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National Technical University of Athens
School of Chemical Engineering
Laboratory of Thermodynamics &
Transport Phenomena

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-G^E 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.

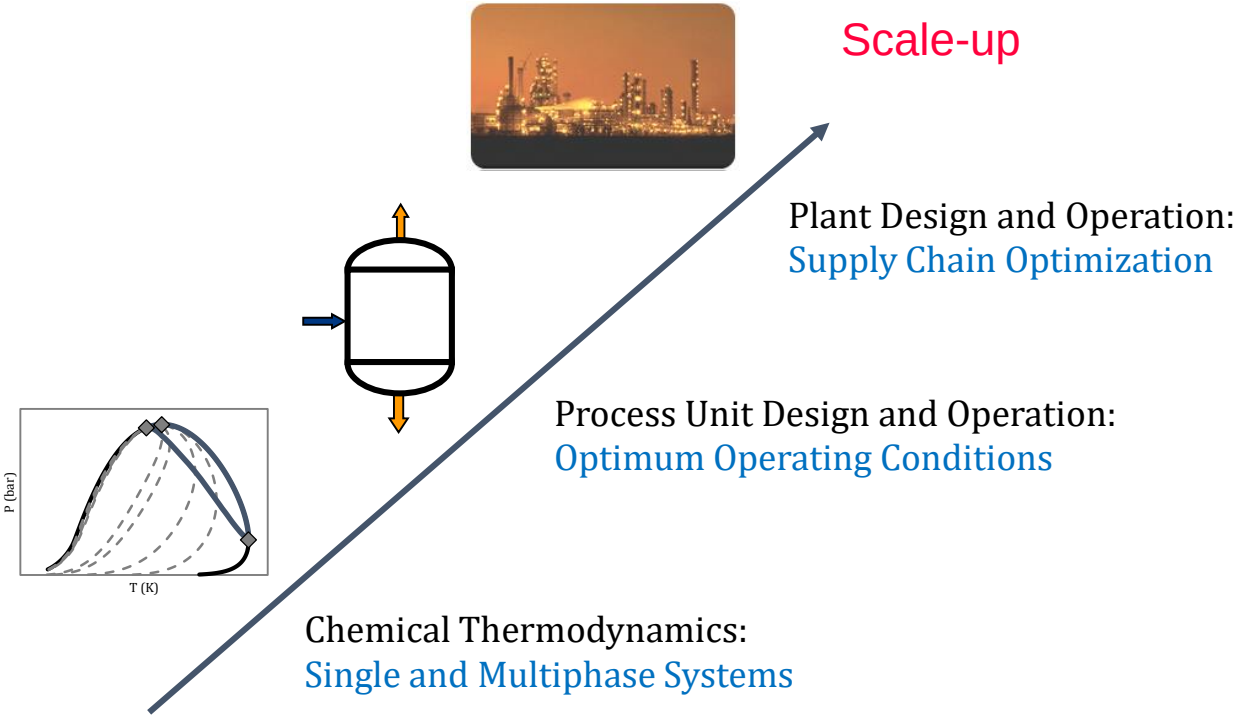
Motivation

Chemical thermodynamics for process optimization

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

Ongoing 10 year collaboration with

equinor



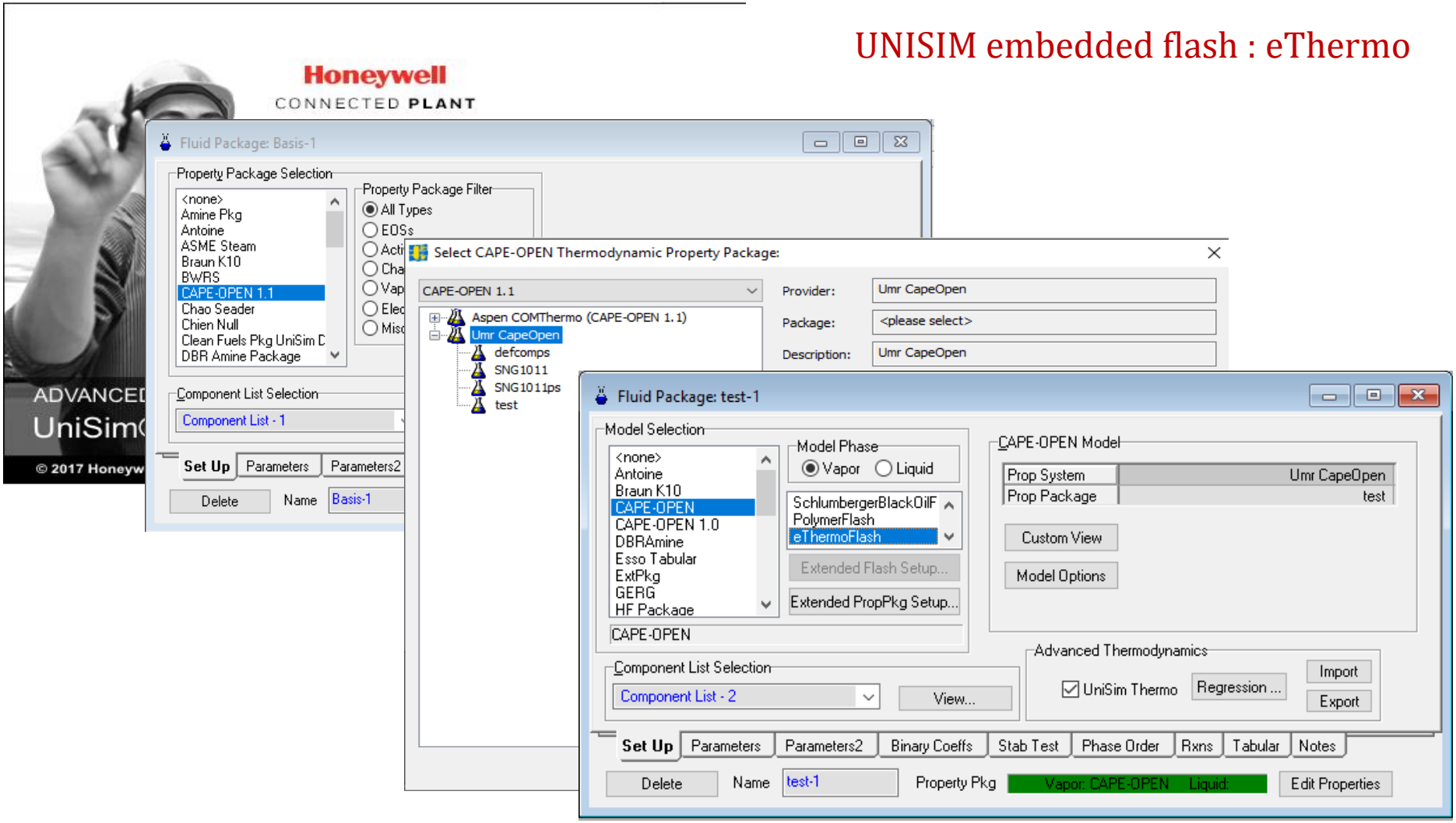
UMR CapeOpen application

PMC :

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

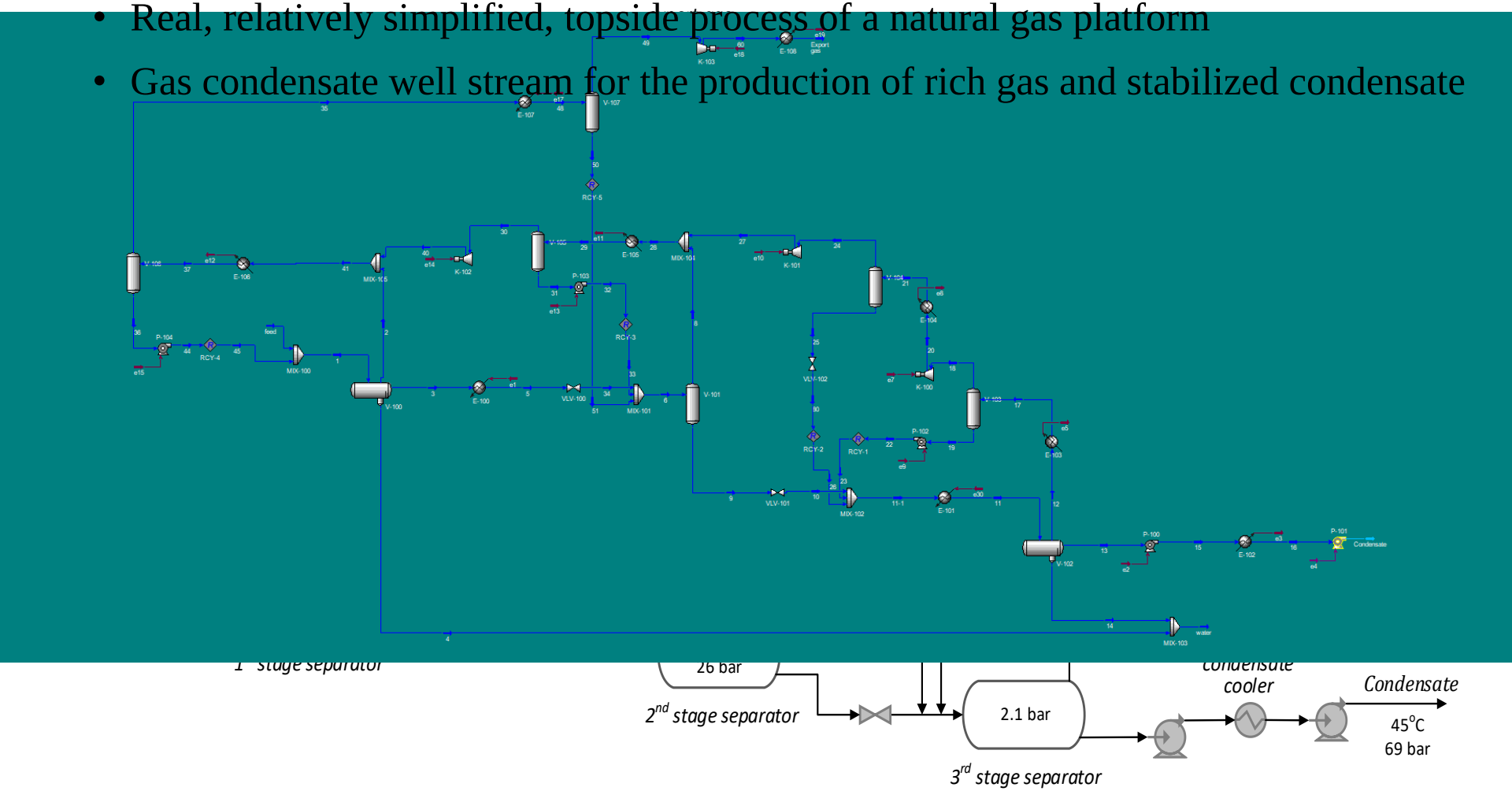
UMR Property Package Setup

UNISIM embedded flash : eThermo



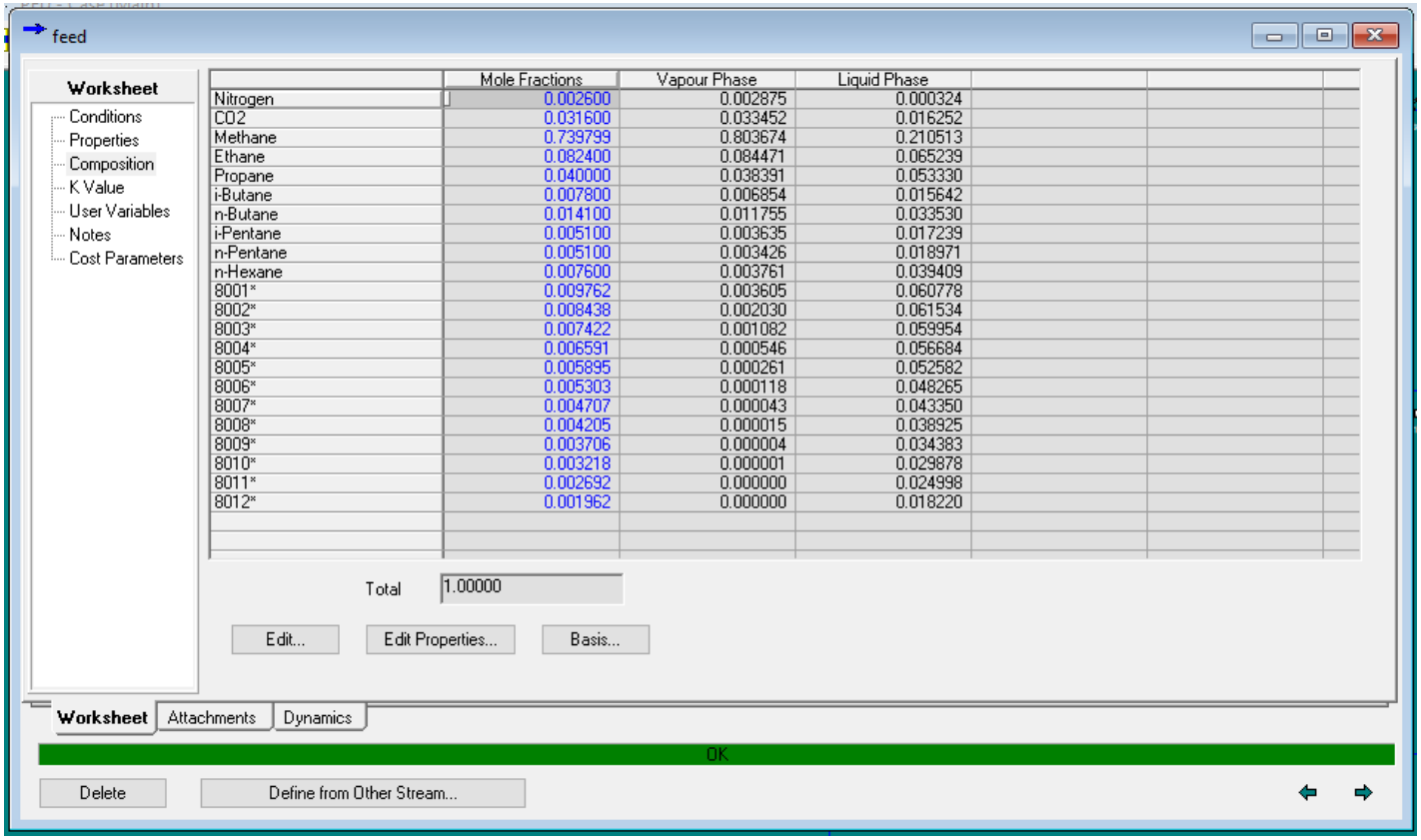
Offshore NG processing

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



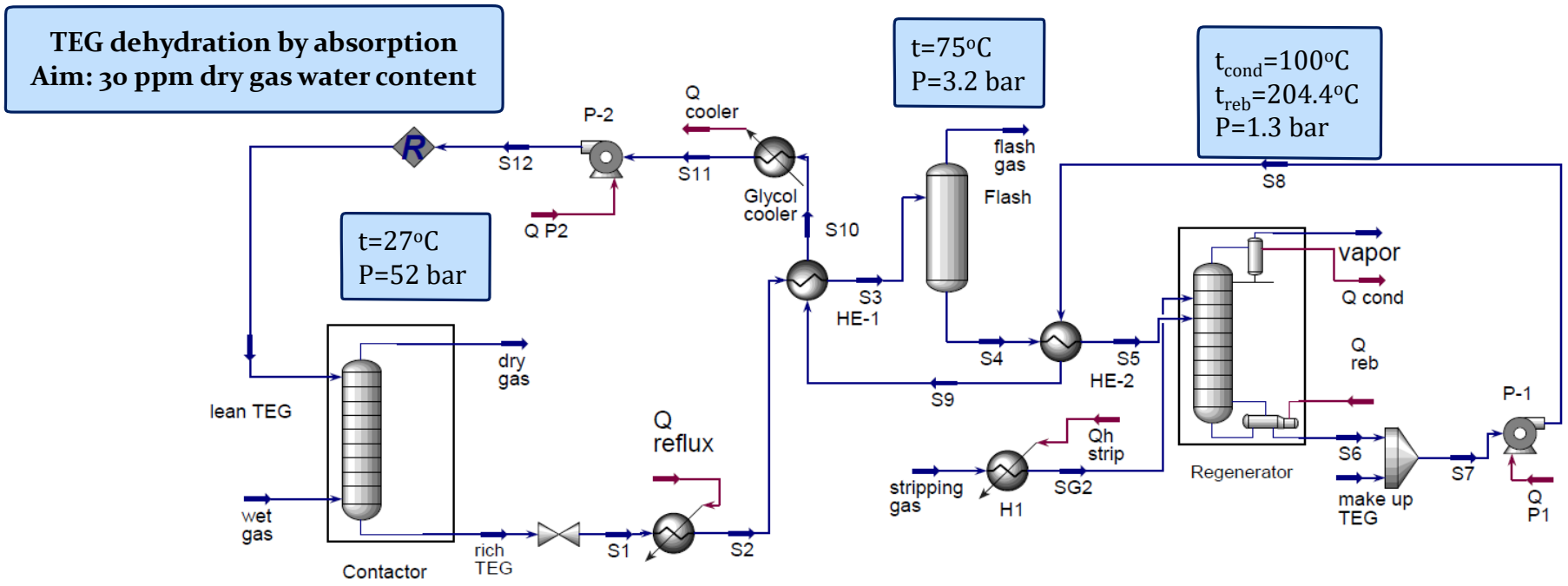
E. Voutsas, N. Novak, V. Vouli, G. Pappa, E. Petropoulou, Ch. Boukouvalas, E. Panteli, E. Skouras, Thermodynamic modelling of natural gas and gas condensate mixtures, in Natural Gas Processing from Midstream to Downstream. 2019.

Feed fluid



Feed fluid contains pseudocomponents!

TEG dehydration

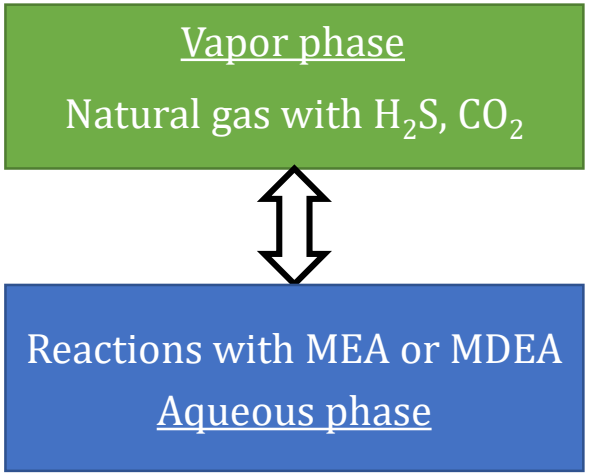


- UMR-PRU yields identical results in HYSYS and Unisim
- Comparison with HYSYS Glycol package (TST/NRTL)
  - ➢ Better prediction of thermodynamic properties with UMR-PRU implies more accurate simulation results

Acid gas/alkanolamine/water mixtures

- Extended UMR-PRU (PR + extended UNIQUAC)
- Acid gases: CO_2, H_2S
- 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?