were obtained in the simulations at other flow velocities and hence not shown here. It is very clear from the contours that the velocity through the inlet and outlet is more because these tubes have smaller cross-sectional area of flow as compared to annulus. There is non-uniformity in the flow at the entrance of annulus region due to sudden expansion

and change in direction of flow. The flow is uniform through the annular region of interest (i.e. middle annular region of length 450 mm).

V. Conclusion

The hydrodynamic of aqueous solution of Rhodamine B in annular reactor under various operational conditions has been investigated using CFD method. The results of CFD modeling have been compared with the results of mathematical. The velocity distribution and average velocity predicted by CFD were in close agreement with the outcome of mathematical modeling of annular reactor. It was found that CFD also provides local values of the parameters of interest in addition to the average values for the simulated geometry. In the present study, detailed local information (velocity profiles) was obtained using CFD modeling of the system which provided a qualitative understanding of the process to better explain the results. The detailed predicted flow field gave an accurate insight to the fluid behavior and presented information which cannot be obtained from correlations and experiments. It has been observed that CFD modeling is capable of predicting the hydrodynamics for annular geometry under laminar flow conditions.

Nomenclature

$\vec{v}$ Velocity vector (m s^{-1})
$\mathbf{P}$ Pressure (N m^{-2})
∇ Divergence (m^{-1})
v_z Axial velocity (m s^{-1})
$< v_z >$ Average velocity (m s^{-1})
r Radius (m)
l Length of the annulus (m)

Greek symbols

ρ Density (kg m^{-3})
$\bar{\bar{\tau}}$ Stress tensor (N m^{-2})
μ Viscosity (kg m^{-1} s^{-1})
κ Dinsionless ratio (r_i/r_o)

Acronyms

CFD Computational Fluid Dynamics

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