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Enhanced mass and heat transfer in catalytic reactors

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ABSTRACT

Mass and heat transfer in square ducts with one side containing a porous wall were simulated using large eddy simulation (LES). Increased wall normal turbulent intensity was observed along the porous wall compared to the smooth wall. Depending on the wall permeability the fluid elements penetrated to different depth resulting in enhanced mass and heat transfer rates. The larges effect was obtained for mass transfer in liquids with up to 20 times larger mass transfer rate, compared to smooth surfaces. An increased penetration into the porous wall was obtained with more open porous structure and with fluids having high density and low viscosity. Most benefit of the porous walls is obtained for fluids with high ρ/μ ratio and high Pr or Sc numbers i.e. for mass transfer in liquids.

1. Introduction

Mass and heat transfer are often the rate limiting steps in chemical processes. Most process flows are turbulent since mixing at turbulent conditions is very effective. However, the viscous layer close to the walls limits the mass and heat transfer rates. Many different reactor designs have been proposed to increase the fluid–solid interaction e.g. metal or ceramic foams [1]. The flow in these reactors is usually laminar. Rough surfaces increase turbulence close to the walls and also decrease the critical Reynolds number for transition from laminar flow to turbulence and a significant increase in the mass and heat transfer to the wall has been observed. For a porous wall there is an additional benefit from allowing the turbulent flow structures to penetrate the wall and Kuznetsov et al. [2] has shown that introducing porous walls increase the heat transfer rate.

Suga et al. [3] investigated the effects of the wall permeability on turbulence near a porous wall. They used particle image velocimetry (PIV) and measured the turbulence in the bulk outside a porous wall in channel flow. They observed an increase in the near-wall turbulence with decreasing flow resistance in the porous wall, i.e. with larger wall permeability. They also observed that the increased turbulence at the porous wall increased the flow resistance and made the average flow distribution in the channel asymmetrical. The objective with this article is to make a more detailed study of how gas and liquid turbulence penetrate porous walls and affect the mass and heat transfer rates.

2. Model description and validation

Detailed characterization of the flow and turbulence through different size rectangular channels, with one side containing a porous wall and with the opposite wall smooth with constant concentration and temperature and the remaining sides with non-permeable surfaces, was done according to Fig. 1. Most simulations were done for square channels with side length of 3 mm or 10 mm but a few simulations were also done with rectangular cross-section to validate the LES simulations with the experimental data from Suga et al. [3]. We kept the design with one porous and one non-porous wall made by Suga in order to directly compare the mass and heat transfer to a solid and a porous wall. However, this design gives asymmetric velocity, temperature and concentration distribution that made mixed cup averaging for mass transfer uncertain. Different porous flow resistances and surface areas were simulated as seen in Tables 1 and 2. The solid material in the porous wall was aluminum for heat transfer, and for mass transfer the wall boundary conditions and the properties were selected to obtain constant concentrations on the surface of the solid and porous walls.

The bulk flow was simulated using dynamic large eddy simulations (LESs) with periodic boundary conditions. The wall boundary conditions were constant temperature and concentration. In the porous volume viscous and inertial resistances were added as a source term according to Breugem et al. [4]. They simulated turbulent flow in a combined open fluid and porous material channel and found that LES worked fine in the porous material when the viscous and inertial resistances were added according to

$$\frac{dP}{dx_i} = -\alpha\mu U_i - \beta\frac{\rho}{2}|U|U_i \quad (1)$$

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Fig. 1. The simulated square channel with a porous wall.

where the coefficient α and β can be estimated from e.g. the Ergun or Poiseuille equation depending on the structure of the porous material. Fine porous structure was simulated in this work and only the viscous term α was important. The heat transport in the open bulk flow was modeled with periodic boundary conditions with an average of 400 K at the inlet. The periodic boundary for flow and heat transfer will correspond to fully developed boundary layers. An effective heat conductivity and diffusivity in the fluid based on the molecular transport and the subgrid viscosity with a turbulent subgrid Prandtl or Schmidt number was used

$$k_{eff} = k + \frac{\mu_{SGS} c_p}{Pr_T} \quad \text{or} \quad D_{eff} = D + \frac{\mu_{SGS}}{\rho Sc_T} \tag{2}$$

where the subgrid Prandtl and Schmidt numbers are $Pr_T = Sc_T = 0.85$.

The heat transport in the porous volume was modeled using the two temperature model according to d'Hueppe et al. [5]. In their model the fluid and the solid have different temperature, and the heat transfer between the phases is modeled by adding a source term $q = -h_p a_p (T_f - T_s)$ with $h_p = \mathrm{Nu} \cdot \lambda / d_p$ and $a_p = 6(1-\varepsilon)/d_p$ where h_p is the heat transfer coefficient and a_p is the surface area density assuming that the porous wall consists of particles a diameter of d_p. For a more open structure e.g. ceramic foam the corresponding models can be used. It has been observed that these materials may have more than 10 times higher mass and heat transfer coefficients for the same flow resistance. In this article we have selected specific viscous flow resistances, α, that scales with particle size or pore openings as $\alpha \propto 1/d_p^2$ i.e. $d_p \propto \sqrt{1/\alpha}$. The heat transfer with constant Nu scales as $h \propto 1/d_p$ and the specific contact area $a \propto 1/d_p$ i.e. $h \cdot a \propto 1/d_p^2 \propto \alpha$ and decreases with decreasing α as seen in Tables 1 and 2. We have varied the mass transfer resistance in the porous wall to visualize the effect on fluid–porous wall mass and heat transfer. An analog model was used for mass transfer with the source term $r = -k_C a (C - C_S)$ with constant surface concentration C_s and by adjusting for the constant background concentration this corresponds to a mass transfer limited chemical reaction for $C' = C - C_S$ i.e. infinite fast reaction on the porous surface. The estimation of the effective diffusivity in turbulent flow corresponding to Eq. (2) above may not be valid for liquids since the mass diffusivity is four orders magnitude lower in liquids than in gases. However, the grid resolution was very high and the dominating mass transport mechanism in the liquid bulk was the resolved turbulent convection. The flow in the porous wall was well resolved and no correction for mass transport of non-resolved turbulent scales was required.

At high Sc numbers the mass transfer from the fluid to the solid within the porous volume becomes important. Miyabe et al. [6] measured fluid solid mass transfer in a HPLC system with 50.6 μm porous silica gel particles and found that the model by Wilson and Geankoplolis [7] could predict the Sherwood number within ±20%.

$$\mathrm{Sh} = \frac{1.09}{\varepsilon_e} Re^{1/3} \mathrm{Sc}^{1/3} \quad (0.0015 < Re < 55) \tag{4}$$

where ε_e is the porosity and Re the superficial Reynolds number in the porous material.

The flow simulation was validated with measurement data from Suga et al. [3]. As shown in Fig. 2a the asymmetric mean flow profile is in very good agreement with the measurements. It is also concluded that the wall normal turbulent fluctuations, which characterizes the turbulent transport of momentum, mass and heat to the porous wall are in excellent agreement with the measurements, Fig. 2b. Fig. 2 shows the results for a viscous resistance $\alpha = 3 \times 10^7$ [m^{-2}] and an inertial resistance $\beta = 550$ [m^{-1}].

3. Simulation results and discussion

Gas and liquid flows with different Prandtl and Schmidt numbers were simulated using different flow resistances in the porous volume. On the average more than 90% of the turbulent kinetic energy was resolved with LES giving the average subgrid viscosity to molecular viscosity ratio below 0.05 and the maximum local ratio below 0.7.

Fig. 3 shows the penetration of turbulence into the porous wall. The root mean squares of the wall normal turbulent velocity show a strong dampening outside the porous wall, but an almost linear decrease inside the porous wall.

Heat and mass is transported by resolved turbulence convection and molecular transport in both air Pr = 0.74 and water Sc = 700. The subgrid transport has an effect at higher Schmidt number (Sc = 700) mainly in the open channel, but the subgrid turbulence is dampened very fast when the flow enter the porous wall and the modeled subgrid transport in the porous material is much less than the convective transport or the molecular diffusion transport.

The simulated heat transfer rate was evaluated by integrating the heat flux to the permeable wall. This was used to calculate the Nusselt number defined as $\mathrm{Nu} = hd/\lambda$ and $q = h(T_{bulk} - T_{surface})$ is the

Table 1
Calculated Nusselt/Sherwood numbers for low Prandtl and Schmidt numbers. In the simulations marked * the heat transfer resistance is dominated by the resistance in the porous wall.

Fluid	Wall permeability	ha	Reynolds number	Pr/Sc number	Nu/Sh number	Correlation Eq. (5)
Air	Solid wall	–	4452	0.74	16.5	17.7
Air	1×10^{11}	1×10^{9}	4452	0.74	16.2	17.7
Air	1×10^{10}	1×10^{8}	3820	0.74	24.2	15.6
Air	1×10^{8}	1×10^{6}	8000	0.74	101	28.2
Air	1×10^{8}	1×10^{4}	8000	0.74	120*	28.2

Table 2
Calculated Sherwood number for high Schmidt number flows. In the simulations marked * the mass transfer resistance is dominated by the resistance in the porous wall.

Fluid	Wall permeability viscous/pore diameter	$k_L a$	Reynolds number	Sc number	Sh number	Correlation Eq. (6)
Water	Solid wall		9300	700	316	338
Water	1×10^{11}	1900	9300	700	820	338
Water	1×10^{10}	190	8200	700	1750	302
Water	1×10^{9}	19	8100	700	5230	298
Water	1×10^{9}	0.19	8100	700	5400*	298