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National Technical University of Athens
School of Chemical Engineering
Laboratory of Thermodynamics &
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UMR-PRU thermodynamic model: application to natural gas processing

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Outline

Introduction

- UMR thermodynamic model
- Motivation

Cape-Open property package

- UMR CAPE-OPEN application
- UMR Property Package Setup

Simulation examples

- Offshore natural gas processing
- TEG dehydration
- CPE in acid gas systems

Challenges

- Speed
- Robustness
- New applications

UMR-PRU thermodynamic model

UMR-PRU is an advanced cubic Equation of State (EoS)

- EoS-GE model, combining Peng-Robinson EoS with UNIFAC
- Thermodynamic properties of fluids (Density, Enthalpy, Heat Capacity, etc)
- Phase equilibria between fluids (Vapor-Liquid, Liquid-Liquid)

Predictive model applicable to the Oil & Gas Industry

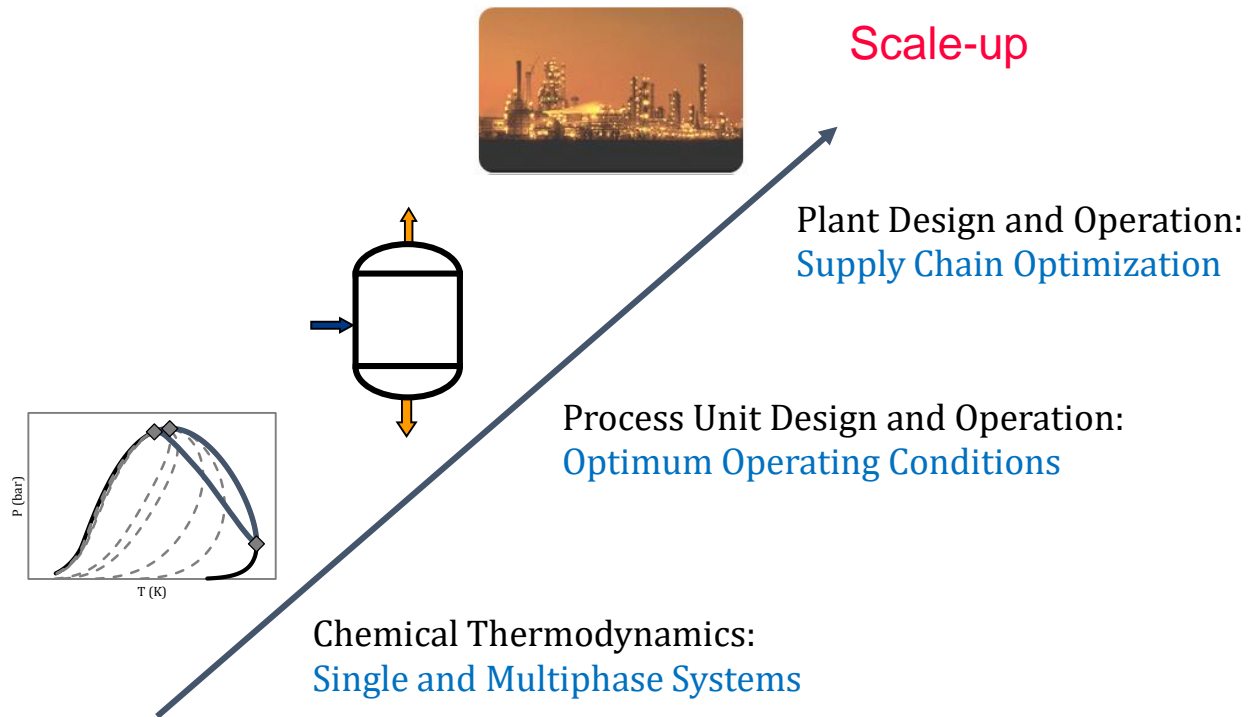
- Phase envelope, flash calculations, liquid dropout, and thermodynamic properties of natural gas and other petroleum fluids
- Mercury, water, acid gases, MEG, TEG, etc.

Motivation

Chemical thermodynamics for process optimization

- ✓ Expand research activity
- ✓ Attract interest from the industry

Ongoing 10 year
collaboration with



UMR CapeOpen application

Process Modelling
Component (PMC)

CAPE-OPEN

Process Modelling
Environment (PME)

PMC :

1. **UMR.dll** : Fortran library for thermodynamic calculations
2. **Wrapper** : C# library acting as a medium between UMR.dll and PME

UMR.dll

Wrapper

CAPE-OPEN

UniSim
Aspen HYSYS
PRO/II

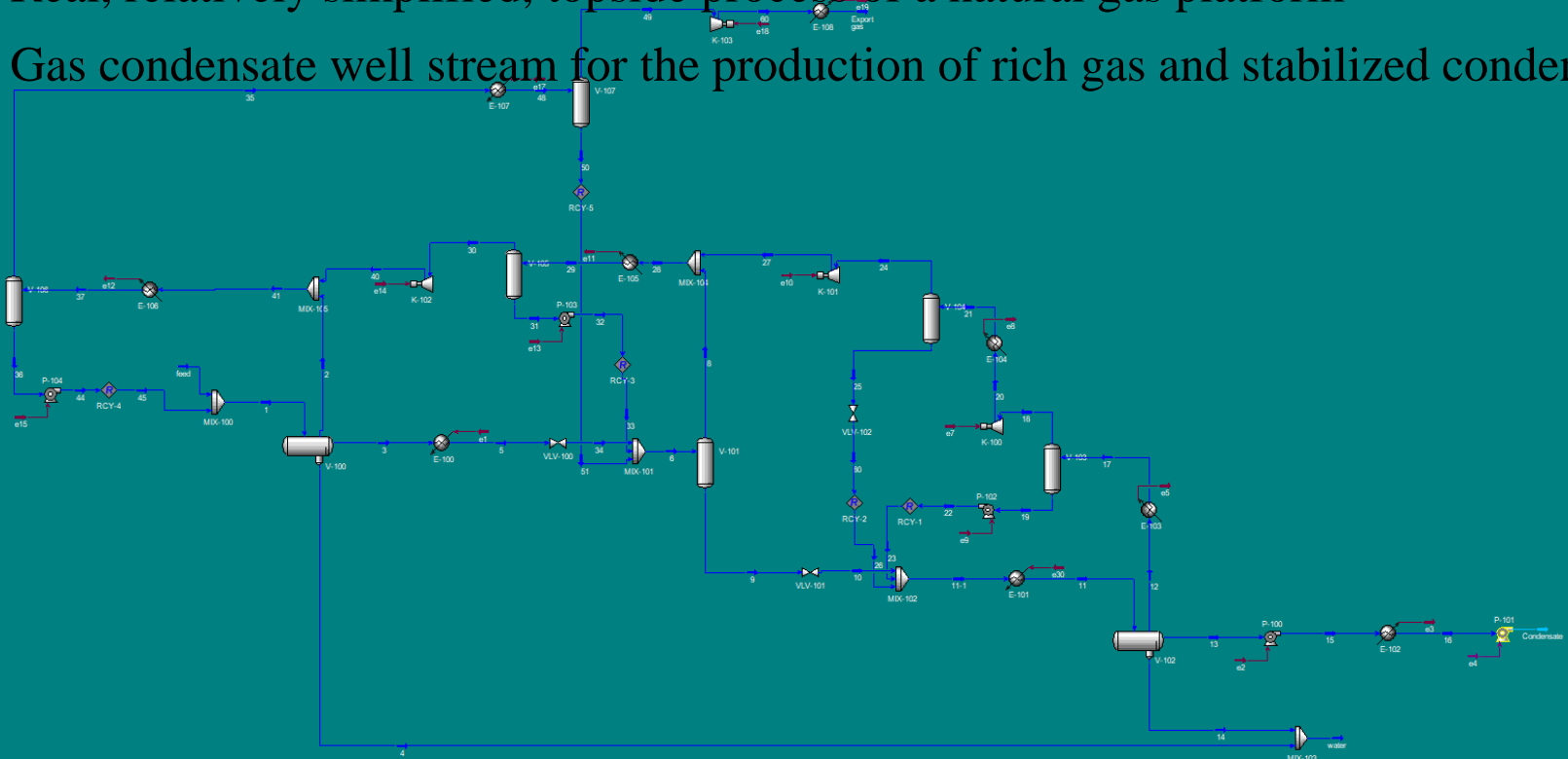
UMR Property Package Setup

UNISIM embedded flash : eThermo

The screenshot displays the Honeywell UniSim software interface, specifically the 'Fluid Package: Basis-1' window. The 'Property Package Selection' list on the left includes 'CAPE-OPEN 1.1', which is highlighted. A 'Select CAPE-OPEN Thermodynamic Property Package' dialog box is open, showing 'Umr CapeOpen' as the selected provider and package. Below this, the 'Fluid Package: test-1' window is visible, showing the 'Model Selection' list with 'eThermoFlash' selected under the 'CAPE-OPEN' model. The 'Model Phase' is set to 'Vapor'. The 'Advanced Thermodynamics' section is checked for 'UniSim Thermo'. The 'Component List Selection' is set to 'Component List - 2'. The 'Set Up' button is highlighted, and the 'Property Pkg' field shows 'Vapor CAPE-OPEN Liquid'.

Offshore NG processing

- Real, relatively simplified, topside process of a natural gas platform
- Gas condensate well stream for the production of rich gas and stabilized condensate



1st stage separator

26 bar
2nd stage separator

2.1 bar
3rd stage separator

condensate cooler

Condensate
45°C
69 bar

Feed fluid

The screenshot displays a software window titled 'feed' with a 'Worksheet' tab selected. The window contains a table with the following data:

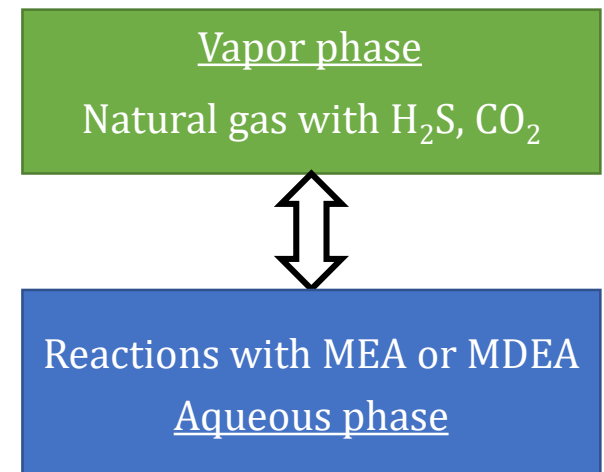
	Mole Fractions	Vapour Phase	Liquid Phase
Nitrogen	0.002600	0.002875	0.000324
CO2	0.031600	0.033452	0.016252
Methane	0.739799	0.803674	0.210513
Ethane	0.082400	0.084471	0.065239
Propane	0.040000	0.038391	0.053330
i-Butane	0.007800	0.006854	0.015642
n-Butane	0.014100	0.011755	0.033530
i-Pentane	0.005100	0.003635	0.017239
n-Pentane	0.005100	0.003426	0.018971
n-Hexane	0.007600	0.003761	0.039409
8001*	0.009762	0.003605	0.060778
8002*	0.008438	0.002030	0.061534
8003*	0.007422	0.001082	0.059954
8004*	0.006591	0.000546	0.056684
8005*	0.005895	0.000261	0.052582
8006*	0.005303	0.000118	0.048265
8007*	0.004707	0.000043	0.043350
8008*	0.004205	0.000015	0.038925
8009*	0.003706	0.000004	0.034383
8010*	0.003218	0.000001	0.029878
8011*	0.002692	0.000000	0.024998
8012*	0.001962	0.000000	0.018220
Total	1.00000		

Below the table, there are buttons for 'Edit...', 'Edit Properties...', and 'Basis...'. At the bottom of the window, there are tabs for 'Worksheet', 'Attachments', and 'Dynamics', and a green bar with 'OK' text. At the very bottom, there are buttons for 'Delete' and 'Define from Other Stream...'.

Feed fluid contains pseudocomponents!

Acid gas/alkanolamine/water mixtures

- Extended UMR-PRU (PR + extended UNIQUAC)
- Acid gases: CO₂, H₂S
- Amines: MEA, MDEA
 - ✓ Phase equilibrium
 - ✓ Chemical equilibrium
 - ✓ Simultaneous chemical & phase equilibrium
 - ✓ Chemical equilibrium solved in two sequential flash drums
 - ✓ Comparison of UMR-PRU with Acid-Gas model
 - Better prediction of VLE with UMR-PRU



Challenges

- Speed
 - ✓ The CAPE-OPEN simulation is tiresome compared to built-in thermodynamic models
- Simulation robustness
 - ✓ 3 phase flash and phase stability may return artifacts
 - ✓ False labeling of phases as Liquid or Vapor
- New applications
 - ✓ Trace components
 - ✓ 4 phase flash
 - ✓ Hypothetical solids

Thank you for
your attention

Questions?