

Modeling and Simulation of Forced Circulation Evaporation Crystallizer

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ABSTRACT

Crystallization is an effective process of forming a solid phase from solution and crystallizer is the equipment used for industrial crystallization operations. In present work flow behavior, solid suspension distribution, population density and mean crystal growth studies have been carried out for the forced circulation evaporation crystallizer (FC crystallizer) by CFD simulations using software package; Ansys Fluent 13. The FC crystallizer is a continuously operating mixed suspension mixed product removal (MSMPR) type crystallizer used in salt, sugar and pharmaceutical industries for crystal production. In the present work simulation has been carried out in isothermal and non-isothermal conditions to characterize the hydrodynamics and population balance model to explain the population density.

Keywords : ANSYS Phase Separation, Solid Suspension, Crystal Size Distribution

I. INTRODUCTION

Crystallization is the (natural or artificial) process of formation of solid crystals precipitating from a solution, melt or more rarely deposited directly from a gas. It is considered as important and effective solid-fluid separation process (Essemiani et al., 2004). This process occurs due to phase transformation of one or more substances from a liquid, amorphous solid or gaseous condition to a crystalline state (Tangtongsakulwong et al., 2006; Geankoplis, 2007). The recovery of sodium chloride in solid crystalline form from water by using evaporative crystallization phenomena is one of the ancient known separation operations (Wohlk and Hofmann, 1987; Seader et al., 2011). Majority of the industrial crystallization processes carried out from solutions (Perry, 2009).

Generally in case of solution crystallization a species crystallizes from its liquid mixture when the solute (species) concentration has become more than its solubility. The term used for this condition of solution is supersaturation, so it is an important factor for crystallization. In crystallization supersaturation can be achieved by the processes such as cooling, evaporation, vacuum, pressure, and reaction, or in some conditions combination of these processes (Geankoplis, 2007). Evaporative crystallization is the most common crystallization process used in maximum industrial crystallizers. In this process the mixture is heated to reach the condition of supersaturation by the evaporation of solvent. Crystallization is required for the manufacturing of a large range of materials from bulk commodity

chemicals to very distinctive chemicals and pharmaceutical products.

a. Application of crystallization

- ✓ Crystallization shows the important role in the pharmaceutical industry as it is started from intermediates separation process and the final manufacture step as active pharmaceutical ingredients (APIs).
- ✓ The crystallization used to provide the production requirements as crystal size and purity in fertilizer products such as ammonium sulfate, potassium chloride, potassium sulfate and potassium nitrate
- ✓ The crystallization process is used in paper and pulp industry for black liquor concentration and in Chloride Removal Process.

II. MATERIALS AND METHOD

a. Computational Geometry

The first step in CFD study is the flow geometry creation where the computational domain of the physical system is created. In the present work the computational geometry of FC crystallizer has been generated using Design Modeler in ANSYS Workbench.13. The computational geometry of FC crystallizer used for numerical simulation is a model of the pilot scale FC crystallizer, used by Essemiani et al. (2004) for their simulation work. Modifications in inlet and vapor outlet position have been done to see the main effect on flow behaviour (Bamforth, 1965).

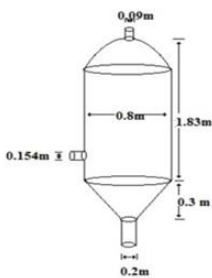


Fig. 1. Schematic representation of force circulation crystallizer.

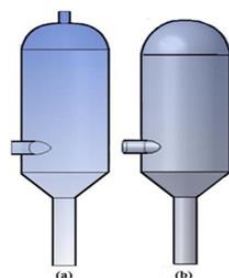


Fig. 2. Computational 3D geometries of FC crystallizer for simulation (a) Isothermal, Non-isothermal and population density simulation, (b) Solid suspension simulation.

The FC crystallizer (Fig. 1) used for the study is cylindrical in shape with conical bottom and semi spherical head. Internal diameter of crystallizer is 0.8 m and total height 2.13 m. The height of conical bottom and semi spherical head is 0.3 m and cone angle is 45°. Inlet

b. Physical properties

The physical properties of dilute solution with NaCl [liquid], water-vapor [vapor] and solid particles for simulation are presented in Table 2. All properties of water-vapor are available in ANSYS FLUENT 13 and all properties of water solution with NaCl at 298 K have been taken from Essemiani et al. (2004).

Table 1 : Number of nodes and elements presents in the mesh of different geometries

Geometry	Number of Nodes	No of Elements
Inlet at 0.5 m	9679	47232
Inlet at 0.7 m	9641	46955
Inlet at 0.9 m	8988	43152
Inlet at 1.1 m	9584	46852
Solid suspension model (without vapor outlet)		
Inlet at 0.5 m	7209	34317
Inlet at 0.7 m	8954	42952
Inlet at 0.9 m	9050	43426
Inlet at 1.1 m	8921	42730
Population balance model		
Inlet at 0.5 m	15496	76268

c. Boundary conditions

Boundary conditions are specifications of properties or conditions on the surface of domains and are required to fully define the flow simulation. The fluid boundary conditions are available for the present work in ANSYS FLUENT 13 as; inlet, outlet and wall.

Inlet boundary condition used is mass flow rate for liquid and vapor and outlet boundary condition is mass out flow but for population balance model inlet boundary condition is velocity inlet and outlet is defined as pressure outlet. Temperature condition is isothermal except for non-isothermal simulation and population balance. Wall boundary conditions are no slip and adiabatic (no heat exchange from wall). The vapor mass flow rate is used in proportion to the solution mass flow rate for maintaining stoichiometric vapor volumetric concentration. Operating conditions used in the present study are listed in Table 2 (Essemiani et al., 2004; Dutta, 2009);

Table 2 : Properties of the system and operating conditions

Isothermal and Non-Isothermal simulation		
	Phase	
Physical properties	Liquid (15% NaCl solution)	Vapor
Density, kg/m ³	1063	0.59
Viscosity, kg/s-m	0.0013	0.0000124
Surface tension, N/m	0.077	-
Thermal conductivity, W/m-K	6.48	0.025
Mass flow rates, kg/s	27.5, 47.8, 67.5, 87.5	0.0102, 0.0176, 0.0249,
Operating pressure, kPa	101.325	
Temperature, K	379.5 (Non-Isothermal simulation)	
Heat, kW/m ³	3000 (for solution)	
Solid suspension simulation		
	Liquid phase (water)	Solid particles (second)
Density,	998	2600

kg/m ³		
Particles sizes, μm	50, 500, 900	
Liquid mass flow rates, kg/s	27.5, 47.5, 67.5, 87.5	
Operating pressure, kPa	101.325	
	Population balance simulation	
	Liquid (15% NaCl solution)	Crystals
Density, kg/m ³	1063	2156
Liquid inlet velocity, m/s	2.4	
Crystals sizes (5 - sizes), m	0.0002 to 3.2e-05	
Volume shape factor	0.523	
Nucleation Rate, No. of nuclei/m ³ -s	3.20E+08	
Growth Rate, m/s	3.33E-08	

III. RESULTS AND DISCUSSION

3.1 Isothermal Simulation

The vapor is assumed to form in an external heat exchanger before being fed into the crystallizer. This situation has been modeled by an isothermal process in order to reduce the computation time and model complexity.

Flow Rates

Fig.3 shows the solution volume fraction that solution volume fraction is not uniform through-out the crystallizer; it is more near the wall because of centrifugal force by swirl flow. Fluid velocity is an important characteristic of the hydrodynamic study

because changes in fluid velocity affect the phase distribution. Fig. 4 shows contour of solution velocity inside the FC crystallizer for mass flow rate of 27.5 kg/s. The solution velocity magnitude is found to be higher near the wall; it is because of tangential inlet which induces circular motion of the fluid. The velocity at the center is low and increase with radius but it is zero at the wall because of no-slip boundary condition for the solid wall. The circular motion increase holding time of solution which is good for crystal growth.

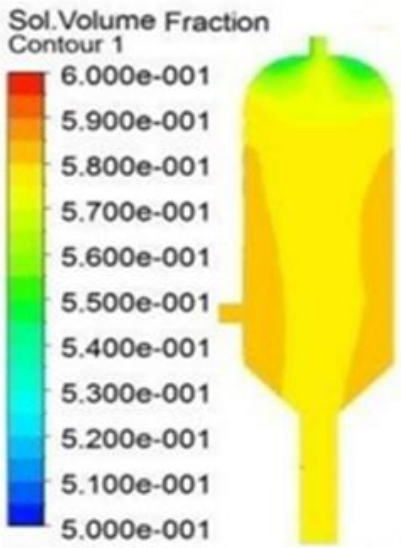


Fig. 3 Contour of solution volume fraction at solution mass flow rate of 27.5 kg/s with inlet position of 0.5 m.

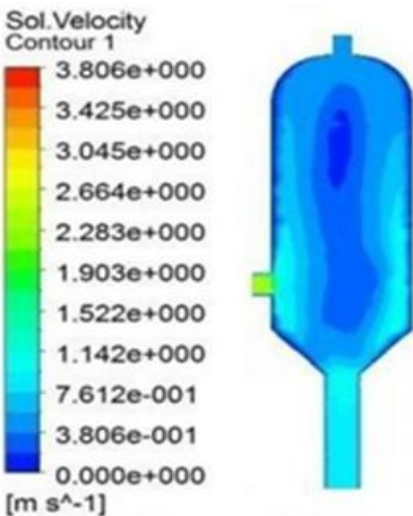


Fig. 4. Contour of solution velocity at solution mass flow rate of 27.5 kg/s with inlet position of 0.5 m.

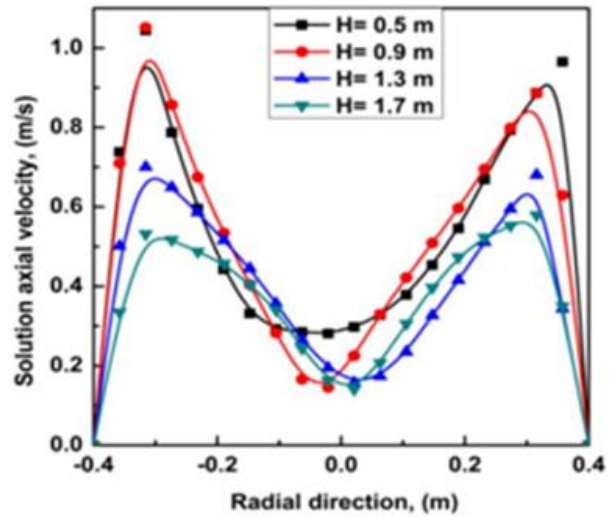


Fig. 5 Variation of solution axial velocity in radial direction for mass flow rate of 27.5 kg/s at inlet position of 0.5 m.

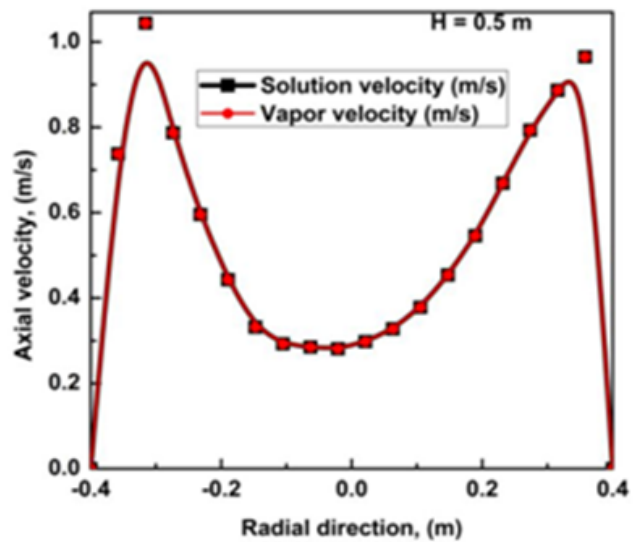


Fig. 6 Plot of solution and vapor velocities varying in radial direction for solution and vapor mass flow rates 27.5 and 0.0102 kg/s at inlet height of 0.5 m.

From Fig 5 is found that solution axial velocity pattern is same for all heights, but the magnitude of linear flow velocity decrease with height. It may be because of gravitational force. The solution velocity profile obtained in the present study is different from the one obtained by Essemiani et al. (2004). The difference in flow profile may be due to tangential inlet in the present work which is normal in the work of Essemiani et al. (2004). Fig. 6 shows the plot of the

axial velocity profile of solution and vapor varying radially at height of 0.5 m. It is observed that the velocity profile of vapor is same to that of solution, which is because of higher solution density and mass flow rate of solution compared to that of vapor. The vapor flows along with the liquid as an entrapped phase. The vapor phase follows the path of the solution.

The following Fig. 7 shows the cross sectional view of velocity vectors of solution at different axial positions. These velocity vectors confirm that flow of solution is circular in pattern (swirl flow) and low velocity zone is forming at the center and the position of low velocity zone position found to change from top to bottom, not coinciding with the geometrical center. Pressure variation is not significant and does not affect the crystallization (except vacuum which cause crystallization at low temperature) but in the hydrodynamics study pressure is an important factor, because due to pressure difference flow varies.

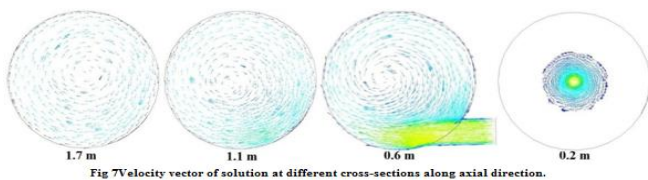


Fig 7 Velocity vector of solution at different cross-sections along axial direction.

IV. CONCLUSION

The *Isothermal simulation*; vapor volume fraction is more at center and solution volume fraction is more near the wall and both increase in there zone with increase in inlet flow rate and inlet height. Solution velocity magnitude is high near the wall (zero at the wall) at less at the center. The solution velocity is found to increase with inlet flow rate, which decrease slightly with elevation of inlet position. The maximum solution velocity is found to increase from 3.8 m/s to 9.374 m/s for increase in flow rate from 27.5 kg/s to 67.5 kg/s. The vapor and solution velocity magnitude is found to be same in the crystallizer. Pressure change is according to hydrostatic law, it increases with flow rate, the axial difference of

solution static pressure is found to be more with at higher inlet height. Turbulence in flow field is found to increase with flow rate.

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Cite this article as :

C. Mahesh Babu, L. Balasubramanyam, "Modeling and Simulation of Forced Circulation Evaporation Crystallizer", International Journal of Scientific Research in Science, Engineering and Technology (IJSRSET), Online ISSN : 2394-4099, Print ISSN : 2395-1990, Volume 6 Issue 4, pp. 294-300, July-August 2019.

Journal URL : <http://ijsrset.com/IJSRSET196438>