ALTA 2024 28
27 - 31 May | Perth, Australia

MODELLING AND SIMULATION OF NICKEL SOLUTION PURIFICATION IN INDUSTRIAL JAROSITE AUTOCLAVES

By

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ABSTRACT

This paper describes how a hybrid first-principles – machine-learning (FP-ML) modelling and simulation platform can help to understand and improve complex industrial processes. Nickel solution purification, predominantly via ammonium jarosite precipitation in a series of autoclave stages, is used as a case-study example to demonstrate the benefits of this approach to the industry. It also provides an implementation platform where these benefits can be made accessible to a wider technical team in an operational environment.

The model inputs are the logged inflow stream flows and upstream block states. An initial modelling phase identified info gaps in the operational chemical suite, which prompted a short sampling campaign to measure the key species profiles over a pre-selected case-study period. Since precipitation mechanisms are complex and difficult to interpret via batch experimentation, only this plant data and the hybrid modelling approach were used to digitally capture the key information.

The FP modelling construct is based on acausal mass-energy balance equations, which take care of the dynamic interactions of each inventory block with its neighbouring blocks. Within this FP framework, phenomenological equations were added, and ML algorithms trained to capture the observed case-study period behaviour. This workflow methodology is discussed in the paper and only relies on basic chemistry, measurement and understanding. The advantage of this approach is that the data science blocks can deal with the microscopic-scale complexities, while the combined model generalises the behaviour so that it becomes predictive.

Measured vs predicted trends are presented in the paper, demonstrating that this model qualifies as a true digital twin (DT) and that it can be used to optimise control and improve operating strategies, amongst others. A compiled application product (App) version of the DT, with user-friendly front-end, was therefore packaged and distributed to the plant engineers for use on a day-to-day basis.

Keywords: hybrid modelling, simulation, digital twin, jarosite precipitation, nickel purification