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Evaluation of longitudinal dispersion coefficient in open-cell foams using transient direct pore level simulation

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HIGHLIGHTS

- The axial dispersion within a sponge structure is function of pore diameter and porosity.
- The axial mixing length is recommended as the characteristic length.
- Peclet numbers of sponges are approximately equal to the Peclet number of packed bed.

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ABSTRACT

A new method to analyze fluid flow in open-cell foams is given by the rise in computational speed, which makes it possible to calculate the heat and mass transport within these structures even with conventional CFD methods. In the present study, air flow through several structures has been explicitly calculated using the standard Navier–Stokes equations. Together with the flow, the dispersion of an initial tracer jump is tracked through the structures and analyzed with respect to effective diffusivity coefficients. The structures comprises a broad range of open-cell ceramic foams which were reconstructed from tomographic data obtained by means of MRI and μ-CT scans.

1. Introduction

Solid sponges made of ceramic, metal or polymeric material are highly porous, monolithic materials with excellent mixing properties. Their open-cell structure consists of stiff, interconnected struts building a continuous network. In literature, these structures are typically named as foams. But, as foam is defined consisting of closed bubbles, its void phase is not continuous but dispersed (Reitzmann et al., 2006). Therefore, the explicit term sponge is used in the present work, having in focus particularly ceramic sponges. Because of the high volumetric porosity, such structures exhibit a relatively small pressure loss and provide good mixing properties and thus, are an interesting material for chemical process engineering purpose. Additionally, sponges made of ceramics, depending on the bulk material bear temperatures up to 1700 K and can be utilized in porous burners in order to enhance the volumetric heat release by enhancing the thermal and mass transport processes. Dispersion can be described considering a fluid flow in such a porous medium, where a fraction of the fluid is labeled as tracer. The tracer mixes with the unlabeled fluid through a non-steady, irreversible process known as hydrodynamic dispersion. The theory of dispersion for porous media from its historical development is presented by Bear (1972) and several relevant theoretical predictions are given by Koch and Brady (1985). As described by Boon et al. (2000) hydrodynamic dispersion is analogous to the turbulent diffusion phenomenon, where the porous matrix plays the role of eddies in dispersing the flow. A macroscopic description of the phenomenon was derived by Carbonell and Whitaker (1983) from the convection–diffusion equation by volume averaging in a porous medium

$$\phi\frac{\partial^2 Y}{\partial t}+\nabla\cdot(\phi\mathbf{u}Y)=\nabla\cdot(\phi D\cdot\nabla Y) \tag{1}$$

where Y is the tracer concentration, ϕ is the fluid volume fraction, $\mathbf{u}$ is the pore velocity, and D is the hydrodynamic (macroscopic) dispersion tensor. The relative importance of molecular diffusion and hydrodynamic dispersion for spreading the tracer is described by the Peclet number, $Pe_m = ud/D_m$, where u is the average pore velocity, d denotes a characteristic length of the porous medium, and D_m is the relevant coefficient of molecular diffusion. For increasing Peclet numbers, the influence of hydrodynamic dispersion too

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increases. The phenomenon of hydrodynamic dispersion has been investigated by many researchers in the past, Maier et al. (2002) give a good overview over these investigations together with more recent investigations that have been conducted using new experimental methods (e.g., pulsed-gradient spin echo NMR) and new numerical methods like the lattice Boltzmann (LB) methods on the pore level. Delgado (2007) in his recent review analyses vast data on dispersion in porous media that are available in the literature and formulates simple correlations for the prediction of longitudinal and transversal dispersion coefficients for gaseous and liquid flow. For relatively high Pe_m numbers (>60), the longitudinal component D_L of the macroscopic dispersion tensor D has been found to asymptotically approach a linear function of Pe_m. Instead of using the most common representation of dispersion coefficients that show the dependence of the ratio D_L/D_m as a function of Pe_m, Delgado (2007) uses the definition of a macroscopic Peclet number in longitudinal direction $Pe_L = ud/D_L$ in order to better resolve the data found in the literature. For gaseous flow in porous media at high Pe_m numbers, an asymptotic value of $Pe_L = 2$ can represent the data for beds with spherical elements in good accordance. Despite the vast amount of the data available in the literature, dispersion coefficients for highly porous media like sponge structures are scarce. This is due to the fact that the dispersion is subject to the internal structure of the porous media and therefore cannot be described without taking this structure into account. In addition, such data usually is not available from the suppliers of the commercially available ceramic sponges. Thus, the present work aims in calculating the effective axial dispersion coefficients of various sponge structures.

2. Numerical setup

Assuming air to be a Newtonian fluid having a constant density and with requirement of unsteady flow, the governing equations of mass and momentum conservation is written using Einstein's summation rule as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}(\rho u_k) + \frac{\partial}{\partial x_j}(\rho u_j u_k) = -\frac{\partial p}{\partial x_k} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_k}{\partial x_j}\right) \tag{3}$$

whereas x_j and u_j denote the spatial coordinate and velocity in j-direction, p is the static pressure and μ stands for the dynamic viscosity of the air. Besides the underlying assumptions of the Navier–Stokes equations, no simplifications are necessary. Within the limits of the numerical truncation error (i.e., mesh refinement) and the accuracy of geometrical representation (i.e., statistical variations), *direct pore level simulation* (DPLS) approaches the exact solution. The boundary conditions at the inlet and outlet are specified using constant gas velocity at the inlet and static pressure together with zero gradient condition for the velocity at the outlet. The domain surfaces perpendicular to the flow direction are given with translational periodic boundary conditions. The structure surfaces are modeled using wall boundary conditions. The flow domains were described based on the reconstructed surfaces of the real probes (Habisreuther et al., 2009). The computational grids were produced using ANSYS ICEM CFD 10 requiring approximately 8 h each on a 2 Quad-core processors with 8 GB RAM. The resulting grids consisted of 4–6 million tetrahedral cells and approximately 0.8–1.1 million grid points. ANSYS CFX employs the finite volume method of a cell-centered storage arrangement. The applied discretization for the momentum equations was based on a bounded linear scheme. The flow is presumed to be laminar, and so no turbulent model has been used. Considering the extreme spatial and temporal resolution (1–4 million grid points for approximately 18000 mm^3, i.e., more than 50 points/mm^3 and a time-step of 1 μs) the simulation could be regarded as a direct numerical simulation.

3. Numerical procedure

Starting point is the simulation of the stationary flow of air through the void phase of sponges. Using the converged stationary solution as a starting condition, a transient calculation is performed, where the incoming fluid is suddenly changed from air to tracer air having same properties as that of air and with molecular diffusion coefficient $D_m = 1.3 \times 10^{-5}$ m^2/s. The tracer air is then transported by convection and diffusion through the sponge structure. In order to calculate an effective dispersion coefficient from CFD simulation, the instantaneous three-dimensional mixture fields are reduced into one-dimensional ones using mass flow average over N cross-sectional planes perpendicular to the main flow direction

$$\overline{Y(x_k,t)} = \frac{\sum_{i=1}^{M}\left(Y_i(t)\cdot \rho u_i A_i(x_k)\right)}{\sum_{i=1}^{M} \rho u_i A_i(x_k)} \tag{4}$$

$\overline{Y(x_k,t)}$ denotes the mass flow averaged tracer mass fraction at the k-th cross-sectional plane at position x_k and for the time t, $\rho u_i A_i(x_k)$ stands for the mass flow in the plane with the i-th grid cell, M is the number of grid cells and $Y_i(t)$ is the tracer mass fraction value in the i-th grid cell at time t. The result of this procedure yields the progress of the one-dimensional dispersion field in time. Fig. 1 shows the positions of surfaces with constant mass fraction of tracer $Y=0.5$. Following an approach similar to the one of Maier et al. (2002) the dispersion coefficient is evaluated from the time history of the mass fraction profiles of a tracer species which is introduced into the flow through the porous media. In contrast to a similar method used in Hackert et al. (1996) and more recently in Pereira et al. (2005), in the present work, the longitudinal dispersion coefficient was evaluated using a sudden concentration jump at the inlet of the flow system. The transient one-dimensional transport of concentration jump by advection and diffusion is analytically described in a frame of reference moving with the mean flow velocity ($x' = x - u\cdot t$) by Fick's law with the differential equation

$$\frac{\partial Y}{\partial t} = D\frac{\partial^2 Y}{\partial x'^2} \tag{5}$$

where Y is the tracer concentration and D denotes the dispersion coefficient. The analytical solution of this differential equation is well known and can be found in standard text books

$$Y = 1 - erf\left(\frac{x'}{2\sqrt{D\cdot t}}\right) \tag{6}$$

As an example the calculated mass fraction profiles for the dispersion in a 20 PPI SiSiC 85% porosity sponge with this time behavior are shown in Fig. 2. In order to evaluate the effective dispersion coefficient, it is more convenient to analyze the gradient of the concentration profiles $\partial Y/\partial x$

$$\frac{\partial Y}{\partial x} = -\frac{2}{2\sqrt{\pi\cdot D\cdot t}}\exp\left(-\frac{x'^2}{4tD}\right) \tag{7}$$

Assuming that the simulated concentration gradient is of Gaussian type, the dispersion coefficient is evaluated fitting the width of the gradient curve of the analytical solution to the one of the simulation results, which is approximated using a central difference scheme

$$\frac{\partial \overline{Y(x,t)}}{\partial x} = \frac{\overline{Y(x_{k+1},t)} - \overline{Y(x_{k-1},t)}}{x_{k+1} - x_{k-1}} \tag{8}$$