Research of the rotation effect upon the hydrodynamics and heat and mass transport in a chemical reactor

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Abstract. The subject of this research is a chemical reactor for producing tungsten. A physical and mathematical model of fluid motion and heat and mass transfer in a vortex chamber of the chemical reactor under forced and free convection has been described and simulated using two methods. The numerical simulation was carried out in «vortex – stream function» and «velocity – pressure» variables. The velocity field, the mass and the temperature distributions in the reactor were obtained. The influence of a rotation effect upon the hydrodynamics and heat and mass transport was showed. The rotation is important for more uniform distribution of temperature and matter in the vortex chamber. Parametric studies on effects of the Reynolds, Prandtl and Rossby criteria on the flow characteristics were also performed. Reliability of the calculations was verified by comparing the results obtained by the methods mentioned above. Also, the created model was applied for numerically solving of the classical test problem of the velocity distribution in an annular channel and that of a rotating infinite disk in a stationary liquid. The study findings showed a good agreement with the exact solutions.

1. Introduction
The industry development requires improving the quality of materials. This determines the interest of science to refractory metals having very high durability. One of the most demanded refractory metals in different branches of industry is tungsten. However, the tungsten production and making the products desired shape are very difficult. Therefore necessity of development of new ways of tungsten isolation from its compounds exists. One such promising method is chemical vapor deposition from tungsten fluorides and chlorides. The stoichiometry of tungsten deposition from the mixture of tungsten hexafluoride and hydrogen is

\[ \text{WF}_6 + 3\text{H}_2 \rightarrow \text{W} + 6\text{HF}. \]

This reaction can start at a temperature of about 300° C and allow to obtain any thickness of tungsten blanket.

2. The reactor operation scheme
Modeling of viscous gas dynamics and heat transfer is considered in a vortex chamber that present a cylindrical chamber (see figure 1).
The carrier gas flow having axial velocity \( U_0 \), temperature \( T_0 \) and concentration \( C_0 \) enters from the pipe along the axis above, flows over the rotating disk and exits through the annular channel at the periphery of the top of the vortex chamber. The top and bottom walls of the apparatus are rotating with an angular velocity \( \omega \). The bottom wall is maintained at a temperature \( T_1 \), and other walls are considered as heat-insulated.

3. Mathematical model

A mathematical model of the processes being considered consists of partial differential equations which includes the fluid dynamics as well as heat and mass transport phenomena along with boundary conditions, incorporating all chemical and physical processes.

3.1. The equations for flow in a vortex chamber

3.1.1. System of equations in «velocity – pressure» variables. By virtue of relatively small velocities and temperature differences, gas is assumed to be incompressible and density change is taken into account only in terms that includes the force of gravity and besides density difference is proportional to the temperature difference with the opposite sign according to the Boussinesq approximation. From above, non-dimensional transport equations of momentum, heat and mass and continuity equation in cylindrical coordinates in the assumption of axial symmetry in angular direction in «velocity – pressure» variables are follows:

\[
\frac{\partial u_r}{\partial t} + \frac{\partial (u_r u_r)}{\partial r} + \frac{\partial (u_r u_z)}{\partial z} = -\frac{\partial p}{\partial r} + \frac{1}{\text{Re}} \left( \frac{\partial^2 u_r}{\partial r^2} + \frac{h u_r}{r} + \frac{\partial^2 u_r}{\partial z^2} - \frac{u_r^2}{r} \right) + \frac{u_r^2}{r} - \frac{u_z^2}{r}; \tag{1}
\]

\[
\frac{\partial u_z}{\partial t} + \frac{\partial (u_z u_z)}{\partial r} + \frac{\partial (u_z u_z)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{\text{Re}} \left( \frac{\partial^2 u_z}{\partial r^2} + \frac{h u_z}{r} + \frac{\partial^2 u_z}{\partial z^2} \right) - \frac{u_r u_z}{r} + \frac{Gr}{\text{Re}^2} \theta; \tag{2}
\]

\[
\frac{\partial u_\theta}{\partial t} + \frac{\partial (u_\theta u_\theta)}{\partial r} + \frac{\partial (u_\theta u_\theta)}{\partial z} = -\frac{2 u_r u_\theta}{r} + \frac{1}{\text{Re}} \left( \frac{\partial^2 u_\theta}{\partial r^2} + \frac{h u_\theta}{r} + \frac{\partial^2 u_\theta}{\partial z^2} - \frac{u_\theta}{r^2} \right); \tag{3}
\]

\[
\frac{\partial u_r}{\partial r} + \frac{\partial u_r}{\partial z} + \frac{u_r}{r} = 0; \tag{4}
\]
\[
\frac{\partial \theta}{\partial t} + \frac{\partial (u, \theta)}{\partial r} + \frac{\partial (\hat{u}, \hat{\theta})}{\partial z} = \frac{1}{Pr \cdot Re} \left( \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} + \frac{\partial^2 \theta}{\partial z^2} \right) \frac{\hat{u}, \hat{\theta}}{r}; \tag{5}
\]

\[
\frac{\partial C}{\partial t} + \frac{\partial (u, C)}{\partial r} + \frac{\partial (\hat{u}, \hat{C})}{\partial z} = \frac{1}{Pr_{p} \cdot Re} \left( \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2} \right) \frac{\hat{u}, \hat{C}}{r}. \tag{6}
\]

The dimensionless form of equations is obtained by using the following scales: vortex chamber radius \( R_0 \), axial velocity at the input \( U_0 \), density at the input \( \rho_0 \), temperature and concentration at the input \( T_0 \) and \( C_0 \) respectively.

The system of equations obtained contains criteria of Reynolds, Prandtl, Schmidt (Prandtl diffusion) and Grashof:

\[
Re = \frac{\rho_0 U_0 R_0}{\mu}; \quad Pr = \frac{c_p \mu}{\lambda}; \quad Pr_{w} = \frac{\nu}{D}; \quad Gr = \frac{g \beta}{(T_1 - T_0) \rho_0 (R_0)^3}. \tag{7}
\]

The dimensionless temperature is determined as \( \theta = \frac{(T - T_0)}{(T_1 - T_0)} \).

In addition, the following notations are introduced: \( u_r \) is radial velocity component, \( u_\phi \) is peripheral velocity component and \( u_z \) is axial velocity component, \( p \) is pressure.

3.1.2. System of equation in «vortex – stream function» variables. For equations in «vortex – stream function» variables to obtain, one introduce the stream function \( \psi \) and vortex \( \Omega \):

\[
u_r = \frac{1}{r} \frac{\partial \psi}{\partial z}, \quad u_z = -\frac{1}{r} \frac{\partial \psi}{\partial r}, \quad \Omega = \frac{\partial u_z}{\partial z} - \frac{\partial u_r}{\partial r}. \tag{8}
\]

By using these expressions one can transform the set of equations (1) – (6) to the following identical system:

\[
\frac{\partial \Omega}{\partial t} + \frac{\partial (u, \Omega)}{\partial r} + \frac{\partial (u, \Omega)}{\partial z} = \frac{2 u_\phi}{r} \frac{\partial u_\phi}{\partial z} + \frac{1}{Re} \left( \frac{\partial^2 \Omega}{\partial r^2} + \frac{1}{r} \frac{\partial \Omega}{\partial r} + \frac{\partial^2 \Omega}{\partial z^2} \right) \frac{\Omega}{r^2} \frac{Gr}{Re}; \tag{9}
\]

\[
\frac{\partial u_\phi}{\partial t} = \frac{\partial^2 \psi}{\partial r^2} + \frac{\partial^2 \psi}{\partial z^2} - \frac{1}{r} \frac{\partial \psi}{\partial r} - \frac{r \Omega}{\partial z}; \tag{10}
\]

\[
\frac{\partial u_\phi}{\partial t} + \frac{\partial (u, u_\phi)}{\partial r} + \frac{\partial (u, u_\phi)}{\partial z} = \frac{2 u_\phi u_\phi}{r} + \frac{1}{Re} \left( \frac{\partial^2 u_\phi}{\partial r^2} + \frac{1}{r} \frac{\partial u_\phi}{\partial r} + \frac{\partial^2 u_\phi}{\partial z^2} \right) \frac{u_\phi}{r^2}; \tag{11}
\]

\[
\frac{\partial \theta}{\partial t} + \frac{\partial (u, \theta)}{\partial r} + \frac{\partial (\hat{u}, \hat{\theta})}{\partial z} = \frac{1}{Pr \cdot Re} \left( \frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r} \frac{\partial \theta}{\partial r} + \frac{\partial^2 \theta}{\partial z^2} \right) \frac{\hat{u}, \hat{\theta}}{r}; \tag{12}
\]

\[
\frac{\partial C}{\partial t} + \frac{\partial (u, C)}{\partial r} + \frac{\partial (\hat{u}, \hat{C})}{\partial z} = \frac{1}{Pr_{p} \cdot Re} \left( \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2} \right) \frac{\hat{u}, \hat{C}}{r}. \tag{13}
\]

This system contains five equations instead of six ones since the continuity equation is automatically satisfied by the stream function determination.

3.2. Boundary conditions

For a unique solution to obtain, the boundary conditions in dimensionless form are set. At the input of chamber we have:
\[
\frac{\partial u_r}{\partial z} = 0, \quad u_\phi = 0, \quad u_z = -1, \quad \theta = 0, \quad C = 1;
\]

at the symmetry axis by \( r = 0 \) we have

\[
u_r = 0, \quad u_\phi = 0, \quad \frac{\partial u_z}{\partial r} = 0, \quad \frac{\partial \theta}{\partial r} = 0, \quad \frac{\partial C}{\partial r} = 0;
\]

at the walls of chamber there are no-slip and heat insulation conditions (\( n \) is normal direction):

\[
\frac{\partial u_r}{\partial n} = 0, \quad u_\phi = 0, \quad u_z = 0, \quad \frac{\partial \theta}{\partial n} = 0, \quad \frac{\partial C}{\partial n} = 0,
\]

with the exception of rotating surfaces, for which no-slip condition cause an emergence of another criterion, the inverse Rossby number \( R_\omega = R_0 \omega / U_0 \).

The value of peripheral velocity at the rotating surface is \( u_\phi = R_\omega \cdot r \). We have \( \theta = 1 \) and \( \partial C/\partial z = kC^m \) at the bottom wall, \( k \) is reaction rate constant, \( m \) is reaction order. At the chamber output, the Neumann conditions are used for all functions: \( \partial C/\partial z = 0 \).

### 4. Numerical solution methods

The numerical simulation of a set (1) – (6) was carried out using method of pressure and velocity correction [2]. One can present a system of equations consisting of the momentum equations and the continuity equation in the vector form as follows:

\[
\frac{\partial \mathbf{V}}{\partial t} = - \frac{\nabla p}{\rho} + F(\mathbf{V}); \quad \text{div} \mathbf{V} = 0.
\]  

One can obtain the two equations using time-splitting method for the momentum equation:

\[
\mathbf{V}^{n+1} - \mathbf{V}^n = - \frac{\nabla p^n}{\rho} + F(\mathbf{V}^n, \mathbf{V}^n);
\]  

\[
\frac{\mathbf{V}^{n+1} - \mathbf{V}^n}{\Delta t} = - \frac{\nabla (\delta p)}{\rho},
\]

here \( \delta p \) is the pressure correction which is equal to the difference between the pressures at new \( n+1^{\text{st}} \) layer of time and at the \( n^{\text{th}} \) layer known, \( \mathbf{V}^* \) is an intermediate grid function. After scalar multiplication of the equation (16) by the gradient and taking into account the solenoidality of velocity on the \( n+1^{\text{th}} \) layer, we have obtained the Poisson equation for the calculation of pressure correction as follows:

\[
\nabla^2 (\delta p) = \rho \nabla \cdot \mathbf{V}^*.
\]

One can represent this equation as transient Poisson equation for the convenience of calculation:

\[
\frac{\partial (\delta p)}{\partial \tau} - \nabla^2 (\delta p) = -\rho \frac{\nabla \cdot \mathbf{V}^*}{\partial t}.
\]

In equation (18) \( \Delta \tau = B \Delta t \) is the time step performing the role of iteration parameter which value is chosen to ensure the most rapid convergence of problem solution. For the difference scheme to construct, it is used a staggered grid. The set of equations obtained was being solved by using an evolutionary method of relaxation in time. For each equation in the set obtained to solve, an alternating direction implicit scheme was used [3]. This method has the second order of accuracy in time and it is unconditionally stable. Convective and diffusion terms in transport equations for a staggered grid [4] are represented by means the Exponential Scheme [5] based on the control volume
method. The alternating direction implicit scheme for a non-staggered grid was used for equations (9) – (13) solving, too. Our own program codes for each method were compiled.

5. Reliability proof
The reliability of results obtained was validated with several ways. Figure 2 shows comparison of graphs of flow characteristics obtained by using different solution methods in sections showed at the right figure. Solid lines are the model predictions in «velocity – pressure» variables, points are the «vortex – stream function» variables method results. A congruence of methods results means the solution right.

![Figure 2](image)

**Figure 2.** Comparison of solutions obtained by different methods in the sections in a vortex chamber:  
* a) axial velocity component;  
* b) temperature;  
* c) the sections specified

Figure 3a illustrates comparison of model prediction for velocity distribution in an annual channel at the vortex chamber output with the exact solution (section 4 at the figure 2c) [6].

At the figure 3b the comparison of a numerically solving of the classical test problem of a rotating infinite disk in a stationary liquid with the exact data is shown [7]. Figure 3 shows a good agreement of model results with the exact solutions.

![Figure 3](image)

**Figure 3.** Comparison of the model results with the exact solutions:  
* a) for a velocity distribution in an annular channel  
* b) for a rotating infinite disk in a stationary liquid

6. Results and Discussion
Numerical calculations were performed for the different reactor operating conditions. The rotating effect upon the hydrodynamics and heat and mass transport in a chemical reactor was studied [8,9]. The results of the numerical solution are presented in figure 4, 5 and 6. Figure 4 demonstrates the
stream function for the different rotation degree. One can see that rotation promotes uniform mixing of a matter in the vortex chamber, but too strong rotation can cause precessing core formation.

![Stream function images](image1)

**Figure 4.** The stream function for the different rotation degree at \( Re = 50, Gr = 10^5 \):

- a) \( R\omega = 0 \);
- b) \( R\omega = 1 \);
- c) \( R\omega = 5 \).

Figure 5 illustrates the solution by rotating effect not taken into account and figure 6 shows the solution with rotation by the same parameters and criteria of the flow considered. The figures presented show that a rotation impacts significantly on the flow hydrodynamics. The distributions of temperature and concentration become more uniform near the susceptor so surface reaction on it proceeds more effective.

![Temperature and concentration images](image2)

**Figure 5.** Temperature and concentration distribution in the vortex chamber at \( R\omega = 0 \). Operating parameters are \( Re = 50, Pr = 1, Pr_D = 1, Gr = 10^5, k = 5 \).

**Figure 6.** Temperature and concentration distribution in the vortex chamber at \( R\omega = 5 \). Operating parameters are \( Re = 50, Pr = 1, Pr_D = 1, Gr = 10^5, k = 5 \).
7. Conclusions
The fluid motion and heat and mass transfer in a vortex chamber of the chemical reactor has been studied by dint of mathematical simulation. The numerical calculation code compiled predicts the flow character by different operating conditions. The influence of a rotation effect upon the hydrodynamics and heat and mass transport was considered. The rotation results in a more uniform distribution of temperature and matter in the vortex chamber.

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