

Determination of Residence Time Distribution and Axial Dispersion Coefficient in a Meso-scale Oscillatory Baffled Crystallizer Using a Computational Fluid Dynamics Approach

Emmanuel N Kimuli,¹ Iyke I Onyemelukwe,¹ Brahim Benyahia¹ and Chris D Rielly*¹
¹*Department of Chemical Engineering, Loughborough University, Leicestershire, LE11 3RB, UK*
C.D.Rielly@lboro.ac.uk

Oscillatory Baffled Reactors (OBR) are often reported to show advantages as continuous tubular crystallizers, as they exhibit good radial mixing, but limited axial dispersion, resulting in near plug flow behaviour over a range of oscillation conditions. Moreover, their geometric design produces high heat transfer rates per unit volume and the oscillations produce flow reversals which maintain solid crystals in suspension, even for low through-flow Reynolds numbers. However, little numerical work has been conducted to characterize meso-scale OBRs [1] and hence optimization of the geometry and oscillation conditions have so far relied on trial and error experimentation. Crystallisation processes may be affected by local hydrodynamics, as these influence, for example the wall heat transfer rates and mass transfer between the solution phase and a growing crystal; these in turn affect the temperature profile in the OBR and the rate of solute depletion and hence they determine the local supersaturation, which is the main driving force for many of the crystallization kinetic processes. The hydrodynamics also have an effect on agglomeration, breakage and other crystal growth mechanisms [2]. Computational Fluid Dynamics (CFD) provides in-depth information about the flow at a local level, making it possible to characterise mixing, mass transfer and heat transfer in a system.

In this work, a meso-scale oscillatory baffled crystalliser (meso-OBC) of 5 mm inside diameter, with smooth periodic constrictions, was characterized using CFD as a numerical tool to give an insight into the hydrodynamic behaviour. Simulations were carried out for conditions that were experimentally reported to deliver near plug flow behaviour. To assess the flow characteristics exhibited by the OBC, residence time distribution (RTD) and axial dispersion coefficient were investigated for a range of oscillatory conditions. The numerical results were validated by using experimentally measured RTD data obtained from real time image analysis process analytical tool (PAT). The experimentally determined axial dispersion coefficients were in reasonable agreement with those obtained from CFD data.

- [1]. M. Zheng, R. L. Skelton, M. R. Mackley, "Biodiesel reaction screening using oscillatory flow meso reactors", vol. 85, no. 1998, pp. 365–371, 2004.
- [2]. R. I. Ristic, "Oscillatory mixing for crystallization of high crystal perfection pharmaceuticals", *Chem. Eng. Res. Des.*, vol. 85, no. A7, pp. 937–944, 2007.