"Combining physical models with machine learning and robotic technology to develop complex chemical processes"

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In speciality chemicals, agrochemicals and pharmaceuticals manufacturing chemical synthesis is characterised by poor observability of states, multiple phases, many synthesis and separation steps and many simultaneous criteria for success. As a result, hardly any commercial manufacturing process in these sectors could be judged to be 'optimised'. Traditional PSE tools require a full set of input data and rigorous models, which will never be available for the types of chemical systems we deal with. Hence, our current focus is on hybrid methods of combining physical models with methods based on data - machine learning. To increase access to data we turn to automated experiments - robots, whereas to increase the usability of the data we turn to Bayesian sequential optimisation. In the talk I'll give an overview of the emerging work flow and present some recent tools that are rapidly gaining acceptance, especially in industrial R&D.