CO in KBC and Infochem: Interoperability examples

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This presentation shows two examples of using Infochem's Multiflash software in conjunction with a CAPE-OPEN compliant process simulator.

Examples of Multiflash with KBC's Petro-SIM simulator are the subject of another presentation: CO in KBC and Infochem - Current status and future plans which is also available on the Co-Lan website

Software components

- COFE 2.5.0
  - CO-based process simulator
- Multiflash 4.1
  - Physical property system
  - Used to create CO Property Packages
- Examples
  - Hydrates: eg. cold flow process
  - LNG: optimisation with high-accuracy model

COFE is a free-to-use CO-based process simulator that is made available by amsterCHEM: www.amsterchem.com

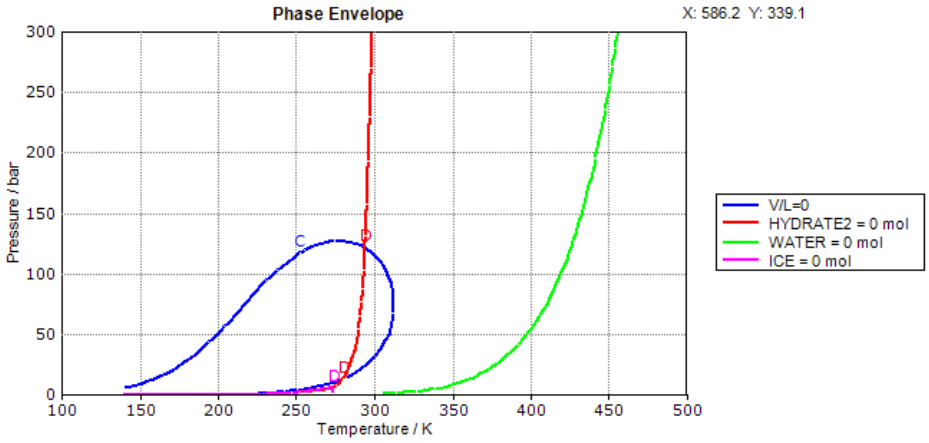
Multiflash is Infochem's physical property system. It includes multiphase fluid and solids phase behaviour calculations, a comprehensive range of physical property models for oil/gas/petrochemical applications and advanced petroleum fluid characterisation procedures.

Multiflash also provides specialist modules for modelling phase behaviour of particular importance in the upstream oil industry including hydrates, waxes, asphaltenes and solid freezeout. See www.infochemuk.com

The presentation highlights two examples. The first involves hydrates and the second uses a high-accuracy thermodynamic property package to model a LNG liquefaction process.

Simple hydrate example

- Methane, propane, butane, water
- Phases: vapour; non-aqueous liquid; aqueous liquid; Hydrate structure II; ice
- CPA fluid model & vdWP hydrate model



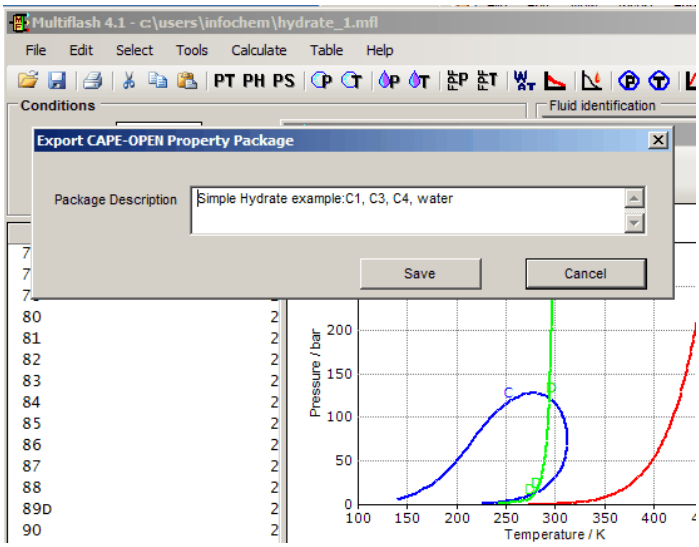
The phase diagram for a natural gas plus water shows the hydrocarbon phase boundary (blue), the water dew point line (green), the hydrate line (red) and the small ice region (magenta). The diagram was calculated using the Phase Envelope tool in the Multiflash user interface (UI).

It is an example of the complex phase behaviour that can be handled by Multiflash.

The CAPE-OPEN Thermo Interface (version 1.1) makes it possible to have the same powerful modelling capabilities in a process simulator.

Simple Hydrate Example

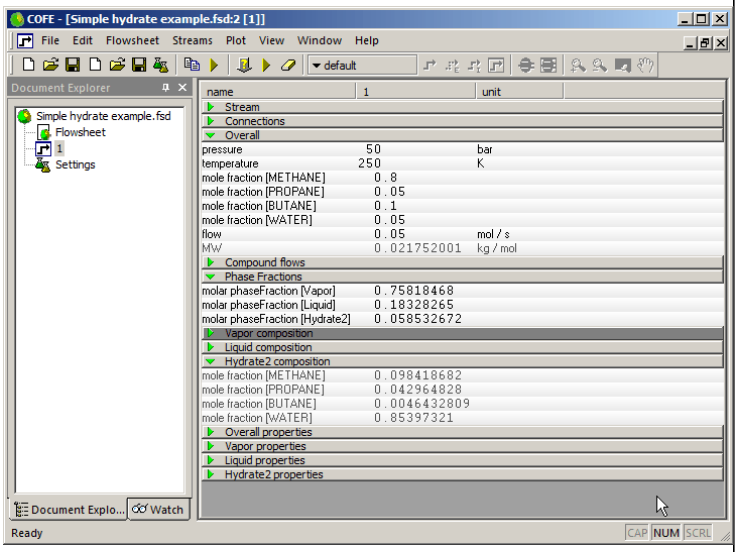
- The Multiflash Property Package can be exported and reused by software that has a CO Thermo socket



Once the physical property models and compounds have been set up in Multiflash the configuration can be exported as a CO Property Package for reuse in a process simulator with a CO socket.

Hydrate example in CoCo

- For example the CoCo simulator
- The flowsheet has just one stream that uses the Multiflash PP
- CoCo is able to handle all the phases in the Multiflash PP including the solid hydrate



In these examples we have used the CoCo simulator from amsterCHEM but it should be possible to achieve the same results in any simulator with a CO Thermo version 1.1 socket.

Although CoCo does not have any native hydrate modelling capability the Multiflash Property Package allows phase behaviour including a solid hydrate phase to be modelled.

LNG C3MR liquefaction process

- Two cycle propane pre-cooled plus mixed refrigerant process
- Example based on Wang et al., Ind. Eng. Chem. Res., **50**, 12630 (2011)
- Published case based on PR eos in Aspen 7.1
- Study carried out by Andras Bulecza (Erlangen) during internship with Infochem
- Invaluable assistance from Jasper van Baten (amsterCHEM)

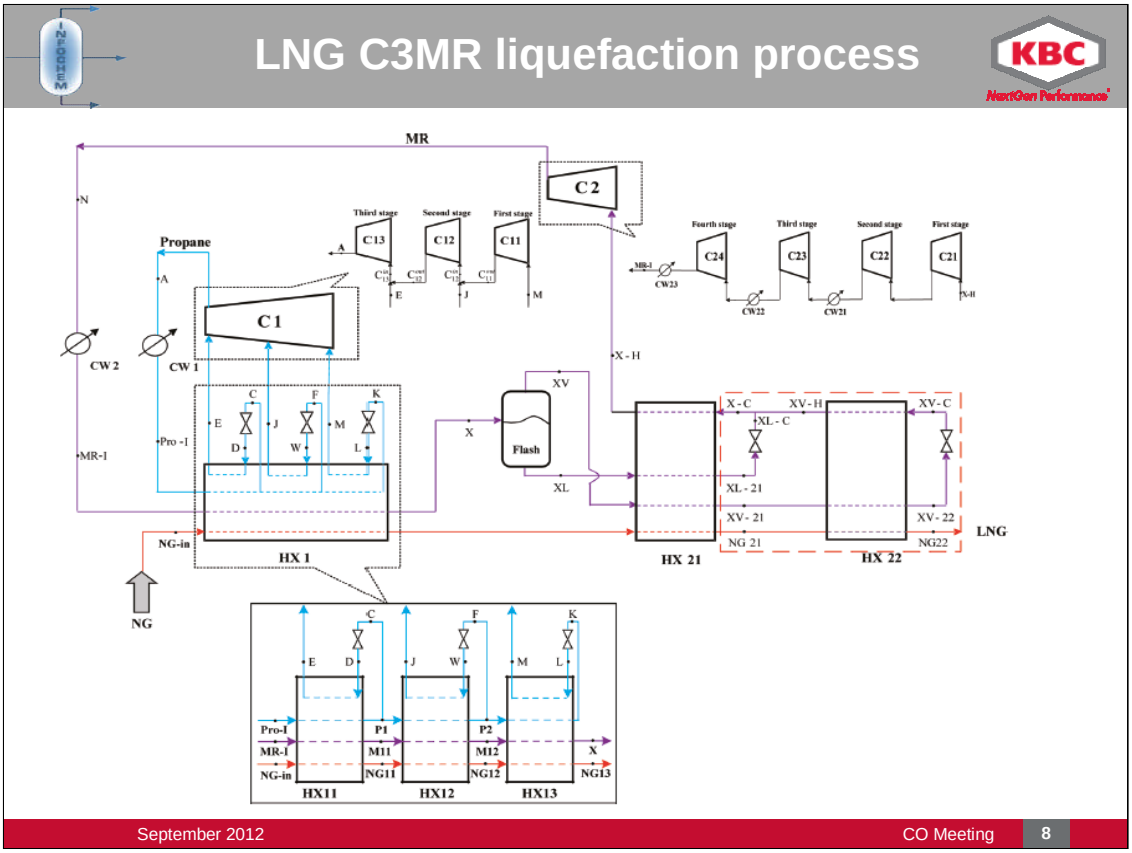
The second example is a LNG liquefaction process that uses two refrigerant cycles: propane and a mixed refrigerant.

LNG C3MR liquefaction process

- Feed: 8 bar, 40 C, Gas, 1 kg/s

	Mol %
N2	0.6
Methane	95.3
C2	3.3
C3	.6
iC4	.09
C4	.06
iC5	< .1
C5	< .1

- Product: 8 bar, -160 C liquid



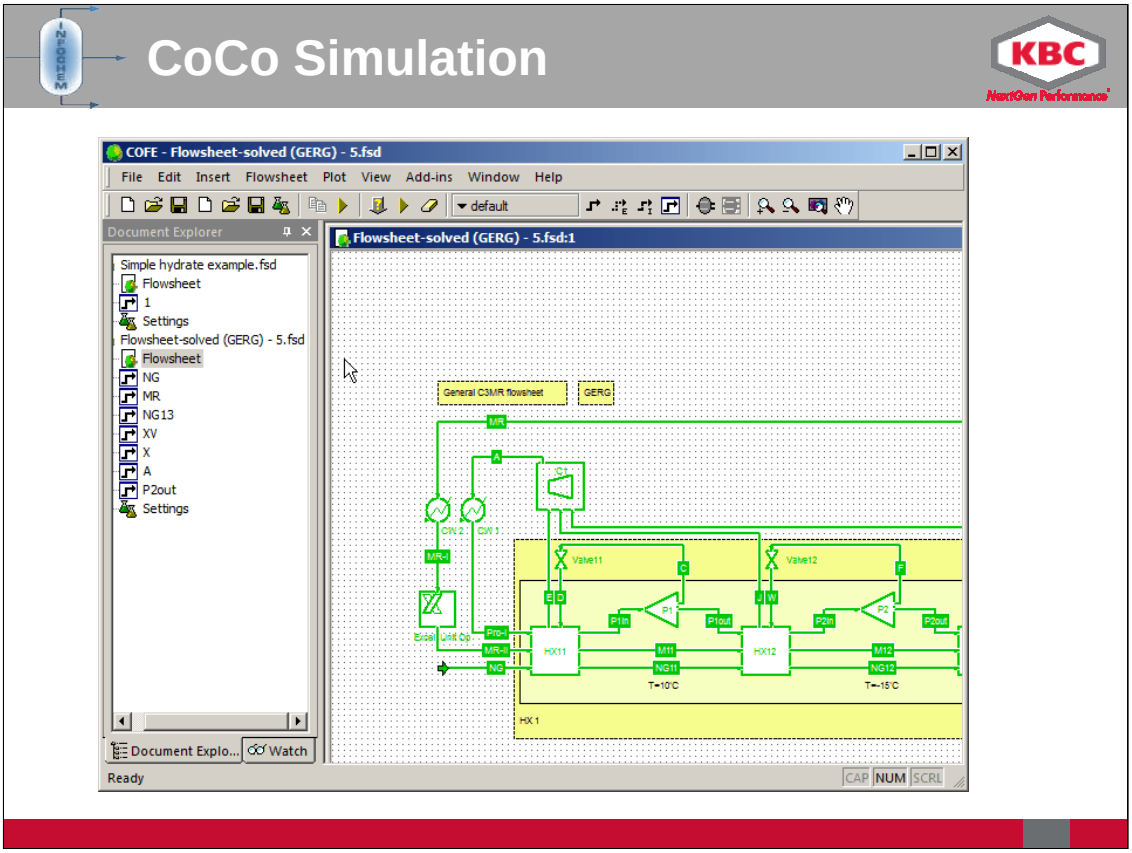
The flowsheet is quite complex and involves sub-flowsheets that model the multi-pass heat exchanger

LNG C3MR liquefaction process

- Compare RKSA and GERG-2008 property packages
- RKSA
  - enhanced RKS eos
- GERG-2008
  - ISO standard for natural gas properties
  - High accuracy for all thermodynamic properties but very complex
- Objective: reduce compressor power (and cooling load)

The GERG-2008 equation of state is a high-accuracy method specifically developed for natural gas.

The GERG 2008 model in Multiflash is compared with a simple cubic equation of state.



This is the flowsheet in CoCo

Some results

- Base case

	RKSA	GERG
Compressor power/kW	2065	2014
Cooling load/KW	3134	3011

- Improved design

	RKSA	GERG
Compressor power/kW	1907	1865
Cooling load/KW	2975	2862

Conclusions

- CO makes it possible to reuse specialised physical property models from Multiflash in any CO-compliant process simulator