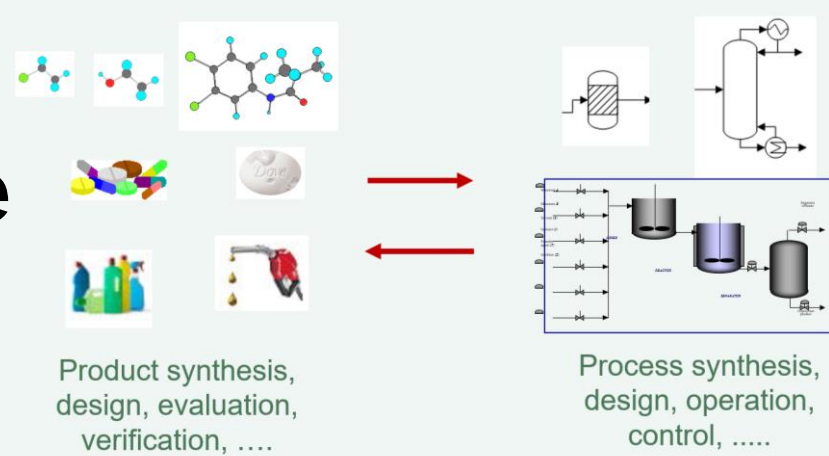


Fast, Efficient & Reliable Problem Solution

A series of six webinars on different topics related to process and product engineering



About the webinars

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:



3-days workshop
on sustainable chemical
(and biochemical) process design



4-hours workshop
on pure component and
mixture properties estimation



3 hours workshop
on refrigerant design



3 hours workshop
on different aspects of
chemical substitution



4 hours workshop
on general computer aided
chemical product design



4 hours workshop
on computer aided
modelling.

- Highlight important issues, various problem definitions, systematic work-flow and data-flow needed to solve the problems.
- Brief overview of the specific computational methods and tools needed to solve the problems.
- The step by step problem solution (discussion plus software demonstration, where use of a suite of computer aided tools will be highlighted).

Course Organization

Lecture & Tutorial Sessions

- Lecture modules (35-40 min) where the basic concepts, methodology overview & solution steps will be highlighted, followed by brief problem solution sessions (demonstrations of the solution steps)
- Case studies with detailed problem solution (35-40 min). Documentation (lecture slides; tutorial problem formulations & solutions; software tool manuals; etc.) in electronic form will be made available for free download.

Lectures and problem solution sessions will be given by Prof Rafiqul Gani, Dr. Anjan K Tula and personnel of PSE for SPEED Thai-office Orakotch Padungwatanaroj; Nichakorn Kuprasertwong; Kornkanok Udomwong). See also list of invited speakers

Webinar participation is free, but registration is required and accepted on a first-come-first-served basis.

Who should attend?

Engineers, scientists, students, and practitioners interested in the topics.

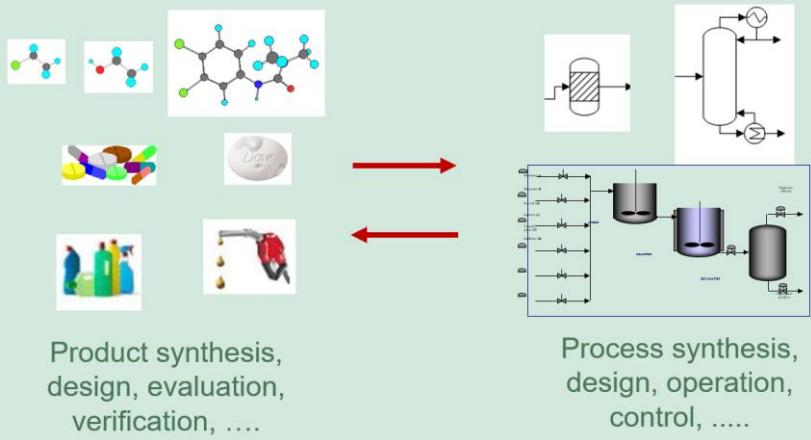
That is, anybody who is interested in one or more of the topics covered in the six webinars.

Registration

Please send an email to webinars@pseforspeed.com indicating name, affiliation, status and the webinars of interest.

Participation

Participants will be provided with a login to join the specific webinar after their registration is received.



Webinar Series 2021: Fast, Efficient & Reliable Problem Solution

WEBINAR 1:

14 - 16 July
14:00 - 18:00 (CET)

Sustainable process design in 12 hierarchical steps consisting of a 3-stage methodology

14 July - Process synthesis stage (general overview, hierarchical method superstructure optimization; hybrid process group-contribution)

15 July - Process design-analysis stage (equipment design, process simulation; analysis (cost, LCA, etc.), hot-spot identification & define targets for improvements.

16 July - Process innovation stage (generate & test alternatives that match desired targets through hybrid, intensification, etc., schemes)

Tools to be used:
ProCAFD & associated tools (Super-O; Pure; Process simulator (ProII, ICAS); LCSOFT, ECON, & etc.)

WEBINAR 2:

27 July
14:00 - 18:00 (CET)

Property estimation in 4 simple steps

- Giving molecule-mixture data
- Selecting/retrieving data-model
- Properties estimation
- Verifying or fine-tuning solution

Tools to be used:
ProCAPE and associated tools (Database-P; MoT; Pure; Mixture; etc.)

WEBINAR 3:

16 August
14:00 - 17:00 (CET)

Refrigerant design, selection, verification

- Database search
- Refrigerant property estimation
- Refrigerant substitution
- Cycle simulation
- etc.

Tools to be used:
ProREFD and associated tools (database-R, MoT, Pure, Mixture, etc.)

WEBINAR 4:

25 August
14:00 - 17:00 (CET)

Chemical substitution

- Database search for harmful effects
- Missing property estimation
- Product analysis to identify harmful chemical
- Harmful effect score
- Chemical substitution

Tools to be used:
ChemSub and associated tools (database-CS, pure, mixture, etc.)

WEBINAR 5:

9 September
14:00 - 18:00 (CET)

Systematic and reliable chemical product design

- Introduction to general chemical product design
- Methods and tools for chemical product design
- Case studies

Tools to be used:
ProCAPD and associated tools (Database-CP, pure, etc.)

WEBINAR 6:

16 September
14:00 - 18:00 (CET)

Systematic & rapid model development

- Define model objective
- Create-transform- solve- apply created models (examples of various types of models)

Tools to be used:
ModFrame (MoT, etc.)

Confirmed Invited speakers

- Prof Ignacio Grossmann on Process synthesis, 14 July (Carnegie-Mellon University)
- Prof Mario Eden on Process design-analysis, 15 July (Auburn University)
- Prof Stratos Pistikopoulos on Process Innovation, 16 July (Texas A&M University)
- Prof John O'Connell on Property estimation, 27 July (Emeritus Professor of Chemical Engineering at University of Virginia)
- Prof Nick Sahinidis on Refrigerant design, 16 August (Georgia Tech University)
- Prof Andre Bardow on Chemical product design, 9 September (ETH-Zurich)
- Prof Fengqi You (Cornell University) and Prof Jay H Lee (KAIST) on Model development and use, 16 September

Fast, Efficient & Reliable Problem Solution
Short description of the special tools in the webinar workshops

Webinar 1: ProCAFD

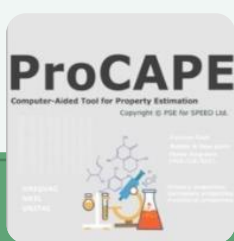
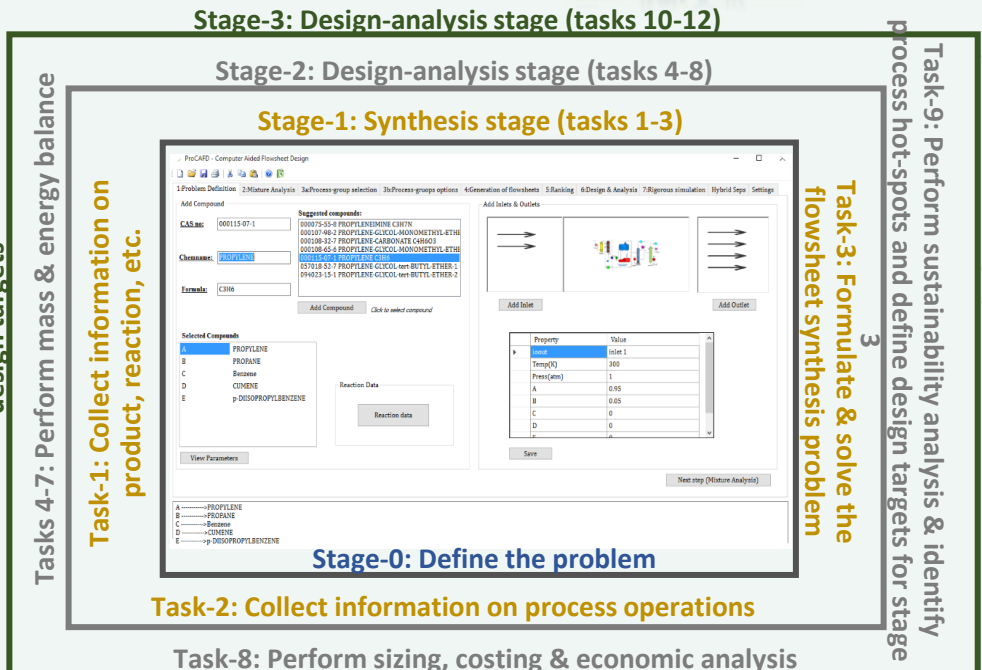


Computer Aided Flowsheet Design

(Database; Super-O; Pure; Process simulator (ProII, ICAS); LCSOFT, ECON, & etc.)

ProCAFD employs the three stages and 12 tasks methodology to obtain sustainable process designs. After problem definition, Stage-1 consists of steps 1-3 related to process synthesis employing simple models (heuristic, superstructure optimization and process-groups methods are available). If a process flowsheet is already available, this step is not needed. Stage-2 performs process design and analysis for a given process flowsheet. The analysis includes economics, LCA and sustainability issues to identify process hot-spots, which help to define process improvement targets. Stage-3 generates alternatives that match the design targets and thereby finds more sustainable designs. Hybrid and process intensification concepts are applied.

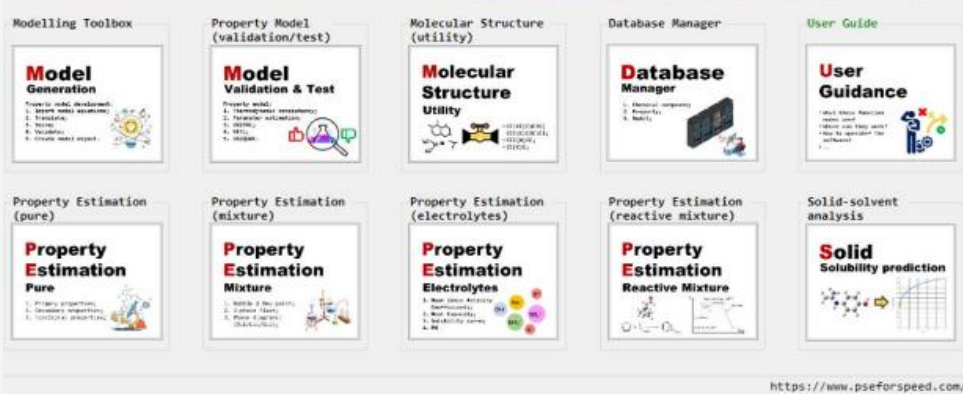
Task-10: Perform heat & mass integration to match design targets



Webinar 2: ProCAPE

Computer Aided Property Estimation

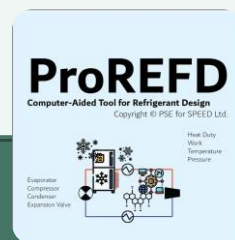
(Database; MoT; Pure; Mixture; etc.)



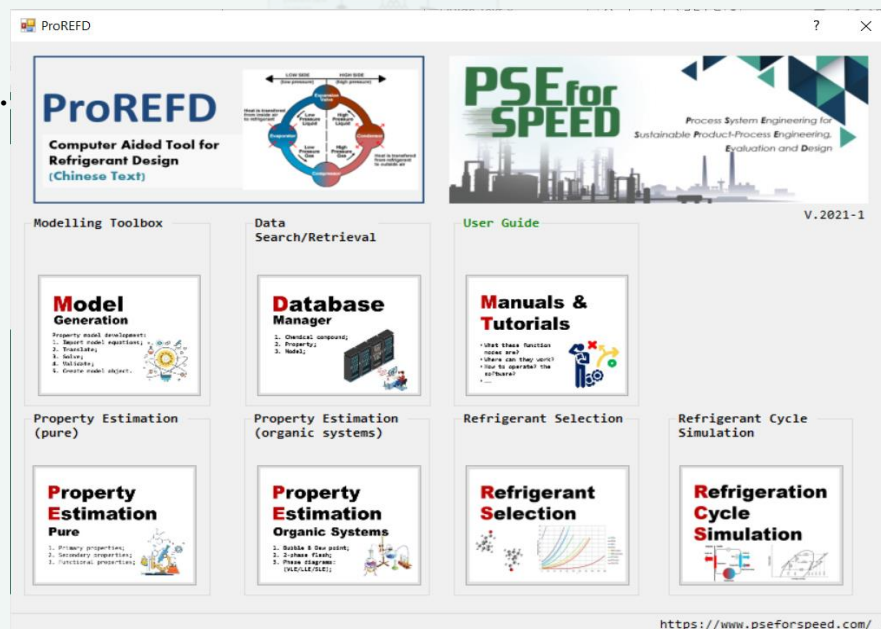
- Model Generation - Create and retrieve property models (UNIFAC, PC-SAFT, SRK EOS,..) from library
- Model Validation - Estimate, fine-tune, validate model parameters
- Molecular Structure Utility - Give molecular description, get groups, connectivities, etc., representation
- Solid Solubility - SLE predictions for wide range of organic systems
- Database: Retrieve property data (chemicals, solvent, lipids, ...)
- Property Estimation-Pure - Give molecular description, get 57 single value and 9 function properties (new updated models plus ML-based models)
- Property Estimation - Mixture - Give mixture description, get VLE, SLE, LLE, phase diagrams, saturation (bubble or dew) points, driving force, ...

Webinar 3: ProREFD

Refrigerant design, selection & verification



- Modelling Toolbox (MoT) - In-house algebraic equations solvers, integrators, ordinary differential equation solvers and optimizers for model development.
- Database Manager - Search and retrieval engine for the refrigerant properties, measured binary mixture phase equilibrium experiments and azeotropic data.
- Property Estimation (Pure) - Pure properties prediction tool consists of 60 different pure component properties.
- Property Estimation (Mixture) - Properties prediction tool for refrigerant (organic) mixtures, phase equilibrium properties (VLE), and saturated data.
- Refrigerant Selection - The tool for designing, replacing and optimizing refrigerants for a specific application based on requirements.
- Refrigerant Cycle Simulation - Perform a refrigeration cycle of compounds, Thermodynamic diagrams (cycle operation embedding), sensitivity analysis.



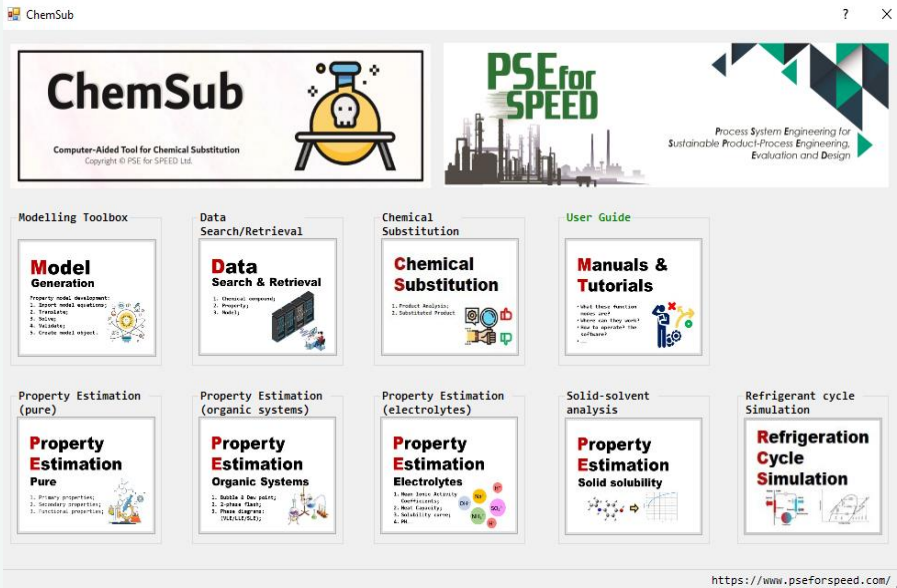
ChemSub

Computer-Aided Tool for Chemical Substitution
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Webinar 4: ChemSub

Chemical substitution (harmful chemicals analysis)

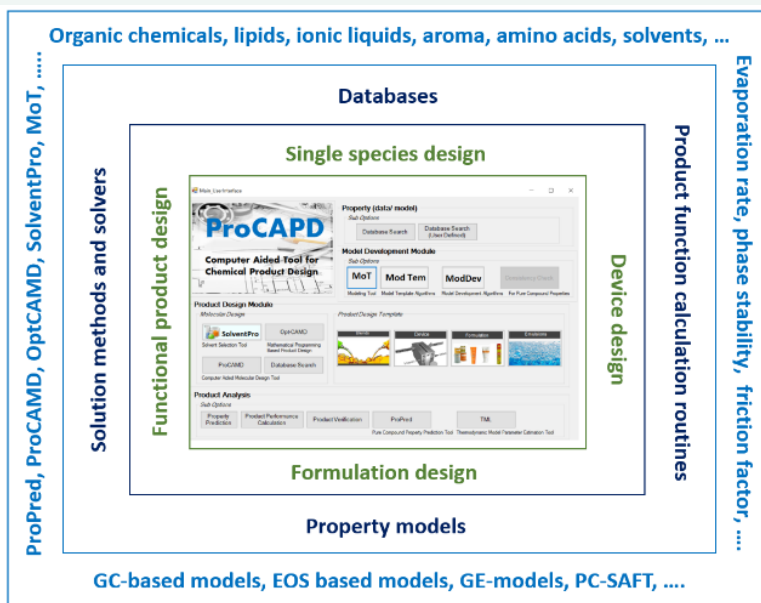


ChemSub is a tool for analysis of chemical products and substitution of chemicals that has unacceptable health, safety and environmental hazards with chemicals with acceptable properties. There are two main functions in chemical substitutions

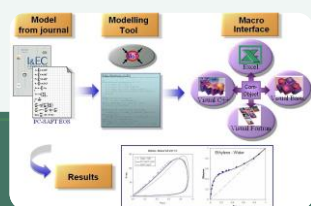
- **Database Manager** - Properties, Hazardous Effects, Chemical Uses, Chemical Types and User Databases are available for search options.
- **Chemical substitution**
 - **Product Analysis** : Analyzes products in terms of hazardous effects of the product and identify the chemicals that need to be substituted because of the hazardous effects.
 - **Substituted Product**: Performs search for alternatives to the identified harmful and evaluate the new product with the substituted chemicals.

Webinar 5: ProCAPD

Computer Aided Product Design



- The first and only computer aided tool, similar in concept to process simulators, available for users in industry as well as academic
- Useful for single molecule design, formulation design and mixture-blend design using design templates
- Allows various types of problem definitions and solution strategies (database search, generate & search (ProCAMD) , direct optimization (OptCAMD) and special tool for pharmaceutical industry (SolventPro for solvents and solid solubility).
- Supported by a collections of databases; property prediction tools and modelling tools



Webinar 6: ModFrame

Computer Aided Modelling

- Fast and flexible model creation (type equations with simple syntax, import text-files, other formats)
- Performs model analysis and equation ordering before solving
- Allows us of different model solution strategies plus links to in-house numerical solvers
- Provides options for model reuse, export and development of model-based systems
- Provides optimization features for model-based process optimization as well as regression of model parameters
- Features for sensitivity analysis with different methods

