21 & 22 SEPTEMBER 2022
@ Pullach (Munich), Germany & Online

PROGRAM

CAPE-OPEN 2022 ANNUAL MEETING

21 September 2022

09:00 **Welcome | Oliver KOCH ([Linde](#)) & Michel Pons ([CO-LaN contractor](#))**

09:10 **[Methods & Tools SIG](#) [progress report](#) | Michael Hlavinka (BR&E)**
Contributor: Bill Barrett (US Environmental Protection Agency)
Michael is Technical Director at Bryan Research & Engineering, recipient of the CAPE-OPEN 2016 Award. Michael is active in the Methods & Tools Special Interest Group (SIG) as well as in the UNIT SIG of CO-LaN.

09:35 **[Threading: COM, COBIA, Status, interoperability and challenges](#) Jasper van Baten ([AmsterCHEM](#))**
Jasper is a leading expert in CAPE-OPEN, has developed its own suite of PME and PMCs, is regularly providing consultancy services on the implementation of CAPE-OPEN interfaces, is active in all CO-LaN SIGS. Jasper received the CAPE-OPEN 2006 Award for the creation of the CAPE-OPEN based simulator COCO. He has been contracted by CO-LaN to develop COBIA.

10:05 **[Efforts of developing a CAPE-OPEN COBIA](#) [compliant REST-API](#) Mark Nicholas Jones (Molecular Quantum Solutions ApS)**
Contributor: Lukasz Ruszczynski (Molecular Quantum Solutions ApS)
Mark Nicholas Jones studied chemical engineering at the Karlsruhe Institute of Technology (KIT) and at Technical University of Denmark (DTU), followed by a PhD and postdoc position there. In 2019, together with Lukasz Rusczcynski, he founded the start-up Molecular Quantum Solutions (MQS) to integrate quantum chemistry calculations for property prediction with higher-layer applications such as computer aided molecular design or unit operation modelling.

10:30 Coffee Break

10.50 **[Thermo SIG](#) [report](#) | Jasper van Baten ([AmsterCHEM](#))**
Contributor: Sergej Blagov (BASF SE)
Jasper, together with Sergej who a thermodynamic expert at BASF, co-leads the the CO-LaN Special Interest Group focusing on thermodynamics. Sergej received the CAPE-OPEN 2014 Award.

11:15 **[Exporting Custom Properties](#) to CAPE-OPEN. | Ross Taylor (Clarkson University/[Chemsep](#)) (recording)**
Contributor: Harry Kooijman (Clarkson University)
Ross is the Liya Regel and Bill Wilcox Distinguished Professor of Engineering at Clarkson. He received his Bachelor of Science, master's, and Ph.D. degree from the University of Manchester Institute of Science and Technology. Since joining Clarkson in 1980 the focus of the work of Taylor and his students has been on the development of better computer models for the simulation and design of distillation and absorption processes. He is the co-creator – with H.A. Kooijman – of the software package ChemSep, winner of the 2017 CAPE-OPEN Award. Ross received the Computing and Chemical Engineering Award from the American Institute of Chemical Engineers (AIChE) in 2004. In 2020 he was named a Fellow of the AIChE. The book "Multicomponent Mass

Transfer" authored by Taylor and R. Krishna, published by John Wiley & Sons in 1993, has won wide acclaim as an authoritative textbook on this subject and one that has changed the way mass transfer is taught.

11.30	**Developing fast and accurate thermodynamic packages for the green transition with Q-props	Bjørn Maribo-Mogensen (Hafnium Labs)**

Bjørn is the co-founder of Hafnium Labs that develops simulation software to bring state-of-the-art research in thermodynamics, physical properties, and computational methods to industrial application. Bjørn received the EFCE Excellence Award in Thermodynamics and Transport Properties 2015. Bjørn is a guest member of the EFCE Working Party for Thermodynamics and Transport Properties (WPTTP). Hafnium Labs is also involved in several research projects aimed at improving thermodynamic models for electrolyte systems such as the ERC-Electrothermo (DTU) and Elether 2 JIP (IFPEN).

11:55	**Field Report – Using CAPE-OPEN to couple HTRI's Xchanger Suite with Linde's General Multiphase Property System** **Stefan Gewald (Linde GmbH, Linde Engineering Division)**

Stefan is an equipment process design expert and is mainly responsible for the design of shell & tube heat exchanger and coil-wound heat exchanger. He is also involved in R&D activities that aim at the further development of Linde in-house design programs and methods. Stefan participates in vendor audits and reviews offers from suppliers. Stefan joined Linde in 2014 after he obtained a B.Sc.in chemical engineering and a M.Sc. in energy and process engineering at Technical University Munich.

12:15	Lunch break

13:15	**Annual General Meeting of Members** **CO-LaN activities and perspectives	Richard Baur (Shell)**

Richard is Model Development Lead, within Hydro Processing Research & Development at Shell Global Solutions International BV and is representing Shell in CO-LaN, assuming the role of President of CO-LaN since October 2016.

CO-LaN Financial report | Philippe Arpentinier (Air Liquide)

Philippe is a scientific advisor within Air Liquide and has been assuming the role of Treasurer of CO-LaN since December 2015. Philippe received his B.Sc. in chemical engineering from ENSIC Nancy in 1985 and obtained his Ph.D. from Ecole des Mines de Paris.

14:15	Coffee Break

14:30	**Interoperability SIG report	Malcom Woodman**

Since 2007, Malcolm has been leader of the Interoperability SIG. This Special Interest Group provides tools and advice to support the achievement of CAPE-OPEN interoperability and to carry out interoperability testing where appropriate.

14:45   **Test Suite, demo & next steps for CAPE-OPEN Test Suite**
Malcom Woodman (MR Woodman Consulting)

MR Woodman Consulting Ltd provides engineering related scientific and technical consulting activities. It operates as a private limited compnay and was incorporated in 2016. Malcolm WOODMAN is the director of MR Woodman Consulting Ltd that has supplied services to CO-LaN since 2018.

15:30   **Workshop: feedback on testing | Malcom Woodman**

To discuss both what we have done so far and how we move forward on PME testing. An opportunity for all to criticise, provide feedback and explain what they need (especially for PME testing).

16:15   **Workflow improvements applying CAPE-OPEN amine wash units in process design with UniSim Design at Linde Engineering**
Anna-Maria Fischer (Linde GmbH, Linde Engineering Division)
Contributor: Alexander Prelipceanu (Linde GmbH, Linde Engineering Division)

Anna-Maria is a Senior Process Engineer at Linde Engineering, specialized in Hydrogen- and Synthesis Gas-Plants. In 2010, she obtained her B.Sc. degree in chemical engineering from Technische Universität München.

16:40   **Meeting adjourns**

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08:55   **Welcome of participants**

09:00   **Process synthesis of advanced NH3 and MeOH plants with gas switching reforming (GSR) | Carlos Arnaiz del Pozo (Universidad Politécnica de Madrid)**
Contributors: Ángel Jiménez Álvaro (Universidad Politécnica de Madrid), Schalk Cloete (SINTEF Industry)

09:20   **Using CAPE-OPEN to make a Python package accessible within PRO/II**
**Sebastian Liebschner (Sunfire GmbH)**

Sebastian studied physics at the Technical University of Dresden and Queen Mary University of London. After receiving his MSc in 2016 he did his PhD in particle physics focusing on the simulation of particle collision as studied at the LHC at CERN. Since 2020 Sebastian is working for Sunfire GmbH, where he is responsible for the development and accessibility of a Python package simulating a stack of fuel/electrolysis cells.

09:35   **ProTreat CAPE-OPEN Property Package**
Simon Weiland (Optimized Gas Treating Inc.) (recording)
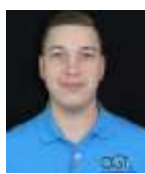
Simon joined Optimized Gas Treating, Inc. as a Software Development Engineer in May, 2014. Following four years of software development experience, Simon became a Technical Applications Engineer in 2018 in which position he is responsible for key accounts, employee and customer training, and workshops. Simon received his B.S. in Chemical Engineering with a minor in German from the University of Oklahoma in 2014. He is expert in fundamentals-based modeling of sulphur recovery operations and is a subject matter expert in sulphur recovery and gas treating.

09:50   Coffee break

10:10   **Learning from flowsheets**
Artur Schweidtmann (TU Delft / Process Intelligence Research)

Artur M. Schweidtmann is a tenure-track assistant professor for chemical engineering at Delft University of Technology and director of the Process Intelligence Research lab (www.pi-research.org). His research focuses on the combination of artificial intelligence and chemical engineering. He received his Master of Science from RWTH Aachen University in 2017 and defended his Ph.D. from RWTH in 2021, both in Chemical Engineering. During his studies, he spent the academic year 2013/2014 at Carnegie Mellon University as a visiting student via the DAAD ISAP program. He performed his Master thesis at the University of Cambridge.

10:35   **Workshop: CAPE-OPEN 2.0 | Michel Pons (CO-LaN contractor)**

Michel PONS started to be involved in CAPE-OPEN back in the mid-90s when the first industrial consortium preparing for CAPE-OPEN was formed: OO-CAPE. Within the CAPE-OPEN project that he formally joined in 1998, he was, on behalf of ELF, in charge of the Work Package targeted at numerics. Within the Global CAPE-OPEN project, he led, on behalf of TOTAL, the work package defining CO-LaN. He serves as Chief Technology Officer of CO-LaN since 2005. Michel holds a B.Sc. in chemical engineering from Université de Lorraine, France, a M.Sc. in chemical engineering from Northwestern University and a Ph.D. in chemical engineering from Université de Lorraine.

11:35   **Prototyping a monitoring tool for an underground gas storage site using Python code and CAPE-OPEN components**
Martin Gainville (IFP Energies Nouvelles)

Martin contributed to the development of CAPE-OPEN Dynamic Unit Operations at IFPEN and was leader of the Hydrodynamic Special Interest Group at CO-LaN during the SIG existence, supervising the development of an interface specification for hydrodynamic modules that was prototyped at IFPEN.

12.00   **End words | Richard Baur (Shell) & Michel Pons (CO-LaN contractor)**