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Hybrid Modelling Framework for on-Line Data-Driven Modelling of Particle Processes

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Abstract

Particles play a key role in many industrial productions, where particle processes are frequently used for removal of insolubles, product isolation, purification and polishing. Because particle processes are quite complex and fundamental understanding of underlying phenomena is lacking, control and monitoring these processes are often challenging tasks. To overcome these challenges, it has previously been examined whether hybrid modelling could capture particle dynamics and be used to optimize these processes. Shallow neural networks have here been used to estimate particle phenomena kinetics and combined with low-order population balance models to produce predictions of particle size evolution. During the last two decades, hybrid models have been employed in various particle processes, including crystallization operations [1,2,3]

and a pharmaceutical milling process [4]. While these models have shown good predictive capabilities, they have been rather case-specific and been trained either using indirect process variables or using fairly small data sets of particle size distributions due to historical limitations of particle analysis methods. With recent developments in particle monitoring tools, such as dynamic image analysis and focused beam reflectance measurements, it is now possible to measure particle properties with a much higher frequency, allowing for better capture of the process dynamics.

In this work, a hybrid modelling framework is presented for particle processes that include all the common particle phenomena, including nucleation, growth, shrinkage, agglomeration and breakage. The hybrid model is trained using time-series data from an on-line/at-line particle analysis sensor, along with other measured process states that may have an impact on the phenomena kinetics. The particle phenomena kinetics are estimated using a deep neural network, where all the available measured and calculated process states are used as inputs. The kinetic model is combined with a medium-resolution discretized population balance model and mass balances, ensuring that physicochemical constraints are not violated. With the high flexibility and the automatic feature selection capabilities of the deep neural network, it becomes possible to model an arbitrary particle process without relying on excessive prior process understanding. The only requirement is that the process dynamics related to the particle phenomena and the particle size distribution can be measured during the process.

The presented modelling approach utilizes automatic differentiation for training of the hybrid model, which significantly speeds up the model training from an order of O(2n) using a finite difference method to O(1), where n is the number of weights in the neural network. This opens up for training the hybrid model in real-time, where new sensor data can be continuously incorporated into the hybrid model during process operation. It furthermore allows for easy scaling of the neural networks to higher complexity without significant additional computational costs.

The versatility of the hybrid modelling framework is demonstrated through three case studies of varying nature and scale, where on-line/at-line dynamic image analysis has been used to measure particle properties during process operation. The case studies include a lab-scale crystallization of lactose, an industrial scale crystallization of an active pharmaceutical ingredient and a lab-scale flocculation and breakage of silica particles. We demonstrate how data quality and quantity affects the model performance and compare with traditional first principles modelling.

It is furthermore illustrated how computational chemistry methods can bring the framework an additional understanding of nanoscale particle interactions [5] by including first-principles model-based soft-sensors as inputs to the deep neural network. This includes estimations of solid-liquid interfacial tension (IFT), which can predict attractive or repulsive forces between particles in a robust way, much faster than experimental measurement of surface forces.

Lastly, a couple of future perspectives are presented, including the use of the hybrid model in model predictive control (MPC) where the hybrid model can be trained in parallel with solving the MPC problem.

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