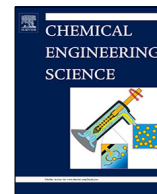


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Editorial

Chemical Engineering Science Danckwerts special issue on Digitalisation



Digitalisation is a hot topic everywhere. Chemical Engineers have been at the vanguard of applying digital approaches and algorithms to problems in manufacturing and environmental systems, and other systems where there is chemical and physical change. What is new today is the huge increase in compute power, the continued development of mathematical algorithmic approaches and in particular the developments in Artificial Intelligence and Machine Learning, in our ability to measure new properties in real time, and in the sheer volume of available data, both static and dynamic often as images as well as point values.

This collection of papers has been brought together as a Special Issue of Chemical Engineering Science to explore the current state of Digitalisation within Chemical Engineering. We have solicited papers from across the range of areas that Chemical Engineers work. We were pleased that the Danckwerts lecture of Prof Morbidelli on 'the integration and digitalization in the manufacture of therapeutic proteins' (see paper by Narayanan et al. <https://www.sciencedirect.com/science/article/pii/S0009250921007247>) fits exactly into the theme which will give more profile to the fast moving area of Digitalization.

The Issue has four invited review papers to address specific parts of the digitalisation challenge. The review of Pan et al. on 'Data-centric engineering: integrating simulation, machine learning and statistics. Challenges and opportunities' <https://www.sciencedirect.com/science/article/pii/S0009250921008368> shows the range of data centric approaches that are coming to fruition. Some of the emerging areas such as digital twins and hybrid models are 'old wine in a new bottle' as they say but the enhanced capabilities really give them new life, while others like probabilistic numerics open up new directions. It also points to the need for data science to be part of the chemical engineer's training and how organizational barriers can be overcome by 'the democratization of simulations'. Machine learning as a tool is becoming more important and this is the topic of the paper by Thebelt et al. <https://www.sciencedirect.com/science/article/pii/S0009250922000537>. They explore four distinct characteristics of data in Chemical Engineering problems and how machine learning is being developed to tackle them. Smart measurement is also one of the characteristics of Digitalisation and the paper by Meng <https://www.sciencedirect.com/science/article/pii/S000925092100837X> reviews the contributions from tomography, a particularly versatile and powerful imaging tool used by engineers in research but also increasingly in operations. The challenges in the detecting signal and hardware are discussed but also very much in the algorithmic reconstruction of the required measurements from the streams of data. Digitalisa-

tion also has a potential significant impact in operations. The review by Vandrangi et al. <https://www.sciencedirect.com/science/article/pii/S0009250921007703> explores data driven approaches to diagnostic systems for the detection of leaks in multiphase flows, particularly from pipelines, and the prediction for determining the magnitude of a fault.

The remainder of the articles come under two headings: data driven methods and artificial intelligence approaches.

The availability of much greater amounts of data, sometimes of variable quality, has spawned a significant amount of research developing new data driven methods to best us this data in design and operations. Sundaramoorthy et al. present a probabilistic approach to data reconciliation accounting for model inaccuracies that give rise to uncertainty <https://www.sciencedirect.com/science/article/pii/S0009250921005613>, Van den Berg et al. <https://www.sciencedirect.com/science/article/pii/S0009250921007004> present methods for data driven optimization focusing on derivative free approaches, Williams et al. <https://www.sciencedirect.com/science/article/pii/S0009250921009258> present a classifier based tool to efficiently obtain surrogate models using only input and output data, Xiang et al. <https://www.sciencedirect.com/science/article/pii/S000925092100926X> a new approach for predicting properties with small datasets, Esche et al. <https://www.sciencedirect.com/science/article/pii/S0009250922000434> use semi-supervised regression to construct robust soft sensors, Yuan et al. a neural network based method for time series data with irregular sampling, Kelley et al. <https://www.sciencedirect.com/science/article/pii/S0009250922000525> a data driven linear formulation for scheduling, and Dai et al. <https://www.sciencedirect.com/science/article/pii/S0009250921005364> a data driven approach specifically for crude oil scheduling under uncertainty.

With respect to Artificial Intelligence approaches Sildir et al. <https://www.sciencedirect.com/science/article/pii/S0009250921008381> present a new method for training neural networks using a piecewise linear model solved using MILP making the most of the non-convex formulation, Bhakte et al. <https://www.sciencedirect.com/science/article/pii/S0009250921009386> present a way of using deep learning to identify those variables in the neural network that lead to the fault classification, Zhang et al. <https://www.sciencedirect.com/science/article/pii/S0009250922000513> further explore fault diagnosis using semi-supervised learning extracting temporal data and effectively use unlabeled data, and Karka et al. <https://www.sciencedirect.com/science/article/pii/S0009250921009040> present a way of

using machine learning to streamline Life Cycle Analysis of bio-based process technologies ahead of process design.

One further article by Wang et al. <https://www.sciencedirect.com/science/article/pii/S0009250922000331>, in the core Process Systems Engineering topic of using optimization for process operations, transforms the energy optimization of ethylene production into a distributed optimization problem giving more efficient and robust optimization.

The Special Issue brings together some very recent research aimed at making Digitalisation of the Process Industries efficient and effective through the latest algorithms and methods and exploiting the massive datasets with data driven approaches.

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