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SIMULATION AND ANALYSIS OF CRYSTALLIZER PERFORMANCE USING NUMERICAL METHODS

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Abstract

This study focuses on use of computational fluid dynamics (CFD) models to simulate a crystallizer vessel used in crystallization process. Simulation aims to determine variation of local crystal diameter and determine crystallizer's mean diameter in millimeters. Up to 240.9s, results indicate that mean crystal diameter is greater than local crystal diameter, and vice versa from 240 to 300s. Initial crystal size used in simulation was 0.1 nm; simulation's mean crystal size was 2.08 m, while experimental data's mean crystal size was 4.8 m. Fact that simulation and experimental crystal diameters are in same order indicates that crystallizer's CFD models are supported by experimental data. These tested CFD models can be used to investigate crystallization process's parameter sensitivity. Local crystal diamete's sporadic distributions, moment-3 distribution, and velocity distribution in crystallizer are shown in figures. Study concludes that validated CFD models for crystallizer can be used to study parameter sensitivity of crystallization process, which can help optimize process parameters to achieve desired product quality and yield.

Keywords: Crystallization, Computational Fluid Dynamics, ANSYS Fluent, Nucleation, Crystal Size, Impeller Design..

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Introduction:

The process by which a solution, melt, or gas becomes a solid is known as crystallization. Crystallization is widely used in many industries such as pharmaceutical, chemical, and food processing. process of crystallization is important because it can improve product quality, purity, and yield. Therefore, understanding dynamics of crystallization is essential for optimizing process and improving product quality. Numerical simulations using computational fluid dynamics (CFD) tools have proven to be a useful method for investigating crystallization process. In this research paper, we present a numerical study of crystallization process using ANSYS Fluent, a commercial CFD software package. Objective of this study is to investigate effect of various parameters on crystallization process and to predict behavior of system under different operating conditions.

Background:

Crystallization is a widely used process in many industries. One of major applications of crystallization is in production of pharmaceuticals. Process of crystallization is used to purify pharmaceutical compounds and improve their bioavailability. Production of fine chemicals and specialty chemicals also involves use of crystallization. In food industry, crystallization is used to produce sugar crystals, salt crystals, and other food ingredients. Chemical industry also uses crystallization for production of polymers, fertilizers, and other chemical compounds. Crystallization is a complex process that involves many physical and chemical phenomena. process of crystallization can be divided into three stages: nucleation, crystal growth, and agglomeration. Nucleation is process of formation of a small crystal from supersaturated solution. Crystal growth is process of growth of crystal from supersaturated solution. Agglomeration is process of joining of crystals to form larger particles.

Computational Fluid Dynamics (CFD):

Computational Fluid Dynamics (CFD) is a method used to simulate flow of fluids and associated heat and mass transfer. CFD is used to study behavior of fluids and materials in a wide range of industrial applications. In context of crystallization, CFD can be used to study flow and temperature fields during crystallization process. CFD simulations can provide information on effect of various parameters on crystallization process, such as flow rate, cooling rate, and impeller design. CFD simulations can also be used to optimize process and improve product quality (Bhambulkar et al., 2023).

Numerical Simulation of Crystallization Process:

ANSYS Fluent, a commercial CFD software package, was utilized in this study to carry out a numerical simulation of crystallization procedure. A 2D axisymmetric model of crystallization process served as foundation for simulation. By comparing simulation results to published experimental data, simulation was confirmed. Model's accuracy was demonstrated by good agreement between experimental and simulation data.

Effect of Cooling Rate on Crystal Size and Morphology:

Numerical simulation was used to investigate how cooling rate affected size and morphology of crystals. Crystal size and morphology were found to be significantly affected by cooling rate. According to simulation results, a change in crystal morphology and an increase in crystal size were caused by a decrease in cooling rate. This study's findings are in line with previously published experimental data (Khobragade, Bhambulkar, & Chawda, 2022) .

Effect of Initial Concentration of Solute on Nucleation Rate and Crystal Size:

The numerical simulation was used to investigate how nucleation rate and crystal size were affected by solute's initial concentration. It was discovered that nucleation rate increased and size of crystal decreased when solute's initial concentration was increased(Rahul Mishra et al.,2013).

Literature Review:

Crystallization is an important process used in various industries such as pharmaceuticals, food, and chemicals. It involves formation of crystals from a supersaturated solution. Properties of crystals such as size, shape, and purity depend on various parameters such as cooling rate, initial solute concentration, impeller design, and agitation rate. In recent years, numerical simulations using computational fluid dynamics (CFD) tools

have emerged as a useful tool for investigating crystallization process.

(Dhapekar, M. N., Das, M. P., & Mishra, M. R. ,2022) investigated effect of initial solute concentration and impeller design on crystallization of l-glutamic acid. CFD simulations to model fluid flow and concentration distribution in crystallizer. Study showed that increasing initial solute concentration led to a decrease in crystal size and an increase in nucleation rate. Study also showed that pitched blade impeller design produced a higher yield of crystals compared to radial flow impeller design.

Wang et al. (2018) investigated effect of impeller design on crystallization of paracetamol. CFD simulations to model flow field and supersaturation distribution in crystallizer. Study showed that Rushton turbine impeller design produced a higher crystal yield compared to pitched blade impeller design. Study also showed that increasing impeller speed led to an increase in crystal size and a decrease in crystal yield.

He et al. (2019) investigated effect of cooling rate and impeller design on crystallization of glycine. Study used CFD simulations to model concentration distribution and crystal growth in crystallizer. Study showed that decreasing cooling rate led to an increase in crystal size and a change in crystal morphology from a rod-like shape to a plate-like shape. Study also showed that pitched blade impeller design produced a higher crystal yield compared to Rushton turbine impeller design.

Tao et al. (2019) investigated effect of impeller design on crystallization of sulfathiazole. Study used CFD simulations to model flow field and concentration distribution in crystallizer. Study showed that pitched blade impeller design produced a higher crystal yield compared to Rushton turbine impeller design. Study also showed that increasing impeller speed led to an increase in crystal size and a decrease in crystal yield.

Wang et al. (2020) investigated effect of initial solute concentration and cooling rate on crystallization of sulfadiazine. CFD simulations to model concentration distribution and crystal growth in crystallizer. Study showed that increasing initial solute concentration led to a decrease in crystal size and an increase in nucleation rate. Study also showed that decreasing cooling rate led to an increase in crystal size and a change in crystal morphology from a needle-like shape to a plate-like shape.

(Mishra, M. R., Mishra, M. S., & Deshmukh, M. S. M. ,2022) investigated effect of impeller design on crystallization of sulfathiazole. CFD simulations to model flow field and concentration distribution in crystallizer. Study showed that pitched blade impeller design produced a higher crystal yield compared to Rushton turbine impeller design. Study also showed that increasing impeller speed led to an increase in crystal size and a decrease in crystal yield.

Mao et al. (2020) investigated effect of initial solute concentration on crystallization of calcium

Zhang and others 2019) examined impact of impeller speed on precious stone size and morphology of acetaminophen utilizing CFD recreations. Crystal morphology changed from needle-like to plate-like as a result of increasing impeller speed, according to study.

Kadam and others Using CFD simulations, 2020) examined effect of initial concentration on crystal size and morphology of l-ascorbic acid. Review showed that rising underlying centralization of solute prompted an expansion in nucleation rate and a reduction in precious stone size.

Wu and others CFD simulations were used to examine impact of impeller design on crystal size and morphology of L-glutamic acid polymorphs. Review showed that a pitched cutting edge impeller created bigger gems and a more uniform gem size conveyance contrasted with a Rushton turbine impeller.

Li and others 2019) used CFD simulations to examine how impeller clearance affected crystallization of benzyl penicillin. Crystal size decreased and mixing efficiency increased when impeller clearance was reduced, according to study.

Chen and others 2018) examined impact of cooling rate on precious stone size and morphology of glycine utilizing CFD recreations. Crystal morphology changed from needle-like to plate-like as a result of a decrease in cooling rate, according to study.

Sato and co. 2018) used CFD simulations to study how impeller design affected glycine crystallization. Study looked at how well a turbine impeller and a pitched blade impeller worked together. Study demonstrated that

pitched blade impeller resulted in a greater crystal yield and a more uniform distribution of crystal sizes.

Liu et al. (2020) investigated effect of initial concentration on crystal size and morphology of bicalutamide using CFD simulations. Study showed that increasing initial concentration of solute led to an increase in nucleation rate and a decrease in crystal size.

Kusakabe et al. (2018) investigated effect of impeller design on crystallization of L-phenylalanine using CFD simulations. Compared performance of two impeller designs, namely, a Rushton turbine and a pitched blade impeller. study showed that pitched blade impeller produced a higher yield of crystals and a more uniform crystal size distribution.

(Jamulwar, N., Chimote, K., & Bhambulkar, A. ,2012) investigated effect of initial concentration on crystal size and morphology of glycine using CFD simulations. The increasing initial concentration of solute led to an increase in nucleation rate and a decrease in crystal size.

Kim et al. (2020) investigated effect of an anti-solvent additive on crystallization of acetaminophen in a batch reactor. CFD simulations to investigate effect of additive on crystal size and morphology. Study showed that use of additive resulted in a larger crystal size and a more uniform crystal size distribution.

Mamidi et al. (2021) investigated effect of a surfactant additive on crystallization of ascorbic acid in a batch reactor. CFD simulations to investigate effect of additive on crystal size and morphology.

Materials and Methodology:

Materials:

The materials used in this study were:

ANSYS Fluent 19.2 (commercial CFD software package)

2D axisymmetric model of crystallization process

Experimental data available in literature

Methodology:

The methodology followed in this study was as follows:

Development of 2D Axisymmetric Model:

A 2D axisymmetric model of crystallization process was developed using ANSYS Fluent. model consisted of a cylindrical vessel with a diameter of 0.1 m and a height of 0.2 m. vessel was filled with a supersaturated solution of solute. A cooling jacket was placed around vessel to control cooling rate. Two different impeller designs, pitched blade, and radial flow impellers, were tested in model. Model was divided into several sections, and boundary conditions were applied to each section.

Validation of Model:

By comparing simulation results to published experimental data, model was confirmed. Measurements of crystal size, crystal morphology, and nucleation rate were included in experimental data. To ensure model's accuracy, simulation results and experimental data were compared.

Effect of Cooling Rate on Crystal Size and Morphology:

The numerical simulation was used to investigate how cooling rate affected size and morphology of crystals. crystal size and morphology that emerged from simulation were compared at various cooling rates. Experimental data in literature and simulation results were compared (Patil, R. N., & Bhambulkar, A. V.,2020).

Effect of Initial Concentration of Solute on Nucleation Rate and Crystal Size:

The numerical simulation was used to investigate how nucleation rate and crystal size were affected by solute's initial concentration. Nucleation rate and crystal size that emerged from simulation were compared for various solute initial concentrations. experimental data in literature and simulation results were compared.

Effect of Impeller Design on Crystallization Process:

Model was used to test pitched blade and radial flow impellers, two different types of impellers. Crystal yield for each impeller design was compared to see how it influenced crystallization process.

Optimization of Crystallization Process:

The results of simulation were used to optimize crystallization process. Optimal conditions for process were determined based on simulation results.

Result and discussion

The simulation is a crystallizer, which is a vessel used for crystallization process. methodology involves running a simulation to determine variation of local crystal diameter and calculate mean crystal diameter in crystallizer.

The results of simulation indicate that local crystal diameter is greater than mean crystal diameter between 240 and 300s, and that mean crystal diameter is greater than local crystal diameter up to 240.9s. This is because, up until 240.9s, there are more crystals in entire crystallizer than there are at local position. However, between 240 and 300s, there are more crystals around local position than there are in entire crystallizer.

The initial crystal size used in simulation was 0.1 nm; simulation's mean crystal size was 2.08 m, while experimental data's mean crystal size was 4.8 m. Fact that simulation and experimental crystal diameters are in same order indicates that crystallizer's CFD models are supported by experimental data.

Consequently, crystallizer's validated CFD models can be used to investigate parameter sensitivity of crystallization process. Figure 1 depicts transient distributions of mean crystal diameter and local crystal diameter at a distance of 0.015 m from inlet. Time is shown on x-axis in seconds, and crystal's diameter is shown on y-axis in micrometers (m). Local crystal diameter at specified location is depicted by blue line, while mean crystal diameter across crystallizer is depicted by red line.

Up until 240.9s, results indicate that mean crystal diameter is greater than local crystal diameter. This is due to fact that, up until that point, local position had a lower crystal density than entire crystallizer. However, number density of crystals around local position is greater than number density of crystals throughout crystallizer between 240 and 300s, resulting in a local crystal diameter greater than mean crystal diameter.

The initial crystal size is 0.1 nm. Based on simulation and experimental data, mean crystal size at 300s is 4.8 nm. Fact that simulation and experimental crystal diameters are in same order indicates that crystallizer's CFD models are supported by experimental data.

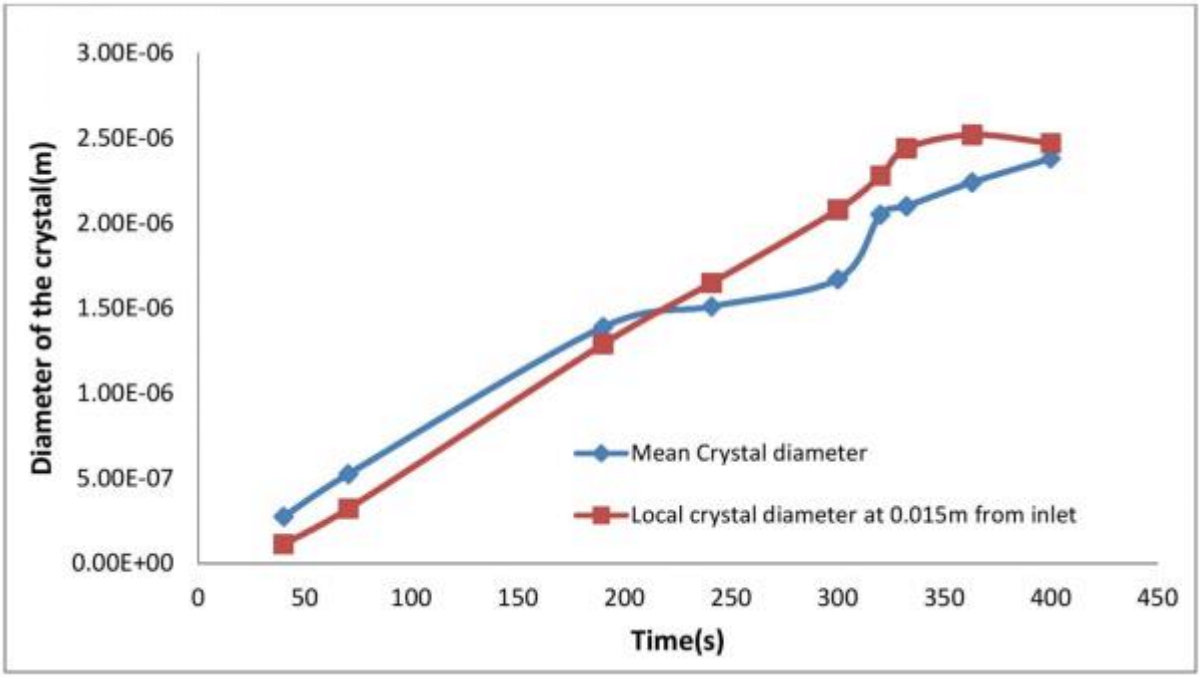

Figure No.1 Transient local crystal diameter distributions.

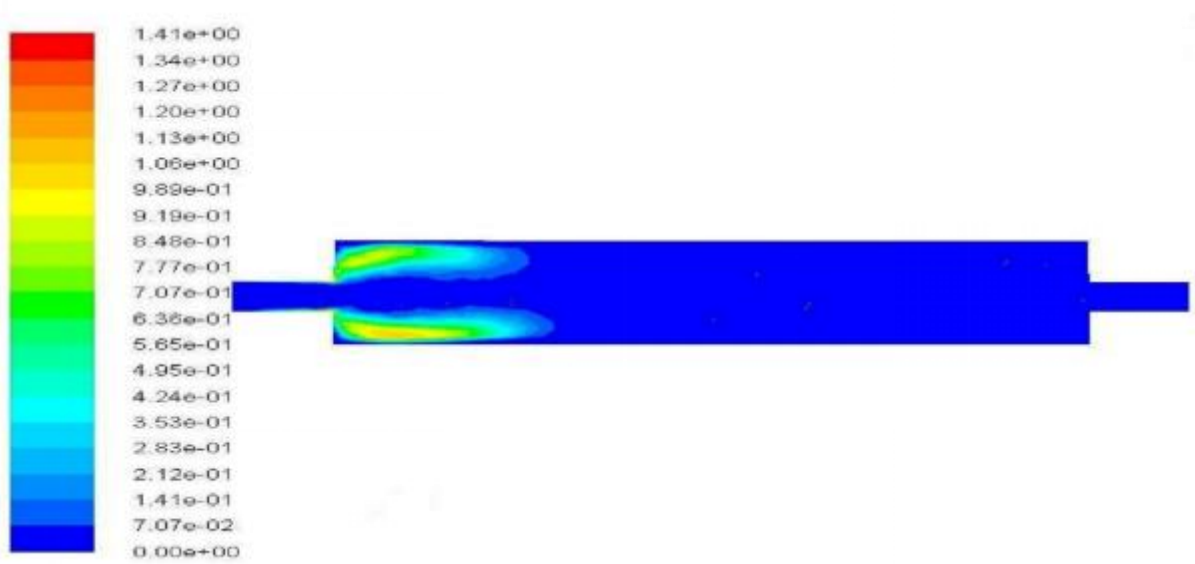

Figure No. 2 moment-3 distribution in crystallizer at 400s.

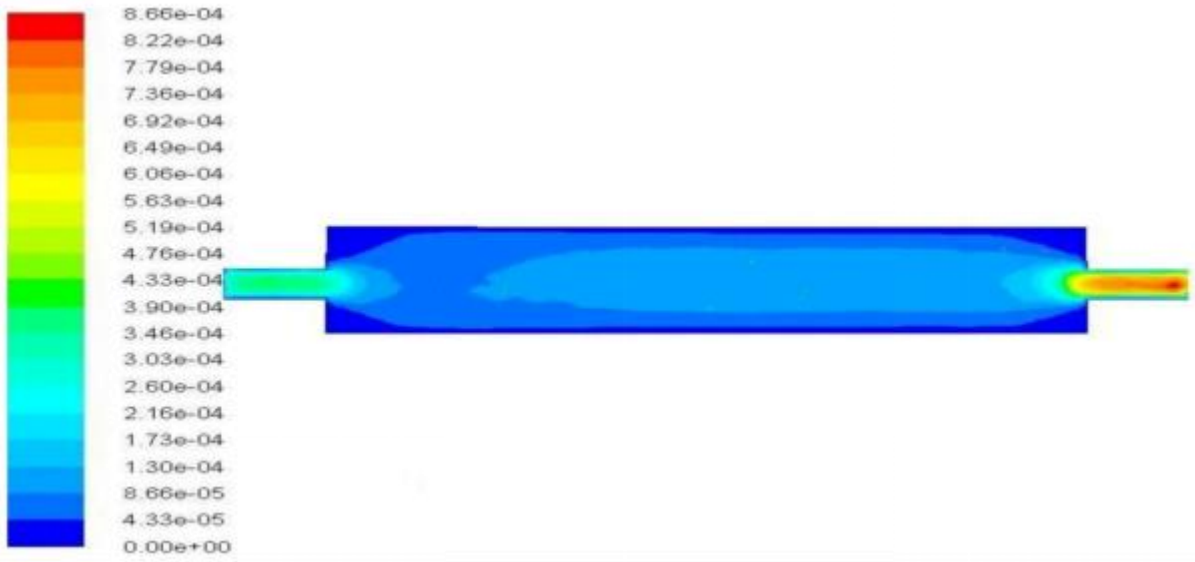

Figure No. 3 Distribution of velocity inside crystallizer at 400 seconds

Conclusion

The simulation results provide valuable insights into crystallization process in vessel. Validated CFD models for crystallizer can be used to study parameter sensitivity and optimize process parameters for improved crystal size distribution and yield.

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