Optimization of Aluminium Hydroxide Seeded Crystallization Using Predictive Model

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Abstract

UC RUSAL is currently testing a system for optimized precipitation control, which enables stabilization of gibbsite particle size distribution and improved liquor productivity. The current version features a predictive mathematical model represented by an artificial neural network. The neural network has been trained using the historical data and functions well under normal conditions; however, optimizer application requires better adaptability from the model while maintaining the same accuracy. A population balance model (PBM) of gibbsite mass crystallization allows for the development of an adaptable model with strict dependencies between the process parameters and explainable predictions, but this model works slowly and requires manual adjusting. On the other hand, a neural network model performs almost immediate predictions but the results are not always explainable. A surrogate model can be a compromise solution between these options. A PBE-based prototype surrogate model of gibbsite mass crystallization has been developed in similar way as a physics-informed neural network. Laboratory test results show that the model can be used to describe agglomeration and growth of gibbsite crystals in pregnant liquor.

Keywords: Alumina size control, Population balance model, Neural network, Predictive model, Process optimization.

1. Introduction

The particle size distribution (PSD) in aluminium hydroxide production at low A/C filling liquor is controlled by adjusting the supersaturation in precipitators because the absence of fine seed agglomeration at low A/C does not allow direct control of particle size and number of particles.

An adequate model must be developed for automated control of the aluminium hydroxide PSD. The correlation between the size and number of particles in the crystallization process is most accurately described by the population balance Equation 1:

$$\frac{\partial n}{\partial t} + G \frac{\partial n}{\partial L} = B - D \tag{1}$$

where:

n numerical density function expressing the derivative of the number of particles dN within the interval from L to L+dL in the slurry volume unit, m⁻⁴

L particle size, m

 $\partial n/\partial t$ rate of change of numerical density in time in the slurry volume unit, $1/(m^4 \cdot s)$

G linear growth rate of crystals, m/s

B and *D* rates of formation and disappearance of particles within the interval resulting from their generation and transition between size grades respectively, $1/(m^4 \cdot s)$

Despite the high accuracy and fine development of the mathematical theory of population balance for precipitation, its complexity and the need for manual adjustment limit its use as part of the automated control system.

2. 1st Generation Optimal Control System

The control objective is to ensure stable PSD of aluminium hydroxide particles at maximum liquor productivity. Model Predictive Control (MPC) is more suitable than other methods because it enables control of the process while accounting for future conditions. MPC requires a predictive model of the process as well as an optimisation algorithm.

The developed predictive model is based on deep neural networks due to their high performance. For neural network training we used an array of 4700 data points obtained from over 20 years of observation of the precipitation area. The best training results were achieved using two-layer neural networks of LSTM (long short-term memory) type with 20–60 neurons per layer.

A sensitivity study of the neural network model showed that, within the established boundaries of parameter changes, the following parameters had the strongest influence on the optimisation function (see Figure 1): temperature of head precipitators (T1 from 61 to 68 °C), solid content in the slurry (Cs from 700 to 800 g/L) and temperature of last precipitators (Tn from 48 to 50 °C). Liquor flowrate per all lines of precipitation area (Ql from 475 to 600 m³/h) and amount of unclassified seed slurry pumping out (Qp from 0 to 80 t/day) had less of an impact.



Figure 1. Degree of influence of factors on the response function.

PSD control in precipitation can be represented by a multi-parameter optimisation problem with nonlinear constraints of equality and inequality types:

$$\min f(x,z)$$

under conditions:

$$a_{j} \ge h_{i}(x, z) \ge b_{j} \quad \text{(inequality)}$$

$$g_{i}(x, z) = c_{i} \quad \text{(equality)}$$

$$(2)$$

where:

x set of control parameters (see Figure 2-d)

z set of unregulated parameters (see Figure 2-c)

f(x, z) optimisation function (see Figure 2-a)

i and j sets of constraints of equality and inequality types respectively

 $g_i(x, z)$ and $h_i(x, z)$ functional constraints (see Figure 2-b)

 a_j, b_j and c_i constants or functions

4. Conclusions

We have demonstrated that a predictive multi-parameter model of aluminium hydroxide precipitation can be based on a deep neural network like LSTM if sufficient extensive historical data is available to train said model.

The precipitation control setpoint optimization method, which combines a preliminary gradient search with gradient-free genetic solution improvement, performs well in finding the optimal point in a multidimensional constrained space.

The principle of using star points allows for significant reduction in the dimensionality of the factor space of the optimal problem and provides for smooth regulation.

Testing of the optimal control system in the precipitation area at the UAZ alumina refinery demonstrated its ability to control the PSD and liquor productivity, but revealed some drawbacks related to the insufficient generalization ability of the neural network model trained on actual industrial data.

The possibility of building a surrogate model of the precipitation process is shown based on PINN-type neural networks. The next stage of the work is developing robust hybrid models, in which industrial data is supported by the physics of the process.

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6. References

- 1. A.S. Bramley et al., Aggregation during Precipitation from Solution: A Method for Extracting Rates from Experimental Data, *Journal of colloid and interface science*, Vol. 183, 1996, 155-165.
- 2. Jorge Nocedal and Stephen J. Wright, *Numerical Optimization*, Second Edition, Springer, 2006, 664.
- 3. E.T. White and S.H. Bateman, Effect of caustic concentration on the growth rate of Al(OH)₃ particles, *Light Metals* 1988, 157–162.
- 4. M. Raissi, P. Perdikaris and G.E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, *J. Comput. Phys.*, 378 (2019), 686–707.
- 5. S. Kollmannsberger et al., Physics-Informed Neural Networks, *Studies in Computational Intelligence, Springer International Publishing, Cham* 2021, 55–84.
- 6. E. Haghighat et al., Tensorflow wrapper for scientific computations and physics informed deep learning using artificial neural networks, *Comput. Methods Appl. Mech. Engrg.*, 373, 113, 552.
- 7. *TensorFlow*, https://www.tensorflow.org/ (Assessed on June 01, 2024).
- 8. I. Livk, D. Ilievski, A macroscopic agglomeration kernel model for gibbsite precipitation in turbulent and laminar flows, *Chem. Eng. Science.* 2007, Vol. 62, 3787–3797.