OPTIMIZATION OF CRYSTALLIZATION PROCESS IN AN INDUSTRIAL CONTINUOUS DRAFT TUBE BAFFLE CRYSTALLIZER THROUGH CFD WITH POPULATION BALANCE MODEL

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Abstract

The population balance framework has been accepted for some time as the most fundamental approach for modeling particulate, droplet, or bubble dynamics in multiphase systems. The coupling of computational fluid dynamics (CFD) with the population balance models (PBM) is a powerful tool in evaluating the design of particulate related equipment such as crystallizers. In this work, a CFD based population balance model is tested in a continuous draft tube baffle (DTB) crystallizer, which is an existing industrial DTB crystallizer located in Qinghai salt lake plant of China, with KCl productivity of 0.1 million tons per year. In this CFD model, the population balance in DTB crystallizer where 1) nucleation, 2) growth, 3) aggregation, and 4) breakage are taking place separately is solved by the quadrature method of moments (QMOM).

Keywords

Population Balance Model, Computational Fluid Dynamics, Industrial Crystallization.

Introduction

The population balance model was developed from pipe reactor experimental data. Population balance modeling (PBM) takes into account particle growth, aggregation, breakage and nucleation and accommodates the dependence of velocity and mass transfer on particle size. The coupling of computational fluid dynamics (CFD) with population balance models (PBM) is a possibility in this direction and has a great potential.

Classical solution methods of the PBM that have been used for CFD-PBM coupling in the literature are the classes methods (CM) based on the fixed-pivot technique of Kumar and Ramkrishna(1996) and the quadrature method of moments (QMOM), the direct quadrature method of moments (DQMOM)(McGraw, 1997), and the sectional quadrature method of moments(SQMOM)(Marchisio, 2005). The QMOM method provides an attractive alternative to the SMOM method for size dependant growth, size dependant aggregation and breakage. The quadrature method of moments (QMOM) is a recent technique of solving population balance equations for particle dynamics simulation (Bin, 2006).

Population balance model used in crystallizer has developed these days. Heiko Briesen(2009)formulated a two-dimensional population balance model. The model accounts for size and shape of the crystals dependent process behavior. Christian Borchert(2009)investigated the multidimensional population balance framework extract shape distributions in a steady state continuous crystallizer for two different cases.

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The crystal size distribution and the coefficient of variation of crystal product were studied based on the CFD simulation of two-phase flow model(Song, 2010), and CFD-PBM coupling model was validated as well(Hang, C. Ze S. 2014). In this work, a CFD coupled with population balance model is tested in a continuous draft tube baffle (DTB) crystallizer, which is an existing industrial DTB crystallizer located in Qinghai salt lake plant of China, with KCl productivity of 0.1 million tons per year.

Mesh and Solver

The GAMBIT software release 2.2 is used to generate these structured and unstructured meshes. The total meshes divided in the DTB crystallizer consist of near a million cells for CFD simulation, shown Figure 1,2. With these fine structured and unstructured meshes, the steady numerical solution for the fluid flow field can be obtained using FLUENT6.3 software with the converging precision 10^{-6}. The multiple reference frame (MRF) method is used in CFD simulation for the industrial DTB in stirring process.

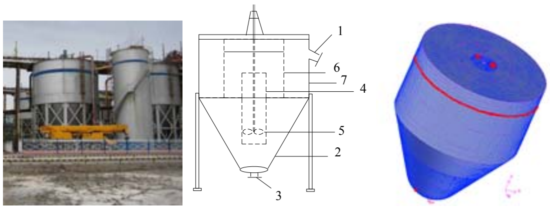

Figure 1. The structure of DTB crystallizer and typical hexagonal and tetrahedral mesh in industrial crystallizer

Results and Discussion

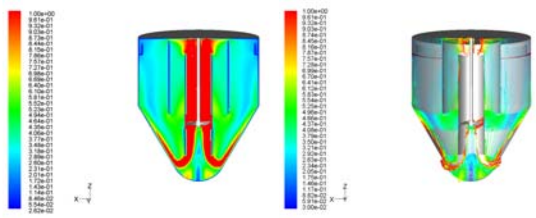

Figure 2. Typical flow field in industrial crystallizer

Figure 2 demonstrates the typical fluid flow field in the existing continuous DTB industrial crystallizer with propeller, calculated by the CFD solver. As mentioned above, the DTB crystallizer with an external fines dissolution vessel has the KCl productivity of 0.1million tons per year. Because of the strong agitation of propeller, there exists a negative pressure drop between upside and downside of propeller, which results in a partial amount of fluid circulating directly from the draft tube to the baffle tube. The most amount of fluid from draft tube will go down the bottom of the crystallizer, and circulate to the clarification zone due to the block of a coniform under-part of the crystallizer.

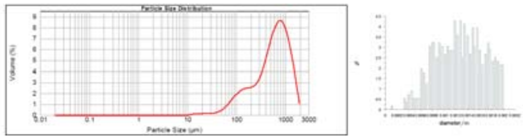

Figure 3. Typical particle size distribution in industrial crystallizer and typical particle size distribution in the CFD calculation with PBM

Figure 3 demonstrates the typical particle size distribution in the real industrial crystallizer and in CFD calculation with PBM. The percentage of product with crystal size larger than 2 mm is raised from 50% to 90%; the amount of natural gas consumption is decreased from 22 to 15 m^3 per ton of crystal product.

Conclusion

Computational fluid dynamics (CFD) is a powerful simulation tool that can be successfully used to investigate mixing, turbulence, shear stress, and crystal size distribution in an industrial DTB crystallizer.

In the paper, the population balance model was used to simulate the crystallization process in DTB crystallizer where nucleation, growth, aggregation, and breakage are taking place.

References

Kumar, S.; Ramkrishna, D (1996). On the solution of population balance equations by discretizations-I. A fixed pivot technique. Chem. Eng. Sci. 51, 1311-1332.

McGraw, R (1997). Description of aerosol dynamics by the quadrature method of moments. Aerosol Sci. Technol. 27, 255–265.

Marchisio, D. L.; Fox, R. O. (2005) Solution of population balance equation using the direct quadrature method of moments. J. Aerosol Sci. 36,43-73.

Bin W.;Terry A.R(2006). Verification of SMOM and QMOM population balance modeling in CFD code using analytical solutions for batch partivalate processes. China Particuology., 4, 243-249.

Heiko B(2009). Two-dimensional population balance modeling for shape dependent crystal attrition. Chem. Eng. Sci. 64, 661-672.

Christian B.;Nandkishor N.; Doraiswami R.; Andreas V.; Kai S(2009). On the prediction of crystal shape distributions in a steady-state continuous crystallizer. Chem. Eng. Sci. 64, 686-696.

Xingfu S.; Menghua Z.; Jin W.; Ping L.; Jianguo Y (2010),. Optimization design for DTB industrial crystallizer of potassium chloride. Ind. Eng. Chem. Res. 49, 10297-10302.

Hang C., Ze S., Xingfu S., and Jianguo Y(2014). Key parameters prediction and validation for a pilot-scale rotating disc contactor by CFD-PBM simulation. Ind. Eng. Chem. Res. 53 (51), pp 20013–20023