COMPARTMENTAL MODEL OF GAS-LIQUID PRECIPITATION IN A STIRRED TANK REACTOR

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Abstract

The compartmental model is introduced to estimate the influence of fluid field on the gas-liquid precipitation in a stirred tank reactor. The fluid field calculated by the computational fluid dynamics is coupled with mass transfer model and population balance model to predict the local gas-liquid absorption rates. Specific mass transfer area (a) is a time-dependent variable during the first 10 minutes. Local volumetric mass transfer coefficient (k_La) near the impeller is 100 times higher than in the suspension region. The compartmental model is capable of combining the fluid field and detailed reaction, precipitation, mass transfer, and population balance models with a relatively low computational cost.

Keywords

Gas-liquid precipitation, Fluid field, Compartmental model.

Introduction

Gas-liquid precipitation is a widely used process to produce fine chemicals and pharmaceuticals. Several models have been proposed to predict the influence of hydrodynamic on the gas-liquid precipitation in the bubble column (Rigopoulos and Jones, 2001). However, the investigation of gas-liquid precipitation in the stirred tank is still a challenging task due to the intensive breakage and coalescence of both bubbles and crystals. The local energy dissipation (ε) and volumetric gas-liquid mass transfer coefficient (k_La) vary considerably in different regions of the stirred tank. Computational fluid dynamics (CFD) is a method to provide a vital insight into the fluid field which governs the overall precipitation rate and crystalline properties. The chemical reaction, mass transfer and population balance (PB) of both bubbles and crystals should be coupled with convective terms during the calculation of flow field. A full CFD computation can be demanding due to the high number of cells required for the discretization of the domain. Therefore, a compartmental model is introduced for the sake of compromise between the accurate details of flow region and the efficient coupling of hydrodynamics and precipitation mechanisms.

Compartmental model

Firstly, the fluid field is solved without detailed chemistry. Then, the flow domain can be divided into high and low mixing region with only a limited number (10-100) of compartments, as shown in Fig 1.

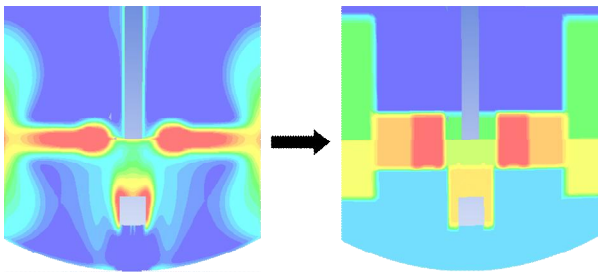

Figure 1. Compartmentalization of fluid field according to the energy dissipation rate profile (ε)

Next, the precipitation mechanism can be combined with the fluid field, as illustrated in Fig 2.

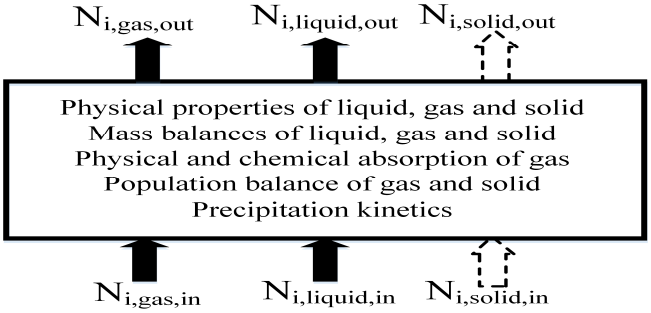

Figure 2. The combination of fluid field and precipitation mechanism in the i-th compartment.

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Meanwhile, the boundary conditions of each compartment are recalculated based on the precipitation model and updated. The two-way coupling algorithm gives reasonable predictions of the interaction between the hydrodynamics and the precipitation. The population balance equation including nucleation, growth, inflow, outflow, breakage and coalescence is solved by high-order moment-conserving method of classes (Alopaeus et al., 2006) for both bubbles and crystals in each compartment.

Results and discussion

A gas-liquid system of $H_2O(l)$-$Ca(OH)_2(l)$-$CO_2(g)$ was considered as our study case. The mass transfer and population balance model of CO_2 bubbles were firstly tested in the compartmental model. Gas-liquid mass transfer determines the supersaturation which is the driving force of precipitation. The overall specific mass transfer area (a) needs to be calculated by the PB model of bubbles. The non-uniform distribution of energy dissipation results in various breakage and coalescence rates of bubbles in different regions. The results of a and k_La at one operating condition are shown in Fig 3 and Fig 4.

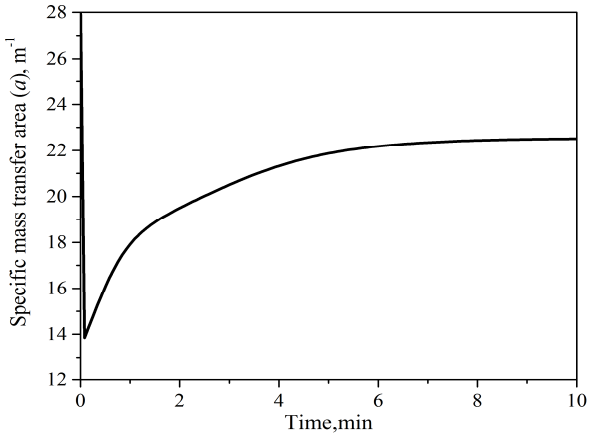

Figure 3. Overall specific mass transfer area (a), m^{-1}

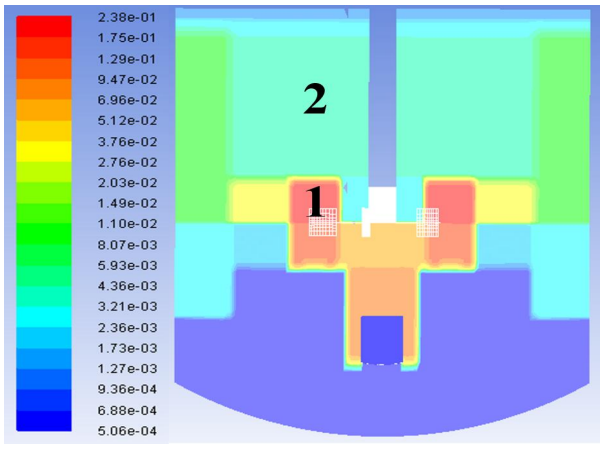

Figure 4. Local volumetric mass transfer coefficient (k_La) at 10 mins, s^{-1}

The mass transfer area during the first few seconds corresponds to the arbitrary initial size distribution of bubbles in Fig 3. Then the fluid field and PB model will govern the value of a. The result shows that a is a time - dependent variable at the beginning of mixing.

The local volumetric mass transfer coefficient at 10 mins is shown in Fig 4. k_La in the impeller compartment (block 1) is 100 times higher than in the suspension compartment (block 2). The local size distributions of bubbles in these two regions are shown in Fig 5, the bubbles in the high turbulence region are significantly smaller than in the low turbulence region. The fast mass transfer rate near the impeller will lead to high supersaturation of the following precipitation. It can be deduced that a large amount of nucleus could appear and finally determine the size distribution of particles.

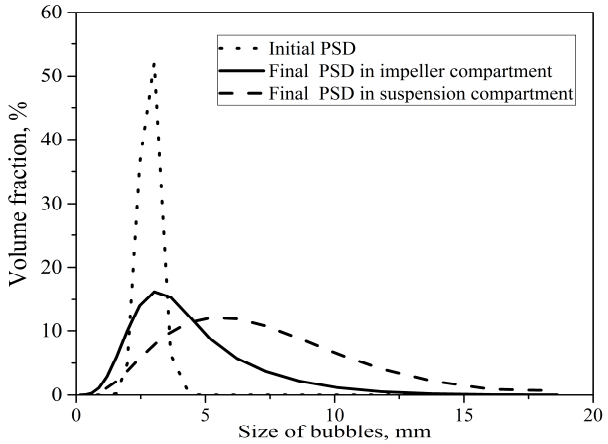

Figure 5. The initial and final size distributions of bubbles in different compartments

Simulation time for the compartmental model is approximately three times faster than the real time with regular PC, which is several orders of magnitude faster than a full CFD computation. The compartmental model is a reasonable and efficient method to combine detailed fluid flow and detailed chemistry.

Acknowledgments

Financial support from the Finnish Academy, project FLUKI (no. 13259597) is gratefully acknowledged

References

Rigopoulos, S., Jones, A. G. (2001). Dynamic modelling of a bubble column for particle formation via a gas-liquid reaction. *Chem. Eng. Sci., 56, 6177.*

Alopaeus, V., Laakkonen, M., Aittamaa, J. (2006a). Solution of population balances with breakage and agglomeration by high order moment conserving method of classes. *Chem. Eng. Sci., 61, 6732.*