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Hydrodynamic modeling of porous hollow fiber anti-solvent crystallizer for continuous production of drug crystals

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Abstract

This study introduces a Computational Fluid Dynamics (CFD)-based hydrodynamic model for a novel porous hollow fiber-based anti-solvent crystallizer (PHFAC). Here the anti-solvent, *water*, is introduced from the hollow fiber lumen into the *acetone-based* feed solution *of a drug* flowing on the shell side where crystals *of the drug Griseofulvin* are formed and swept away. Such a device is very useful for achieving continuous anti-solvent crystallization with significant crystal size control. It is necessary to predict the hydrodynamics and other mixing characteristics of the PHFAC device to facilitate optimization and prediction of their behavior. In this study, a 3D physical model for a PHFAC device was first constructed using *the* software GAMBIT. After meshing and optimization, a 3D computational simulation-based modeling was conducted by *the* CFD software FLUENT for understanding the hydrodynamics and the mixing characteristics of a miscible aqueous-organic system in the PHFAC module *without any drug being present*. Different combinations of characteristic parameters e.g., *inlet* flow rates of the shell side and tube side and numbers of hollow fiber membranes, were *investigated* to optimize the conditions

[1] Dr. Chen and Dr. Wang contributed equally to this work and should be considered as co-first authors.