



## Webinar Series 2021: Fast, efficient & reliable problem solution

A series of six webinars on different topics related to process and product engineering has been organized by PSE for SPEED. The series will consist of the following webinars: 1) 3-days workshop on sustainable chemical (and biochemical) process design; 2) a 4-hours workshop on pure component and mixture properties estimation; 3) a 3 hours workshop on refrigerant design; 4) a 3 hours workshop on different aspects of chemical substitution; 5) a 4 hours workshop on general computer aided chemical product design; 6) a 4 hours workshop on computer aided modelling. See the table below for the date and time (in Central European Time) for the webinars.

### Program for Webinar 5: Systematic and Reliable Chemical Product Design

The objective of this workshop is to give the participants a view on various aspects related to chemical product design, their sustainable production as well as their application. Sustainability of modern society depends very much on chemicals-based products that are used from the time a person wakes up in the morning to the time the person goes to sleep. Design and development of chemicals-based products is broadly classified into those that are process centric and those that are product centric. While significant advances have been made in the development of systematic model-based techniques for process design including optimization and control, much work is needed to reach the same level for chemical products. In terms of current challenges and opportunities, issues related to integrated product-process design, modelling related to product properties and functions, and how to find novel, innovative and better products need to be addressed. To achieve this, an integrated model-experiment based design approach employing a systematic computer-aided framework with built-in design templates is necessary.

In Webinar 5, methods for systematic and reliable chemical product design will be highlighted in terms of background theory, product classification, problem definition and solution approaches. Also, uses of a chemical product simulator, ProCAPD (Computer Aided Product Design), will be highlighted for design, analysis and verification of different types of chemical products.

The guest speaker for Webinar 5 is Professor André Bardow from ETH-Zurich and he will talk about CAMPD (Computer Aided Molecular Product Design) methods based on PC-SAFT and quantum chemistry.

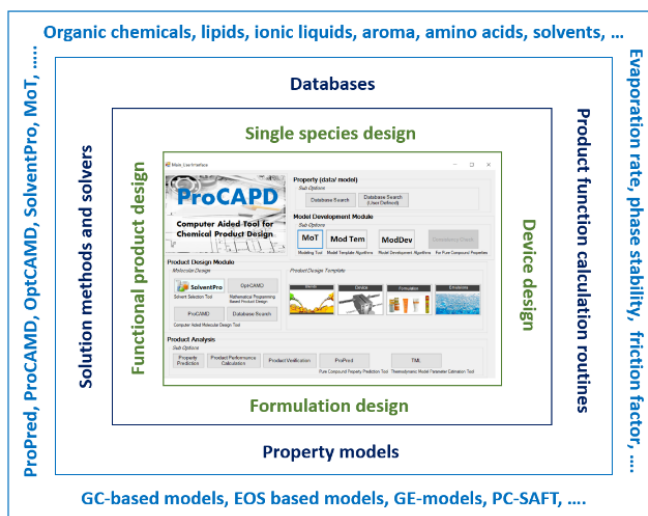
### Course Organization

The Webinars are being organized by the PSE for SPEED office in Bangkok, Thailand. All confirmed registered participants will be sent a link to join the Webinars. The time indicated for each lecture includes Q&A after the lecture. The problem solution lectures will include step by step demonstration of selected problem solutions. There will be Q&A at the end of all lectures and also at the end of the problem sessions. Selected recorded presentations will also be available to subscribers to the PSE for SPEED YouTube channel and Webinar participants will be able to download copies of the presentation slides from the link:

<https://www.pseforspeed.com/webinar-lecture-and-recorded-video/>

Please direct all your questions to the PSE for SPEED in Bangkok to Ms. Orakotch Padungwatanaroj (P.orakotch@gmail.com).

## Webinar 5: Systematic and reliable chemical product design (9 September)



- Similar to the concept of process simulator, ProCAPD helps users to design, analyze and verify different types of chemical-based products;
- The current version can be used for single molecule design, formulation design and mixture-blend design employing product specific design templates;
- Users can select different solution approaches, such as, database search, generate & search (ProCAMD), direct optimization (OptCAMD) and a special tool for pharmaceutical industry;
- Links to other tools developed by PSE for SPEED are also available

Lecture	Time (CET)*	Topic	Speaker
1	13:00 – 14:00	Chemical Product Design: Introduction (theoretical background, product classification, solution approaches, ...)	Rafiqul Gani
2	14:00 – 15:00	Chemical product design case studies (single molecules, blends, formulations, functional products)	Rafiqul Gani
3	15:00 – 16:00	CAMPD methods based on PC-SAFT & quantum chemistry	Prof André Bardow
4	16:00 – 17:00	Problem solution using ProCAPD (database features, product design examples: single molecule, blends, formulations) plus Q&A	Orakotch Padungwatanaroj; Siriporn Jalernsuk

\*The change in time (start time is 13:00 CET, Central European Time)

*Next PSE for SPEED Webinar is on 16 September on Systematic & Rapid Model Development (Webinar 6, starting at 13:00 CET)*