Numerical Simulation of the Spatial Distribution of Mean Residence Time in Complex Flows through Porous Media

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In this paper, a numerical method for obtaining theoretical predictions of mean residence time spatial distributions in flows through porous media is presented. The simulation sequence consists in solving first continuity and momentum conservation equations, possibly coupled with turbulence quantities transport equations, using the finite volume method. Once the flow configuration is calculated, the simulation consists in solving the additional transport equation of a passive scalar, the local mean age of the fluid, which is the average time that takes a fluid particle to reach any point of a domain from a supply inlet. The result obtained is a spatial distribution of the local mean age of the fluid, which may be displayed as isocontours in the space domain considered.

§1. Introduction

The determination of residence time distributions is of major interest in the design and characterization of most physicochemical and biochemical processes in chemical engineering, where a proper and homogeneous fluid distribution is often essential.[1] This residence time distribution is for instance required in order to design the optimal geometry of a reactor or to calculate the yield of reactions with kinetic parameters. With regard to flows through porous media, most chemical and environmental engineering applications, such as for instance petroleum engineering (secondary oil recovery), mineral processing, and water treatment are concerned, but also food, biological or pharmaceutical engineering applications are to be noticed. The analysis of dispersion processes in porous media is also of great practical interest in miscible displacement, chromatography columns, fixed-bed chemical reactors and pollutant transport. The objective of this paper is to present a modeling approach which provides information about the spatial distribution of the mean residence time of a fluid in a porous medium. Solving conservation (mass and momentum) and coupled transport equations linked to the turbulent nature of the flow provides, using classical Computational Fluid Dynamics (CFD) techniques such as the finite volume method, the spatial distribution of relevant variables which describe the basic flow. Once these variables have been determined, a decoupled approach may be used in order to determine the spatial distribution of the mean residence time. This approach consists of solving the steady transport equation of a passive scalar, the local mean age of the fluid or local mean residence time,[2] which is the average time that a fluid particle takes to reach any point of the domain from a supply inlet, even if the path of the particle includes porous media. Different simulations of mean residence

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time spatial distributions have been already performed[3),4)] and validated[5)] in complex geometries using the finite volume method, but only in the case of non-porous flows. In this paper, the transport of this scalar incorporates the time linked to the movement due to laminar and possibly turbulent diffusion, and also the source of residence time attributable to the porous medium, characterized by its porosity and tortuosity. The result obtained is a spatial distribution of the local mean age of the fluid, which may be displayed as isocontours in the space domain considered. The determination of zones wherein the mean residence time is greater than in the vicinity enables modifications in the design of the geometry in consideration to be made in order to reduce the dispersion of the residence time.

§2. Model development

The fluid mechanics core model basically consists of mass (2·1) and momentum (2·2) conservation equations :

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0, \tag{2·1}$$

$$\frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i - \frac{\mu}{\alpha_i}u_i - \frac{1}{2}\rho C_i \, \|\boldsymbol{u}\| u_i + \frac{\partial}{\partial x_j}(\rho \overline{u_i' u_j'}) \tag{2·2}$$

and turbulence quantities transport equations if the flow is not laminar. In Eqs. (2·1) and (2·2), ρ is the fluid density, u_i is the velocity component in the x_i direction, p is the pressure, τ_{ij} is the viscous stress tensor, g_i is the gravitational acceleration in the x_i direction, α_i is the permeability of the porous medium in the x_i direction, C_i is the inertial resistance factor of the porous medium in the x_i direction and F_i is a possible body force component in the x_i direction. The fifth and sixth terms on the right-hand side of Eq. (2·2) only appear in the flow occurs in a porous medium, and represent respectively the microscopic viscous shear stress Darcy term and the microscopic inertial force term, also called Ergun inertial term or microflow development term. There is no need in the present case to include a turbulence modeling for this term in the porous cells since it is actually taken into account in the value of the parameter C_i. For turbulent flows, if there is no need in the present case to include a turbulence modeling for this term in the porous cells since it is actually taken into account in the value of the empirical parameter C_i, one nevertheless needs to introduce the term $\rho \overline{u_i' u_j'}$, which represents the so-called Reynolds stresses, related to the mean flow by the so-called Boussinesq hypothesis :

$$\rho \overline{u_i' u_j'} = \rho \frac{2}{3} k \delta_{ij} - \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{2}{3} \mu_t \frac{\partial u_i}{\partial x_i} \delta_{ij} \tag{2·3}$$

necessitates the determination of additional turbulence quantities, which, when using a second order closure model, for instance the classical and basic $k - \epsilon$ model, are respectively the turbulent kinetic energy k and the dissipation rate ϵ :

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_j}{\partial x_i} - \rho \epsilon, \tag{2·4}$$

$$\frac{\partial}{\partial x_i}(\rho u_i \epsilon) = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_i}\right] + C_{1\epsilon}\frac{\epsilon}{k}\mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_j}{\partial x_i} - C_{2\epsilon}\rho\frac{\epsilon^2}{k}. \quad (2\cdot5)$$

The turbulent viscosity μ_t, related to k and ϵ, is given by

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}. \quad (2\cdot6)$$

In Eq. (2·3), δ_{ij} is the Kronecker symbol. The coefficients $C_{1\epsilon}$, $C_{2\epsilon}$, C_μ, σ_k and σ_ϵ are empirically determined constants.[6)] Since the concept of the average age of fluid[2)] was introduced, the concept of local average résidence time has been thoroughly treated.[7),8)] This variable represents physically at a given point the time that has elapsed on average since the particle of fluid which is located at this point entered the domain at one of its inlets. It can be measured experimentally at any point of the domain, for example by injecting a pulse of tracer gas into the inlet at time $t = 0$ and by recording continuously the concentration of the tracer gas at the point under consideration. Its distribution function $f_{\bar{t}}$ is defined by

$$f_{\bar{t}} = \frac{C(\boldsymbol{x},t)}{\int_0^\infty C(\boldsymbol{x},t)dt}, \quad (2\cdot7)$$

where $C(\boldsymbol{x},t)$ is the concentration of the tracer injected into a domain inlet, at a point $\boldsymbol{x}$, at time t. The local average residence time $\bar{t}$ is the first moment of $f_{\bar{t}}$ and can be defined as :

$$\bar{t}(\boldsymbol{x}) = \frac{\int_0^\infty C(\boldsymbol{x},t)tdt}{\int_0^\infty C(\boldsymbol{x},t)dt}. \quad (2\cdot8)$$

A steady state solution of this variable may be obtained directly from a transport equation,[7)] and may be rewritten as :[5)]

$$\frac{\partial}{\partial x_i}(\rho u_i \bar{t}) = \frac{\partial}{\partial x_i}\left[\left(\rho D_{AA} + \frac{\mu_t}{\sigma_t}\right)\frac{\partial \bar{t}}{\partial x_i}\right] + \rho, \quad (2\cdot9)$$

where $D_{AA} + \frac{\mu_t}{\sigma_t}$ is an estimation of the local actual diffusivity, wherein D_{AA} is the self-diffusivity of the fluid,[9)] which is the diffusivity of the fluid in itself, and which may be expressed by the ratio $\frac{\mu}{\sigma}$ where σ is the laminar Schmidt number, and σ_t is the turbulent Schmidt number. This self-diffusivity equals 3.03 10^{-6} m^2s^{-1} for water,[10)] and the assumption $\sigma_t = 1$ is adopted since this value has been validated in a previous study in the case of non porous 2D flow.[5)] In the particular case of the flow through porous medium, one may take into account both the fifth and sixth terms (negative sources of momentum) in the Navier-Stokes equations (2·2), and the alteration of the mean residence time transport equation (2·9) attributable to the porous medium. The first modification in this last equation consists in rewriting the diffusion term. The molecular diffusion term D_{AA} in Eq. (2·9) has to be divided by the tortuosity factor, τ^2, where the tortuosity τ is the actual ratio of pore length over the superficial diffusion path.[11),12)] The definition of the tortuosity factor accounts for the effect of altered diffusion path lengths in the porous medium. As far as the flows considered in this study are concerned, the Reynolds number (based on particle diameters and superficial velocity) is less than the transitional Reynolds number limit (about 110 to 150) [13] for which the contribution of the turbulent motion to the diffusion coefficient is expected to be important. Therefore, the diffusion term for the residence time in the porous media only consists of the modified molecular diffusion term. In CFD codes, use is made even in the porous cells of a local macroscopical velocity, the so-called superficial or filter velocity, which is not equal to the actual fluid velocity, the pore velocity or interstitial velocity, but which in average is related to the latter by the Dupuit-Forchheiner relation, that expresses that the ratio between these two velocities is in average equal to the porosity ϕ of the porous medium. This relation accounts for the modification (constriction) in average of the cross-section area in the pore system. Since the superficial velocity is kept in Eq. (2·9), the transport equation of $\bar{t}$ has to incorporate the effect of the mean pore velocity and is finally rewritten as :

$$\frac{\partial}{\partial x_i}(\rho u_i \bar{t}) = \frac{\partial}{\partial x_i}\left[\rho\left(D_{AA}\frac{\phi}{\tau^2}\right)\frac{\partial \bar{t}}{\partial x_i}\right] + \rho\phi. \tag{2·10}$$

The set of parabolic partial differential equations is solved using the finite volume discretization method, which is appropriate for solving sets of conservation equations. Use is made of the Fluent commercial software package, [14] and of the SIMPLE algorithm [15] with interpolation on cell faces (upwind scheme for density, momentum weighted for pressure and linear for velocity). The classical power law scheme [15] is used as the differentiating scheme. A multigrid algorithm accelerates convergence for the calculation of pressure and the resolution of the transport equation of the mean residence time. A test on the nature of the cell (whether it is porous or live) is performed and depending upon the result, Eq. (2·9) or Eq. (2·10) is used. The source code of the Fluent package [14] was modified and recompiled in order to implement the calculation of the transport of the additional mean residence time variable.

§3. Example of application

An example is given in order to set out in concrete form the potential and the relevance of this approach. The application is chosen in the domain of water treatment, mainly because the determination of residence time distributions is in this case always essential, and consists in the simulation of the bidimensional flow of water through a real geometry containing a filter composed of activated carbon granular packed bed. The bidimensional geometry considered is rectangular. Its length equals 18 m and its heigh equals 3.5 m. The height of porous medium in the fixed bed equals 2.5 m. The upper boundary is a free surface. The water enters the domain through an inlet situated at the right-hand side, upper the fixed bed, and exits the filter through 17 outlets regularly distributed on the bottom side (see the streamlines patterns in Fig. 1). Excepted two vortices, which are detected by the model at the vicinity of the domain inlet, the flow configuration is rather simple. The porosity ϕ of the fixed bed equals 0.26 and its tortuosity τ equals 1.5. The flow is turbulent and driven by gravitation. Use is made of the $k-\epsilon$ second order closure model, which is appropriate [16] (the use of a more precise model is not necessary since the transport of $\bar{t}$ is essentially convective and since

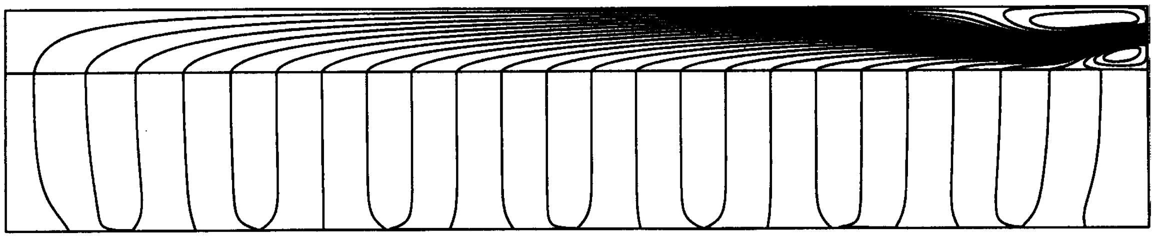

Fig. 1. Streamlines.

Fig. 2. Isovalues of the mean residence time in the space domain.

turbulent diffusion can be neglected in the porous region[13]). The grid contains 45 580 cells and the results presented hereafter are grid-independent. The mean residence time is set to zero at the domain inlet and a condition of zero-flux is imposed at the solid boundaries. Its spatial distribution is displayed in Fig. 2. The mean residence time varies from zero at the inlet (at the right-hand side upper corner) to 1968 s at the left-hand side lower corner, where a significant gradient is observed. The modification of the direction of the gradient of the mean residence time when the flow enters the porous medium is attributable both to the streamlines curvature (their direction becomes vertical, see Fig. 1) and to the decrease of the diffusion coefficient of this scalar (Eq. (2·10) is used instead of Eq. (2·9) in the porous medium). In the present case, the dispersion of the residence time distribution is mainly attributable to the slowing down of the particles in the boundary layers and to the different possible path lengths between the flow inlet and the different flow outlets. This dispersion may be displayed by quoting the averaged mean residence times at the different outlets (see Fig. 3, where the outlet 1 is at the right-hand side of the domain, on the inlet side, and the outlet 17 is at the left-hand side). The averaged mean residence time at the domain outlets is noticeably wide-ranging from 283 s to 1493 s. The transport of the mean residence time is essentially convective in the porous region and its diffusion is not sufficiently effective to account for a global significant spatial averaging process. The location of the maximum of the mean residence time is not situated at a domain

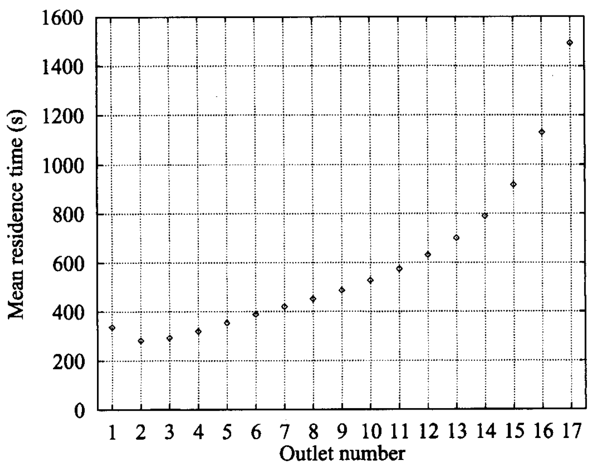

Fig. 3. Mean residence time (s) at outlets.

exit but is located in the left lower corner of the domain. This method can be used for the assessment of geometric configurations and for engineering purpose, to set out modifications of the flow geometry in order to meet requirements linked to the reduction of the dispersion of the residence time distribution at the domain outlets.

§4. Conclusion

A model for the transport equation of the mean residence time in porous media was presented and was solved with the finite volume method using a Computational Fluid Dynamics commercial software, Fluent, that was modified and recompiled. The spatial distribution of the mean residence time was predicted in a complex turbulent flow in a space domain containing porous media. The feasibility of predicting the spatial distribution of such a variable, considering its importance in the field of chemical, pharmaceutical, food and environmental engineering, is of great potential, and should be considered in the design or the assessment of installations and vessels where a homogeneous fluid distribution is essential. This method of simulation provides the instantaneous determination of the geometric characteristics of a flow boundary that contribute to the dispersion of the mean residence time, and its appropriate use should enable undesirable phenomena linked to the dispersion of residence time, such as short circuiting and dead spaces, to be prevented in a large range of engineering flows.

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