Advances in Process Simulation of Agglomeration in Bayer Precipitation

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Abstract

Developing a Bayer precipitation circuit model with accurate predictive capability requires comprehensive physical models for the fundamental processes occurring and, importantly, a structured approach to tuning the model to available plant data. A new agglomeration size kernel has been constructed based on agglomeration kernels developed by René David et al. for different types of eddies within turbulence. The new kernel takes account of the fact that two types of eddies are of practical relevance to agglomeration in precipitation circuits, namely small laminar eddies whose behaviour is dominated by viscous forces and larger eddies whose behaviour is dominated by inertial forces. As well as simulating the chemical and physical processes underlying agglomeration, the kernel offers flexibility in its application due to the inclusion of various adjustable parameters. This facilitates model calibration for accurate prediction of particle size distribution (PSD) in the discharge flows from tanks in the precipitation circuit where complex particle interactions take place under a variety of hydrodynamic conditions. The kernel has been implemented into the Precipitator 3 unit model of the SysCAD process simulation software. A systematic procedure for calibration has been developed for obtaining the closest approach to the target PSD whereby various combinations of kernel parameters are tested with simultaneous tuning of constants for growth, nucleation, and agglomeration rates on their respective targets. Aspects of supersaturation, growth rate, nucleation rate and agglomeration rate are reviewed in the context of calibrating predictive established relationships.

Keywords: Process simulation, Agglomeration, Nucleation, Growth, Calibration.

1. Introduction

Product quality and production rate are ongoing concerns in alumina refineries. Uncertainties often arise about the best way to resolve product quality issues with the least impact on production or how to optimise plans for production improvements. In these cases it is useful to have a tool which can predict changes in particle size distribution (PSD) around the white-side circuit as a consequence of changes in operating parameters, circuit configuration or equipment conditions.

Recently a new agglomeration size kernel has been added to the SysCAD process simulation software. The kernel offers a large degree of flexibility in calibrating a precipitation circuit model to an existing plant circuit such that each tank in the model has the right set of parameters producing the correct gibbsite mass with the correct PSD. This paper discusses this new kernel and the method of calibration. In this context, attention is also paid to fundamental aspects of growth rate, nucleation rate and agglomeration rate.

Agglomeration of $Al(OH)_3$ (gibbsite or hydrate) crystals in the Bayer process has been extensively studied in Australian research institutions. In the early 2000 s a collaborative research project was executed within CSIRO Minerals under the direction of AMIRA. Dean Ilievski and Iztok Livk were the leading scientists on this project and published important results, conclusions and correlations, including an agglomeration kernel that is available in SysCAD. Their experimental

work was conducted in two types of reactors: an in-house developed reactor for simulating laminar flow conditions and another for simulating turbulent flow conditions [1]. Regarding the latter it was recognised that the agitator power input, thus shear rate, per reactor volume unit was an order of magnitude greater than in real-world precipitators. To overcome this issue, the conclusions from both the laminar and turbulent reactors were considered in constructing an agglomeration kernel.

In this paper a more pragmatic approach is presented whereby the actual precipitators in a plant serve as kernel parameter development reactors. In this approach, scientific findings regarding agglomeration under laminar and turbulent flow conditions are used, but a degree of flexibility has been incorporated into the kernel to account for the actual plant environment.

2. New Agglomeration Kernel

2.1 Microscales of Turbulence

The new kernel is based on expressions from publications by René David et al. [2, 3, 4] about their research into the agglomeration of adipic acid crystals. These expressions relate to the hydrodynamic and orthokinetic conditions within the turbulence in a tank, where different types of eddies can be distinguished. Turbulent energy is added at the largest length scales. The vortices or eddies created are distorted and broken into continually smaller eddies. Of interest here are eddies at the smaller scales, where agitator energy input is ultimately dissipated as heat via viscous action. The Taylor microscale, λ_g, is the scale at which viscous effects start to become important, while turbulent inertia through flow fluctuations in magnitude and direction is still present. Below the Kolmogorov microscale, λ_k [5], viscous effects dominate and motion is laminar.

$$\lambda_k = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \tag{1}$$

$$\lambda_g = \theta \cdot \left(\frac{60\nu}{\varepsilon}\right)^{1/2} \tag{2}$$

where:

λ_k	Kolmogorov microscale of turbulence, m
λ_g	Taylor scale of turbulence, m
ν	Kinematic viscosity, $m^2\ s^{-1}$
ε	Energy dissipation rate per unit mass, $J\ s^{-1}\ kg^{-1}$
θ	Fluctuating average component of the local velocity, $m\ s^{-1}$

The Taylor and Kolmogorov microscales are typically within the hydrate particle size range of Bayer circuit precipitators. These scales can vary from tank to tank and from location to location within a tank. It is worth noting that turbulence is a characteristic of the flow situation, not a property of the fluid, and that these scales are not exact dimensions but representative dimensions.

2.2 The Process of Agglomeration

The Kolmogorov microscale is an important transition point for particle behaviour. The motion of particles smaller than the Kolmogorov microscale is dominated by viscous forces. These particles have little motion relative to the fluid. They tend to move parallel to each other in the laminar flow elements. Collisions between these small particles only occur because particles catch up with each other as a result of a viscosity related, shear induced velocity gradient. The chance of collision as a function of particle size is described by Smoluchovski [6]. Particles larger than the Kolmogorov microscale tend to follow more diverse individual flow patterns and exhibit varied velocity fluctuations and trajectory changes. They have a much greater chance of being involved in collisions, e.g. with each other, or with the smaller particles crossing their path.

7. References

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