



## Interoperability with CAPE-OPEN.

A demonstration to re-use a MATLAB® unit model in different process simulators.

Oliver Koch, Linde Engineering  
Robert Kender, TU Munich  
Munich, 04.06.2019



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*Linde*

# Agenda



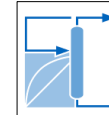
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1. Motivation
2. What is CAPE-OPEN?
3. Who is CO-LaN?
4. How does interoperability work with CAPE-OPEN?
5. Why is CAPE-OPEN important for Linde Engineering?
6. Why is CAPE-OPEN important for you?



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## Current Situation

- CO-LaN develops and promotes the CAPE-OPEN standard
- CAPE-OPEN standard allows interoperability between different engineering tools
- CAPE-OPEN is actually implemented in many commercial and academic engineering tools
- Industrial engineers have a rather low awareness about CAPE-OPEN
- Linde is member of the non-profit organization CO-LaN
- CAPE-OPEN is part of Linde Engineering's IT strategy

## Objective

- Create awareness about CAPE-OPEN and CO-LaN
- Introduce into capability and applicability of CAPE-OPEN
- Introduce into business cases for Linde Engineering
- Show up business cases for industrial and academic engineers

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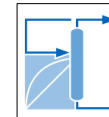


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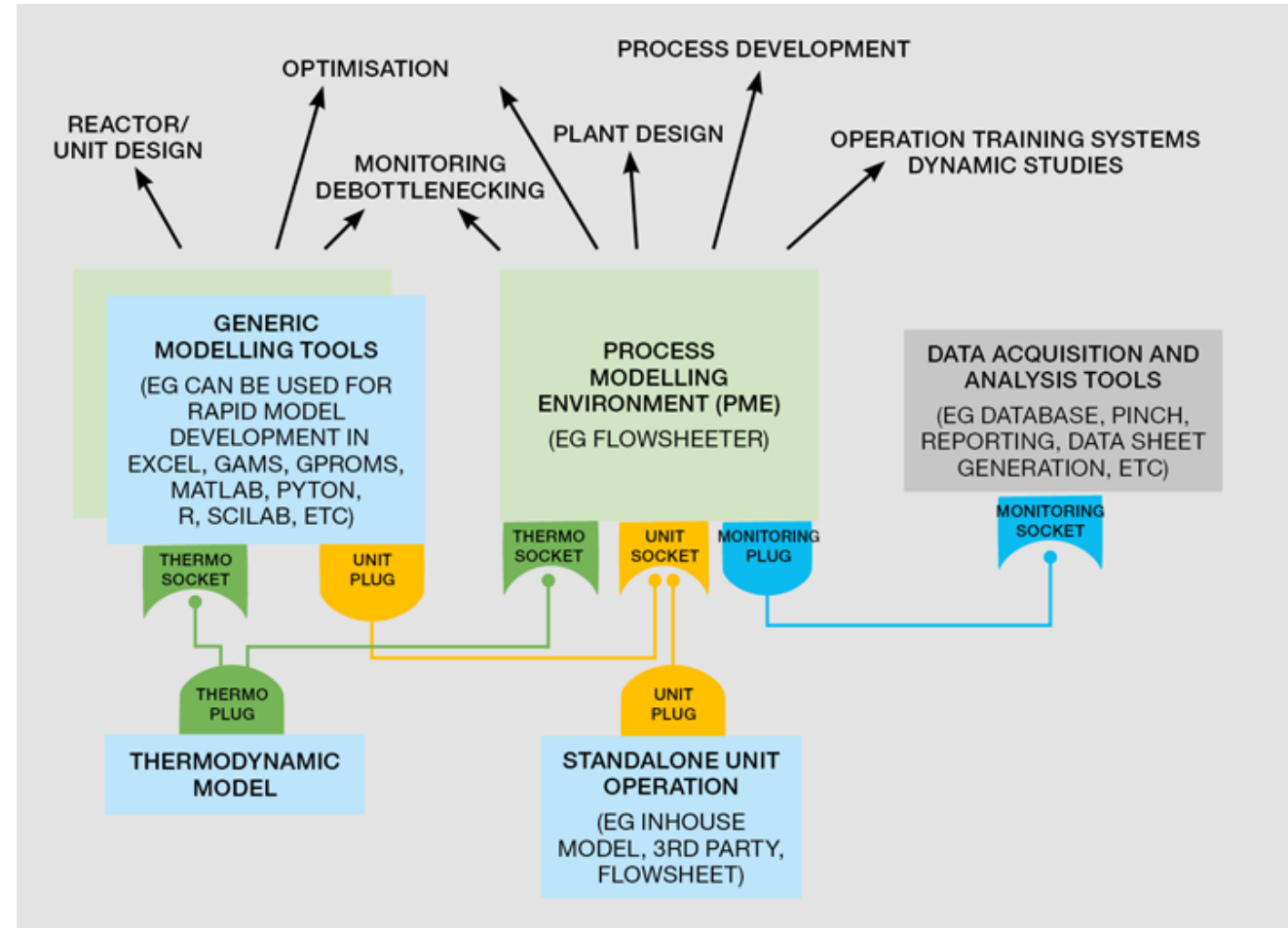


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# What is CAPE-OPEN?



- The CAPE-OPEN standard defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate
- CAPE-OPEN defines currently these (business) interface specifications:
  - Partial Differential Algebraic Equations
  - Numerical solvers
  - Thermodynamics and Physical Properties interface specification
  - Unit Operation interface specification
  - Petroleum Fractions
  - Chemical Reactions
  - Physical Properties Data Bases



Picture from The Chemical Engineer (11<sup>th</sup> January 2019)  
<https://www.thechemicalengineer.com/features/better-together/>

# Where is CAPE-OPEN implemented?



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## Process Modeling Environments (selection)

- Scilab
- Aspen HYSYS
- COFE
- IndissPlus
- ProMax
- Simulis Thermodynamics
- BatchReactor
- gPROMS
- BatchColumn
- ProSimPlus
- Petro-SIM
- COMSOL
- UniSim Design
- VALI
- PRO/II
- Aspen Plus
- MOSAICmodeling
- XChanger Suite

## Process Modeling Components (selection)

- MATLAB® Unit Operation
- REFPROP CAPE-OPEN
- MEMSIC
- CAPCO2
- VMGThermo
- COUSCOUS
- TEA
- Simulis Thermodynamics
- Aspen Properties
- Gas-Liquid Cylindrical Cyclone
- MultiFlash
- ChemSep
- IK-CAPE
- Shortcut
- Cosmotherm
- Scilab Unit Operation
- Xchanger Suite

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## Who is CO-LaN?



- CO-LaN is a non-profit organization founded in 1995 (EU project)
- Membership is free for associate members (software vendors, universities and individuals)  
<http://www.colan.org/category/member/2-corporate-associate-member/>  
<http://www.colan.org/category/member/3-individual-associate-member/>
- Corporate full members (“industrial CAPE-OPEN users”) pay an annual fee and are represented in the management board  
<http://www.colan.org/category/member/1-corporate-full-member/>



The missions of CO-LaN are:

1. Promote cooperation among CAPE software vendors to ensure that the CO standards actually translate into commercially valuable interoperability according to users priorities
2. Promote CAPE-OPEN standard to end-users and distribute CAPE-OPEN information and technology internationally
3. Maintain and develop CAPE-OPEN interface specifications
4. Supply testing facilities to support development of components and interoperability of PMC and PME vendors
5. Provide training, guidelines and tools for CAPE-OPEN development

## Selected Additional References to CO-LaN and CAPE-OPEN



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- CAPE-OPEN on Wikipedia  
[https://en.wikipedia.org/wiki/CAPE-OPEN\\_Interface\\_Standard](https://en.wikipedia.org/wiki/CAPE-OPEN_Interface_Standard)
- CO-LaN Homepage  
<http://www.colan.org>
- MATLAB® Unit Operation potential improvements for academic use  
<http://www.colan.org/presentation/matlab-uo-in-aspen-plus/>
- A Rate-Based Equation-Oriented Parallel Column Model: Application to Dividing Wall Columns  
<http://www.colan.org/presentation/chemsep-dwc/>
- AmsterCHEM  
<https://www.amsterchem.com/>

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Software components needed for demonstration:

1. CAPE-OPEN compatible process simulator  
<http://www.colan.org/category/process-modeling-environment/>
2. MATLAB® CAPE-OPEN Unit Operation  
<https://www.amsterchem.com/matlabunitop.html>  
License needs to be requested, but free-of-charge for non-commercial use
3. MATLAB®  
[www.mathworks.com](http://www.mathworks.com)

# MVP Lesson 4: Kinetic Reactor Unit in MATLAB®



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## Input to MATLAB® model

### Feed Conditions

$$T = 392 \text{ } ^\circ\text{C}$$

$$p = 1.013 \text{ bar}$$

$$\dot{N}_{\text{CO}} = 0.0025 \frac{\text{mol}}{\text{s}}$$

$$\dot{N}_{\text{H}_2\text{O}} = 0.0015 \frac{\text{mol}}{\text{s}}$$

$$\dot{N}_{\text{CO}_2} = 0.0001 \frac{\text{mol}}{\text{s}}$$

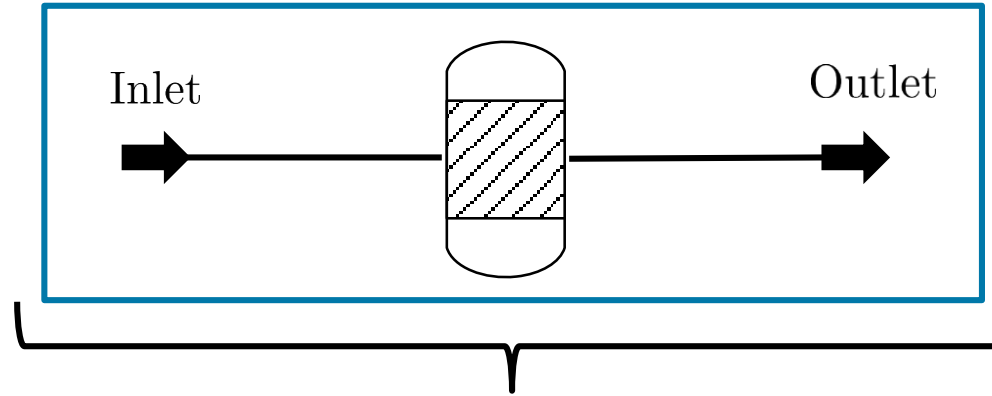
$$\dot{N}_{\text{H}_2} = 0.0002 \frac{\text{mol}}{\text{s}}$$

### Reactor Geometry

$$d = 2.54 \text{ cm}$$

$$L = 7.5 \text{ m}$$

$$\rho_{\text{Sch}} = 4.6 \times 10^6 \frac{\text{g}_{\text{Kat}}}{\text{m}^3}$$





## Input to MATLAB® model

### Feed Conditions

$$T = 392\text{ }^{\circ}\text{C}$$

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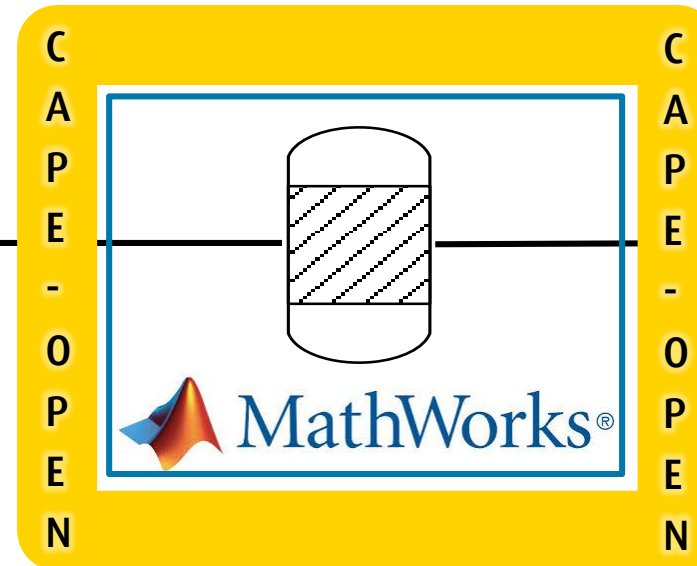
$$L = 7.5\text{ m}$$

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**Honeywell**

Inlet



Outlet

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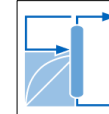
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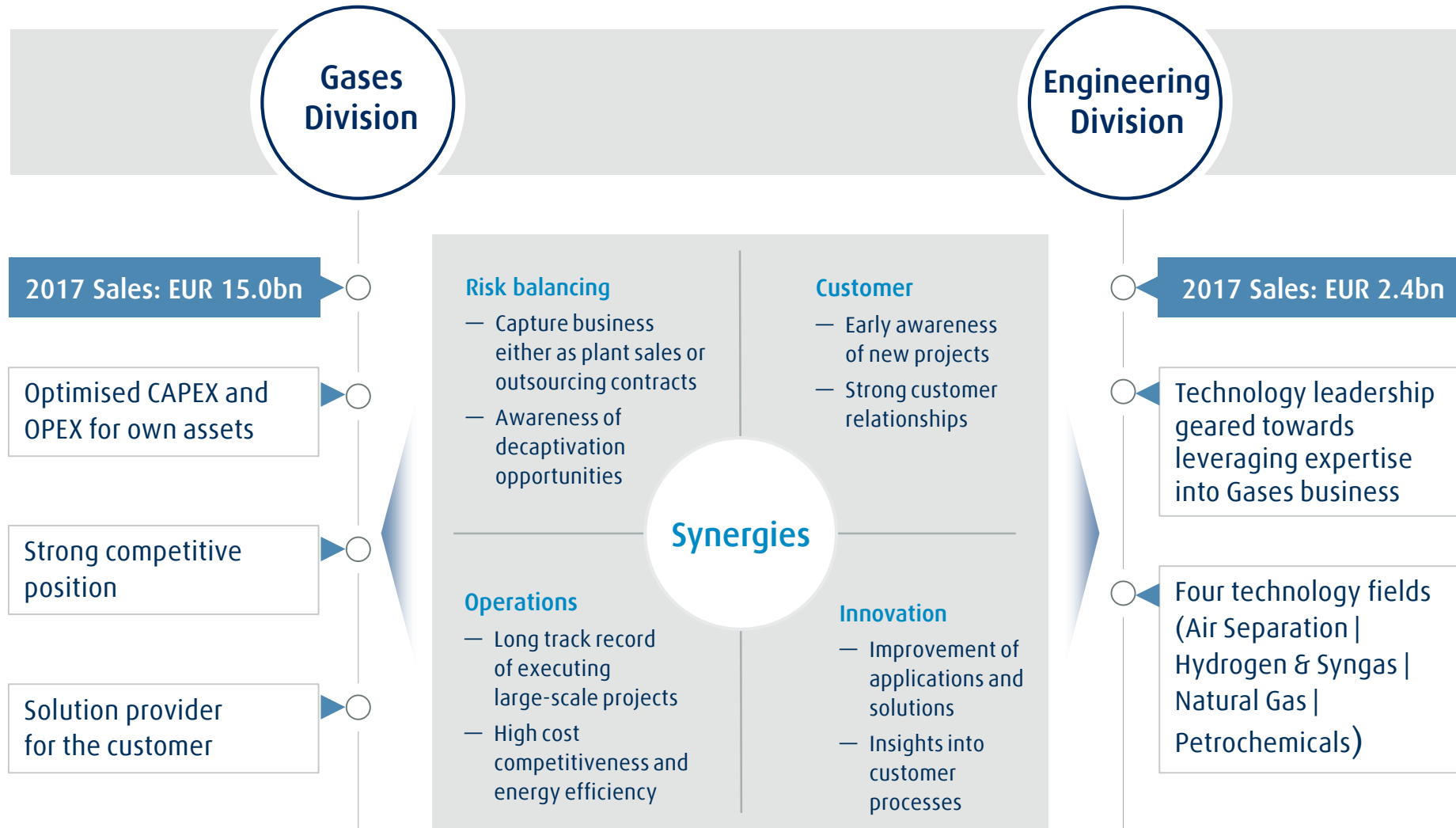
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# Integrated Gases & Engineering model

## Synergies built on strong Engineering foundation



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# Engineering Division

Core competence in gas processing applicable to full portfolio



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6,144 employees\*

3,000 engineers

1,000 process engineering patents  
**Expertise & experience**

4,000 completed plant projects

## Feedstock

Air  
Hydrocarbons  
Tail gases  
Natural gas  
Exhaust gases

Liquefaction

Separation

Thermal Cracking

## Products

Hydrogen  
Rare gases  
Carbon dioxide  
Nitrogen  
Carbon monoxide  
Olefins  
Oxygen  
Synthesis gas

## Offerings

Components

Standardised plants

Customised plants

Services

### Air separation plants



### Hydrogen and Syngas plants



### Petrochemical plants



### Natural gas plants



For Linde Gas & third-party customers

For the chemical & energy-related industries

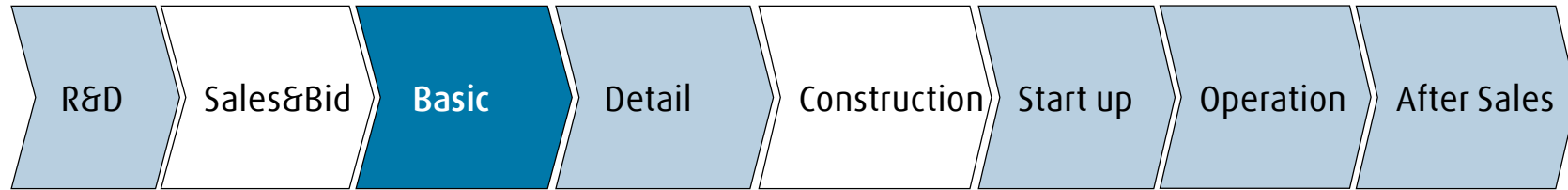
\*Status: 31/12/2017

# Process Simulation

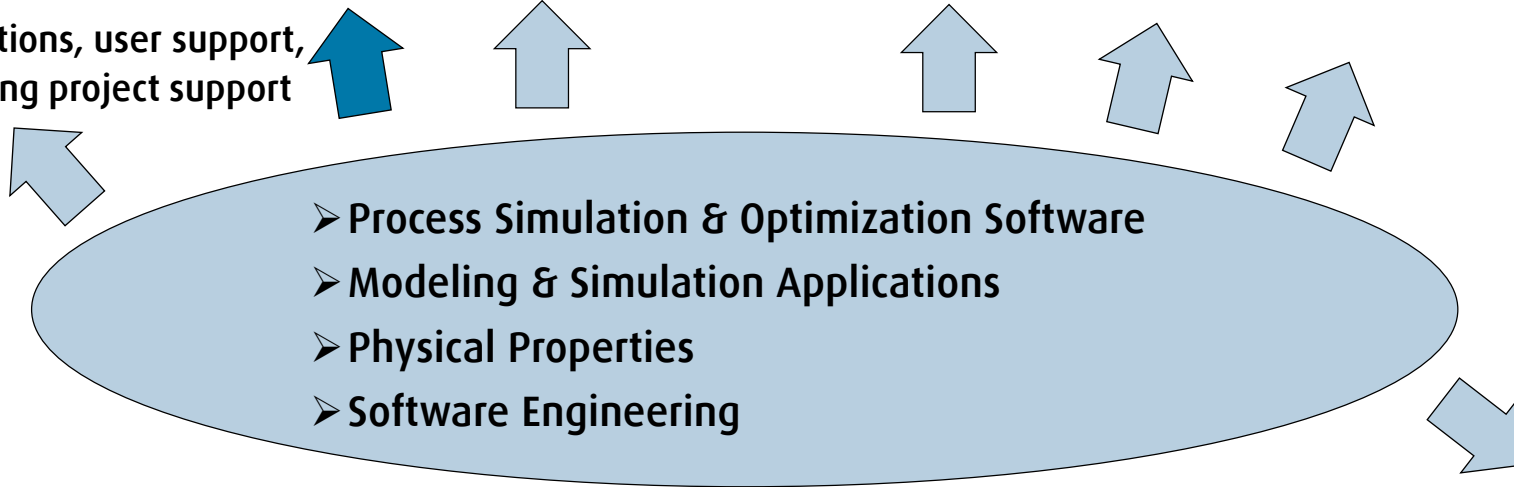
## Overview – IT for Process Design & Control



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IT applications, user support,  
engineering project support



Linde Engineering

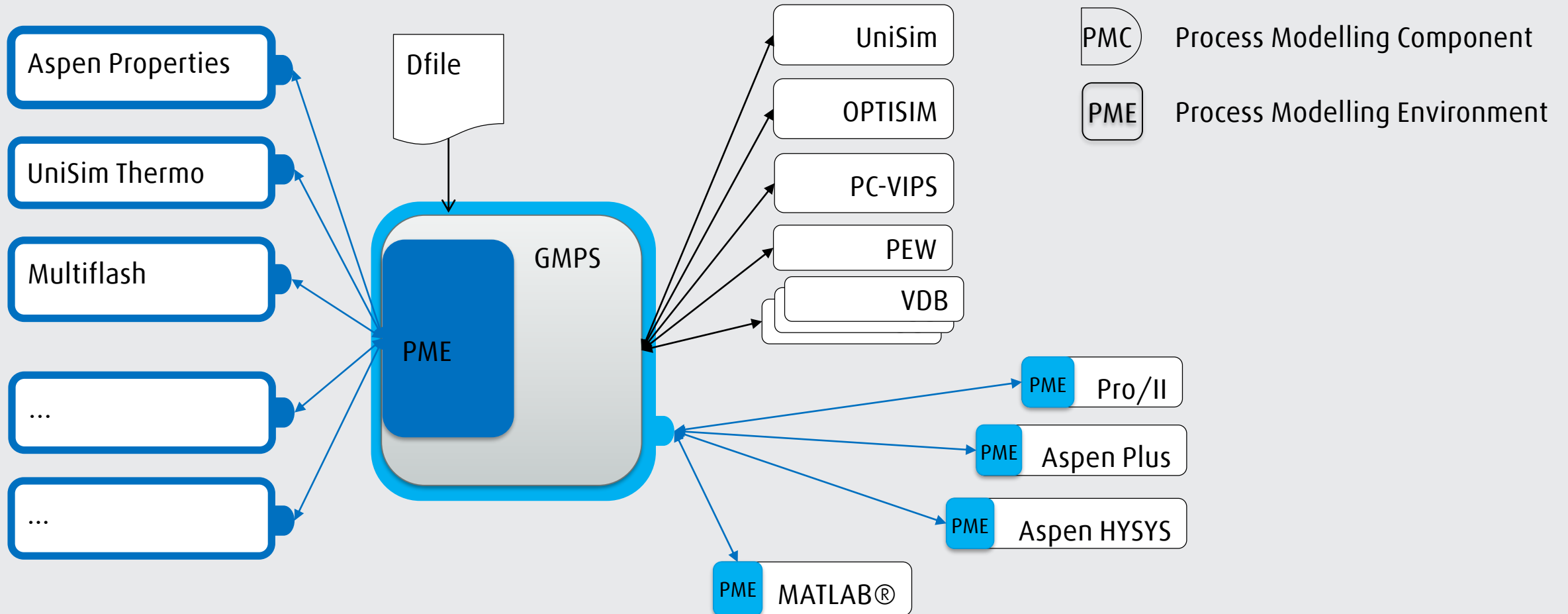
Linde Gas



# CAPE-OPEN Thermo Interfaces to Linde's Thermo Package



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Applications  
&  
Process simulation tools

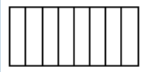
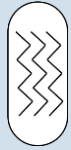
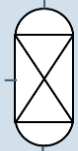

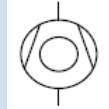
**PdM**

**OPTISIM**

**PC-VIPS**

**UniSim & OTS**



Process unit models  
&  
Physical properties










**GMPS**

Plate Fin Hex, Coil Wound Hex, Column, Membrane, Turbo compressor,  
Cracking furnace, Cracked gas heat recovery, Reformer


Modeling software




SW engineering tools




Microsoft





Microsoft





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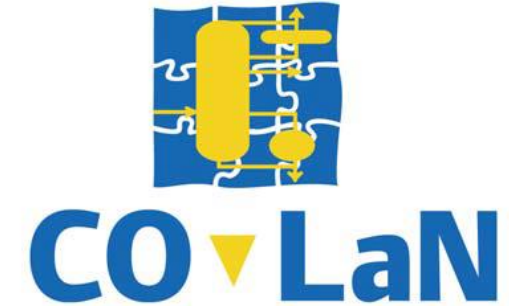


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## Why is CAPE-OPEN important for me?



- CAPE-OPEN is the bridge to attach your unit or thermo model to other platforms  
[https://en.wikipedia.org/wiki/CAPE-OPEN\\_Interface\\_Standard](https://en.wikipedia.org/wiki/CAPE-OPEN_Interface_Standard)
- CO-LaN maintains and develops CAPE-OPEN standard  
<http://www.colan.org>
- CAPE-OPEN allows to create even more complex models based on existing pieces
- CAPE-OPEN can save you a lot of time and money by avoiding to re-invent the wheel







**The whole is more than the sum of its parts**  
**Aristotle (384 – 322 BC)**



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