PROCESS
SYSTEMS ENGINEERING
NL

Symposium

PSE-NL Summer Symposium

A dive into digitalization

Friday June 28th 2024
from 12:30 to 18:00

at **Wageningen University & Research**

These are PSE-NL's industrial members:

Corbion, Royal Cosun, Fluor, Unilever, Ketjen, Danone

Process Systems Engineering NL is a knowledge network that aims to offer a platform for sharing the best practices and scientific advancements in the PSE area. The systems approach has a strong track record of usage in industry to improve the decision making, to optimize plant configurations, chemical process conditions, molecular synthesis routes, and to control biological synthesis. The role of PSE is even more relevant now in the context of transition to bio-based raw materials and renewable energy. PSE-NL can help bolster the interests and careers of members, as well as initiating and carrying out industrial projects, making contributions to technology development and application projects with industry, while fostering academic research.

Venue: Wageningen University & Research, Leeuwenborch Building no. 201, Room B0062
Visiting address: *Hollandseweg 1, 6706 KN, Wageningen*

Program:

12:30 – 13:15	**Lunch**
13:15 – 13:30	**Word of welcome** (PSE-NL Chair)
13:30 – 14:00	**Modelling the Transformation of the (full) Dutch Energy System** *by Rutger de Mare (Founder QuO Mare)*
	If needed, 15 min time slot for questions, remarks, and short discussions
14:15 – 14:35	**Pitch for each PhD thesis nominated for the Johan Grievink PSE Award** *by the nominees (~5-10 min each)*
14:35 – 15:05	**Simulation-driven Predictive Decision Support for Batch Production** *by Dominik Wolff, INOSIM*
	If needed, 15 min time slot for questions, remarks, and short discussions
15:20 – 15:40	**Coffee break**
15:40 – 16:10	**Real-time biomolecular sensing for smart process control** *by Prof. Dr. Ir. Menno Prins, TU/e & Helia Biomonitoring*
	If needed, 15 min time slot for questions, remarks, and short discussions
16:25 – 16:55	**RoboChem – The Robots are Coming to the Lab** *by Aidan Slattery, University of Amsterdam, Van 't Hoff Institute for Molecular Sciences*
	If needed, 15 min time slot for questions, remarks, and short discussions
17:10 – 17:20	**Announcement of the Johan Grievink PSE Award winner for an outstanding PhD thesis in PSE** *by the Chairmen of the Jury Committee*
17:20 –	**Closure and social event**

Please register your attendance by email at pse-nl@outlook.com before **Friday 23th June 14:00**. The participation fee is **25 EUR** for non-PSE-NL members.

Abstracts

Modelling the Transformation of the (full) Dutch Energy System *by Rutger de Mare and Jan van Schijndel*

Preparing for a net-zero emission and circular economy within 20-30 yr is a complex and highly ambitions task for the entire industry. Short-term pathways to reach our targets in 2030 are challenging and reasonably well-known. Many decisions have already been taken or are imminent. But creating a clear outlook beyond the 2030 horizon will take quite an effort. Fundamental changes are needed on how we deal with alternatives for fossil feedstocks, that currently drive almost everything in society. Opportunities are numerous, but challenges and uncertainties are also large. The development of industry within planetary boundaries requires a more comprehensive approach. The industrial transition calls for innovation of the system – the way all our production resources transform and get connected to each other and to new, renewable, and emission-free energy sources. This requires that we understand the interplay and interactions between production technologies and circular raw material flows, green power production systems and the infrastructure for power, hydrogen and CO_2 that connect all these. And all this while restricted by limited availability of land. In 2018, the Dutch Energy System used 93 mln ton of fossil resources (natural gas, crude oil, coal). Power-generation units and refineries converted 70 mln tons of these resources into heat, power, transportation fuels and cracker feeds to meet demand set by Residential, Mobility, Agriculture, and Industry Sectors. Some 23 mln tons of crude was refined for export. In 2018, the Dutch CO_2 emissions amounted to 200 megaton CO2-equivalent. Transformation of the Dutch Energy System entails both decarbonisation and recarbonisation of these fossil resources. Decarbonisation can be achieved by electrification, carbon capture & storage and use of waste heat and H2. Recarbonisation needs carbon from biomass, waste streams and/or CO_2. It is estimated that in 2050 the domestic need for sustainable transportation fuels and chemicals will require the equivalent of 19 megatons of renewable carbon. This calls for significant imports of biomass and waste streams as the Dutch production potential for biomass and waste is limited. Furthermore, annually some 4 to 8 megatons of H_2 are expected to be needed. A portfolio of renewable-carbon-based technologies complementing, partly replacing the current set of refineries needs to be built and commissioned for this recarbonisation challenge. These technologies are electrolysis, pyrolysis, gasification, oxy-firing, fermentation, Fischer-Tropsch synthesis, methanol synthesis, and auto-thermal reforming with carbon capture. *TDES is a decision support framework developed by QuoMare that supports this transformation challenge. Based on mathematical programming, TDES guides the development of an 'optimal transition pathway' towards a fully de-/re-carbonised system with zero CO_2 emissions by 2050 at lowest costs. In this lecture Rutger de Mare and Jan van Schijndel will describe TDES modelling approach and explain how it supports the development of pathways towards an effective and efficient transformation of the Dutch Energy System towards 2050.* Two transformation scenarios are presented: the Net-Zero CO2 Case and the Fossil Free Case.

RoboChem – The Robots are Coming to the Lab *by Aidan Slattery, University of Amsterdam, Van 't Hoff Institute for Molecular Sciences*

The field of synthetic organic chemistry has long been a cornerstone of scientific innovation, yielding discoveries in medicines, materials, and fine chemicals [1]. However, despite its advancements, traditional methodologies rooted in manual labor persist, posing barriers to accessibility and efficiency. Our research group is dedicated to pushing the boundaries of synthetic organic chemistry by harnessing technology to its fullest potential [2]. As a specific example: through the integration of flow technology, automation, and machine learning, we have developed RoboChem—an autonomous laboratory aimed at revolutionizing reaction optimization [3]. RoboChem employs a combination of readily available hardware, customized software, and Bayesian Optimization algorithms to streamline the optimization, intensification, and scale-up of complex photocatalytic reactions. By operating autonomously, RoboChem reduces the need for extensive expertise in photocatalysis, making it accessible to a wide range of researchers. In this lecture, we will showcase the capabilities of flow chemistry and self-driving labs in advancing synthetic organic chemistry. Additionally, we will address the ethical considerations surrounding the use of such powerful technology and strategies for preventing its misuse. [1] Campos et al. (2019), Science 363 (6424); [2] Capaldo et al. (2023), Chem. Sci., 14, 4230-4247; [3] Slattery et al. (2024), Science 383 (6681)

Simulation-driven Predictive Decision Support for Batch Production *by Dominik Wolff, INOSIM*

Modern batch production plants are complex, with multiple parallel batches, various dependencies, shared resources and variability in routes and parameters. This is mostly handled by conservative planning and reduced flexibility to mitigate potential risks like unexpected downtimes, resulting in a throughput lower than the theoretical maximum. But what if you knew the future? You could foresee the consequences of your decisions and react to problems before they even occur. INOSIM's novel solution Foresight uses real plant data from various sources to initialize detailed simulation models, to visualize the results, and to ultimately provide decision support to the right stakeholders at the right time. This talk will showcase how Foresight already helps operators to prioritize manual interactions and how it enables production managers to analyze the impact of delays, breakdowns, short maintenance breaks, or rush orders.

Real-time biomolecular sensing for smart process control *by Prof. Dr. Ir. Menno Prins, TU/e & Helia Biomonitoring*

Food, biotech, and biopharma companies need to deal with variations of bioprocesses, which cause fluctuations of quality, yield, productivity, and costs. This gives dilemmas of running manufacturing processes with either costly conservative process settings (over-engineering, set for the worst-case variation that may occur) or with high product loss rates. The dilemma can be resolved by implementing real-time measurements, because real-time data can enable adaptations of process settings, to deal with variations and run processes always at optimal conditions. Real-time measurements of biomolecular concentrations are possible with optical spectroscopic sensors such as NIR and Raman, however, the achievable sensitivity and specificity are limited. Here, I will present an affinity-based real-time sensing technology called Biosensing by Particle Motion (BPM) that we are developing to quantify specific biomolecules, at low concentrations, in real time (see www.heliabiomonitoring.com/publications). I will present the BPM sensing technology and will discuss how the sensor can be applied in downstream processing (DSP) and upstream processing (USP).

Speakers

Rutger de Mare is expert consultant at Quo Mare. He founded this company in 2016 and provides to the customers solid answers to their complex optimization challenges in logistics, manufacturing, and finance. He worked and provided consultancy for different governmental institutions, political parties, various industries, TSO's/DSO's, port authorities, and logistics in maritime transportation in over 30 projects related to the energy and materials transition. Rutger and Quo Mare aim to apply optimization technologies to challenges with a high societal impact. For example, during covid-19 pandemic he provided consultancy to GGD on planning and optimization of the COVID-19 vaccination program for the Netherlands, support on predicting demand at test centers and intensive care optimization. The advised Minister of Healthcare and the chairman of the National Acute Care Network on debottlenecking the manpower of the Dutch intensive care units. Rutger graduated in 2006 from Erasmus University Rotterdam with an MSc in Econometrics and Management Science.

Aidan Slattery was born in Cork, Ireland. He obtained his B.Sc(Hons) degree in Chemistry of Pharmaceutical compounds in 2019 from University College Cork. His final year project was carried out on the topic of α-diazo-β-cyanoamides in asymmetric catalysis under the supervision of Prof. Anita Maguire. Following his undergraduate he joined Snapdragon Chemistry Inc., Waltham, MA, USA. His work there involved the characterization of the Snapdragon IRIS photoreactor, as well as working with clients on process intensification through flow chemistry. Currently, he is a Ph.D. candidate at the Van't Hoff Institute for Molecular Sciences under the supervision of Prof. Timothy Noël. He is now working on the development of a high-throughput experimentation platform for the photocatalytic functionalization of organic molecules.

Dominik Wolff graduated as a bio-chemical engineer at the Technical University Dortmund, Germany. He joined INOSIM in 2016 as a process simulation consultant, providing services around their simulation software suite, like building models, offering support and different trainings. Starting in 2018, a cross-functional team at INOSIM started to build a prototype of what is now known as Foresight – a solution that allows models to be initialized with real-time data to predict the immediate future behaviour of a production plant. For several years now, Dominik is co-lecturer for the Bioprocess simulation course at TU Dortmund and since early 2023, he is heading the Consulting team at INOSIM.

Menno Prins received a PhD in physics and worked for nearly 20 years at Philips Research. Since 2014 he has been professor at Eindhoven University of Technology, in the Molecular Biosensing group in the departments of Biomedical Engineering and Applied Physics (www.tue.nl/mbx). He investigates technologies for the continuous monitoring of biomolecules. He founded and organizes SensUs, the annual international student competition on sensors for health (www.sensus.org). He co-founded Helia Biomonitoring (www.heliabiomonitoring.com), a spin-off company that develops continuous sensing technologies for real-time industrial process control.