Equivalence of Growth Rate and Yield Methods

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Abstract

There are two approaches to modeling trihydrate alumina production in precipitation modeling. *Yield methods* relate the rate of change of plant measurable properties (typically Alumina concentration, A or A/C ratio) to key parameters such as temperature, supersaturation and caustic concentration; such methods have been tuned by plant operators to accurately represent plant performance. *Growth rate* methods such as White or Veesler-Boistelle determine an actual growth rate (either as a deposition rate or particle diametral growth), again as functions of a similar set of parameters. Yield methods are suitable for simplified precipitation circuit models and have been modified to include effects of additional observable parameters such as organics levels or free caustic. For full particle size balance simulation in circuits with recycle, a true growth rate method is necessary to determine the size distribution change through the precipitation row, but such methods are typically derived from laboratory experiments with synthetic liquors and may not incorporate parameters that plant operators have found to be important. We discuss how typical yield methods can be rewritten as true growth rate equations, allowing their use in full PSD circuit modeling.

Keywords: Precipitation circuit modeling, particle size distribution, growth rate.

1. Historical Overview

The analysis described here results from the historical development of the general-purpose process simulation SysCAD package. The original implementation of an alumina model precipitator was for a simple steady-state continuously stirred tank reactor (CSTR) based on the yield model and a simple empirical yield equation. The model required that the *Specific Surface Area* (SSA) and temperature be specified for each tank in a precipitation row — the model could then predict the solids concentration and composition for the inter-tank flows. Further refinements included adding reaction heats and various cooling and environmental heat loss options, so that energy balance could be included, and the row temperature profile predicted as well.

SysCAD incorporates general purpose programming capability, and the overall rate constant in the yield equation can be adjusted for the influence of other process parameters. At the request of various users, additional parameters were incorporated into the yield equation and users tuned these parameters to provide successful predictive yield models.

With increasing computing power, further development of the model into two areas became feasible. Various proprietary PSD models have been available, and SysCAD has always had PSD capability aimed at comminution and separation operations, so the underlying framework for incorporating full PSD into the precipitator model was available. Early implementations of PSD simulation in SysCAD had a separate precipitator unit operation which used a White growth model. Full PSD models can now predict the change in SSA between tanks in the precipitation row, and using cyclone and classifier models can close the circuit, something impossible to achieve with the SSA yield models.

At the same time, there was interest in dynamic simulation for purposes of operator training, commissioning optimization and upset recovery. Rather than having separate dynamic and PSD unit operations, we were aiming at a single unit operation that could operate with PSD and in either steady state or dynamic modes with the same process parameters. Such a model could be tuned for steady state yield conditions, then used in a dynamic or full PSD model, effectively maintaining compatibility with the original yield model.

To achieve this, it was necessary to recast the yield model as a true growth rate equation, allowing it to be used in these new areas. The key observation is that the SSA yield equation implies a growth rate — by distributing the precipitated material over available surface area.
In section 2 we review the yield model and discuss some of the limitations to be overcome in moving to dynamic and full PSD modelling. Section 3 discusses briefly the standard growth models and various forms and shows the equivalence of growth and yield methods. We conclude with discussion some of the other parameters incorporated into yield models that imply influences on particle growth rates.

2. Yield Method Theory

Yield methods have been around for many years, and are useful in modelling single tank operation. They are easily derived from steady state operational plant data, since they are tuned by — and predict — readily observable plant parameters.

Looking at a single precipitation tank, we can measure the feed A_F and product A_P alumina concentrations in grams per liter (gpl), the difference $\Delta A = A_F - A_P$ is simply the solids yield, also in gpl. Since the volume flow is also measurable, we can determine the total solids Trihydrate Alumina (THA) production as

$$Q_v(A_F - A_P) = Q_v\Delta A = Q_v C\Delta \mathrm{AC}$$

We work with AC since it is a dimensionless quantity and was the basis of the original SysCAD implementation. Subsequently, we will drop the product subscript; all the parameters influencing the yield equations are understood to be at the product (or tank) conditions.
The change in alumina to caustic ΔAC is then correlated against the supersaturation driving force to give us the *Yield Equation*:

$$\Delta\mathrm{AC} = K(\mathbf{P}) \times \exp\left(\frac{-\Delta E}{RT}\right) \times \mathcal{C}_\mathrm{S} \times \sigma \times t_R \times (\mathrm{AC} - \mathrm{AC}^*)^2$$

Here K is an overall “constant” that depends on any number of observable tank parameters represented as **P**; different plant operators have found various quantities that may influence the yield, such as ionic strength, caustic concentration, and free caustic. The four other driving terms are the solids concentration C_S, the SSA σ, the residence time t_R, and the supersaturation. Empirically, more solids, higher SSA, and longer residence times translate proportionally to higher yield, while the effect of supersaturation (the primary driving force) is quadratic. All quantities are measured at tank (ie product) conditions. In practice, the contributions of the main terms may not be precisely linear, and the supersaturation dependence may not be quadratic, and additional exponents or functional forms may be introduced, but we will work with this form to illustrate the main points here.

For modelling a single tank we know the feed conditions and the tank volume, but we don’t know the product conditions. It is straightforward to solve numerically, analytical solutions for simplified cases do exist, but in reality, internal or external cooling, reaction heats, and other complications in determining the steady state tank temperature make such analysis pointless.

4.1 Organics

The presence of organic compounds, as measured for example by TOC, has been found to inhibit yield with a suggested correction

$$K_{\mathrm{TOC}} = \exp(-n_{\mathrm{TOC}} \times \mathrm{TOC})$$

4.2 Caustic

The growth rate equation shows a C^{-1} dependence on caustic concentration, the White equation has no caustic dependence, a variant due to White and Bateman [6] has a dependence $C^{-3/2}$. The general yield method allows all these via a caustic rate correction $K_C = C^{nC}$.

4.3 Free Caustic

Another White variant due to King [2] includes a factor for Free Caustic, so we can incorporate a further factor $K_{FC} = \mathrm{FC}^{n}{}_{\mathrm{FC}}$

In implementing a precipitation model based on the generalized yield equation, we can include each of these factors; if the corresponding exponent is set to zero, then the parameter has no effect on the rate. These empirical factors from the yield methods indicate forms for generalized growth equations.

Our overall growth rate factor $K_G = K_{FC} \times K_{\mathrm{TOC}} \times K_C$. We can add further corrections as needed — for example the supersaturation dependence may not be precisely quadratic, and the SSA dependence nonlinear.

5. Summary

We have shown how the empirically derived yield methods can be converted to true growth rate equations, allowing simulation software to incorporate such methods along with other standard previously available growth rate formulae. The resulting growth equation has a form similar to many others that have been proposed, but can be easily fitted to plant data — indeed a number of refinery operators have "tuned-up" variants of the yield equation available. These can then be used in full PSD and dynamic modelling, obtaining results consistent with previous models which only use SSA.

6. References

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