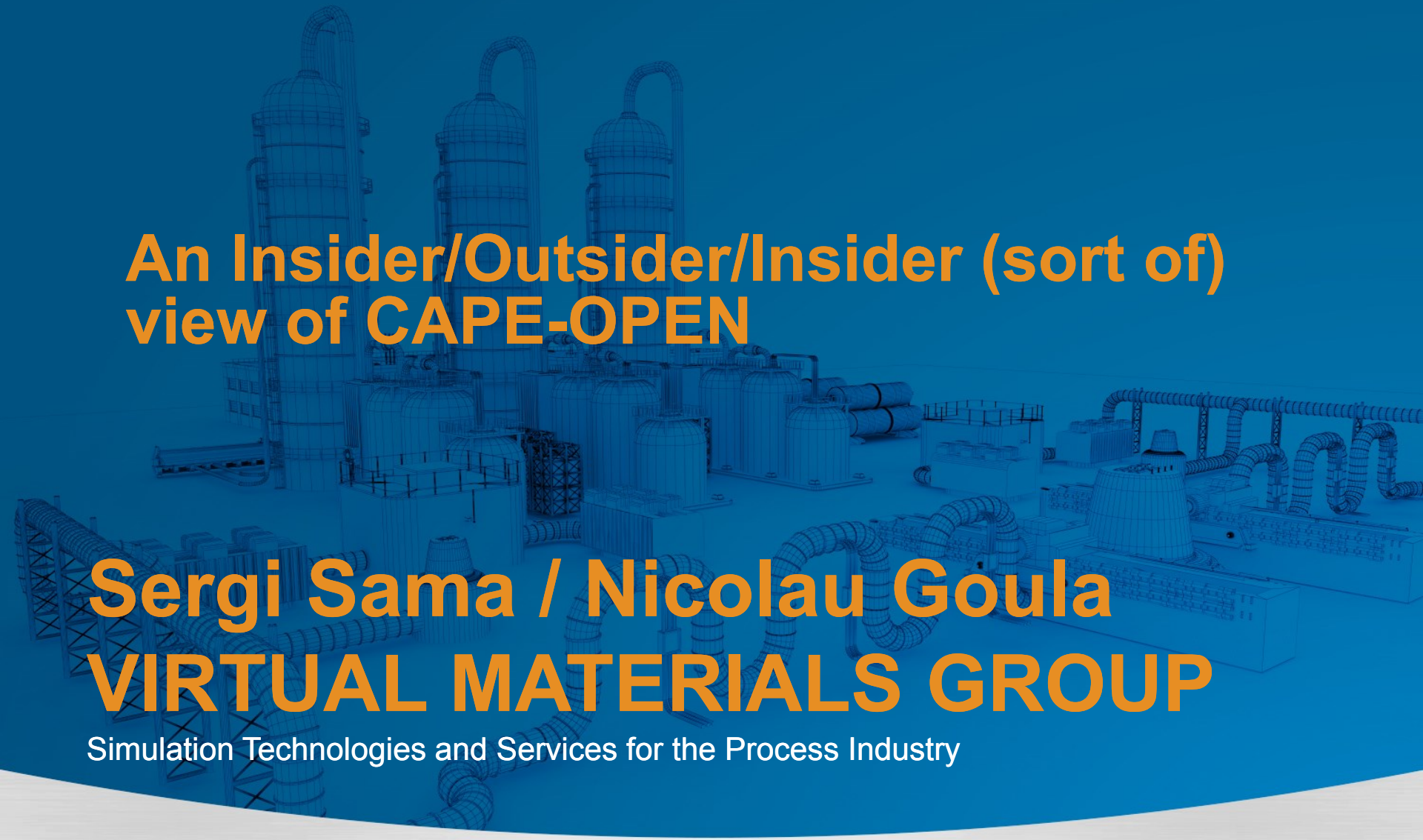
An Insider/Outsider/Insider (sort of) view of CAPE-OPEN



Sergi Sama / Nicolau Goula

VIRTUAL MATERIALS GROUP

Simulation Technologies and Services for the Process Industry

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WHO IS

VIRTUAL MATERIALS GROUP

VMG is a group of technology innovators that service the oil, gas & petrochemical industry with advanced process simulation solutions.

Founded in 1999 Head Office: Calgary, Canada

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VIRTUAL MATERIALS GROUP

……engineers helping engineers

GLOBAL CENTERS

Head Office
- R & D
- Corporate Admin
- Licensing
- JV participation

Head Office:
Subsidiaries:
Sales & Support:

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VMG Europe

European subsidiary established in 2012

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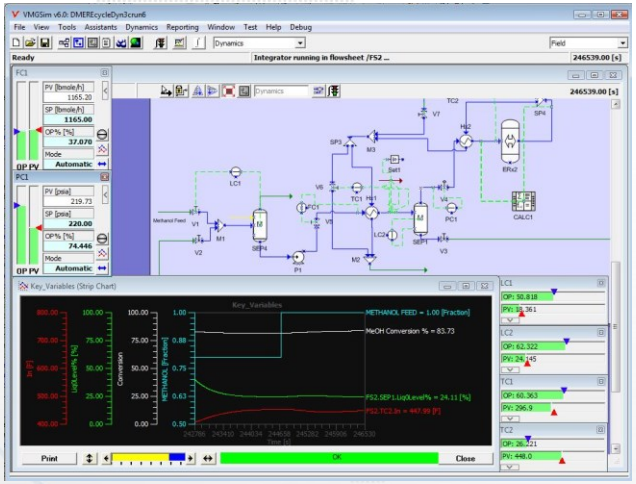
sales@virtualmaterials.com
support.europe@virtualmaterials.com

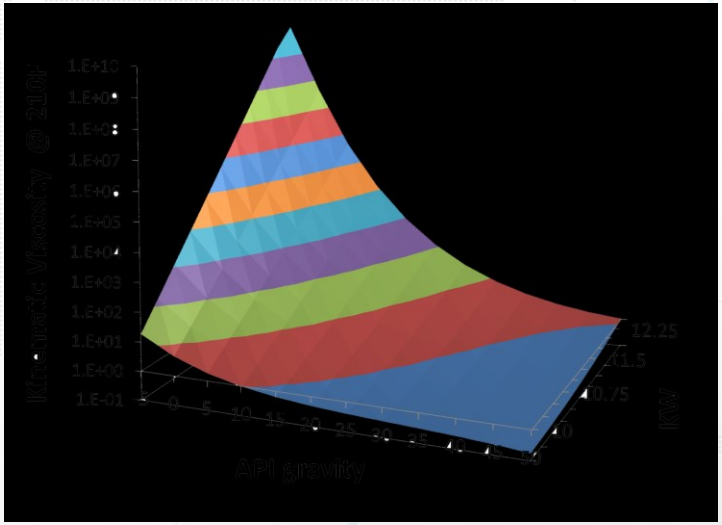
Main **PRODUCTS**

VMGSim™



Fully interactive steady-state and dynamic process simulator

VMGThermo™



Robust thermo-physical property calculation engine

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Sergio Sama Rubio

Managing Director and co-founder

Sergi brings 20+ years of experience in the world of industrial software. After graduating from the Institut Químic de Sarrià (Chemical Institute of Sarria) with a dual degree in Chemical (1990) and Industrial (1992) Engineering.

Sergi joined m2r (since 2000 part of Aspen Technology) as a developer of manufacturing execution systems. In 1995, Sergi joined Hyprotech Europe, where he held various positions involving process simulation with HYSIM and HYSYS (Tactical Developer, Tactical Development Manager, and Technical Services Manager). After the acquisition of Hyprotech by Aspen Technology in 2002, Sergi focused on the applications of process simulation in the Upstream Oil & Gas sector. In 2009 Sergi joined Halliburton as Practice Manager for software systems for Integrated Operations, including model-based operations decision support tools. Sergi also holds a postgraduate degree in executive management by IESE Business School.

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Nicolau Goula i Masllorens

Technical Services Manager at Virtual Materials Group Europe

Nicolau brings 10+ years of experience in Process Engineering from both industrial plants and research centres. Nicolau graduated as a Chemical Engineer at Universitat de Barcelona and has a MSc in Process Systems Engineering from Imperial College.

Nicolau started his career as an interim at Air Products while he was a student. After he got his MSc, he worked for 5 years at Catalonian Research and Innovation Centre managing projects for various industries (polymers, chemicals, industrial gases, etc). In 2007 he joined CELSA Group to work as a Process Engineer in the metallurgical industry, developing simulation models for direct Operations decisions and for Process improvement. He also collaborated in the development of the Manufacturing Execution System (MES), bringing the power of optimisation techniques to daily use at plant level.

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Objectives

- Test the maturity of the CAPE-OPEN standard
- Test the maturity of VMG implementation of CAPE-OPEN
- Test the availability of tools

Constraints

- Simple, yet, showing some valuable application

Test description

- Use COCO/COFE
- Use VMGThermo

- Port a sample simulation case (shipped with our process simulator VMGSim) to COFE

- Create a CAPE-OPEN thermo property package in VMGThermo

- Run the simulation case in COFE

- Compare results

Value of the test

- Demonstrate interoperability between PMC and PME
- Use “non-std” thermodynamics (solid CO2 formation)
- Identify points for further improvement

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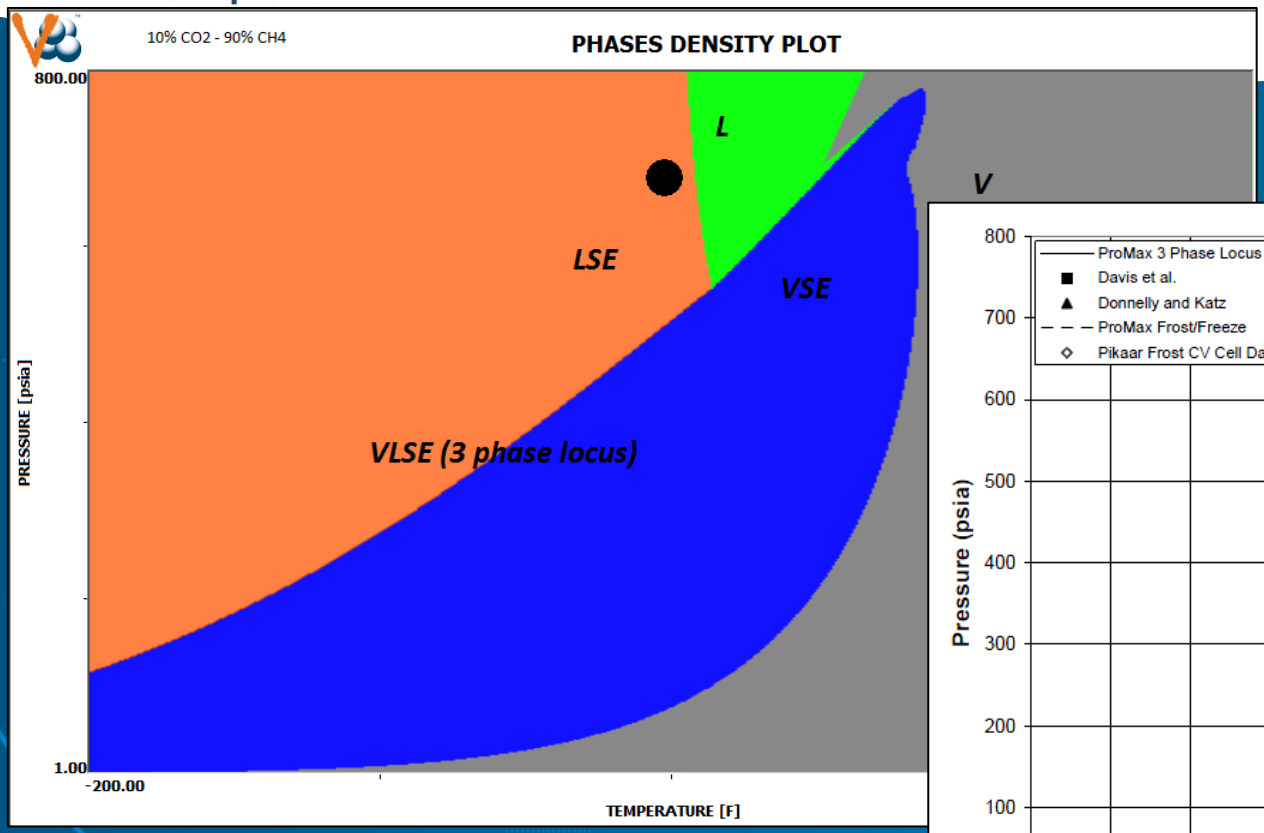

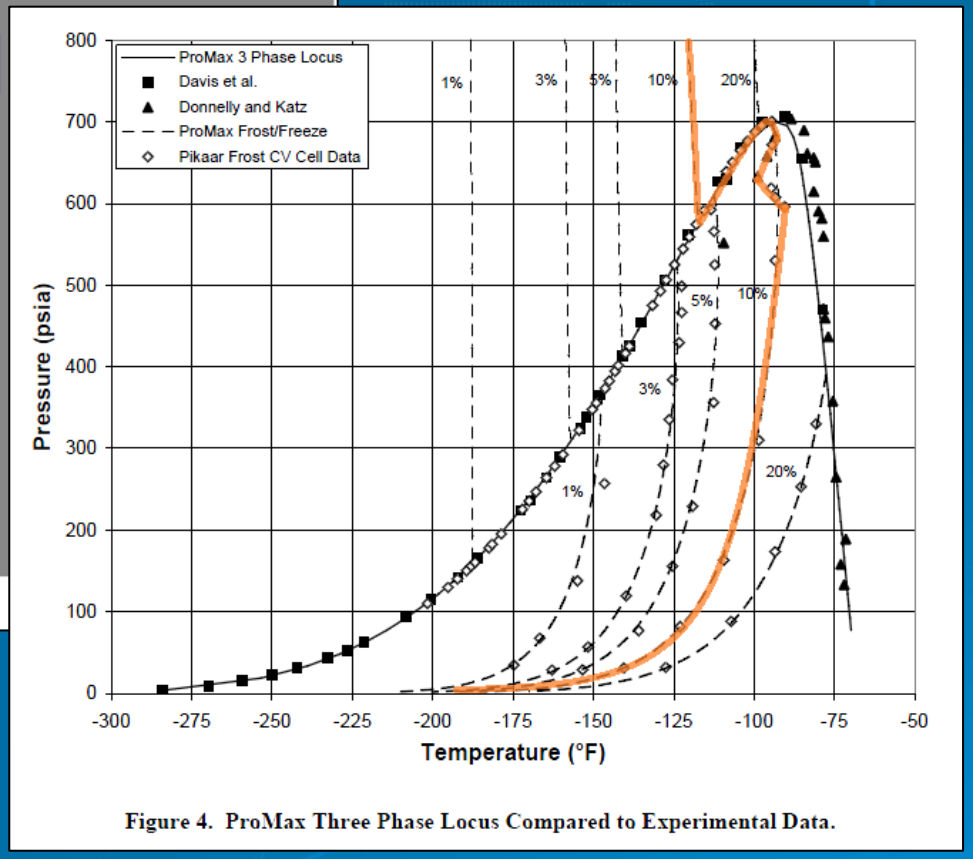

Figure 4. ProMax Three Phase Locus Compared to Experimental Data.

VMGThermo capable to predict CO2 VSE and VLE equlibrium, as well as to locate the three phase locus. 10%CO_2-90%Methane shown (plot from M.W. Hlavinka, V. N. Hernandez "*Proper interpretation of freezing and hydrate predictionresults from process simulation*". Bryan Research & Engineering, Inc.)

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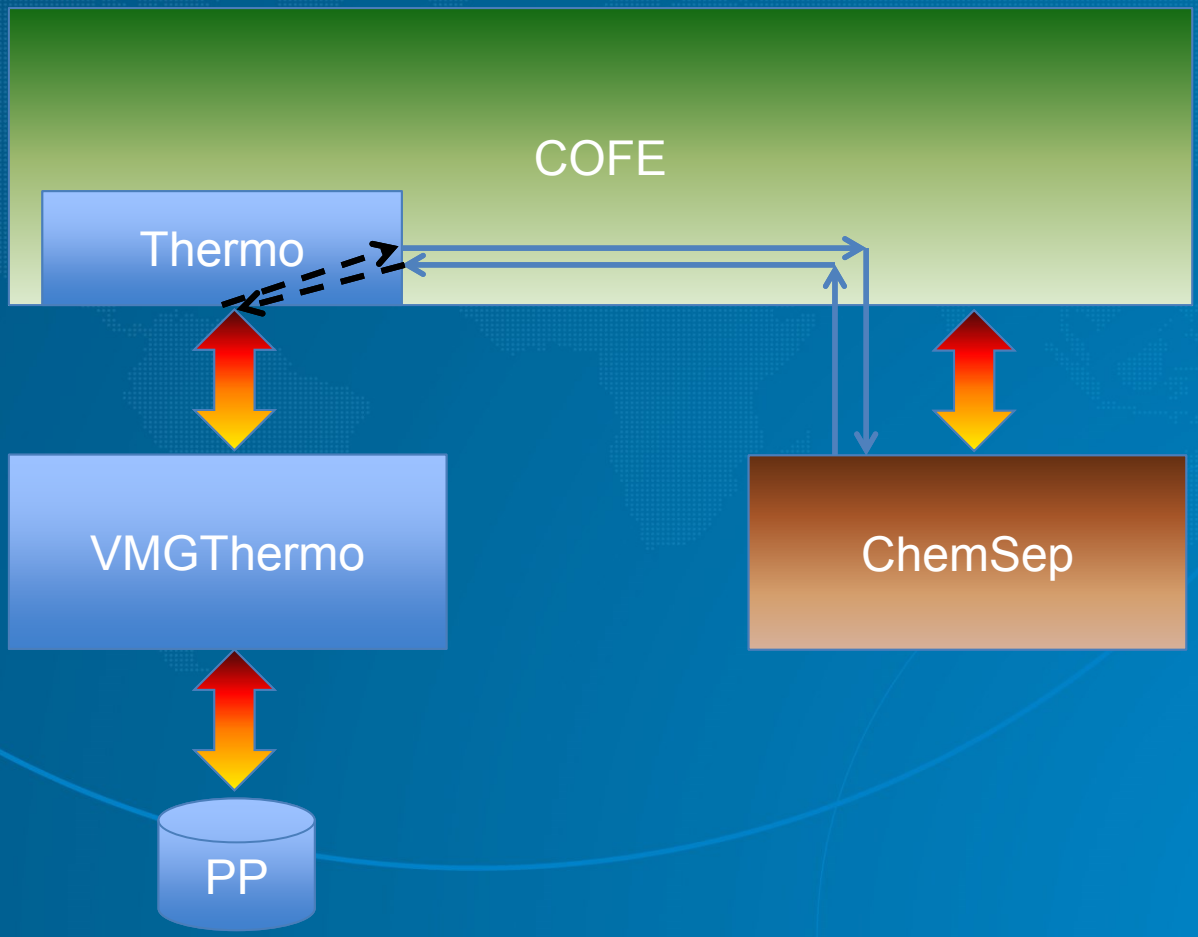
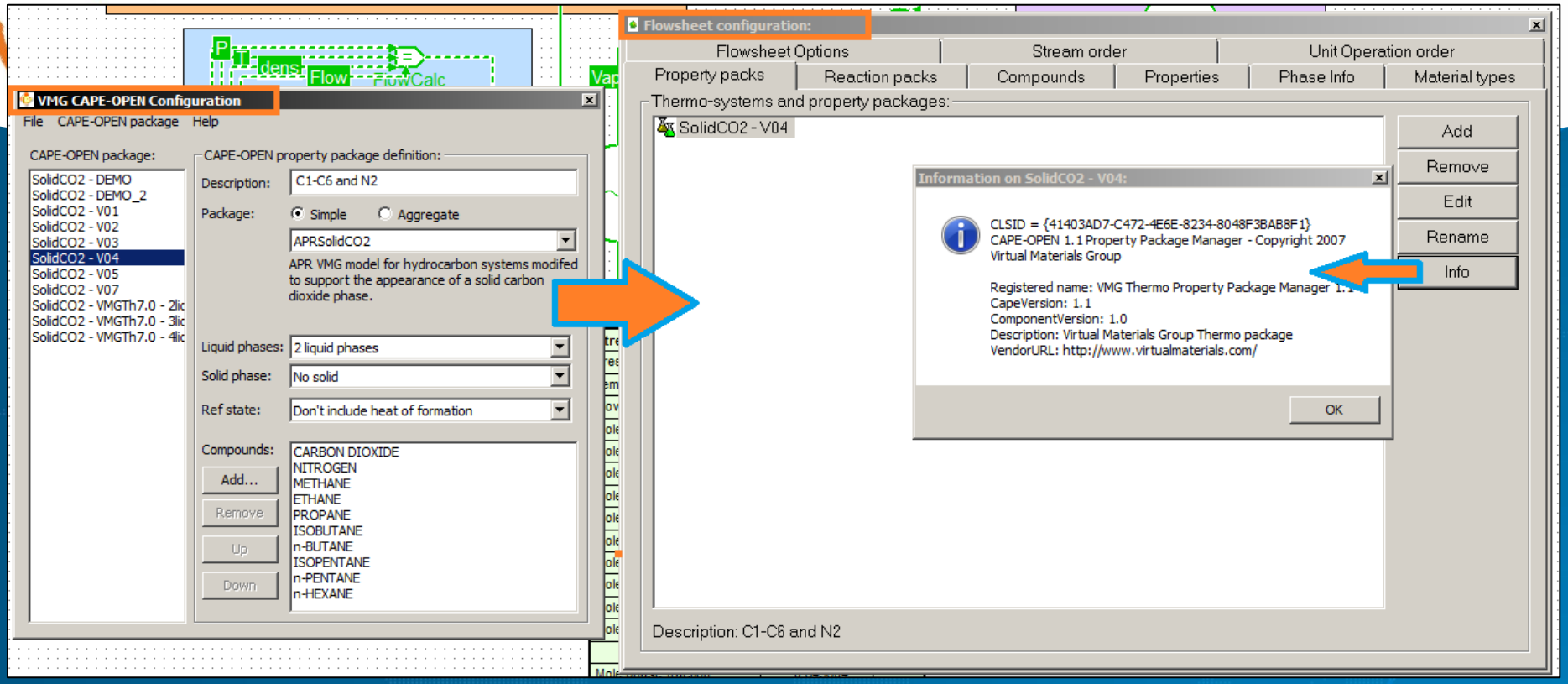
Block Diagram





VMG CAPE-OPEN Configuration utility (on the left) lets the user create a CO compliant Property Package (PP). This PP is available to any CO Simulation Environment (COCO shown on the right).

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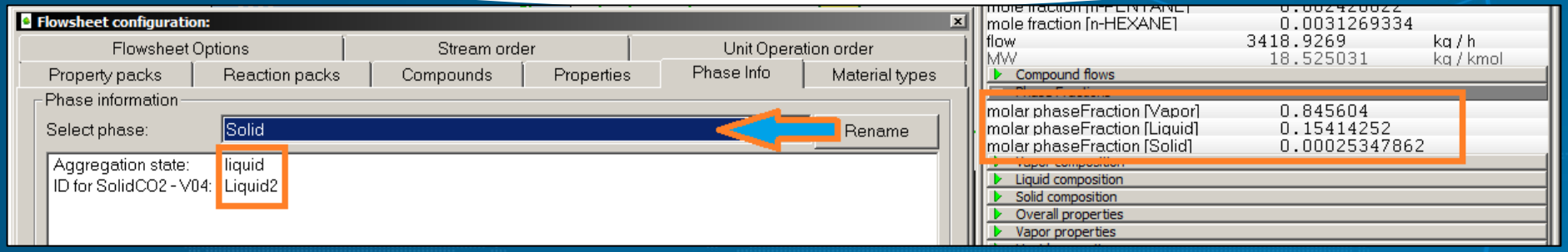
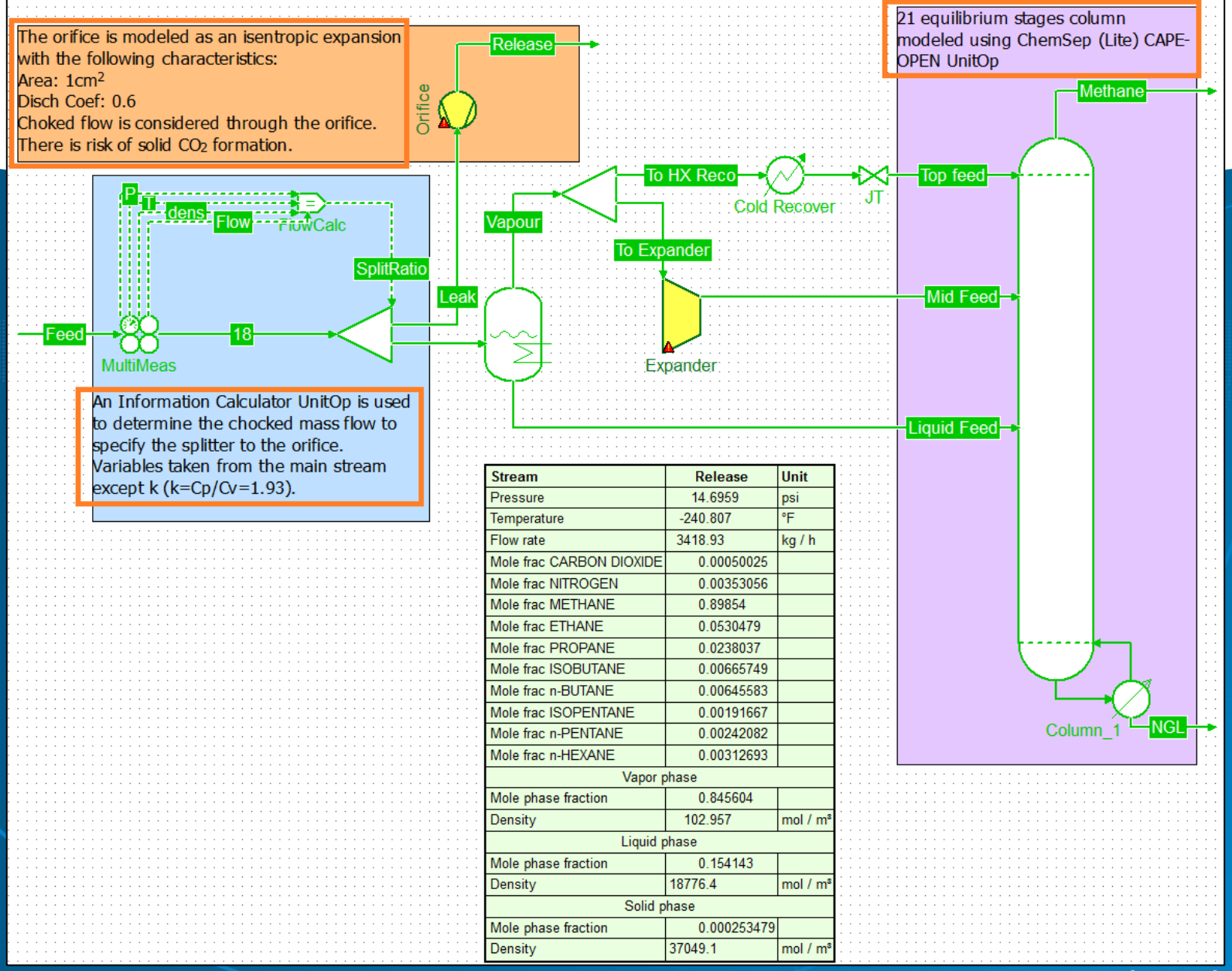


VMGThermo throws the solid CO_2 to the second liquid slot. COCO lets the user rename the phases and any phase starting with “Sol” is actually considered a solid (i.e. solid separator UnitOp).



Stream	Release	Unit
Pressure	14.6959	psi
Temperature	-240.807	°F
Flow rate	3418.93	kg / h
Mole frac CARBON DIOXIDE	0.00050025	
Mole frac NITROGEN	0.00353056	
Mole frac METHANE	0.89854	
Mole frac ETHANE	0.0530479	
Mole frac PROPANE	0.0238037	
Mole frac ISOBUTANE	0.00665749	
Mole frac n-BUTANE	0.00645583	
Mole frac ISOPENTANE	0.00191667	
Mole frac n-PENTANE	0.00242082	
Mole frac n-HEXANE	0.00312693	
Vapor phase		
Mole phase fraction	0.845604	
Density	102.957	mol / m³
Liquid phase		
Mole phase fraction	0.154143	
Density	18776.4	mol / m³
Solid phase		
Mole phase fraction	0.000253479	
Density	37049.1	mol / m³

Cryogenic Demethaniser taken from the Plant Examples folder in VMGSim. A pipe rupture is modelled (orifice) and the possibility of solid CO_2 formation evaluated.

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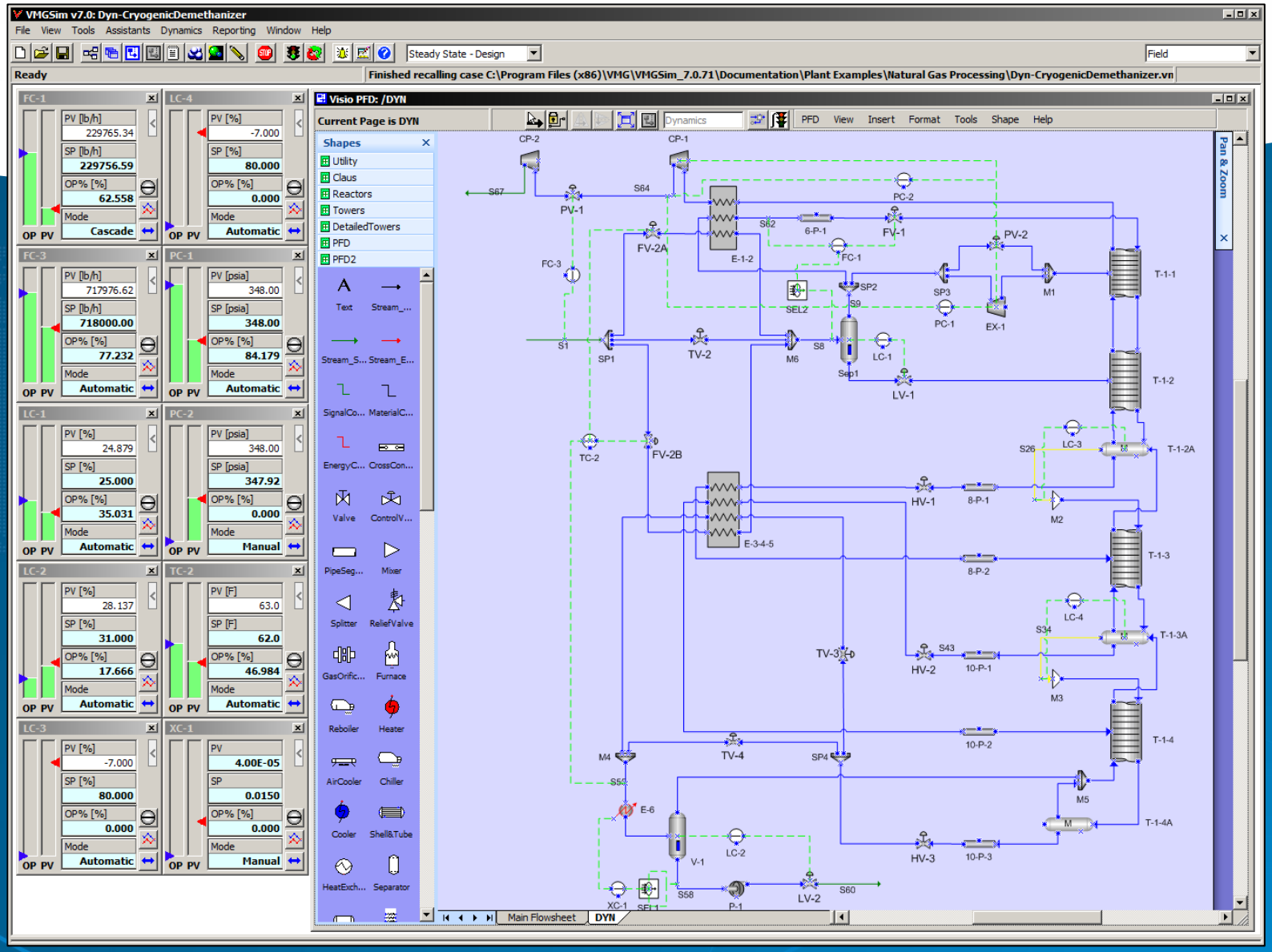

Cryogenic Demethaniser taken from the Plant Examples folder in VMGSim. Dynamic case.

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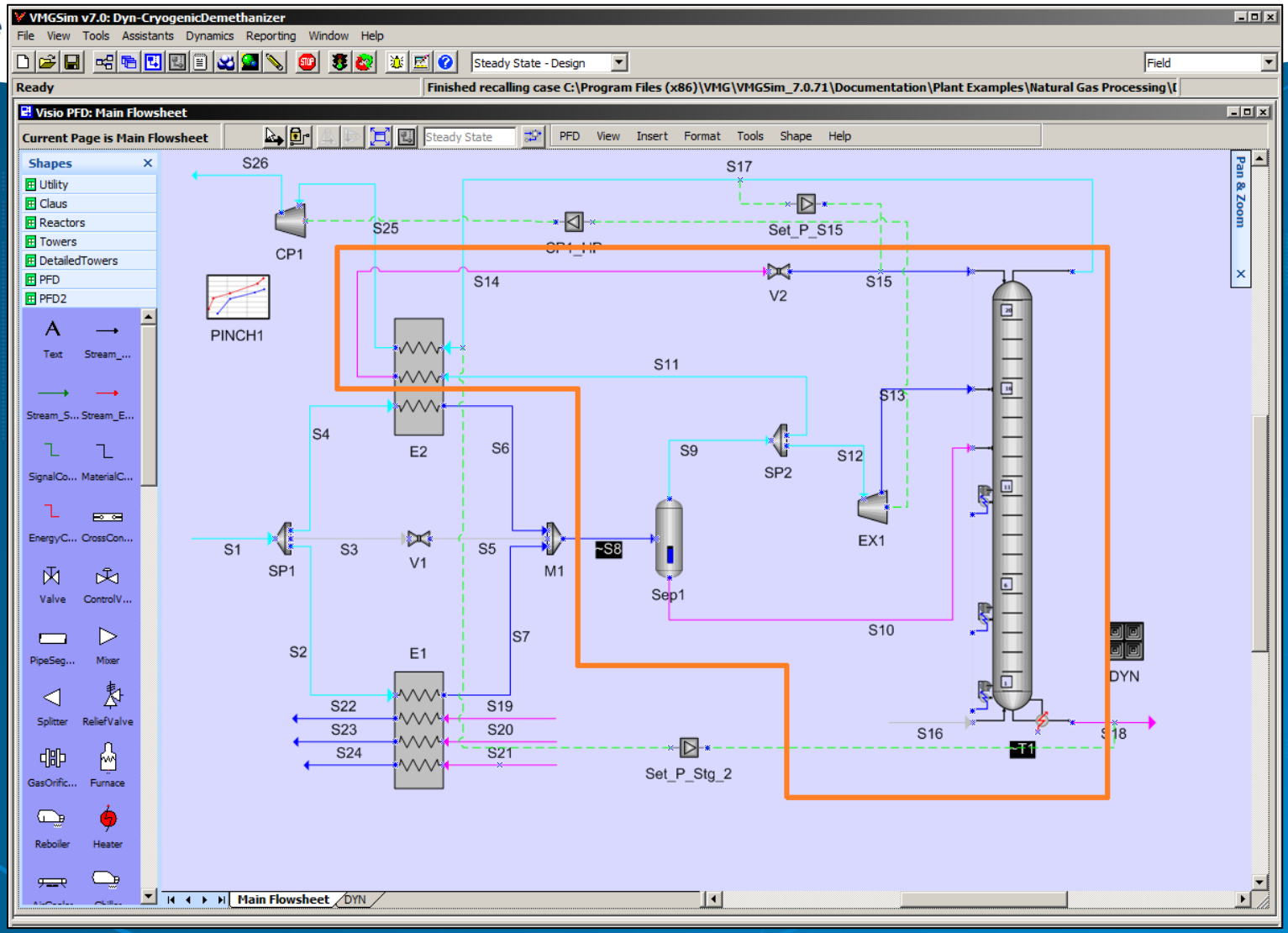

Cryogenic Demethaniser taken from the Plant Examples folder in VMGSim. SS case, part ported into COCO has been highlighted

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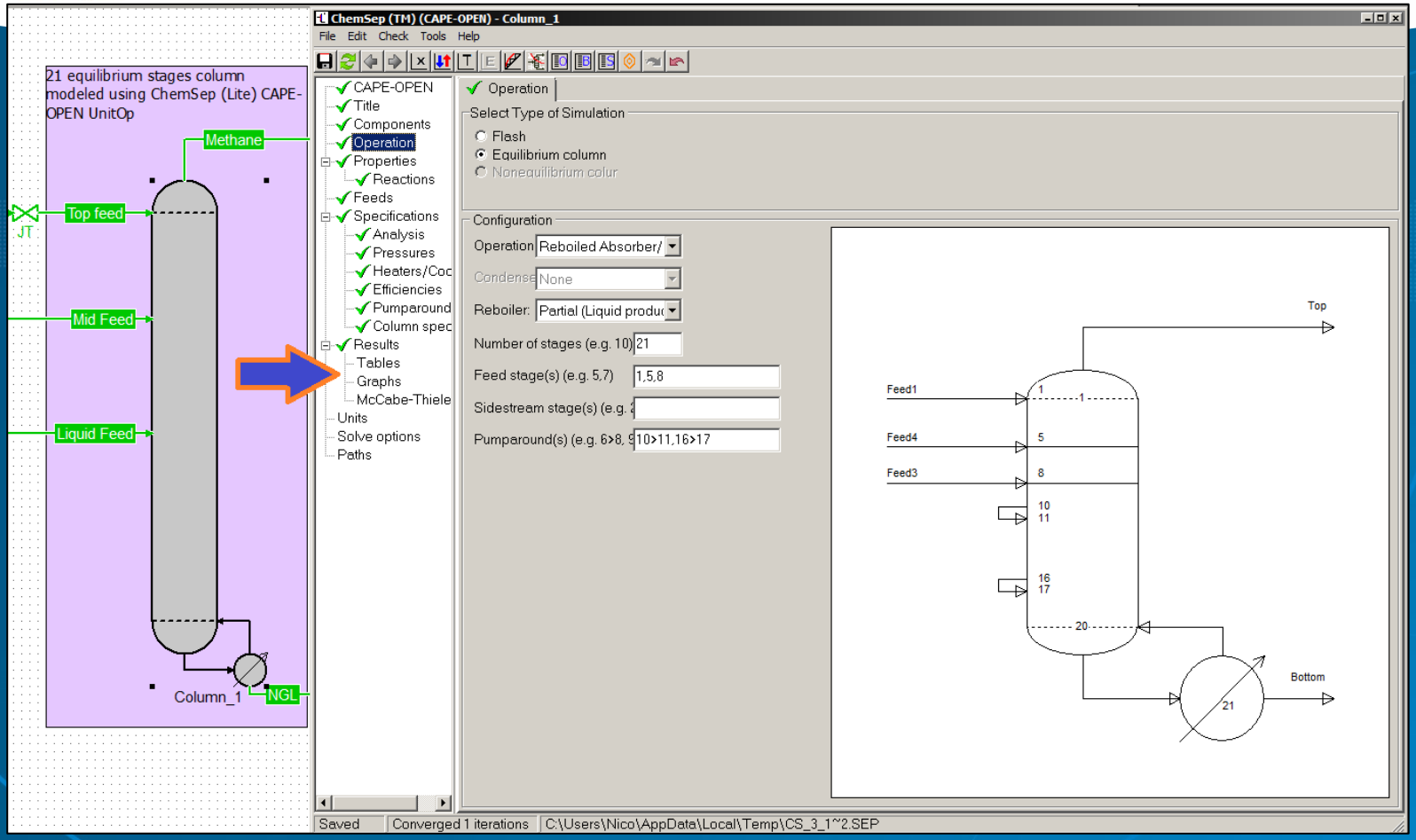
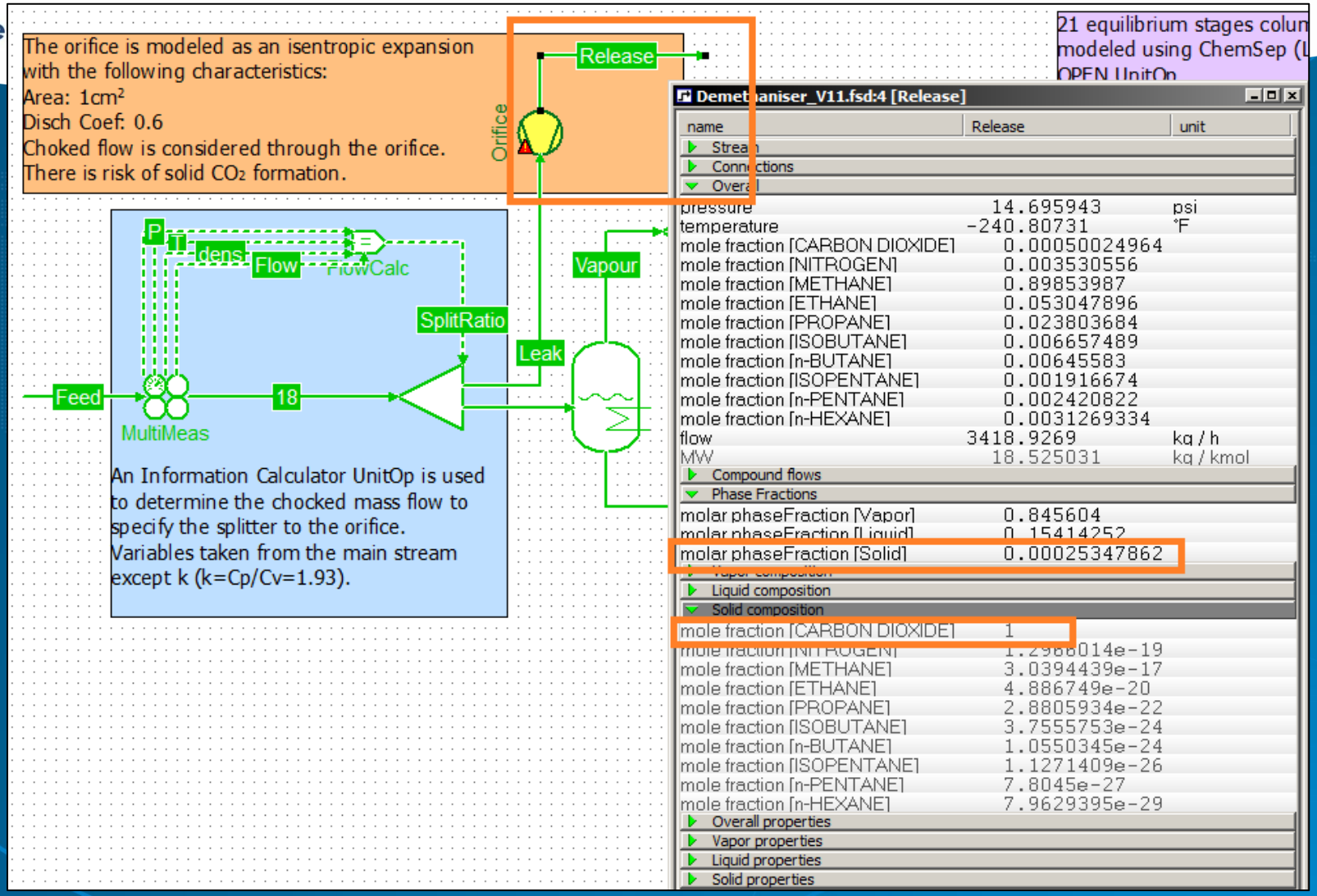


The column is modelled using ChemSep™ (Lite). The thermo to ChemSep™ is provided by COCO (i.e. VMGThermo via VMG CAPE-OPEN)

Live Demo



VMGThermo using the APRSolidCO2 Property Package has predicted the solid CO_2 formation in this release to the atmosphere (from a stream @ 815psia & -18F with C1 to C6, N_2 and CO_2)

Conclusions

- EXCELLENT JOB OF CO-LaN
- Able to connect COFE with VMGThermo easily even with phase mapping
- Able to use non-std thermodynamics and predict solid CO2 formation
- Special thanks to AmsterChem and Jasper van Baten

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Thanks!

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