2nd European Forum on New Technologies – Digitalisation in Chemical Engineering
Frankfurt, Germany, 1 March 2019

Report by the EFCE Scientific Vice President, David Bogle.

Digitalisation has the potential to change the way we work in Chemical Engineering. In particular it is likely to change the way the process industries work with the potential of big data and its analysis making the operations and the supply chain much more responsive. It could also significantly change the innovation process in developing new products and processes.
An EFCE event took place in Frankfurt on 1st March to hear some visionary industrial and academic speakers to discuss the potential effects of digitalisation and to consider the challenges and opportunities. One objective was to see how the EFCE and its Working Parties and Sections might work together to address the challenges.
The programme was in four parts. The Vision for Digitalisation in the Process Industries; The Potential of Digitalisation; the Role of Digitalisation across the Life Cycle: in R&D, Design and Operations. The final section was a round table discussion of challenges and opportunities.

Vision for Digitalisation in the Process Industries

Hergen Schultze from BASF opened the session presenting how BASF see the value of Digitalisation, and in particular Artificial Intelligence (AI) in research for manufacturable new materials with precise properties using the development of a new coating as an example. Digitalisation provides the opportunity for efficient and generic procedures to optimise the research and development process particularly given the amount of uncertainty and noise. While the volume of data constitutes a challenge, the big challenges are really in the variety of forms of data, and its veracity.
Martin Winter from CEFIC outlined how digitalisation could transform our operations across the whole supply chain. The sector is behind other manufacturing sectors and we are noticing a significant step up in R&D in China. Great value can be obtained from advanced analytics particularly in manufacturing operations. Horizon Europe is expected to be an evolution rather than a revolution and will likely offer R&D investment of €15Bn of Digital and Industry, and €9.1Bn for the Digital Europe Programme. CEFIC is a partner in the A-SPIRE partnership with the EC in shaping the Commission's Research Programme. EFCE is also a member of A-SPIRE and of CEFIC's SusChem Sustainable Chemistry platform.
We then heard from Sebastian Carsch (Frauenhofer IVV) about developments in the food industry, often seen as a leader in this domain given its links from farm through manufacturing to the consumer in the shops. The food manufacturing sector has a data intensive platform getting stated 95-99% efficiency although it seems that true efficiency is really 60-70% due to missing process understanding and the very variable raw materials. The industry is looking hard at how to empower unique human skills combining machine learning with human experience. Perhaps the best quote of the day, which came from Elon Musk, was 'humans are underrated'!

The Potential of Digitalisation

Michel Dumontier is Distinguished Professor of Data Science at Maastricht University. Data is the 'world's most valuable resource' and he highlighted examples such as Amazon Go and precision medicine. We need to better link humans and AI (he gave deepdreaminnovator.com as an example). How can our community benefit? He raised a series of issues that we should consider as we develop and exploit data science: identify theft, job substitution, ensuring appropriate technical infrastructure (including FAIR data), the future of education, and how we can establish scalable governance and flexible consent to underpin responsible use of Big Data.

Frode Brakstad (SINTEF) outlined some developments in the use of data analytics and ensuring data quality in the process industry. Unintentional variation is still normal in the process industry. Understanding the root cause is vital and he gave examples showing how data is only valuable when you get insights from the data. There are many challenges around how to ensure the quality of data driven models: missing measurements, missing time lags, and where data is heavily correlated which is often overlooked. The industry of the future will be using big data, smart analytics etc. leading to cognitive plants and tighter interactions in the circular economy.

Representing Siemens, Maurizio Rovaglio gave us a tour of their digital asset portal enabling connectivity and availability of data, asset predictive analytics helping with predictive maintenance leading to 'physics based analytics'. He showed us how this has been used for a challenging problem: the submersible mobile offshore ultra deep water drilling unit.

The chair of the EFCE Energy Section, Francois Maréchal, spoke about the use of smart energy systems particularly in the built environment. This gives opportunities for co-ordination of prediction, pooling, control (particularly model-predictive control) and access to the grid market. Many new technologies are on the horizon including microgrids for decentralised systems and blockchain. The industry is aiming for better systems integration, circular economy concepts, and industrial symbiosis. Energy systems are likely to move towards more open data, shared databases, shared models and the use of AI within integrated renewable energy systems.

The Role of Digitalisation across the Life Cycle: in R&D, Design and Operations

Georgios Tetradis-Meris from Unilever explained how R&D is moving away from traditional linear ways of working. Drivers include the speed o information availability, consumer demographics and trends, increasing costs of raw materials and increasingly global supply chains for some products. Seamless execution and speed to market are critical to business. Digitalisation of R&D enables speed and must embrace all functions. Collaborative working, with internal and external partners, is enabled. This allows capture of structured data, integration of scientific knowledge, and exploitation using predictive models. Digital twins are becoming common especially in process and packaging.

Digital technologies are being used, particularly in design, to change the business model according to Costas Pantelides of PSE Ltd because of increasing competitive pressures. Model based engineering across the life cycle allows engineers to perform individual tasks better, to exploit deep process knowledge, leverage off-line modelling efforts, perform tasks not amenable to first principles modelling, combine tasks, integrate workflows, and to perform tasks previously computationally infeasible. There is much to be gained by using deep knowledge. General digital applications platforms are necessary and feasible but there is work to do. Visualisation is key.

Christoph Herwig, the chair of the EFCE WP on Quality by Design, explained of the need for holistic control strategies for the whole life cycle of the production and distribution process. There will be issues arising from data fusion and data integrity. Blockchain technology will be useful to help assure data integrity. Knowledge management using a systematic approach to acquiring, storing and disseminating information is important and can be enabled by new digital technologies and algorithms. Model centred tools, using digital twins, will enable better design of experiments with adaptive dynamic exploration of uncertainty identifying process parameters that are holistically critical. Increasing automation of model generation and data analytics means engineers must work increasingly in symbiosis with AI.

Our last speaker, Nilay Shah from Imperial College, told us of increasingly integrated supply chains in the process industry requiring decision support tools for planning and operation. The flexible multipurpose plant of the future will be highly automated, optimised, and customised. The process industry is mostly B2B but with a need to better understand and know customer demands. Opportunities for better working include integration and seamless use of data and models, integration across the lifecycle, integration between real time planning and scheduling, real time optimization of the supply chain, adaptive optimisation and customisation, and incorporation of analytics to reduce testing and improve quality and responsiveness. New pressures include becoming more service oriented, vendor managed inventory expectations, more rapidly changing market circumstances, mass customisation, improving and reporting on sustainability, and the ability to anticipate and respond to future regulation and compliance.

Challenges and Opportunities

The discussion ranged across technology, motivations, and threats.

New tools are still needed: for example how to combine first principles models with machine learning models, how to manage different time and length scales, and how to combine different data sources which depends on context and alignment. Are the tools suitable for both for process and for product design? How do we use AI to create first principles models – to enhance understanding and to generate high level conclusions? We need to ensure the safety of workers in the new AI enhanced world. Many IT hurdles exist making it difficult for software products to communicate. We need standards for the sharing of data and metadata. Are there lessons to be learned from digital Chemistry and Biochemistry or other domains?

It was felt that we need better experience and guidance about how best to identify the best tool for specific engineering problems. There were many different ideas about what is appropriate for development and what training is required for future Chemical Engineering professionals which requires further discussion.

Next Steps

The potential is huge and the changes are coming. It is clear that we have some experience in industrial practice and in the research and development done by academic and industry to support. However there is much to be done by our community and opportunities to work together to test existing technology, to devise clearer ideas on what is needed, to influence public and private agencies, and to undertake the research, and to demonstrate and stress test new technologies and approaches.

We had representation from the following EFCE Working Parties and Sections: Mixing, Energy, Product Design & Engineering, Fluid Separations, Computer Aided Process Engineering, Quality by Design, Education, Chemical Reaction Engineering, Sustainability, Multiphase Fluid Flow, Crystallisation, and Thermodynamics and Transport Properties with apologies from others.

EFCE's involvement with A-SPIRE gives us the opportunity to shape the European Commission research priorities but also to find new partnerships to develop ideas and proposals and to carry them out. As Scientific Vice President I aim to help support the development of such networks and to help our community to shape the technology agenda to meet the needs of the process industry in the future.