CFD SIMULATION OF PARTICLE-TO-FLUID HEAT TRANSFER UNDER SUPERCRITICAL CONDITIONS: PRELIMINARY RESULTS

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Computational Fluid Dynamics (CFD) has proven to be a powerful tool to numerically solve the fluid-flow equations so it gives a further insight into the flow pattern of contacting equipment. There has been a fast growing in the study of applications in fluid flow and heat transfer, and several authors have used it to analyze flow patterns in fixed-bed equipment and to predict heat transfer parameters in studied cases. In this work, particle-to-fluid heat transfer is studied in a maximum-occupying-space arrangement of solid spheres in a cylindrical container, in order to simulate via CFD the heat transfer behavior in a supercritical catalytic reactor under steady state conditions. Supercritical CO_2 was chosen as circulating fluid; buoyancy terms were found to be relevant in calculations through a dimensionless analysis done to Navier-Stokes equations, and therefore are used during simulations. C-written programmed modules based on the SRK equation of state and accepted correlations for high pressure properties estimation have been implemented for use with CFD commercial codes in order to estimate the transport properties of the fluid (i.e., density, viscosity, heat capacity and thermal conductivity).

INTRODUCTION

An understanding of the particle-to-fluid heat transfer phenomena in a porous media implies the study of the fluid transport model within the void space; this fact is of fundamental importance to many chemical engineering systems such as fixed bed extraction or catalytic reaction equipment. Experimental and theoretical studies of flow through such systems often treat the porous medium as an effectively homogeneous system and concentrate on the bulk properties of the flow. Such an approach neglects completely the complexities of the flow within the void space of the porous medium, reducing the description of the problem to macroscopic average or effective quantities. The details of this local flow process may, however, be the most important factor influencing the behavior of a given physical process occurring within the system, and are crucial to understanding the detailed mechanisms of, for example, heat and mass dispersion and interface transport.

I - GEOMETRICAL MODEL

An 11-sphere arrangement, with 9 particle-to-wall contact points and 14 particle-to-particle contact points was built. A 4-layer arrangement with a 60^o rotation around the reactor axis within each layer and with a diameters ratio of 3.923 was chosen to be the geometrical model (Fig. 1). Modeled geometry has been constructed following the bottom-up technique (generating surfaces and volumes from nodes and edges) in order to control mesh size around critical points (i.e. particle-to-particle and particle-to-wall contact points), necessary to avoid grid elements skewness, and also to gain computational resources by reducing the number of elements in zones of low interest (i.e. geometrical zones away from contact points).

Figure 1: Generated geometric model.

II - MESH DESIGN AND CFD MODELING

In order to properly understand the transport mechanisms present in the study case, a dimensionless analysis under work conditions of the set of used equations has been developed. Dimensionless equations corresponding to mass, momentum and energy balances are as follows:

$$\frac{\partial r_0}{t_0}\left(\frac{\partial \hat{r}}{\partial \hat{t}}\right)+\frac{u_0}{L}\partial r_o\left(\boldsymbol{u}\cdot\nabla\hat{r}\right)=r_0\frac{u_0}{L}\left(-\hat{r}\nabla\cdot\boldsymbol{u}\right) \tag{1}$$

$$St\left(\frac{\partial \boldsymbol{u}}{\partial \hat{t}}\right)+\hat{r}\left(\boldsymbol{u}\cdot\nabla\right)\boldsymbol{u}=Eu\left(-\nabla\hat{p}\right)+\frac{1}{\mathrm{Re}}\nabla\cdot\left\{\hat{m}\left[\nabla\hat{m}+\left(\nabla\hat{m}\right)^T\right]\right\}+\frac{1}{\mathrm{Re}_T}\nabla\left(\hat{m}^T\nabla\hat{m}^T\right)+\frac{1}{Fr}\left(\hat{r}\hat{f}_b\right) \tag{2}$$

$$St\left(\frac{\partial \hat{T}}{\partial \hat{t}}\right)+\left(\boldsymbol{u}\cdot\nabla\right)\hat{T}=Ec\frac{1}{\mathrm{Re}}\left[\hat{v}\left(\boldsymbol{t}:\nabla\boldsymbol{u}\right)\right]+\frac{1}{\mathrm{Re}}\frac{1}{\mathrm{Pr}}\left(\frac{\hat{m}}{\hat{r}}\Delta\hat{T}\right)+\frac{1}{\mathrm{Re}}\frac{1}{\mathrm{Pr}_T}\left(\frac{\hat{k}_T}{\hat{r}}\Delta\hat{T}\right) \tag{3}$$

The order of magnitude of the dimensionless groups was estimated taking physical-chemical properties values for supercritical CO_2 under the simulation conditions. SRK equation of state was used to estimate density and heat capacity of the fluid [1], Lucas method was used to estimate the viscosity, and thermal excess method was used to estimate the thermal conductivity [2]. Results are shown in table 1.

Dimensionless analysis allows identifying the problem as natural convection heat transfer in laminar flow. Buoyancy terms and pressure drop are found to be relevant for the calculations. Turbulence terms are negligible in calculations. The mesh should be properly defined near to the surface of the spheres, in order to properly capture the boundary layer problem involved. In order to simulate contact points between particles, the spheres drawn have been overlapped in a 1 % of their diameters.

St $[L/t\cdot v]$	**Re** $[L\cdot u\cdot r/m]$	**Eu** $[dP/r\cdot u^2]$	**Fr** $[u^2/L\cdot g]$	**M** $[u/C]$	**Pr** $[C_p\cdot m/k]$	**Br** $[m\cdot u^2/k\cdot T]$
40	15,6	5,48E+21	1,29E-08	3,15E-07	1,79	4,21E-15

Gr$_H$ $[g\cdot b\cdot L^3\cdot dT/v^2]$	**Ra** $[g\cdot b\cdot L^3\cdot \delta T\cdot r/m\cdot a]$	**$Gr_H/Re^2 > 1$**	**$Pr\cdot Gr_H > 10^8$**	**Ec** **[Br/Pr]**
5,67E+08	1,02E+09	2,34E+06	1,02E+09	2,35E-15

Table 1: Dimensionless numbers of the studied case

The boundary conditions of the model equations are as follows:

- Constant temperature and mass flow rate of the fluid at the inlet [330 K; 1 x 10^{-4} kg/s].
- Constant temperature at the particles surface [340 K].
- Adiabatic reactor’s wall.
- Constant operating pressure [1 x 10^7 Pa].

III - MODEL ANALYSIS

Navier-Stokes equations together with energy balance in steady state were solved using commercially available finite volume code software Fluent® 6.0. The fluid was taken to be supercritical CO_2 in a laminar flow regime. C-written programmed modules were incorporated to the CFD code as user defined functions for calculating the transport properties of the fluid. SRK equation of state was used to estimate density and heat capacity of the fluid [1], Lucas method was used to estimate the viscosity, and thermal excess method was used to estimate the thermal conductivity [2].

First order upwind discretization schemes were selected to compute field variables, excepting for the pressure-velocity coupling algorithm, in which a second order discretization scheme was applied. The generated mesh had 120.000 tetrahedral elements, and several processes of mesh adaption and refinement were made in order to avoid large variables gradients that could cause numerical divergence of the solution.

The simulation was run in an HP C3000 Workstation, and the simulation time was approximately 120 hours. Numerical convergence of the model was checked based on the numerical residuals of all computed variables. For a more complete convergence checking, the drag force over the particles surface and the average static temperature, density and viscosity at the bed outlet were also chosen as monitors.

IV – RESULTS AND DISCUSSION

Particle-to-fluid heat transfer phenomena was studied for a selected case. Flowing fluid was taken to be CO_2 at supercritical state in the bed inlet [330 K, 1 x 10^7 Pa], and with a mass flow rate of 1 x 10^{-4} kg/s. Particles were set to be at a constant temperature of 340 K. Simulation was run under steady state conditions. Results and discussion are shown below.

Velocity profiles

Flow maldistribution inside the fixed bed is noticed through the analysis of the velocity profiles obtained. The variation of the velocity values makes clear that the fluid does not have a ‘plug flow’ behavior in any part of the bed. The influence of the gravity forces over the velocity fields inside the packed bed can be noticed in the presence of convective flow due to the temperature and density gradients in the fluid. Figure 2 shows the obtained velocities in the longitudinal axis of the fixed bed. It can be noticed that velocity values are not uniform along the axis.

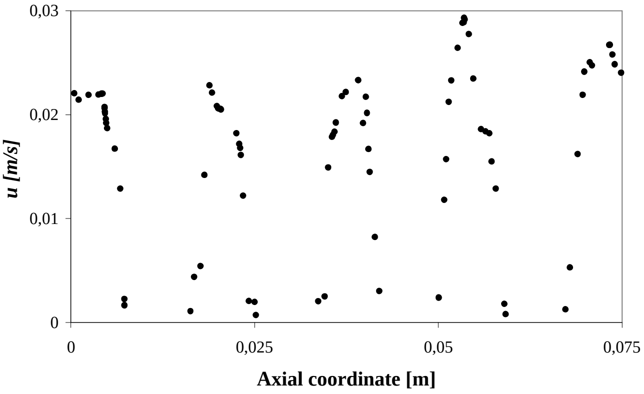

Figure 2: Velocity values in the longitudinal axis of the fixed bed.

Temperature profiles

It can also be noticed that temperature profiles are not homogeneous within the fixed bed. Temperature jump is present near the spheres surface, and the mixing allows the fluid to reach a quasi-homogeneous temperature in the main voids of the bed. This scenario allows thinking that a unique value for heat transfer parameters is not a realistic way to represent the heat transfer phenomena in a fixed bed. Figure 3 shows the obtained temperatures in the longitudinal axis of the fixed bed.

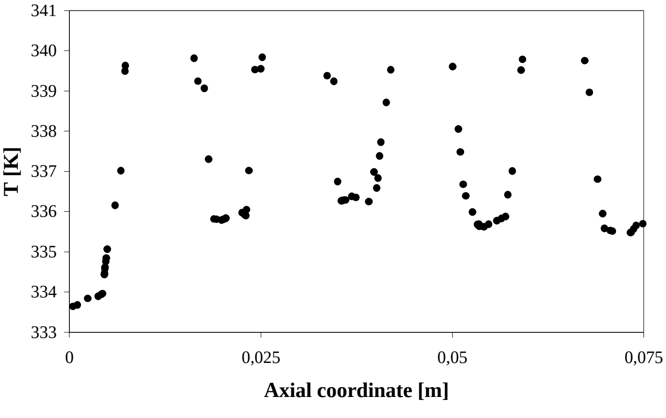

Figure 3: Temperature values in the longitudinal axis of the fixed bed.

Transport properties estimation

Transport properties can be visualized for every point of the fixed bed. The estimation of main momentum and heat transport properties (i.e., density, viscosity, heat capacity and thermal conductivity) is done by means of the implementation of an additional set of equations via user defined functions that are solved together with the momentum, mass and energy balances. Figure 4 shows the density profile for the studied case.

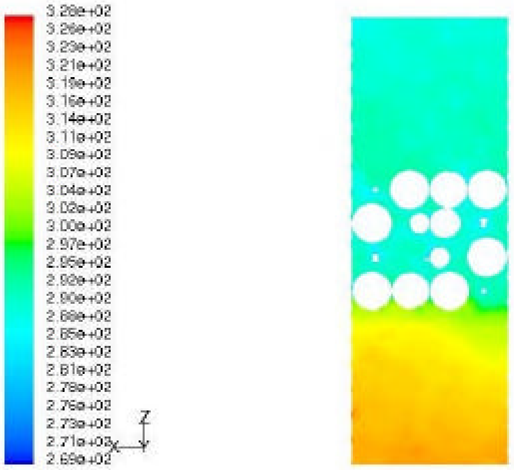

Figure 4: Density profile in an axial cut of the studied case. Density scale expressed in kg/m^3.

Local heat transfer parameters estimation

Local values of Gr_H, Pr and Re were calculated various points inside the thermal boundary layer around the spheres in order to corroborate the heat transfer mechanism present in the fixed bed. Obtained values were compared with Metais-Eckert maps [3] and are shown in Figure 5. As it can be observed, the main heat transfer mechanism inside the fixed bed under the simulation conditions is the free convection in laminar flow regime.

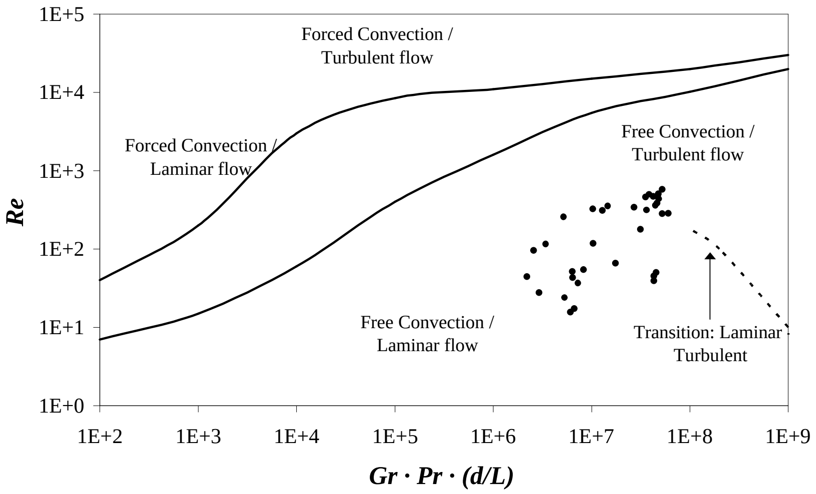

Figure 5: Comparison between simulation data and Metais-Eckert maps

Numerical results of computed variables in the flow channels placed on a longitudinal cut of the fixed bed were taken to calculate local values of Nu_p, Gr_H and Pr inside these channels. Special attention was taken to exclude the boundary layer values in the calculations. Figure 6 shows the behavior of the local Nu_p values with the dimensionless group $Gr_H \cdot Pr$ inside the flow channels of the selected cut of the fixed bed.

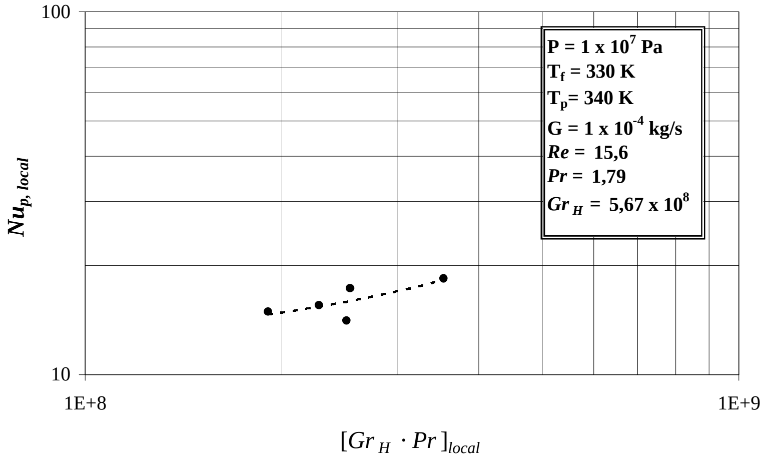

Figure 6: Nu_p vs. $[Gr_H \cdot Pr]$ inside the flow channels of the fixed bed.

CONCLUSIONS

CFD proves to be a useful tool to simulate fluid flow through complex geometries as a fixed bed. The implementation of transport properties estimation parameters via user defined functions into the used equations in commercial available solvers makes possible the idea of using this technique to simulate the behavior of supercritical fluids in fixed bed equipments such as supercritical extractors or fixed bed reactors.

At low values of *Re*, gravity forces become clearly important in the behavior of the flow pattern inside the fixed bed for a supercritical fluid. This makes that the buoyancy terms have to be included into the calculations for momentum, heat and mass transfer parameters when needed.

Free convection in laminar flow regime is the main heat transfer mechanism in the fixed bed under the operating conditions mentioned; therefore, numerical calculations confirm the ideas extracted from the dimensionless analysis of the problem. The numerically obtained local values of Nu_p inside the channels of the fixed bed increase with the dimensionless group $[Gr_H \cdot Pr]$.

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