

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



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



GLOBAL CENTERS

Head Office

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

Head Office:

Subsidiaries:

Sales & Support:

European subsidiary established in 2012

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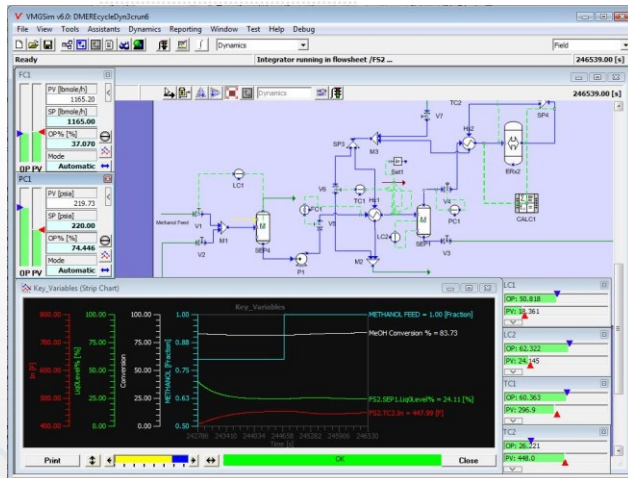
Other:

sales@virtualmaterials.com

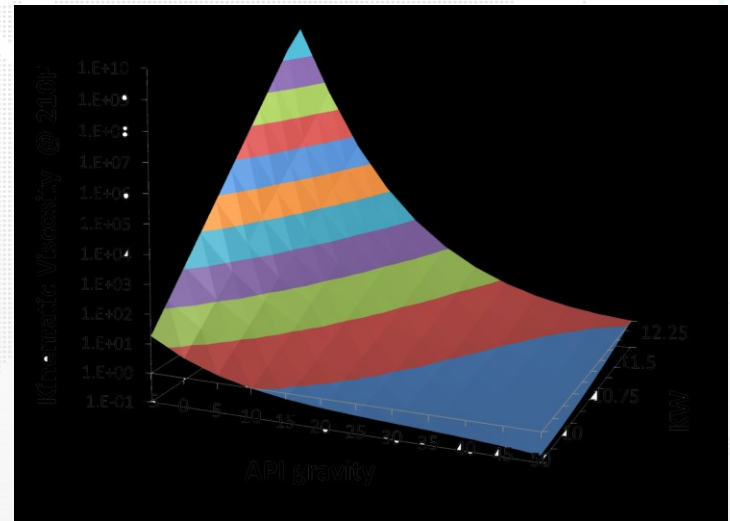
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Main PRODUCTS



Fully interactive steady-state and dynamic process simulator



Robust thermo-physical property calculation engine

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,

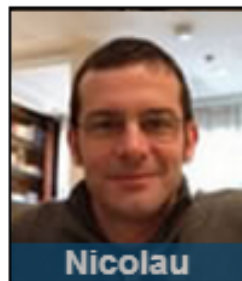
including model-based operations decision support tools. Sergi also holds a postgraduate degree in executive management by IESE Business School.

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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 Catalanian 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

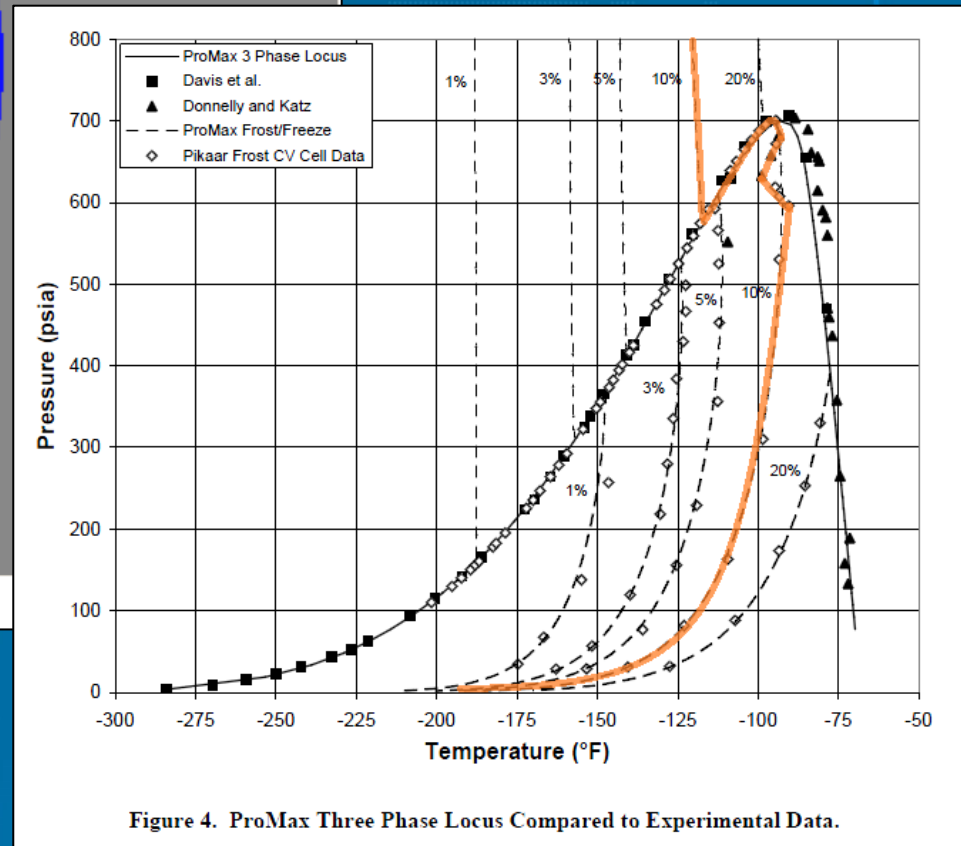
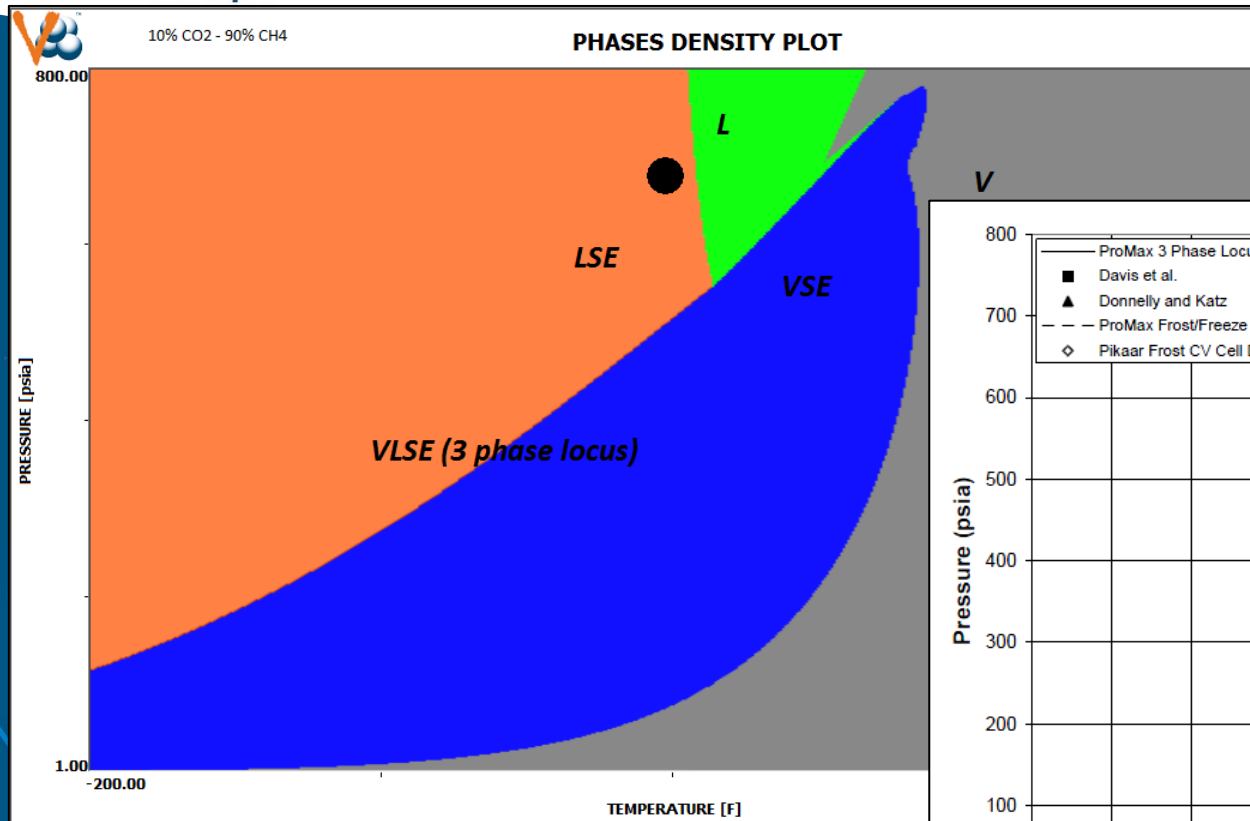
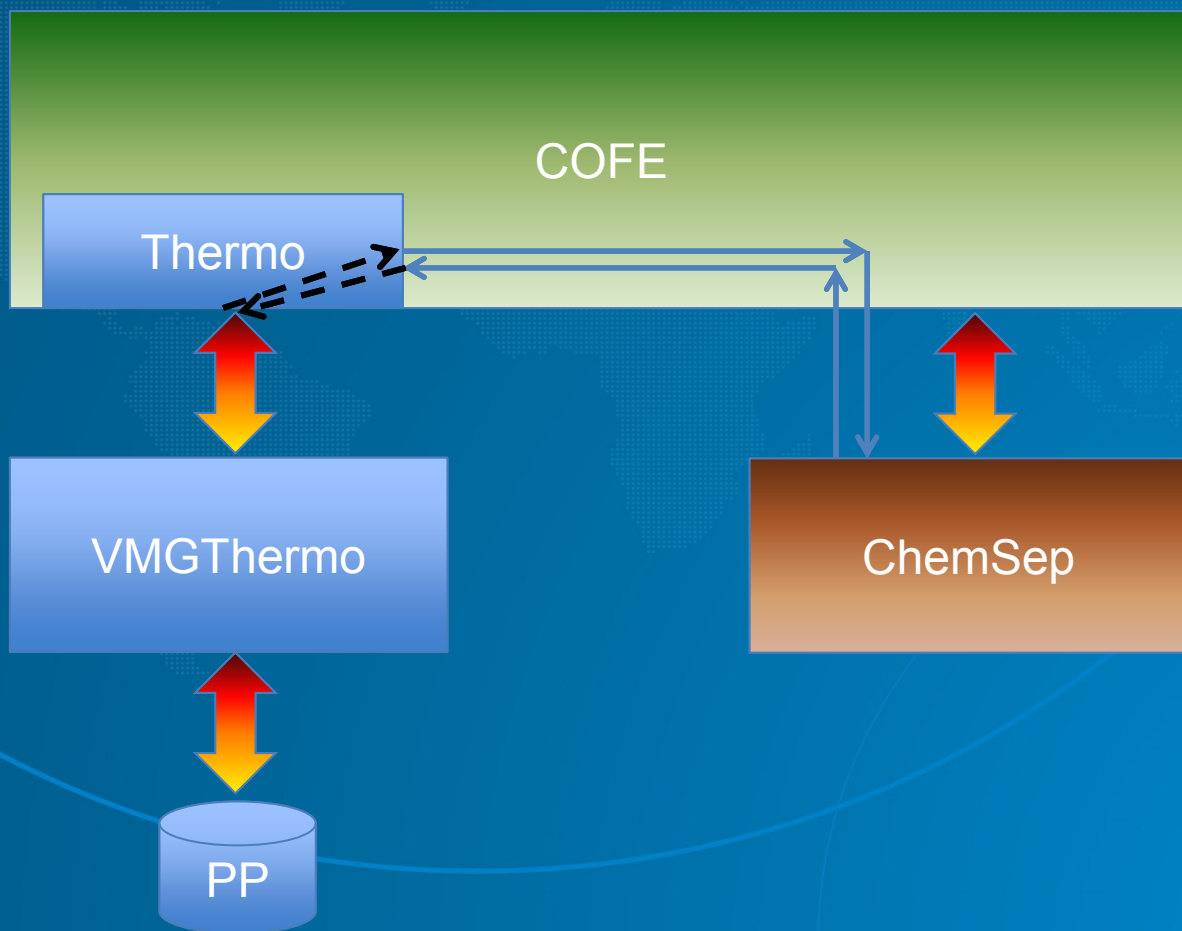
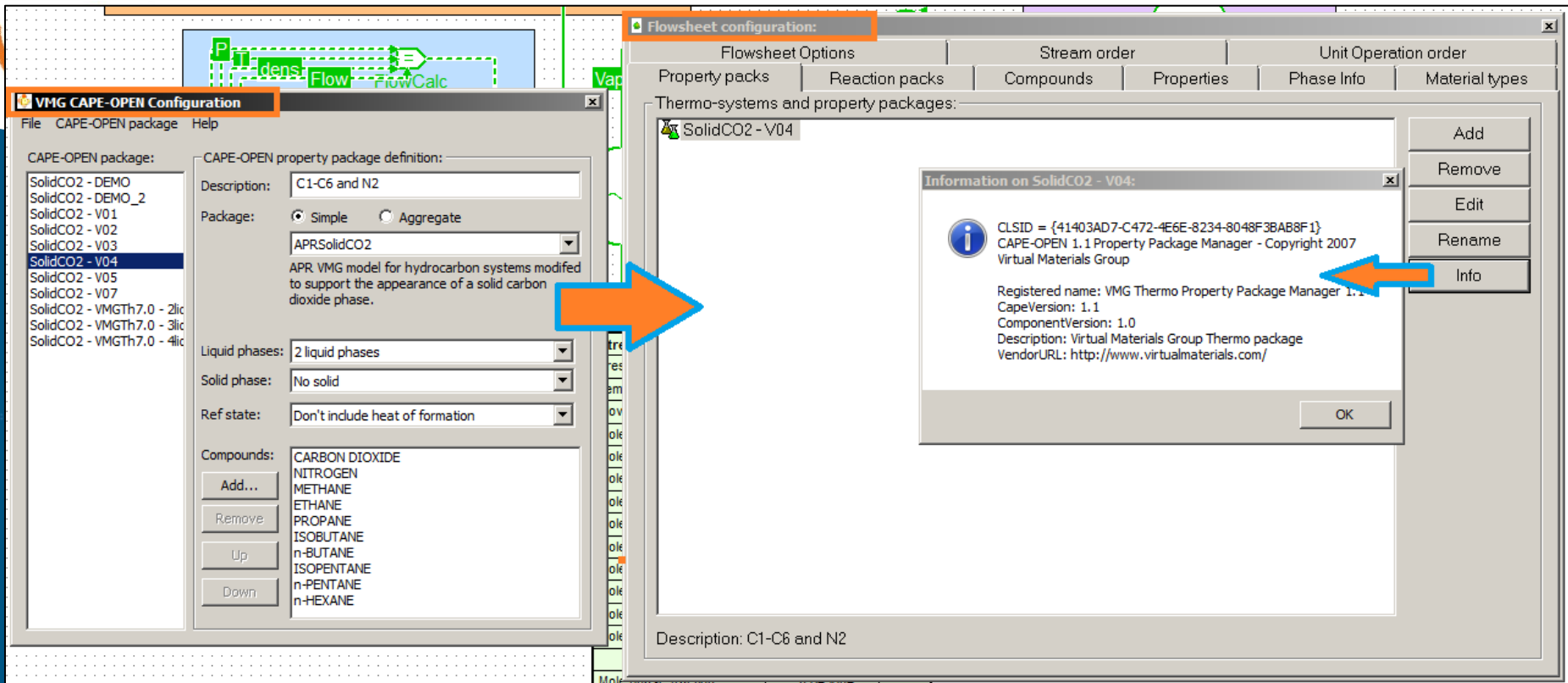


Figure 4. ProMax Three Phase Locus Compared to Experimental Data.

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

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).

Flowsheet configuration:

Flowsheet Options | Stream order | Unit Operation order

Property packs | Reaction packs | Compounds | Properties | Phase Info | Material types

Phase information

Select phase: Solid  Rename

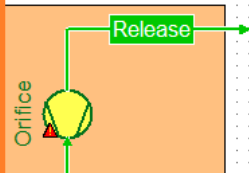
Aggregation state: liquid
ID for SolidCO2 - V04: Liquid2

mole fraction (IMPENTANE)	0.002420022	
mole fraction (n-HEXANE)	0.0031269334	
flow	3418.9269	kg / h
MW	18.525031	kg / kmol
Compound flows		
molar phaseFraction (Vapor)	0.845604	
molar phaseFraction (Liquid)	0.15414252	
molar phaseFraction (Solid)	0.00025347862	
Vapor composition		
Liquid composition		
Solid composition		
Overall properties		
Vapor properties		

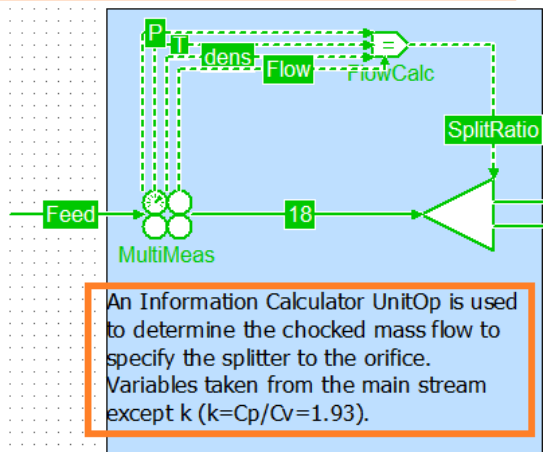
VMGThermo throws the solid CO₂ to the second liquid slot. COCO lets the user rename the phases and any phase starting with “Sol” is actually considered a solid (i.e. solid separator UnitOp).



The orifice is modeled as an isentropic expansion with the following characteristics:
 Area: 1cm²
 Disch Coef: 0.6
 Choked flow is considered through the orifice.
 There is risk of solid CO₂ formation.

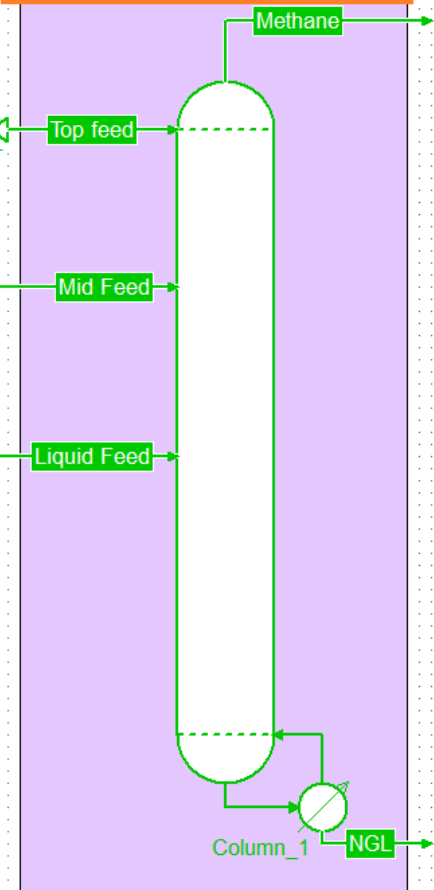


21 equilibrium stages column modeled using ChemSep (Lite) CAPE-OPEN UnitOp

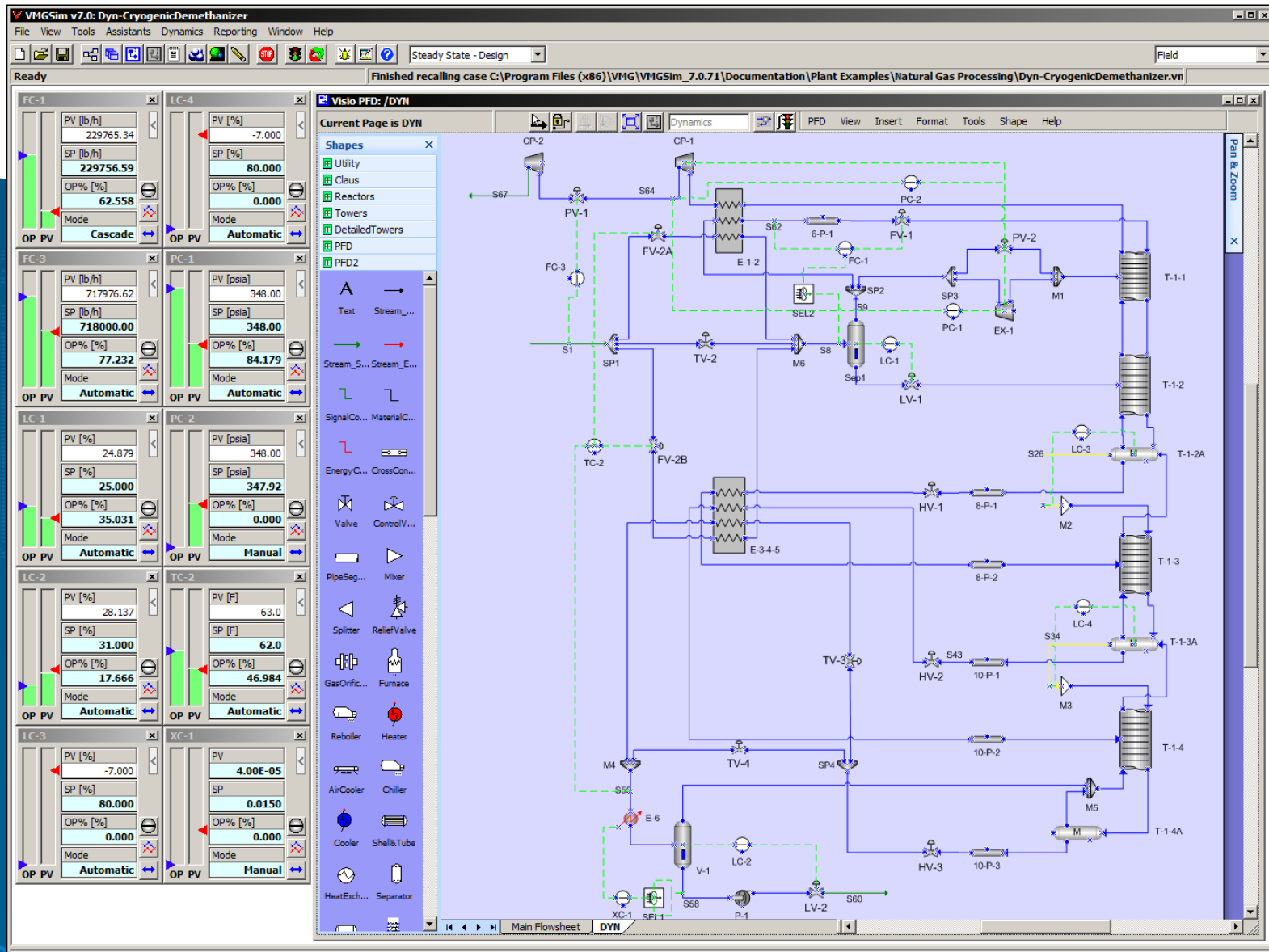


An Information Calculator UnitOp is used to determine the choked mass flow to specify the splitter to the orifice. Variables taken from the main stream except k ($k=C_p/C_v=1.93$).

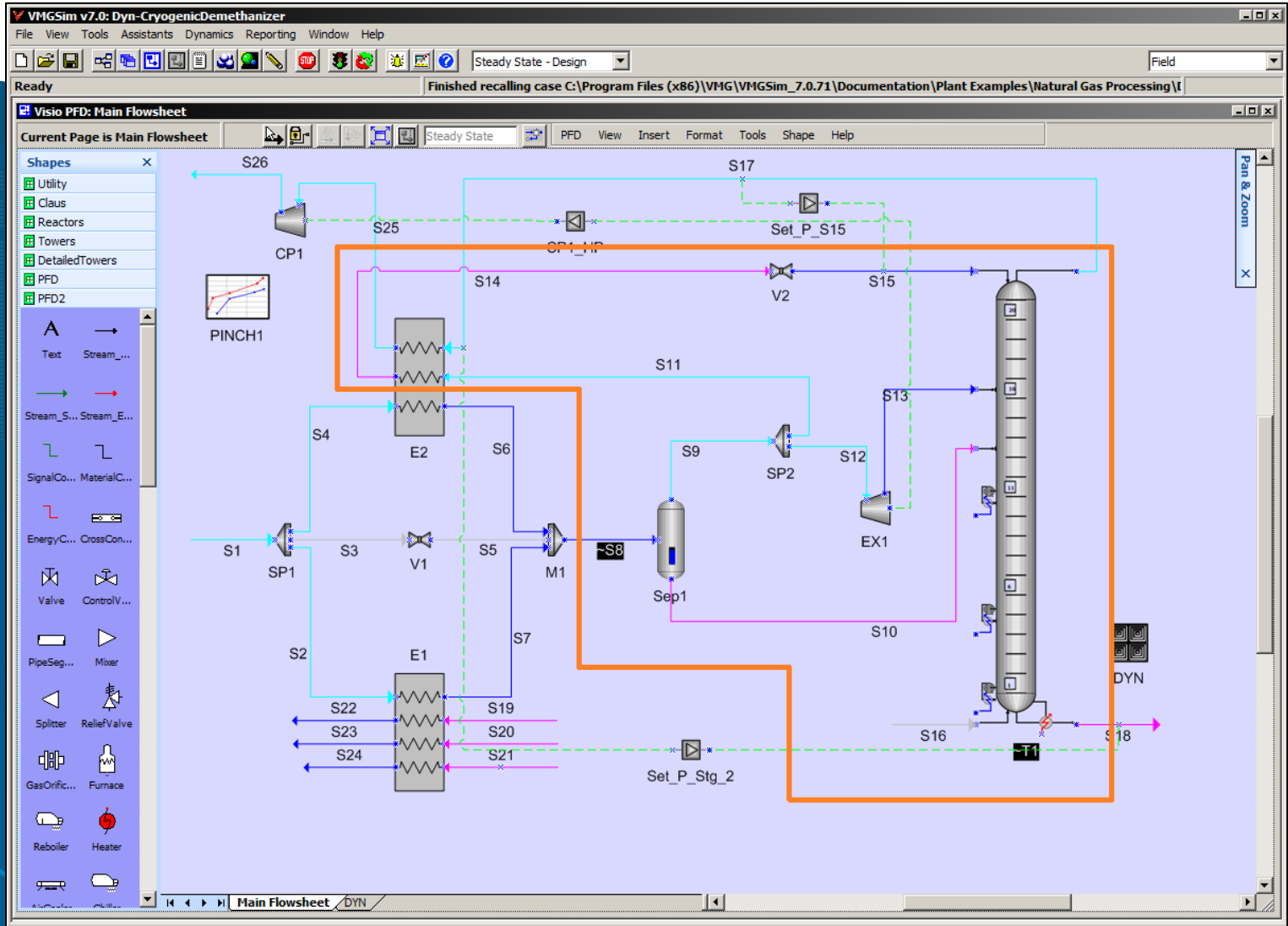
Stream	Release	Unit
Pressure	14.6959	psi
Temperature	-240.807	°F
Flow rate	3418.93	kg / h
Mole frac CARBON DIOXIDE	0.00050025	
Mole frac NITROGEN	0.00353056	
Mole frac METHANE	0.89854	
Mole frac ETHANE	0.0530479	
Mole frac PROPANE	0.0238037	
Mole frac ISOBUTANE	0.00665749	
Mole frac n-BUTANE	0.00645583	
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 / m ³
Liquid phase		
Mole phase fraction	0.154143	
Density	18776.4	mol / m ³
Solid phase		
Mole phase fraction	0.000253479	
Density	37049.1	mol / m ³



Cryogenic Demethaniser taken from the Plant Examples folder in VMGSim. A pipe rupture is modelled (orifice) and the possibility of solid CO₂ formation evaluated.



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



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

ChemSep (TM) (CAPE-OPEN) - Column_1

File Edit Check Tools Help

CAPE-OPEN
 Title
 Components
 Operation
 Properties
 Reactions
 Feeds
 Specifications
 Analysis
 Pressures
 Heaters/Coc
 Efficiencies
 Pumparound
 Column spec

Results
 Tables
 Graphs
 McCabe-Thiele
 Units
 Solve options
 Paths

Operation
 -Select Type of Simulation
 Flash
 Equilibrium column
 Nonequilibrium calor

Configuration

Operation: Reboiled Absorber/

Condense: None

Reboiler: Partial (Liquid produc

Number of stages (e.g. 10): 21

Feed stage(s) (e.g. 5,7): 1,5,8

Sidestream stage(s) (e.g. 4):

Pumparound(s) (e.g. 6>8, 9|10>11,16>17):

21 equilibrium stages column modeled using ChemSep (Lite) CAPE-OPEN UnitOp

Methane

Top feed JT

Mid Feed

Liquid Feed

Column_1 NGL

Top

Feed1 1

Feed4 5

Feed3 8

10 11

16 17

20

21

Bottom

Saved | Converged 1 iterations | C:\Users\Nico\AppData\Local\Temp\CS_3_1~2.SEP

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

Live Demo

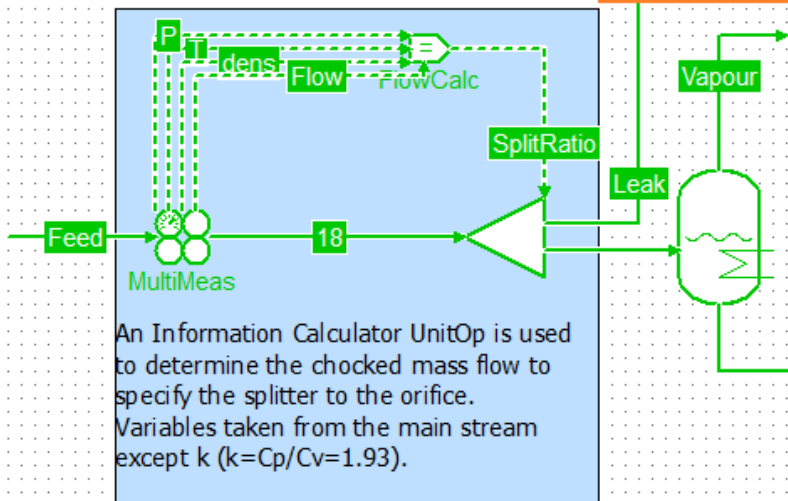
The orifice is modeled as an isentropic expansion with the following characteristics:

Area: 1cm²

Disch Coef: 0.6

Choked flow is considered through the orifice.

There is risk of solid CO₂ formation.



An Information Calculator UnitOp is used to determine the choked mass flow to specify the splitter to the orifice. Variables taken from the main stream except k ($k=C_p/C_v=1.93$).

21 equilibrium stages column modeled using ChemSep (L...
OPEN UnitOp

Demethaniser_V11.fsd:4 [Release]

name	Release	unit
Stream		
Connections		
Overall		
pressure	14.695943	psi
temperature	-240.80731	°F
mole fraction [CARBON DIOXIDE]	0.00050024964	
mole fraction [NITROGEN]	0.003530556	
mole fraction [METHANE]	0.89853987	
mole fraction [ETHANE]	0.053047896	
mole fraction [PROPANE]	0.023803684	
mole fraction [ISOBUTANE]	0.006657489	
mole fraction [n-BUTANE]	0.00645583	
mole fraction [ISOPENTANE]	0.001916674	
mole fraction [n-PENTANE]	0.002420822	
mole fraction [n-HEXANE]	0.0031269334	
flow	3418.9269	kg / h
MW	18.525031	kg / kmol
Compound flows		
Phase Fractions		
molar phaseFraction [Vapor]	0.845604	
molar phaseFraction [Liquid]	0.15414252	
molar phaseFraction [Solid]	0.00025347862	
Vapor composition		
Liquid composition		
Solid composition		
mole fraction [CARBON DIOXIDE]	1	
mole fraction [NITROGEN]	1.2988014e-19	
mole fraction [METHANE]	3.0394439e-17	
mole fraction [ETHANE]	4.886749e-20	
mole fraction [PROPANE]	2.8805934e-22	
mole fraction [ISOBUTANE]	3.7555753e-24	
mole fraction [n-BUTANE]	1.0550345e-24	
mole fraction [ISOPENTANE]	1.1271409e-26	
mole fraction [n-PENTANE]	7.8045e-27	
mole fraction [n-HEXANE]	7.9629395e-29	
Overall properties		
Vapor properties		
Liquid properties		
Solid properties		

VMGThermo using the APRSolidCO₂ Property Package has predicted the solid CO₂ formation in this release to the atmosphere (from a stream @ 815psia & -18F with C1 to C6, N₂ and CO₂)

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

Thanks!