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IMPROVING INTERNAL FLOW OF COILED STIRRED TANKS

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ABSTRACT

Jacketed Stirred Tank Reactors are extensively used in chemical industries. When they are used for highly exothermic reactions, jackets or coils are employed for heat removal. Internal coils considerably affect the flow inside the reactor because their tubes provide a resistance to flow circulation. The aim of this project is to show that the design of coiled vessels can be further improved because many designs today follow very much the geometry proposed by Oldshue and Gretton [7, 13], which is believed to affect the flow considerably. 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. Results show a large gain in performance when small alterations are made specially in the shape of the coil arrangement.

NOMENCLATURE

h_c	heat transfer coefficient between coils and liquid [W.m^{-2}.K^{-1}]
h_{fs}	heat transfer coefficient between liquid and free surface [W.m^{-2}.K^{-1}]
T	tank diameter [m]
D	impeller diameter [m]
Z	liquid height [rn]
Z_c	coil height [m]
C	impeller height [m]
C_c	distance between the bottom of the tank and coil base[m]
D_b	blade length [m]
D_w	blade height [m]
D_c	helix diameter [m]
s	disk thickness [m]
u_z	axial velocity [m.s^{-1}]
u_r	radial velocity [m.s^{-1}]
u_θ	angular velocity [m.s^{-1}]
C_p	specific heat capacity at constant pressure [Jkg^{-1}K^{-1}]
R_s	shaft radius [m]
d	tube diameter [m]
S_c	distance between tubes [m]
k	thermal conductivity of the liquid [Wm^{-1}K^{-1}]
N	power number which describes the non-Newtonian attributes
p	pressure [N.m^{-2}]
T	temperature [K or °C]

GREEK SYMBOLS

ΔH	Heat source term [W.m^{-3}]
μ	Average reaction viscosity [kg.m^{-1}s^{-1}]
μ_0	newtonian viscosity [kg.m^{-1}s^{-1}]
ρ	density [kg.m^{-3}]
τ_{ij}	stress tensor acting on ij section

INTRODUCTION

The performance of stirred tanks is greatly affected by the location of their internals and the mode of operation. When these vessels are used for highly exothermic polymerization reactions, it is common to use either jackets or internal coils for temperature control. Both arrangements have positive influences and drawbacks in controlling bulk temperature, and they should be weighed carefully before deciding which arrangement should be chosen in any design.

For reactions occurring under laminar flow, jacketed vessels have the tendency to affect the flow, mainly at the bottom and walls of the vessel, since the low temperature at these regions causes the fluid to have a higher viscosity in comparison to the rest of the vessel. Coiled vessels are affected much more than jacketed vessels because the coils drag the flow circulation. This means that the number and location of the coils as well as tube radius and helix diameter are important design parameters. All these factors have an influence on the final flow and heat transfer inside the tank.

When jacketed vessels are employed for reactions under laminar flow, there is a temperature peak inside the vessel at the centers of the recirculation zones of the secondary flow, since heat transfer in stirred tanks in these circumstances is dominated by the secondary flow. If coils are used, the temperature peak is not necessarily still at the center of the recirculation zones, because the heat transfer is greatly affected by the coils. The amount of coils and their design will determine the heat transfer area inside the tank. On the one hand, it is desirable to have as many coils as possible for it increases the heat transfer area but, on the other hand, the smaller the number of coils and its diameter is, the better the circulation and mixing inside the tank. An optimun design for coiled vessels would provide an arrangement with a high internal heat transfer coefficient, which means that the heat generated by the reaction would be removed by a small heat transfer area. Since heat transfer is dependent on flow circulation, improvements in design for these systems will depend heavily on a detailed knowledge of how flow is affected by the locations of the internals of the reactor.

Oldshue and Gretton [7] suggested a coiled vessel arrangement which was later presented by Uhl and Gray in a book that has become a reference for reactor design [13]. The primary concern of this research is to show that there are some mechanical limitations for flow circulation and heat transfer in the geometry suggested by Oldshue and Gretton. In their experimental work, Oldshue and Gretton investigated laminar and turbulent conditions. This computational work is only for laminar flow and the results indicating improvement for flow under laminar conditions can not be directly extended to turbulent conditions. However, a point should be made because similar flow patterns are expected for both flow regimes and 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 for laminar flow will provide insights which will be beneficial for understanding how internal flow of helical coiled tanks can be improved in both flow regimes. The results for turbulent flow, however, have to be studied to confirm how much the flow is affected under these conditions.

Street [10], Street and McGreavy [11] and Nunhez and McGreavy [6, 12] have indicated in their work that no coils should be placed at the impeller blades height because fluid circulation is restricted and overall heat transfer is poor, even though there is an excellent local heat transfer in the impeller region. This is due to the fact that the sweeping flow at the impeller region is at a high speed and it looses considerable momentum when it encounters the coils placed between the impeller blades and the wall of the vessel. If no coils are placed there, momentum is lost only at the walls and, as a result, fluid circulation away from the impeller will be greater and overall heat transfer is improved. This aspect, however, has not yet been shown and this work intends to demonstrate it by simulating the momentum, mass and energy equations inside the reactor.

MODELING AND SIMULATION

The problem under investigation is three dimensional and can be applied to both Newtonian and non-Newtonian flow. For a preliminary investigation however, a two-dimensional axisymmetric model will be considered. This means that the radial, axial and angular velocities will be determined on a two-dimensional grid, making this a pseudo three-dimensional model. Even though this is a simple representation for the flow, i.e., a single phase two dimensional model, it is accurate enough to give a good representation for the flow of stirred tanks and indicates how flow can be improved by rearranging the location of internal coils.

The critical part and weakest link of the axisymmetric model is the application of the boundary conditions for the impeller blades in order to give a reasonable representation of the effect of the blades. The approach used by Kuncewicz [3] was adopted. The idea is to apply the momentum generated by the impeller in an averaged sense in the whole swept volume of the impeller. This approach was later followed by Street [10] and Nunhez and MeGreavy [6, 12, 4] and results show that it gives a good representation for the flow patterns and serves as the basis for geometry selection. The reaction at this stage is represented by a heat source which is generated in bulk. These aspects can be further refined at a later stage by both a three-dimensional model and a more detailed reaction model.

The governing equations for the axisymmetric model are:

MOMENTUM BALANCE

radial

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

angular

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

axial

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

MASS CONSERVATION

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

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:

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

$$\sigma_{\theta\theta} = -p + 2\mu \frac{u_r}{r} \quad (7)$$

$$\sigma_{zz} = -p + 2\mu \frac{\partial u_z}{\partial z} \quad (8)$$

$$\sigma_{r\theta} = \mu r \frac{\partial}{\partial r}\left(\frac{u_\theta}{r}\right) \quad (9)$$

$$\sigma_{z\theta} = \mu \frac{\partial u_\theta}{\partial z} \quad (10)$$

$$\sigma_{rz} = \mu\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right) \quad (11)$$

The fluid properties and other important paramenters are:

Density	$\rho = 800$ kg.m^{-3}
Viscosity	$\mu_0 = 1.0$ kg.m^{-1}.s^{-1}
Heat capacity	$C_p = 100$ J.kg^{-1}.K^{-1}
Thermal conductivity	$k = 0.1$ W.m^{-1}.K^{-1}
Heat transfer coefficient (wall)	$h_c = 500$ W.m^{-2}.K^{-1}
Heat transfer coefficient (coils)	$h_c = 500$ W.m^{-2}.K^{-1}
Heat transfer coefficient (free surface)	$h_{fs} = 5$ W.m^{-2}.K^{-2}

Table 1: Fluid properties and some important parameters.

The non-Newtonian viscosity is given by the Power law model:

$$\mu = \mu_0 \gamma^{n-1} \quad (12)$$

$$\gamma = 2\left[\left(\frac{\partial u_r}{\partial r}\right)^2 + \left(\frac{u_r}{r}\right)^2 + \left(\frac{\partial u_z}{\partial z}\right)^2\right] + \left[r\frac{\partial}{\partial r}\left(\frac{u_\theta}{r}\right)\right]^2 + \left[\frac{\partial u_\theta}{\partial z}\right]^2 + \left[\left(\frac{\partial u_r}{\partial z}\right)^2 + \left(\frac{\partial u_z}{\partial r}\right)^2\right] \quad (13)$$

The parameters used are n = 0.5, 1 or 1.5

Figure 1 shows the dimensions used in the tank used by Oldshue and Gretton [7] and Table 2 gives the geometrical dimensions.

Figure 1 shows that Oldshue and Gretton [7] used baffles in their work and this can not be satisfactorily modelled on a two dimensional grid. This aspect has to be considered in more detail on a full three dimensional. Nevertheless, the two dimensional model gives us the main design features that can improve flow circulation.

Tank diameter	T	1.22 m
Liquid height	Z	1.22 m
Impeller height	C	0.41 m
Impeller diameter	D	0.02 m
Impeller disk thickness	s	0.10 m
Blade length	D_b	0.10 m
Blade height	D_w	0.08 m
Helix diameter	D_c	0.87 m
'I'ubes diameter	d	0.05 m
Separation between tubes	S_c	0.09 m

Table 2: Tank dimensions used by Oldshue and Gretton.

BOUNDARY CONDITIONS

Free surface - At the liquid free surface there is no shear stress, which is acceptable for Reynolds numbers below 300 [1]. Therefore a flat surface is assumed and axial velocity is null.

Bottom and walls of the vessel - There is no slip, so the velocity is null.

Coil tubes - There is no slip.

Impeller blades - The approach of Kuncewicz [3], which takes into account the number of impeller blades, is used. He assumes that the blades can be approximated by a momentum which acts equally in the whole swept volume of the blades and he uses a coefficient varying between 0 and 1, which is dependent on the number of blades and can be thought of as a drag coefficient which accounts for the blade effect. This approximation is able to provide a good representation for the flow patterns of turbine impellers.

Coil tubes - It is assumed the there is enough cooling liquid inside the coils to maintain temperature constant at 10 ^{0}C.

Bottom and walls of the vessel - For jacketed arrangements it is assumed that there is enough cooling liquid inside the jacket to maintain temperature constant at 10 ^{0}C.

At the walls, vessel bottom and coils the boundary condition is:

$$q_c = -\left(k\frac{\partial T}{\partial n}\right) = h_c\left(T - T_c\right) \quad (14)$$

and the free surface is:

$$q_{fs} = h_{fs}\left(T - T_{fs}\right) \quad (15)$$

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. It uses the SIMPLEC algorithm by van Doormaal and Raithby [14], which is a variation of the SIMPLE algorithm first developed by Patankar and Spalding [9, 8]. The upwind scheme was applied for the convective and diffusive terms in the model equations.

PRELIMINARY RESULTS AND DISCUSSION

In order to determine a good number of finite volumes, several grids were used and the approach used by Foumeny et al. [2] and Nunhez and McGreavy [6, 5] was adopted. Table 3 presents the results for the temperature in two different mesh densities of 5264 and 10604 control volumes, respectively. The difference between the two meshes gives a maximum of approximately 1.5 ^{0}C for the maximum temperature, and all the other results give a smaller difference. This indicates that results given for the smaller density are satisfactory for this preliminary investigation. Therefore a mesh density of 5264 control volumes is used. Figure 2 show the mesh used for the calculations[1].

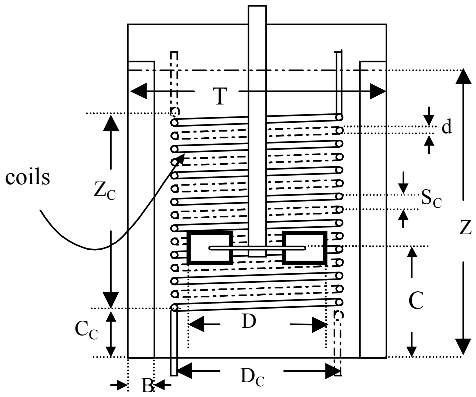

Figure 1: Experimental geometry used by Oldshue and Gretton.

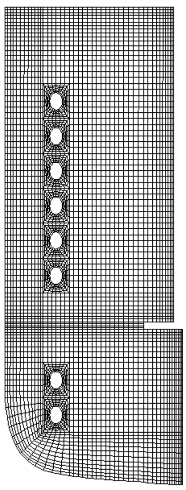

Figure 2: Mesh of 5264 control volumes for a proposed geometry.

[1] Only half section is shown because the other half is symmetric

Figures 3 and 4 show the generated velocity field by both geometries. It is apparent that the flow in the proposed geometry is superior. Flow is specially improved in the regions further away from the impeller and between the coils and the wall. This is because the proposed geometry provides better fluid circulation. Therefore, results show it is beneficial to avoid placing any coil at the impeller blades height. The reason for this is because the presence of coils at the blades height reduces the average flow velocity of the fluid leaving the impeller when it encounters the coils. As a consequence of the reduction in velocity, there is a tendency for the fluid to stagnate between the coils and the wall of the vessel.

Figures 5 and 6 show the temperature contour plot for the experimental geometry used by Oldshue and Gretton and a proposed geometry. The difference in calculated temperatures is shown in Table 4. The maximum and average temperatures for both geometries are very similar, but the temperature distribution in the proposed geometry is much more uniform. The very important point is that the proposed geometry has a considerably smaller heat transfer area because, apart from having two coils less than the experimental arrangement, the diameter of the tube for the proposed geometry is 0.04 m, and the experimental work uses 0.05 m.

Power number	Mesh density	Maximum temperature ^{0}C	Average temperature ^{0}C
0.5	coarse	27.46	21.04
	fine	28.08	21.84
1.0	coarse	27.26	21.33
	fine	28.43	22.52
1.5	coarse	27.92	22.01
	fine	29.59	23.64

Table 3: Comparison of the temperature distributions of between the coarser and the finer mesh.

Power number	Geometry	Average temperature ^{0}C	Heat transfer coefficient $W.m^{-2}.^0C$
0.5	Experimental	19.42	36.36
	This work	21.75	41.28
1.0	Experimental	20.73	31.43
	This work	22.02	40.22
1.5	Experimrntal	22.12	27.48
	This work	22.68	37.85

Table 4: Comparison between the temperature distributions of the proposed geometry and the work by Oldshue and Gretton.

CONCLUDING REMARKS

The pseudo three-dimensional model presented in this work gives a good representation for the flow and temperature fields for disk turbine impellers and helps to determine design features which improve the flow inside coiled stirred tank reactors. Results show that coiled vessels have better fluid circulation if no coils are placed at the impeller blades height and, as a consequence, the internal heat transfer inside the vessel is improved.

At a later stage, a three-dimensional and a turbulent model, as well as a better defined reaction model will be investigated.

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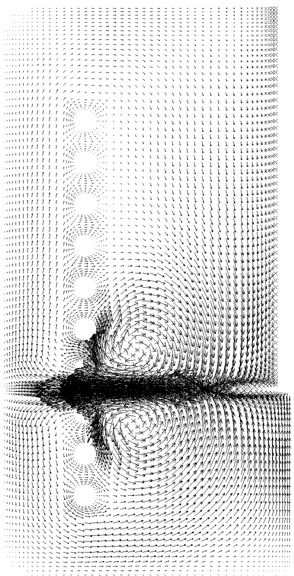

Figure 3: Flow patterns for the experimental apparatus.

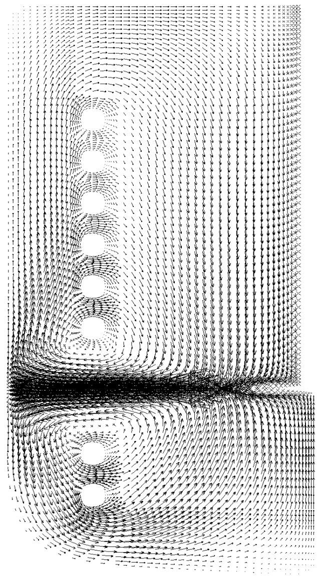

Figure 4: Flow patterns for a proposed geometry.

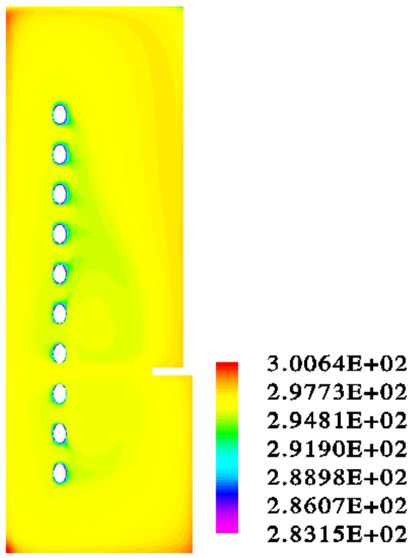

Figure 5: Temperature (K) contour plot for the experimental apparatus.

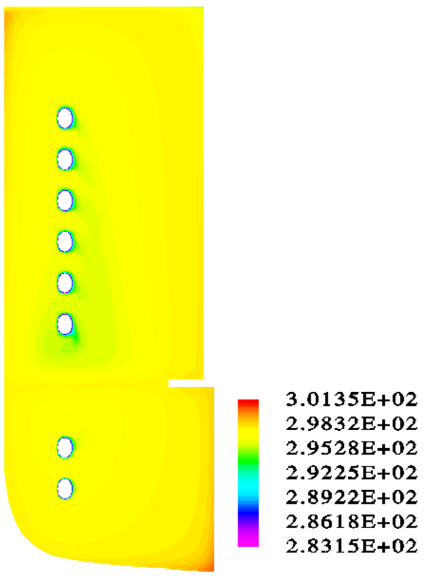

Figure 6: Temperature (K) contour plot for a proposed geometry.

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