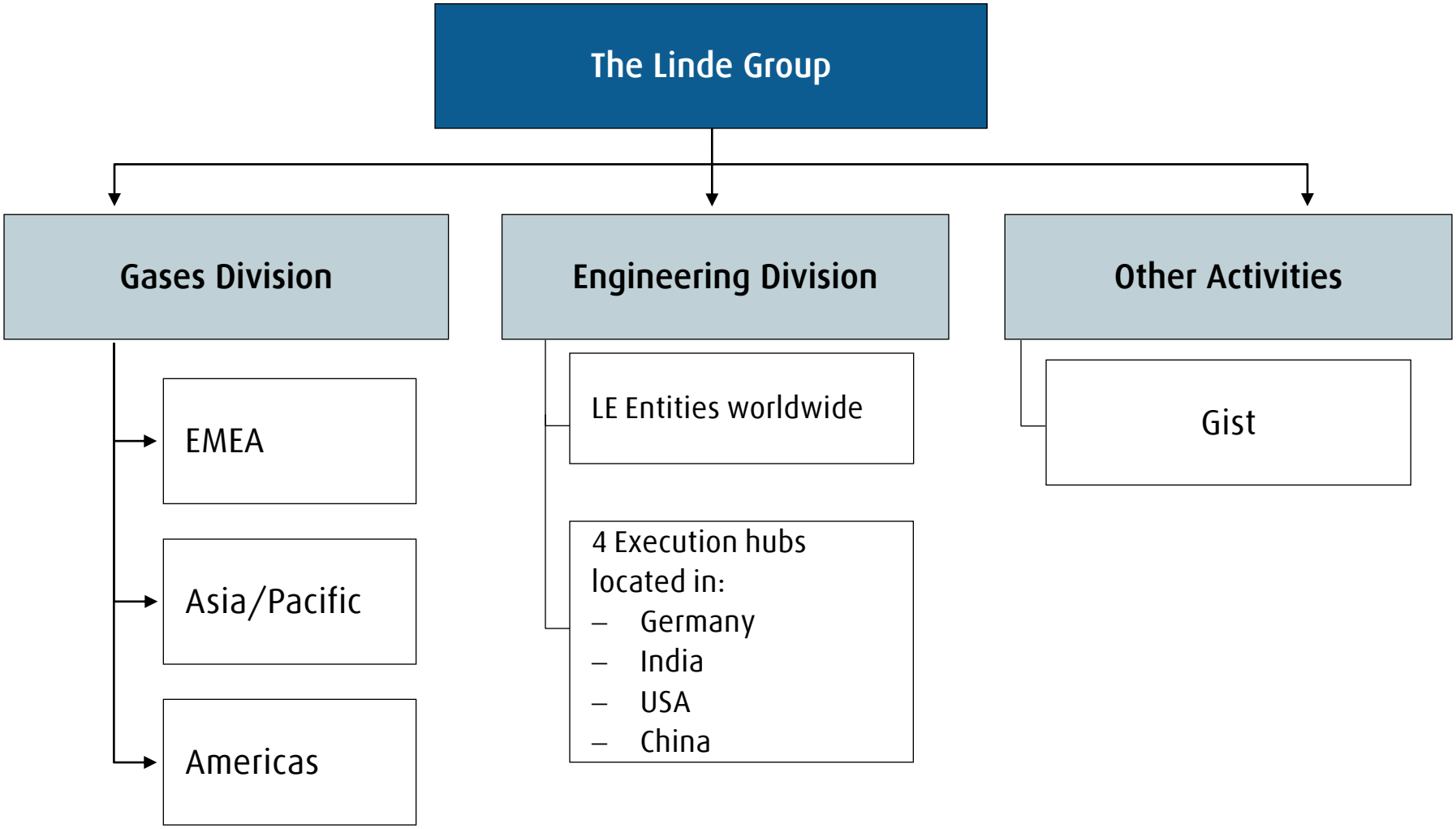
LINDE field report on CAPE-OPEN Thermo

Andreas Grenner, Linde AG, Enigeering Division
CAPE-OPEN 2016 Annual Meeting

THE LINDE GROUP

Linde

Group profile
Organisational structure



Linde heritage

Linde Engineering

Linde Engineering's core competence is the treatment of gases

Air

Natural gas

Hydrocarbons

TailGases

Exhaust fumes

Liquefaction

Separation

Thermal Cracking

Oxygen

Hydrogen

Rare Gases

Nitrogen

Carbon monoxide

Synthesis Gas

Carbon dioxide

Olefins

Proprietary Equipment	Standardised plants	EPC plants	Services
			

Linde Engineering
Leading market position in multiple segments

THE LINDE GROUP

Linde

Air Separation Plants

Hydrogen and Synthesis Gas Plants

Providing plants for Linde Gas and third party customers

Petrochemical Plants

Natural Gas Plants

Providing plants for chemical industry and energy-related industries

With around **1,000 process engineering patents and applications** and about **4,000 completed plant projects,** Linde Engineering is supporting the energy and environment megatrend and leveraging customer relationships for gas projects.

Content

THE LINDE GROUP

Linde

Why CAPE-OPEN @ LINDE?

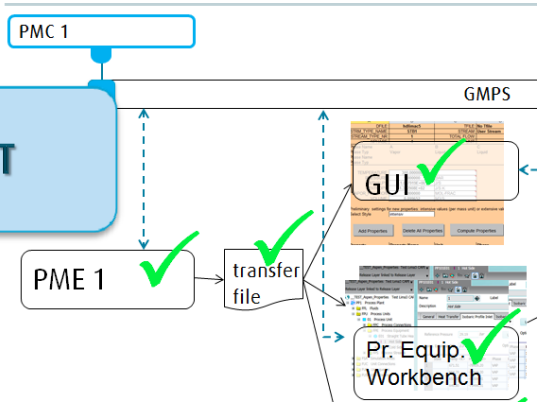
How we want to work with CAPE-OPEN?

CapeThermoLinde

LINDE physical property infrastructure

COGMPS

TEST



Results

- phase naming caused trouble
- n results at phase boundary
- ropy (F, NF)
- of fluid packages files differs for each PME
- memory leak in certain PME-PMC combination
- simulations outside of VLE? Not all PMC support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties
- calculation time (20 – 30 % more)

Why and how CAPE-OPEN @ Linde Engineering?

WHY CAPE-OPEN implementation :

improved cooperation with customers & licensers

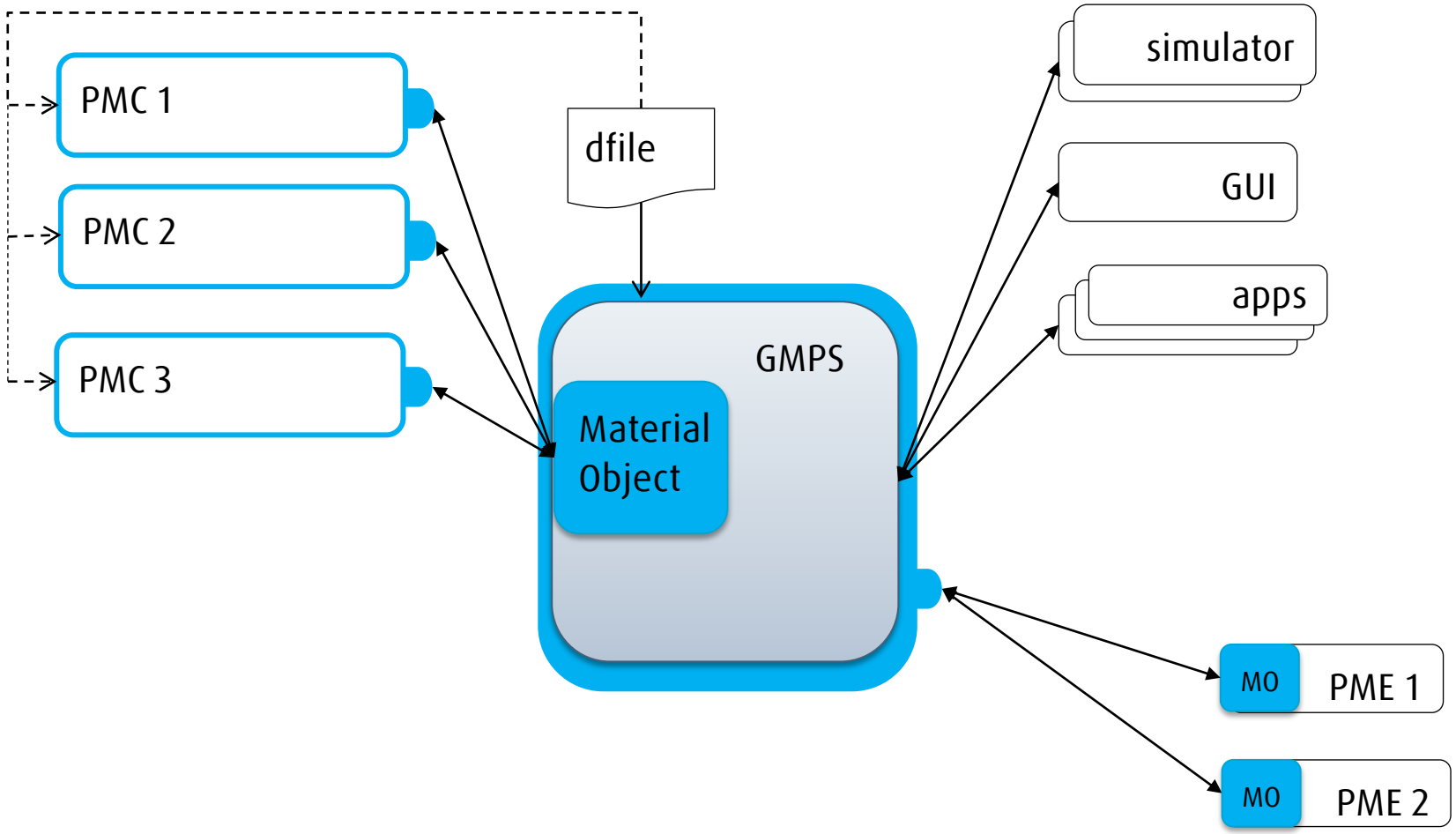
- ability to use 3rd party thermo packages
- handling of licenser processes
- use of various process simulators

HOW we want to work with CAPE-OPEN:

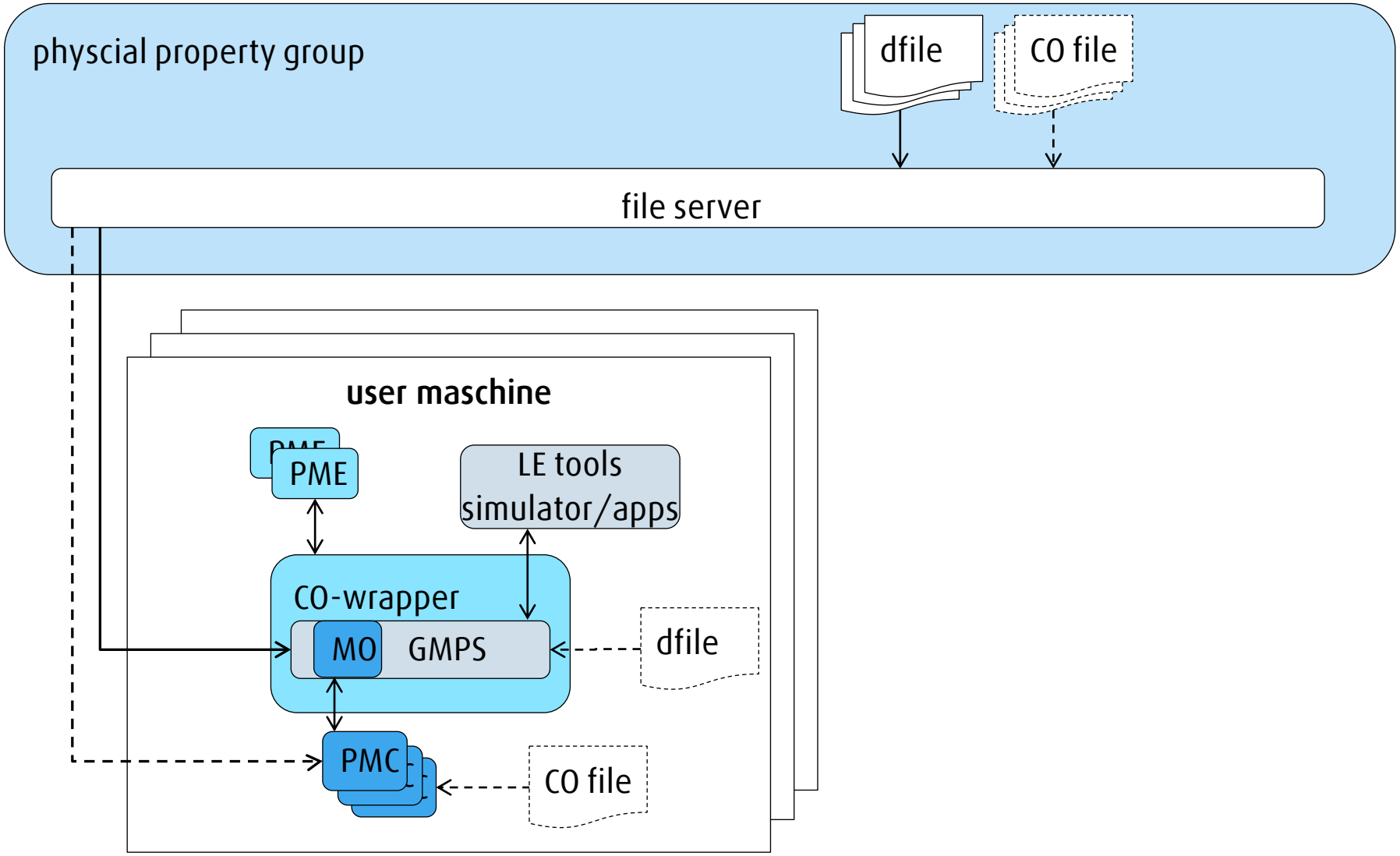
- plug and play usage of different PMCs via LINDE thermo system
- plug and play usage of different PMEs in LE's workflow with LINDE thermo system

⇨ using 3rd party thermo and/or simulator in LINDE's workflow

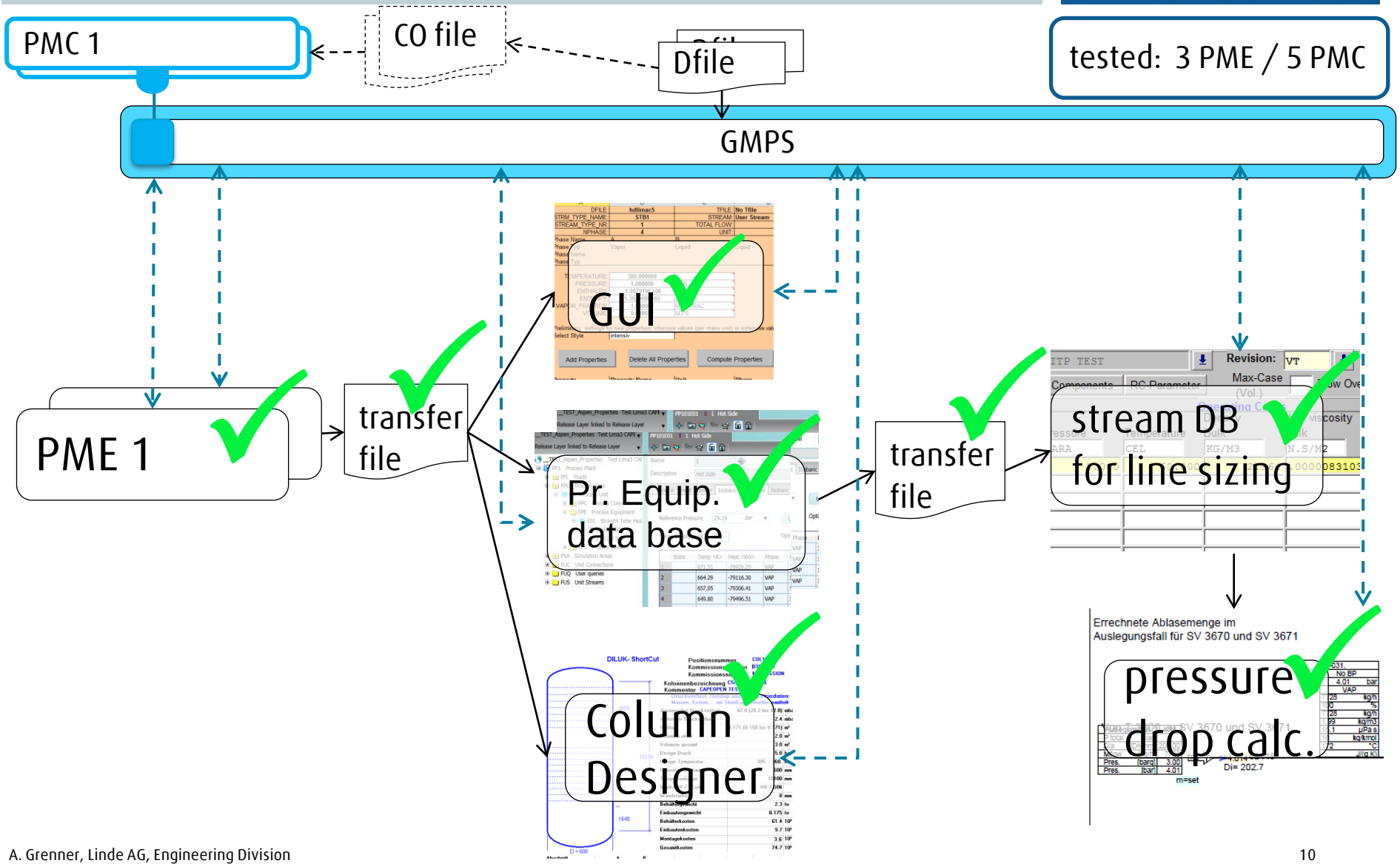
LINDE thermo system



IT infrastructure – process design



CAPE-OPEN test along LE's workflow



conclusion: CAPE-OPEN is not Plug & Play

- phase naming can caused trouble
- odd flash results at phase boundary
- enthalpy, entropy (F, NF)
- without persistence: file structure of fluid packages files differs for each PMC
- memory leak in certain PME-PMC combinations
- simulations besides VLE? Not all PMCs support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties; need for fallback calculations
- calculation time may be higher
- only few PMCs support persistence

phase naming caused trouble

entry on phase list: → LiquidLiquid

3.11 CAPE-OPEN Phase List

3.11.1 Phase Details

Permitted phases have been restricted to the following:

Phase	Description
Vapor	Vapor phase
Liquid	Liquid phase
LiquidX	Liquid phase X
Solid	Solid phase
SolidX	Solid phase X
Overall	All phases

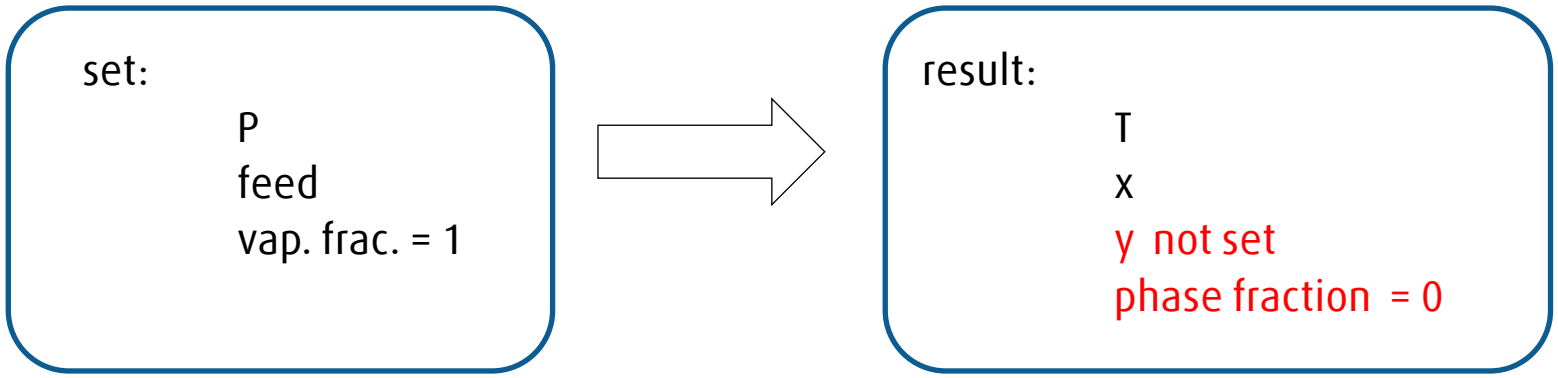
Multiple liquid phases can be achieved by using different names for a liquid. All liquid-phase names must start with "Liquid" so that they can be identified as a liquid. Multiple solid phases can be achieved by using different names for a solid. All solid-phase names must start with "Solid" so that they can be identified as a solid. It is advised to use the name "Liquid" for the first liquid phase, and the name "Solid" for the first solid phase. In the above table, X is a place holder for any name, so "LiquidX" could be for example "LiquidWater", "Liquid2", …

Version	Version 1.08.008

conclusion: CAPE-OPEN is not Plug & Play

- phase naming can caused trouble
- odd flash results at phase boundary
- enthalpy, entropy (F, NF)
- without persistence: file structure of fluid packages files differs for each PMC
- memory leak in certain PME-PMC combinations
- simulations besides VLE? Not all PMCs support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties; need for fallback calculations
- calculation time may be higher
- only few PMCs support persistence

odd flash results for PVF flash (DEWT):



conclusion: CAPE-OPEN is not Plug & Play

- phase naming can caused trouble
- odd flash results at phase boundary
- enthalpy, entropy (F, NF)
- without persistence: file structure of fluid packages files differs for each PMC
- memory leak in certain PME-PMC combinations
- simulations besides VLE? Not all PMCs support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties; need for fallback calculations
- calculation time may be higher
- only few PMCs support persistence

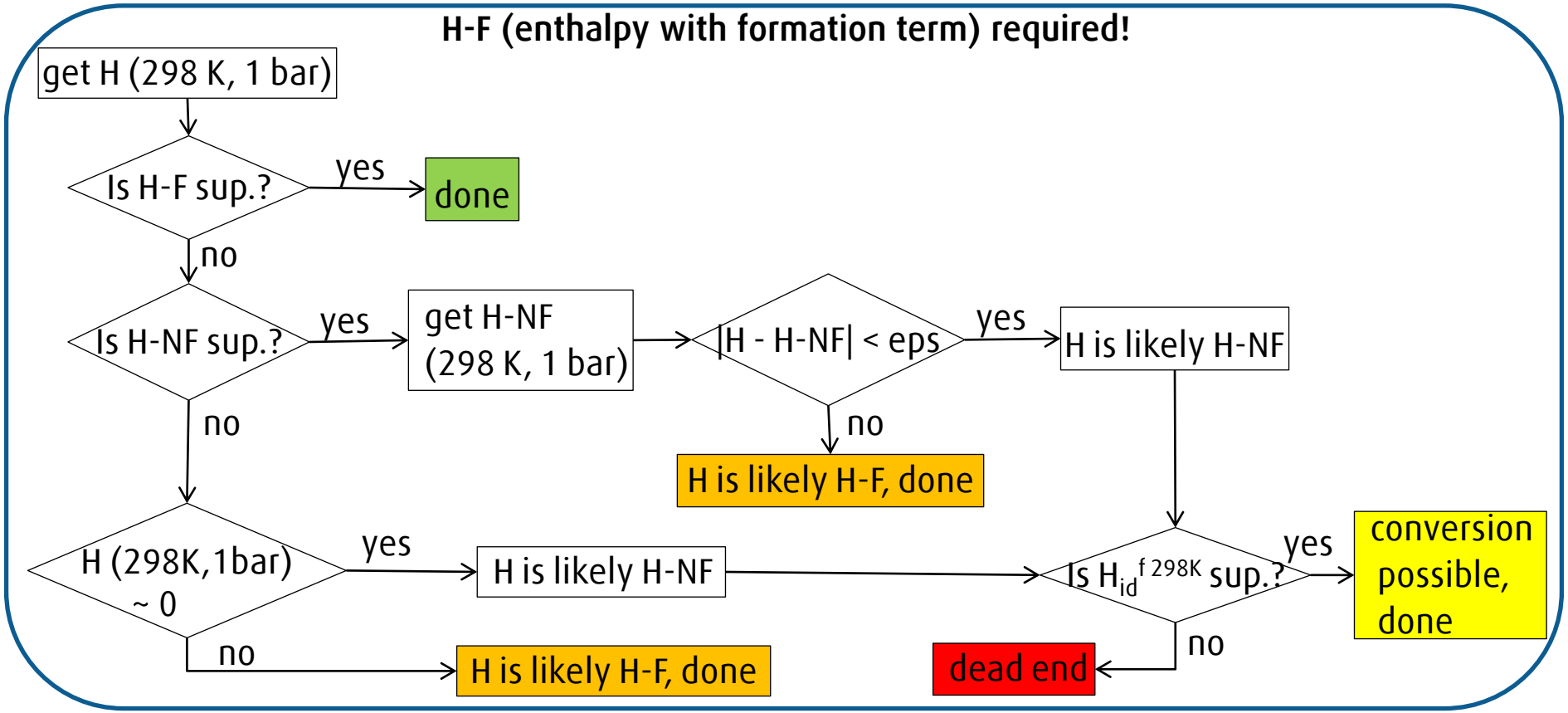
enthalpy with (F) or without formation term (NF)

Trade off using heat of formation in enthalpies:

- heat of formation required for reactors,
- but larger numerical values can cause convergence issues in flowsheet simulation

CAPE-OPEN defines three enthalpies:
H, H-F, H-NF

is required enthalpy supported by PMC ?



conclusion: CAPE-OPEN is not Plug & Play

- phase naming can caused trouble
- odd flash results at phase boundary
- enthalpy, entropy (F, NF)
- without persistence: file structure of fluid packages files differs for each PMC
- memory leak in certain PME-PMC combinations
- simulations besides VLE? Not all PMCs support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties; need for fallback calculations
- calculation time may be higher
- only few PMCs support persistence

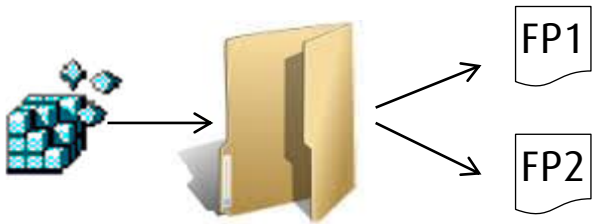
CapeOpen fluid package – file structure e.g.

THE LINDE GROUP

Linde

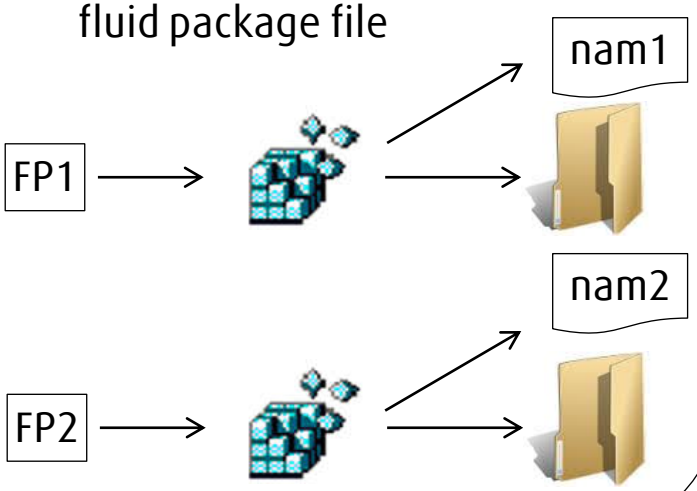
PMC 1

- general registry key contains path were files with fluid package information will be searched



PMC 2

- each CO fluid package must be registered
- registry key contains path with fluid package file



conclusion: CAPE-OPEN is not Plug & Play

- phase naming can caused trouble
- odd flash results at phase boundary
- enthalpy, entropy (F, NF)
- without persistence: file structure of fluid packages files differs for each PMC
- memory leak in certain PME-PMC combinations
- simulations besides VLE? Not all PMCs support VLLE!
- dealing of solid phases - does it work?
- every PMC supports a different set of properties; need for fallback calculations
- calculation time may be higher
- only few PMCs support persistence

summary

- LINDE tested 5 PMC and 3 PME with GMPS (as PME resp. PMC)
- in general tests were sucessfully
- in most cases CAPE-OPEN was not plug & play, several problems discovered

THE LINDE GROUP

Linde

Collaborate. Innovate. Deliver.

Thank you for your attention.