

Special Issue

Modeling, Simulation and Data Analysis of Pharmaceutical Manufacturing Processes

Message from the Guest Editor

Pharmaceutical processing models, whether linear or non-linear, discrete or continuous, static or dynamic, explicit or implicit, deterministic or probabilistic, portray mathematical representations of correlations between manufacturing variables. Pharmaceutical processing models simulate drug and excipient syntheses and their formulations, amongst various other important product lifecycle steps such as analytical testing, packaging, and supply chain management. These correlations underly "ab initio" physio-chemical phenomena such as Mass and Heat Transfer, Mass Flows, Reaction Kinetics and Thermodynamics, setting up "First Principle" models. As real-world situations increase the complexity of the interplay between variables, the system's behavior often deviates from this "knowledge-based" description. Empirical models are therefore recruited to analyze arbitrary correlations of available datasets, creating hybrid optimization threads. These threads may also be delegated by Artificial Intelligence through Neuronal Networks, Machine Learning algorithms, and Data Mining functions.

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