

EFCE SpotLight Talks

from
17 May
to
21 May
2021

by the Working Parties
and Sections

5 Webinars



EFCE

European Federation of Chemical Engineering

Welcome to the second series of EFCE SpotLight Talks.

There will be a series of talks by seven of our Working Parties: Drying, Chemical Reaction Engineering, Loss Prevention and Safety Promotion, Mixing, Multiphase Fluid Flow, Process Intensification, Thermodynamics and Transport Properties. Our previous series proved very popular with 2000 people signing in to one or more of the series of events. This time we are making a small charge for the series to help cover costs for the EFCE but it will remain free for students.

We hope you will find the series stimulating and that it will enable you to sample content from some of our groups that you may not otherwise be able to hear.

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|--------|-------|---|
| 17 May | 14:00 | Emerging Risks and Advanced Modelling within the Process Safety Horizon |
| 18 May | 09:20 | Intensification of mixing and multiphase contacting in continuous flow equipment |
| 19 May | 13:30 | Electrolyte Thermodynamics challenges from industrial needs to academic research |
| 20 May | 15:00 | Recent Developments and Further Demands in Reactive Gas-Liquid Flows |
| 21 May | 09:30 | Drying research: focus on freeze-drying, lyophilization, spray-drying and product quality |

Central
European
Time

Programs



EFCE Spotlight Talks

Working Party on Loss Prevention and Safety Promotion in the Process Industries

17 May

14:00 • 16:15
CET

Emerging Risks and Advanced Modelling within the Process Safety Horizon



The world is changing, the traditional boundaries of engineering are merging and there will be more stringent requirements of energy use, product quality, market adaptability, safety and environmental protection and further higher plant complexity. Advanced techniques are progressively providing reliable support for critical decision making and guiding the industry towards more risk-informed and safety-responsible planning, even though serious safety concerns need to be addressed when adopting digitalization. The role of process engineering should include a critical and balanced application of new developments in data science and digital technology with fundamentals science and engineering principles. Additionally, system thinking and process safety could be a real benefit to entirely different sectors and perhaps unexpected areas, according to cross-fertilizing assumptions and trans-disciplinary research modelling. This webinar will provide you with a vision of new approaches and advanced techniques illustrating the interdisciplinary features of the problem.

World class experts in the field will address a comprehensive discussion on selected themes focusing on four main challenges:

- dynamic risk management approach and system advances from a holistic digitalization perspective;*
- challenges and limitations of machine learning techniques in evaluating the safety level in industrial systems;*
- early warning detection of Covid 19 based on reaction safety methodologies, as an example of a cross-industry learning approach;*
- emerging risks and challenges towards a reliable risk assessment following digitization and system approach.*

PROGRAM

- 14:00 **Welcome and introduction**
Bruno Fabiano, Chair of Working Party on Loss Prevention and Safety Promotion
- 14:10 **Safety of Digital Process Systems**
Faisal Khan, Memorial University of Newfoundland St John's - NF Canada
- 14:35 **Are Big Data taking Industry towards a "No-brainer" Safety?**
Nicola Paltrinieri, NTNU - Norway
- 15:00 **Q&A – discussion**
- 15:10 **From Reaction Safety Modelling towards Pandemic Risk Early Detection**
Giuseppe Maschio, University of Padova - Italy
- 15:35 **What about Emerging Process Risks and Risk Management?**
Hans J. Pasman, Texas A & M University, Texas - USA
- 16:00 **Q&A - conclusions and closing**
Bruno Fabiano, Chair of Working Party on Loss Prevention

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Contact: martine.poux@toulouse-inp.fr
brown@unige.it

EFCE Spotlight Talks

Working Parties on Mixing and Process Intensification

18 May

09:20 • 11:40
am
CET

Intensification of mixing and multiphase contacting in continuous flow equipment



Process intensification is a technological strategy based on innovative process and equipment design that results in substantial benefits in industrial manufacturing processes, including reduced energy consumption, higher product quality, fewer wastes and improved safety. It typically deploys novel continuous flow equipment and/or methods that result in more compact and efficient processes. Process intensifying equipment includes devices that significantly improve the efficiency of mixing, mass and heat transfer. A wide variety of process-intensifying equipment has been developed over the past 20 years, demonstrating considerable enhancement of mixing, mass and heat transfer processes.

This webinar aims at presenting selected types of continuous flow devices and how they can intensify mixing and multiphase contacting for mass transfer and chemical reaction.

PROGRAM

- 09:20 **Welcome and introduction**
Tom Van Gerven, Chair WP Process Intensification
Joelle Aubin, Chair WP Mixing
- 09:30 **High-gravity high shear for intensified chemicals production**
John van der Schaaf, Eindhoven University of Technology – The Netherlands
- 10:00 **Overcoming mixing limitations in microreactors using acoustic streaming**
Simon Kuhn, KU Leuven - Belgium
- 10:30 **Oscillatory flows in mesoscale reactors for low Reynolds number applications**
Jonathan McDonough, University of Newcastle - UK
- 11:00 **Intensifying mixing for CO₂ capture using the NetMIX technology**
José Carlos Lopes, CoLAB Net4CO₂- Portugal
- 11:30 **Conclusions and closing**
Tom Van Gerven, Chair WP Process Intensification
Joelle Aubin, Chair WP Mixing

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Contact: martine.poux@toulouse-inp.fr
joelle.aubin@toulouse-inp.fr
tom.vangerven@kuleuven.be

EFCE Spotlight Talks

Working Party on Thermodynamics and Transport Properties

19 May

13:30 • 15:00
CET

Electrolyte Thermodynamics challenges from industrial needs to academic research

Many applications in the process industry deal with fluids that contain electrolytic species. While thermodynamic models for neutral molecules are now well established, there are still many unanswered issues related to the presence of ions in a fluid mixture. This webinar aims at informing the community about important initiatives that have been taken in order to further the understanding of these systems, both from a fundamental point of view, as applied to typical applications.



PROGRAM

A workflow for setting up an adequate thermodynamic model for process simulation

Jean-Charles de Hemptinne - IFP Energies Nouvelles, France

The EleTher Joint Industrial Project was initiated in order to set up an industrial community for promoting research on electrolyte thermodynamics. Best Practices are being identified based on some case studies that have been submitted by participating members. In this presentation, these best practices are detailed using a three-step workflow: (i) The first step is data analysis. It appears that even for simple systems, significant regions (temperature-composition) remain unexplored experimentally. (ii) The second step consists in extrapolating the data in the range of industrial interest. An example will be given using a simple graphical approach. (iii) In the third step the parameters of a process simulator model must be regressed. The Aspen e-NRTL equation is used as a benchmark to investigate this part. The presentation will summarize the achievements so far and lay some perspectives for future work. The final objective is to promote collaboration in view of a second version of the JIP.

Thermodynamic modeling of electrolyte solutions using the Debye-Hückel theory

Georgios Kontogeorgis - Center for Energy Resources Engineering (CERE), Technical University of Denmark

Electrolyte solutions are present almost everywhere, in numerous applications in chemical, biochemical, geochemical, petroleum engineering as well as in diverse disciplines such as geology, biology and medicine.

Almost 100 years ago (1923), Peter Debye and Erich Hückel published a 20-page long paper entitled "On the theory of electrolytes. I. Freezing point depression and related phenomena". This single manuscript, adopting the (then) pioneering concept (by Bjerrum) of complete dissociation of strong electrolytes, has revolutionized the field of electrolyte thermodynamics. Debye received the Nobel prize in 1936.

The Debye-Hückel theory has since 1923 been cited thousands of times, and mentioned even more without citation, derived and interpreted in numerous ways, approximated, extended, generalized, incorporated in other "more general" electrolyte models, compared to more "modern" approaches (like the mean-spherical approximation), called various things and re-baptized in many names (e.g. Debye-Hückel limiting law, extended law, etc), used (and misused) in many ways and many times. McQuarrie wrote in 1976 in his famous book about Statistical Mechanics "*in spite of the great success of the Debye-Hückel theory, when it was originally proposed its range of validity was not at all clear*". Is it today?

The story of the Debye-Hückel theory was and is under extreme debate with many controversial aspects. In this lecture, I will try to present a modern status of the Debye-Hückel theory and outline both capabilities and limitations, from fundamental and engineering points of view. Future directions will also be briefly outlined.

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Contact: martine.poux@toulouse-inp.fr
susanna.kuitunen@neste.com
jean-charles.de-hemptinne@ifpen.fr

EFCE Spotlight Talks

Working Parties on Multiphase Fluid Flow and Chemical Reaction Engineering

20 May

15:00 • 17:45
CET

Recent Developments and Further Demands in Reactive Gas-Liquid Flows



In order to design climate-friendly and sustainable processes with low resource consumption and reduced emissions, it is necessary to produce chemicals with high yield and selectivity. To achieve this, the transport processes within a reactor and the chemical reaction network must be suitably adjusted and controlled. In many fast gas-liquid reactions, such as oxidations, hydrogenations, or chlorinations, the time scale of transport across the liquid interface, through boundary layers and bubble wakes, and mixing by agitation and buoyancy-driven convection play a dominant role, in addition to the kinetics of the reaction networks. In recent years, tremendous progress has been made with new methods in experiment and numerical simulation, allowing deeper insights and targeted improvement of processes. Such opportunities will be presented and discussed in this spotlight talk and further needs will be addressed. Participants from academia and industry are welcome.

PROGRAM

- 15:00 **Welcome and introduction**
Michael Schlueter, Chair of WP Multiphase Fluid Flow
Olaf Hinrichsen, Chair of WP Chemical Reaction Engineering
- 15:10 **Interaction of reaction and internal fluid dynamics in jet loop reactors**
Erik von Harbou and Ferdinand Breit - University of Kaiserslautern, Germany
Oliver Bey, BASF, Ludwigshafen - Germany
- 15:35 **Hydrodynamics and photon transport in gas-liquid photoreactors**
Simon Kuhn, Process Engineering for Sustainable Systems, KU Leuven - Belgium
- 16:00 **Reactive mass transfer and deposit in the wake of confined bubbles**
Karine Loubiere, Anne-Marie Billet, Nicolas Dietrich - FERMAT, University of Toulouse - France
- 16:25 **Modeling and Simulation of Reactive Mass Transfer across Fluid Interfaces**
Dieter Bothe, Department of Mathematics, Technical University of Darmstadt - Germany
- 16:50 **Controlling and leveraging gas bubbles in electrochemical energy technologies**
David A. Vermaas, TU Delft - The Netherlands
- 17:15 **CO2 absorption/capture modelling by Computational Fluid Dynamics validated with experimental data**
Dr. Yi Ouyang, Ghent University - Belgium
- 17:40 **Conclusions and closing**

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Contact: martine.poux@toulouse-inp.fr
michael.schlueter@tuhh.de
olaf.hinrichsen@ch.tum.de

EFCE Spotlight Talks

Working Party on Drying

21 May

09:30 • 12:30
CET

Drying research: focus on freeze-drying, lyophilization, spray-drying and product quality

Drying is an essential physical unit operation that can be found in a lot of production processes within the chemical, pharmaceutical, and food sectors among others. It is usually considered that about 10 to 15% of the industrial energy consumption is due to drying operation. Besides being an energy intensive operation, drying can be crucial in terms of final product quality. This is why drying research remains an important field, with development related to the design of new or more efficient dryers, the better understanding of the relation between drying operating conditions and product quality, the reduction of the environmental impact, ... based on both experimental and modeling approaches.

The aim of this webinar is to highlight some of the research done in the drying field by PhD students within EFCE members.



PROGRAM

09:30 **Welcome and introduction**

Angélique Leonard, Chair of WP Drying

09:40 **Session 1 - Freeze drying and lyophilization - Modeling**

- Mathematical modelling of heat and mass transfer during freeze-drying using high-throughput vial systems to accelerate the development of new vaccines
Juan Buceta-Correa-De-Borba (Université Paris-Saclay-INRAE-AgroParisTech)
- NIR and IR as monitoring tools for freeze-drying processes
Maite Harguindeguy and Serena Bobba (Politecnico Torino)
- Pore network generation and parameterization based on image data and experiments of freeze-drying
Nicole Vorhauer and Maximilian Thomik (Magdeburg University)
- Modernizing manufacturing of parenteral products: from batch to continuous lyophilization
Merve Adali and Lorenzo Stratta (Politecnico Torino)
- The role of liquid films in drying capillary porous media investigated by 3D pore network models
Hafiz Tariq Mahmood (Magdeburg University)
- Discussion

11:00 **Session 2 - Quality aspects and monitoring in food drying**

- Encapsulation of aroma compounds by spray drying of concentrated asparagus juice
Joanne Siccama (Wageningen University)
- Use of image analysis to evaluate oil-in-water emulsions stabilized with an artichoke by-product before and after spray drying
Mónica Umaña (University of the Balearic, Spain)
- Impact of pulsed electric field pretreatment and ultrasound application in drying kinetics and antioxidant properties of kiwifruit (*Actinidia deliciosa*)
Beatriz Llavata (Universitat Politècnica de València)
- Analysis of solar air heaters for drying applications
Gedion Habtay (Hungarian University of Agricultural and Life Science, Godollo)
- Use of air-coupled ultrasound for the real-time and non-invasive process monitoring. Application to potato air drying
Virginia Sanchez-Jimenez (Universitat Politècnica de València)
- Discussion

12:20 **Conclusion**

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Contact: martine.poux@toulouse-inp.fr
a.leonard@uliege.be