A LAGRANGIAN APPROACH TO PREDICT THE FLOW BEHAVIOUR AND RESIDENCE TIME DISTRIBUTION IN CHEMICAL REACTORS

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Highlights

- Implementation of Smoothed Particle Hydrodynamics (SPH) for predicting RTD in chemical reactors.
- Comparison of flow behavior in different chemical reactors with SPH and CFD.
- Results obtained from SPH methodology are fast and reliable.

1. Introduction

The flow dynamics of chemical species is important for characterizing, analyzing, and designing chemical reactors. Computational fluid dynamics (CFD) provides accurate flow patterns, but this approach can be computationally expensive for large or complex geometries.

To overcome this limitation, we developed a new Lagrangian-based method using smoothed particle hydrodynamics (SPH) [1] to forecast the flow patterns and residence time distribution of two different fluids for various reactor geometries: (laminar, fractal, T-mixer, Hartridge–Roughton mixer and packed bed with a gyroid internal packing) and compared the results with computational fluid dynamics (CFD) simulations.

2. Methods

The fundamental equations, assumptions, and kernel definitions of SPH are described using a scalar field. For a scalar field A and Dirac delta function δ, the following identity holds in the space Ω:

$$A(x,t) = \int_\Omega A(x,t)\delta(x-x')dx' \tag{1}$$

In SPH, the Dirac function is approximated by the kernel function W:

$$A(x,t) \approx \int_\Omega A(x,t)W|x-x'|dx' \tag{2}$$

The kernel must fulfill the following conditions for a first-order approximation:

$$\int_\Omega W|x-x'|dx' = 1 \tag{3}$$

$$\int_\Omega W|x-x'|xdx' = 0 \tag{4}$$

If the integral is approximated by a finite sum and the scalar field is replaced by particle properties such as the mass and density, then

$$A(x,t) \approx \sum_j \frac{m_j}{\rho_j} A(x_j,t)W|x_i - x_j| \tag{5}$$

This is the main equation for SPH, and it shows that the properties of a single particle are influenced by the surrounding particles.

The different reactor models were built parametrically within Grasshopper (Rhino) [2], and the Flexhopper plugin [3] was used to determine the flow and RTD. In addition, we used DualSPHysics [4], which is an open-source SPH code written in C++ and CUDA. The CFD analysis was carried out by using the commercial software ANSYS Fluent 22 R1, which is based on the finite volume method [5].

3. Results and discussion

Figure 1(a) shows a comparison of SPH and CFD methodologies to predict residence time distribution in a laminar flow reactor. The trend obtained by the SPH simulations matched the CFD solution quite well.

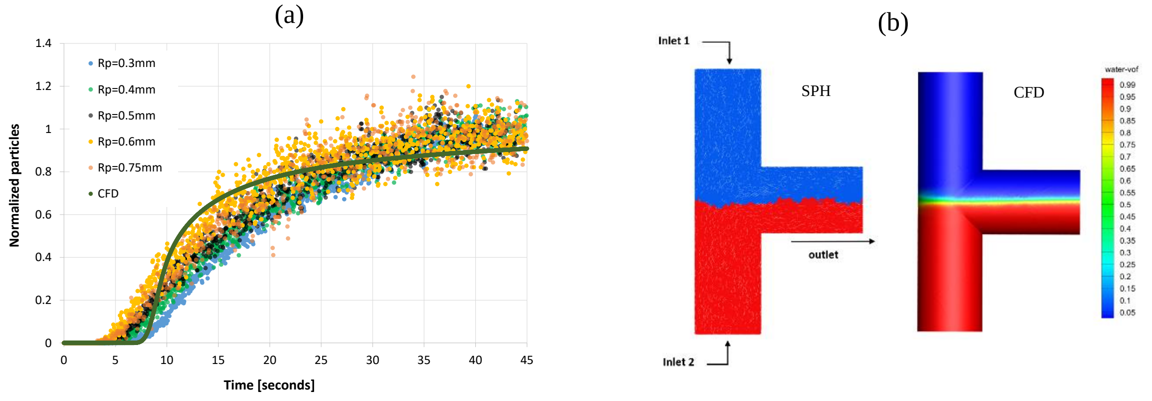

Figure 1. (a) RTDs of index-1 particles with different radii exiting the tubular reactor according to SPH simulations. The solid line shows the numerical solution of the laminar flow reactor obtained by implementing CFD (Finite volume method); (b) a comparison of SPH and CFD simulations for a T-mixer reactor.

SPH simulations were carried out for a two-fluid system (i.e., two different fluids entering the two inlets) under the assumption that the physical properties of the two fluids were equal and the flow regime was laminar. Figure 1 (b) compares the flow patterns obtained using SPH and CFD under similar operating conditions. The flow patterns obtained by SPH and CFD were similar: a clear separation between the two fluids except for a thin strip in the middle of the domain in the lateral direction, where some intermixing took place due to diffusion and/or dispersion.

4. Conclusions

The present study is first of its kind where two different fluids are employed using SPH. The RTD obtained from SPH in a laminar flow reactor for different particle sizes is comparable with the CFD results. The SPH results of the T-mixer reactor are also in good agreement with CFD results. Hence, SPH can be used as an alternative to define certain geometric constrains before using CFD simulations for the final detailed analysis.

References

[1] M. Asif, C. A. Grande, Adv. Theory Simul. 10 (2023) 2300349.
[2] R. McNeel, & others, Rhinoceros 3D, Robert McNeel & Associates, Seattle, WA 2010.
[3] B. Felbrich. FlexCLI: FlexCLI–FlexHopper (Version v1.1.2). Zenodo. http://doi.org/10.5281/zenodo.3355744.
[4] A.J.C. Crespo, J.M. Domínguez, B.D. Rogers, M. Gómez-Gesteira, S. Longshaw, R. Canelas, R. Vacondio, A. Barreiro, O. García-Feal, Comput. Phys. Commun. 187 (2015) 204-216.
[5] ANSYS Inc. User Guide, ANSYS Inc. Canonsburg, PA, USA 2022.

Keywords
Smoothed particle hydrodynamics; residence time distribution; computational fluid dynamics, chemical reactors.