Selection of Optimized Vessel Geometries for Coiled Stirred Tank Reactors

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Abstract

Stirred Tank Reactors are extensively used in chemical industries. It is common to use either jackets or internal coils when the reaction inside these reactors is highly exothermic. Both arrangements have positive influence and drawbacks in controling the bulk temperature.

The design of coiled vessels today follows very much the geometry by Oldshue and Gretton [4] which has been criticized since it affects the flow. Street and McGreavy [6, 5] and Nunhez and McGreavy [3, 7, 2] indicated that if coils are placed in the same height of the impeller blades, internal flow circulation is restricted, even though there is an excellente local heat transfer in the impeller region.

This work aims to show by simulating the momentum, mass and energy equations inside the reactor, that there is great gain in performance if small alterations in the internals location are made. The idea is to simulate the flow for both the experimental apparatus cited above and some proposed geometries to indicate how internal flow can be improved. Preliminary simulations have already shown that there is great gain by avoiding to place any coil at the impeller height.

1 Introduction

It is common to use either jackets or internal coils when the reaction inside stirred tank reactors is highly exothermic. Both arrangements have positive influence and drawbacks in controling the bulk temperature and they should be weighed carefully before deciding which arrangement should be chosen in any design. Reactor performance is greatly affected by the location of the internals and reactor mode of operation. Coiled vessels are even more affected because the coils drag the flow circulation. Important design parameters are coil helix and tube radius, as well as the number and location of coils. All these factors have an influence on the final flow and heat transfer inside the tank.

For laminar flows, when jacketed vessels are employed, there is a maximum of temperature inside the vessel at the centers of the recirculation zones of the secondary flow, since heat transfer in stirred tanks in these circumstances are dominated by the secondary flow. If coils are used, the temperature peak is not necessarily anymore at the center of the recirculation

The primary concern of this research is to show that there are mechanical limitations for flow circulation and heat transfer in the geometry suggested by Oldshue and Gretton [4]. Even though this computational work is only for laminar flow, the results for the flow can be extended to turbulent conditions because similar flow patterns are present for both laminar and turbulent conditions. The same mechanical limitations which are present for laminar flow are also present for turbulent flow. Therefore, studying the fluid circulation inside the coiled tank laminar flow will be of benefit for both flow regimes.

2 Modeling and simulation

The problem under investigation is three dimensional and can be for both Newtonian and non-Newtonian flow. For a preliminary investigation however, it will be considered a two-dimensional axi-symmetric model, even though the radial, axial and angular velocities will be determined on a two-dimensional grid, making this a pseudo tree-dimensional model.

The critical part and weakest link of the axi-symmetric model is the application of the boundary conditions for the impeller blades in order to give a reasonable representation of the blades effect. The approach used by Kuncewics [1] was adopted. This approach was followed by Nunhez and McGreavy [3, 7] and results show it gives a good representation for the flow patterns and serves as a basis for geometry selection which can be further refined at a later stage by a three dimensional model.

The governing equations for the axi-symmetric model are:

2.1 Momentum balance

radial

$$\rho\left(u_r\frac{\partial u_r}{\partial r}-\frac{{u_\theta}^2}{r}+u_z\frac{\partial u_r}{\partial z}\right)=\frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rr})-\frac{1}{r}\sigma_{\theta\theta}+\frac{\partial\sigma_{rz}}{\partial z} \tag{1}$$

angular

$$\rho\left(u_r\frac{\partial u_\theta}{\partial r}+\frac{u_r u_\theta}{r}+u_z\frac{\partial u_\theta}{\partial z}\right)=\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\sigma_{r\theta})+\frac{\partial\sigma_{z\theta}}{\partial z} \tag{2}$$

axial

$$\rho\left(u_r\frac{\partial u_z}{\partial r}+u_z\frac{\partial u_z}{\partial z}\right)=\frac{1}{r}\frac{\partial}{\partial r}(r\sigma_{rz})+\frac{\partial\sigma_{zz}}{\partial z} \tag{3}$$

2.2 Mass conservation

$$\frac{1}{r}\frac{\partial}{\partial r}(\rho r u_r)+\frac{\partial}{\partial z}(\rho u_z)=0 \tag{4}$$

2.3 Energy conservation

$$\rho C_p\left(u_r\frac{\partial T}{\partial r}+u_z\frac{\partial T}{\partial z}\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(k_l r\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(k_l\frac{\partial T}{\partial z}\right)+\Delta H \tag{5}$$

The stress tensors are:

$$\sigma_{rr}=-p+2\mu\frac{\partial u_r}{\partial r} \tag{6}$$

$$\sigma_{\theta\theta}=-p+2\mu\frac{u_r}{\partial r} \tag{7}$$

The equations are solved numerically by the finite volume method and the simulations are performed using the CFX-4 package by AEA which has been successfully used for many flow problems. The boundary conditions are the same used by Street and McGreavy [6, 2] and Nunhez and McGreavy [3, 7].

3 Preliminary results and discussion

Preliminary results have already been obtained and show that there is great gain in modifying coils position inside the vessel and show it is benefitial to avoid placing any coil at the impeller height. This happens because if there are coils at this height, the average flow velocity is reduced when the fluid which leaves the impeller encounter the coils and, as a consequence of the velocity being reduced, there is a tendency of fluid stagnation between the coils and wall of the vessel. Figure 1 shows the velocity vector plot for an axial section of the reactor [1] for the experimental arrangement suggested by Oldshue and Gretton. As already commented, there is a limitation in the fluid circulation because the flow which is generated by the impeller encounters the coils which are present at the impeller blades height. As a consequence, those two coils drag the flow in the intire tank which, of course, impaire the flow in the tank. Figure 2 shows an arrangement having no coils at the impeller blades height. It is apparent from the figure that fluid circulation is greatly improved if the coils at the impeller region are removed. It is specially true for the circulation between the coils and the wall. The two figures are for the same angular velocity of the impeller of 30rpm.

In the actual stage, heat transfer and a non-Newtonian model have been introduced into the model. Reaction is considered as a source of heat in the bulk which has to be removed by either a jacket and/or coils. Several arrangements are being analysed to demonstrate how computational fluid dynamics can be used as a tool for reactor design.

At a later stage, a three dimensional and a turbulent model is aimed to be considered.

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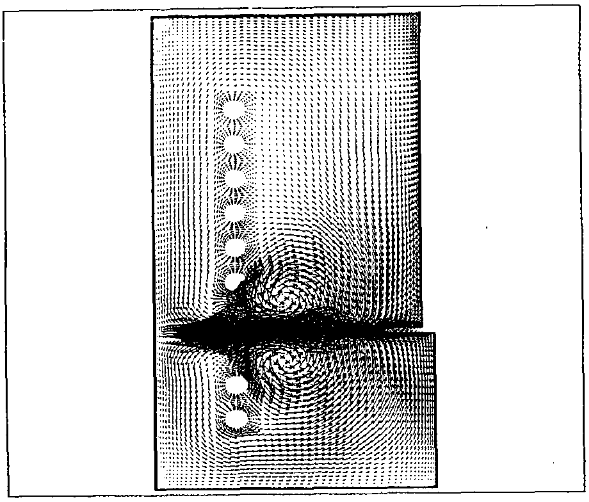

Figure 1: Experimental coiled arrangement by Oldshue and Gretton

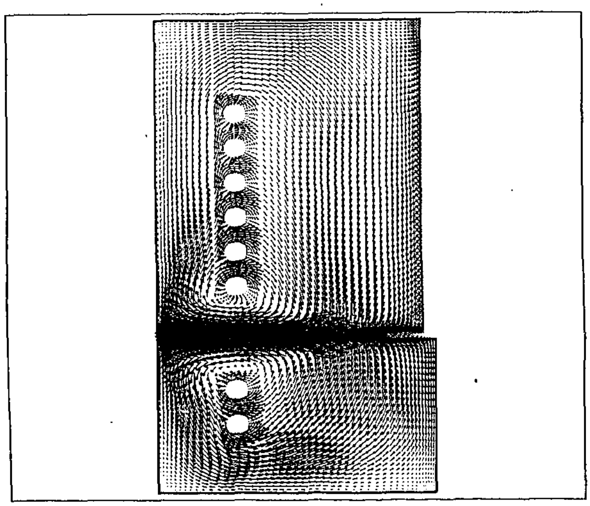

Figure 2: Alternative arrangement having no coils at the impeller height