AVEVA Advisory Group Meeting

NOV.14.2022

Thermodynamic updates/ roadmap

Seiya Hirohama, Thermodynamic Product Manager, AVEVA

Prasad Narasimhan , Thermodynamic Development Manager, AVEVA

For Internal Use Only. ©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA ADVISORY GROUP MEETING

Thermodynamic updates/roadmap

1. **Overview of Roadmap of Therm. Features**
2. **Highlighted New Features/ Items in the Roadmap for;**
   - Design in Chemicals
   - Design in Oil&Gas
   - OTS
   - Commonly Utilized Items

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Overview of Roadmap of Therm. Features

Flexible and Customer Driven

:Items being talked today

Platforms		Yesterday	Today*	Tomorrow
Major Goals		Enable AVEVA™ Process Simulation to cover design in Chemicals except for Polymers Enable AVEVA™ Dynamic Simulation and AVEVA™ Process Optimization to conduct key OTS/RTO Enable AVEVA™ PRO/II Simulation to achieve committed items	Enable AVEVA™ Process Simulation to start covering design in Gas Processing Enable AVEVA™ Dynamic Simulation and AVEVA™ Process Optimization to conduct Enable AVEVA™ PRO/II Simulation to achieve committed items	Enable AVEVA™ Process Simulation to cover design in Polymers and Oil&Gas Drastically accelerate AVEVA™ Dynamic Simulation Enable AVEVA™ PRO/II Simulation to achieve key refinery items
Platforms	AVEVA™ Process Simulation:	**Thermo Methods**: SRKH, PSRK with gE of NRTL. gE of UNIFAC, e-NRTL, LK(enth),HF-Thermo, CO2_SW, Cryo_H2 **Transport prop.**: Pure comp ave. with mixing rules for chemicals **Diagrams /Utilities**: Liquid-Liquid Diagrams, Ternary Charts, Phase envelopes **Integration/Interface**: User Added Thermo Interface (works with DPP of DECHEMA) , Thermo Access Interface, PPDX imp./exp., Data export for HTRI **Thermo Architecture and Flash**: Thermo Data Override, VLLE, Non-Equilibrium Solids, Electrolyte Precipitates	**Thermo Methods:** • Amine (using eNRTL and Reactions), • Electrolyte density • Gas hydrate prediction • Cubic Plus Association (CPA) EOS **Transport prop.:** • TRAPP **Diagrams /Utilities:** • Native REGRESS(being discussed) **Integration/Interface:** • Thermo Access Interface enhance. **Data:** • FILL Options (from UNIFAC) **Architecture and Flash:** • VLLE flash improvements, VLWE flash	**Thermo Methods:** • GERG-2008(being discussed) • LACT with association (being evaluated) • (Elec.)PC-SAFT(being discussed), polymer • Refinery Inspection Properties **Integration/Interface:** • Assay data import (incl. Spiral) **Data:** Electrolyte Species and Reaction Data • FILL options for refineries, • Heavy Oil. water and gas Solubility in oil **Architecture and Flash** • Distil curves, Crude Assay, Characterization • Polymer flash/MW distribution • Enhance solid feature
	(Sim4Me Thermo) • AVEVA™ Dynamic Simulation • AVEVA™ Process Optimization • AVEVA™ PRO/II Simulation:	**Thermo Methods**: HV, TCB, PSRK(UNIFAC), PC-SAFT(2 terms), GPSW.. **Transport prop.:** TRAPP, PETRO, Pure **Refinery-related features:** Distil curves, Crude Assay, Charac., refinery insp.prop. **Diagrams /Utilities:** Ternary LLE Charts, Phase env., Edit/add UNIFAC groups **Integration/Interface:** Interface with OLI, ChemApp, REFPROP **Data**: FILL options (including UNFIAC) **Architecture and Flash**: Open form VLLE and Super-linear Local Model	**Thermo Methods** • Update temp. dep. Eqs. of methods **Diagrams /Utilities** • Update temp. dep. Eqs. of TDM REGRESS **Architecture and Flash** • Improve VLLE flash calculation (continued effort) including Open Form/Super Linear • PRO/II Simulation to have native multi-phase flash (VLSE) of JIP project	**Thermo Methods** • (Native) GERG-2008 or alternative • Cubic Plus Association (CPA) EOS • Gas hydrate prediction • New standard of American Petro. Inst. **Data** • Use of 2DxGC analysis • Heavy Oil, New gas solubility methods **Architecture and Flash** • Thread-safe Sim4Me Thermo • Improve VLLE flash (continued effort)
	Commonly shared data	Updated coefficient of alpha formula, Glycol update (BIPS for Glycol HC pairs), Redistribution of DIPPR Lite	Wilson BIP bank, Update BIPs for ammonia, consistent VLE/LLE of alcohol-HCs, solid precipitation in LNG Cryogenic H2 bank, LNG bank	Databanks for newly implemented methods Databanks for extended number of components

*: As for exact release versions, please check with the product manager of each end-product

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA ADVISORY GROUP MEETING

Thermodynamic updates/roadmap

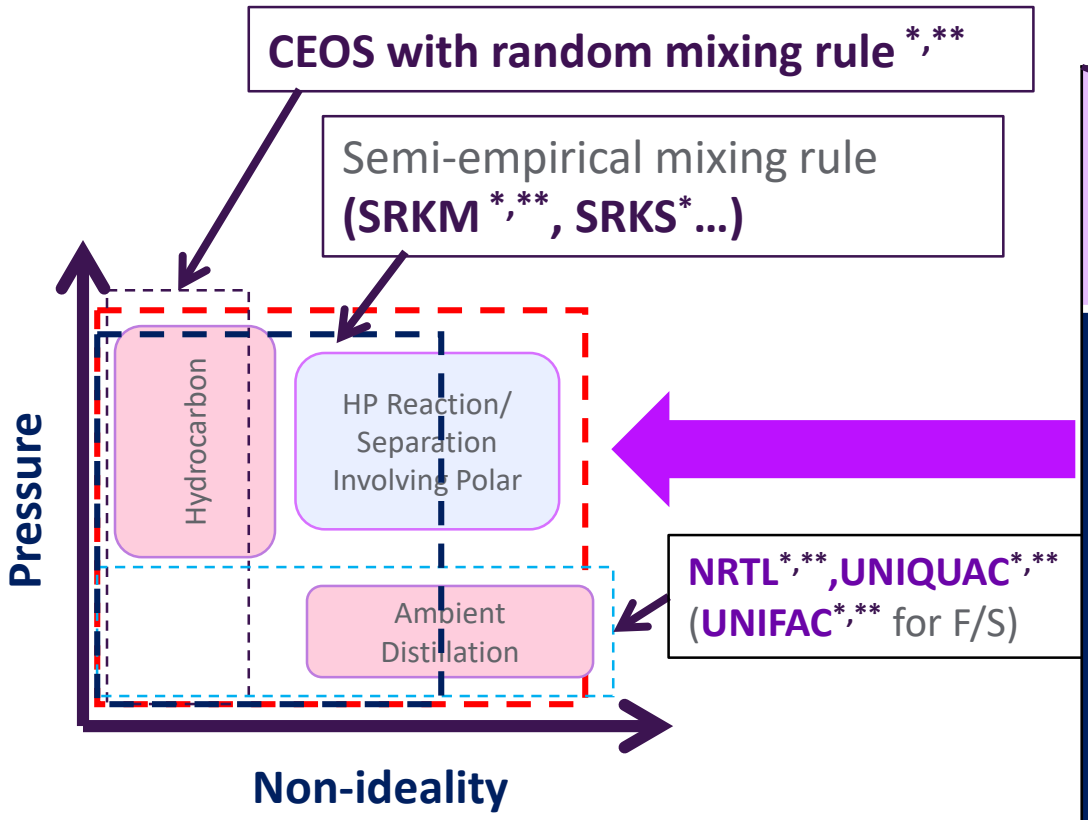
1. **Overview of Roadmap of Therm. Features**
2. **Highlighted New Features/ Items in the Roadmap for;**
   - Design in Chemicals
   - Design in Oil&Gas
   - OTS
   - Commonly Utilized Items

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Thermo Methods for Non-Ideal Mixtures at Elevated Pressures

30% of chemical processes are operated at high pressures!!



Schematic Diagram for Applicable Range of Thermo Methods

Currently Published Methods for High Pressure Non-ideal Mixtures

		Type of Equation of State	
		Cubic	**Non-Cubic**
Type of non-ideality expression	**gE-type**	**Hüron-Vidal*,** **PSRK UNIFAC gE*,**** **PSRK NRTL gE**** **VTPR,** MHV-2, Wang-Sandler **Twu-Bluck-Coon****	(none)
	Association	**Cubic Plus Association (CPA)***	**PC-SAFT (2nd phase)***

*:Already implemented in Sim4Me Thermo
**:Already implemented in AVEVA Process Simulation
***:In the roadmap or being discussed for AVEVA Process Simulation

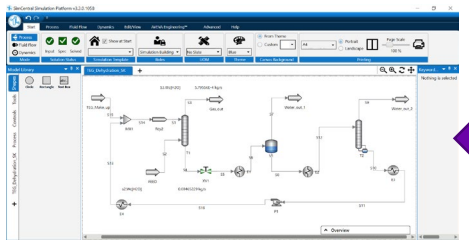
AVEVA

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

Use of SRK+ Holderbaum-Gmehling Mixing Rule (SRK-HG)

Mixing Rule of PSRK. Often uses g^E of NRTL and its parameters determined using experimental data.

Process Simulations



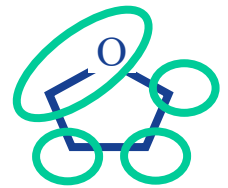
Holderbaum-Gmehling (HG) Mixing Rule*

$$\frac{a_m}{b_m} = \frac{g^E}{C} + \frac{RT}{C}\sum_i x_i \ln\left(\frac{b_m}{b_i}\right) + \sum_i^{Nc} \frac{a_i}{b_i} x_i$$

Done!

g^E of UNIFAC

Molecular Structure



Done!

g^E of NRTL**

$$g^E = \sum_i x_i \frac{\sum_j x_j G_{ji} \tau_{ji}}{\sum_k x_k G_{ki}}$$

$$G_{ji} = exp(-\alpha_{ji}\tau_{ji})$$

$$\alpha_{ii} = 0, \tau_{ii} = 0$$

UNIFAC FILL

Proposed

NRTL Bank

Experimental data

PSRK (SRK-HG + UNIFAC g^E)

SRK-HG + g^E of NRTL

gE of UNIFAC: Available for AVEVA Process Simulation, AVEVA PRO/II Simulation, AVEVA Dynamic Simulation,..
gE of NRTL: Currently available only for AVEVA Process Simulation

* Holderbaum ,T and Gmehling,J.; Fluid Phase Equilibria, 70,2-3, (1991), 251-265
** Renon H., Prausnitz J. M.; AIChE J., 14(1), S.135–144, 1968

AVEVA

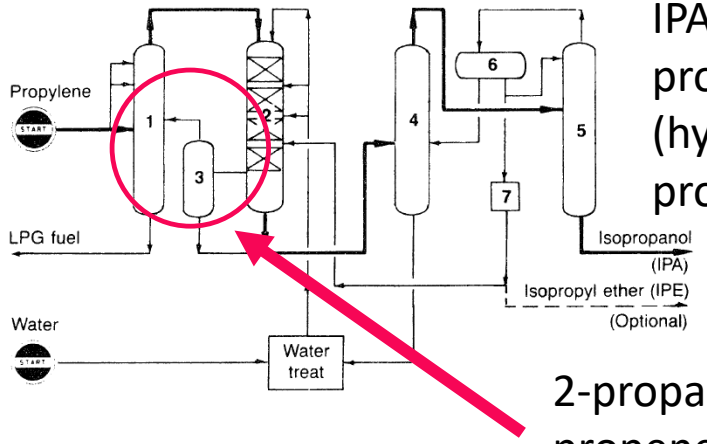
© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

PSRK with gE of NRTL: A Benchmark Test

2-Propanol (IPA) + Propene + Water System

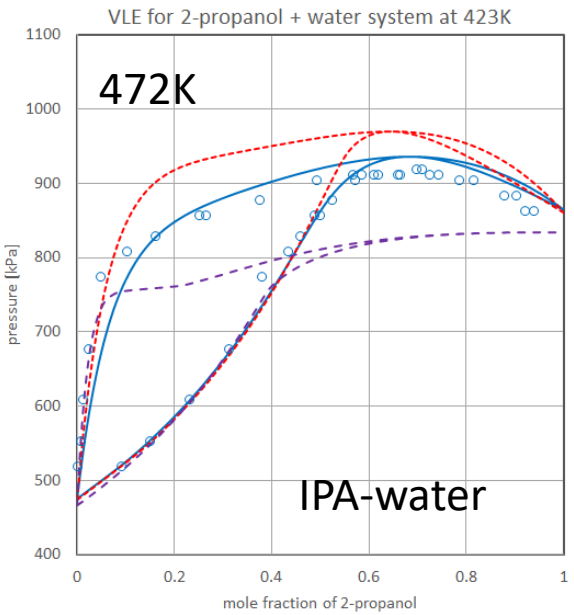
Test at VLE at reactor condition

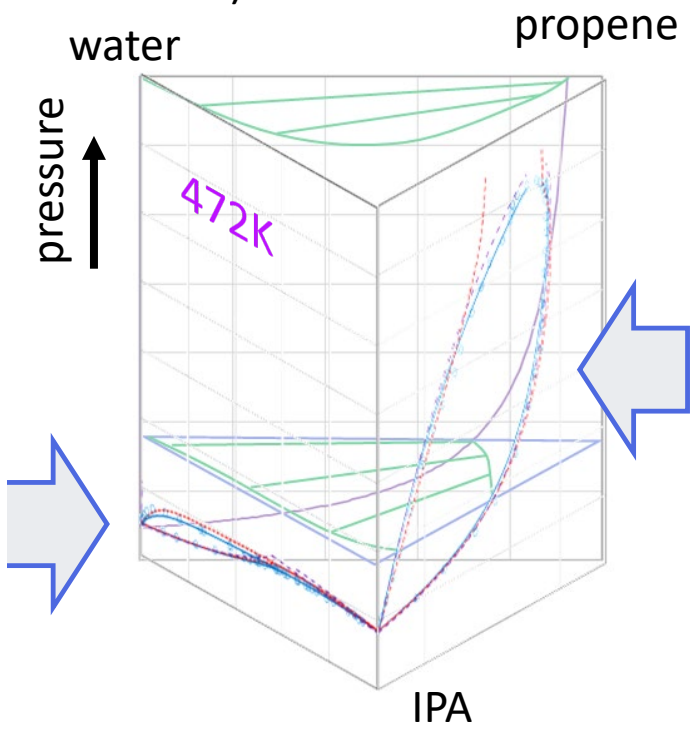
- IPA-water system (moderate press.) : PSRK with gE of NRTL worked well (with BIPs in NRTL bank, determined at lower press. and temp.) , NRTL+RK fairly worked. SRK failed to correlate VLE
- Propene-IPA system (high press.): PSRK with gE of NRTL, SRK worked well , NRTL+RK failed to correlate VLE.
- (BIPs were adjust to experimental data)

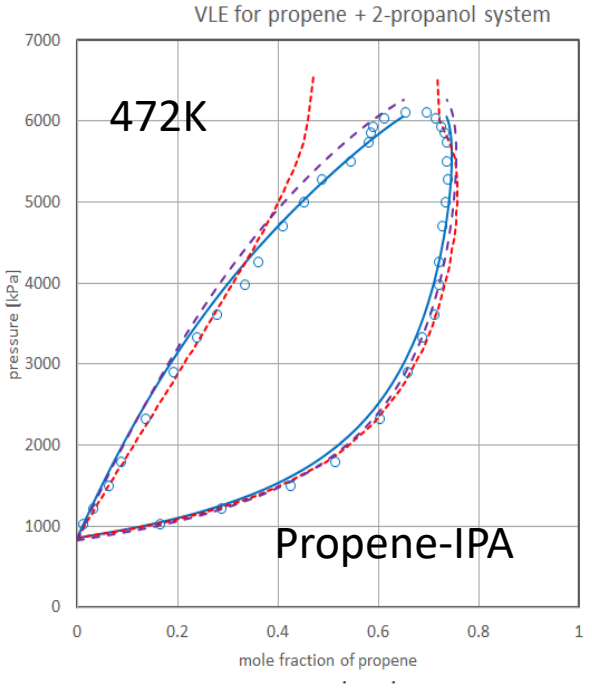


IPA production process (hydration of propene)

2-propanol(IPA) + propene + water







Exp.

Calc.(PSRK with gE of NRTL)

Calc.(NRTL+RK, gamma-phi)

Calc. (SRK)

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

Interface of DPP with AVEVA™ Process Simulation

Done!
(further progress is being made)

Objective and Background

- DECHEMA's Data Preparation Package (DPP) has been widely used by major chemical companies for regression of thermophysical property models.
- Enables users to manage/determine parameters of thermodynamic methods in AVEVA Process Simulation, utilizing the capability of DPP.

Solutions

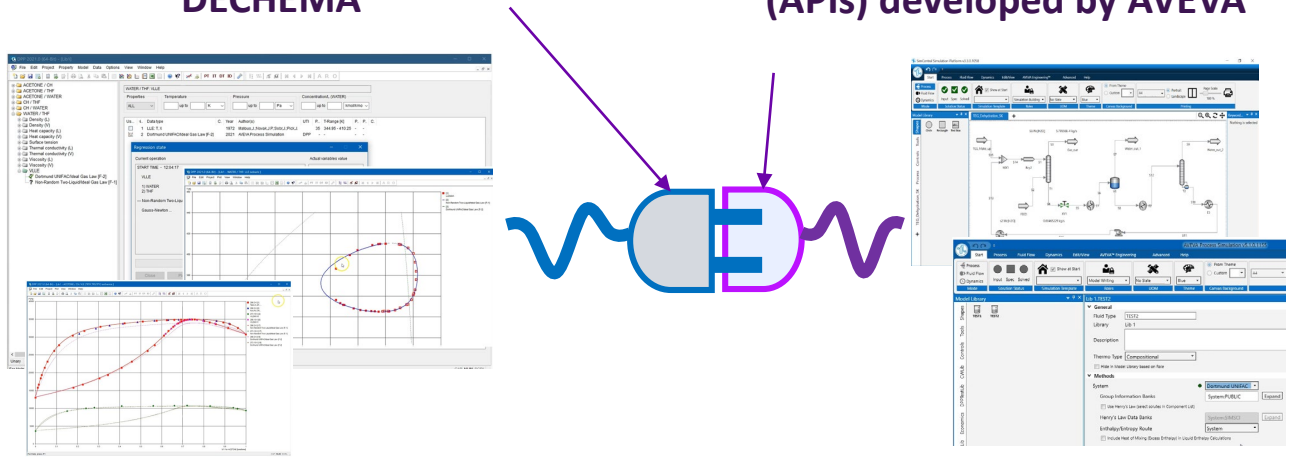
- DECHEMA has integrated DPP to AVEVA Process Simulation using the Thermo Access Interface.
- AVEVA has created the Thermo Access Interface which is a set of APIs of AVEVA Process Simulation so that the 3rd party tools have access to thermodynamic calculation in AVAVE Process Simulation

Delivery

- DPP 2021 "Preview Release" available now and works with AVEVA Process Simulation version for data regressions of Pure Component Data, Ideal, Henry, and NRTL for VLE and VLLE.
- More thermo methods are being available in subsequent versions. PSRK(with gE of NRTL) have been already covered.

Interface developed by DECHEMA

Thermo Access Interface (APIs) developed by AVEVA



DPP of DECHEMA

AVEVA Process Simulation

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

On the roadmap

Cubic Plus Association (CPA) EOS

Outline

- Inventor: Prof. Georgios Kontogeorgis, Chairman of Center for Energy Resources Engineering (CERE-DTU)
- Usage: Heavily used for up-stream in Europe, applicable to chemicals also

Objectives and Background

- Accurately predict phase equilibrium of highly non-ideal mixtures at elevated pressures.

Solutions

- Association term was added to cubic equations (SRK)

Challenges

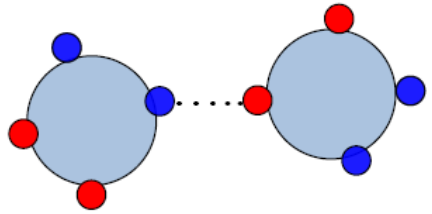
- There are many version of CPA.

Plan

- Select the best version of CPA with helps of DTU and European customers
- AVEVA to implement CPA on AVEVA™ Process Simulation (CY2023)
- Discussing on implementing the same feature for AVEVA Process Optimization

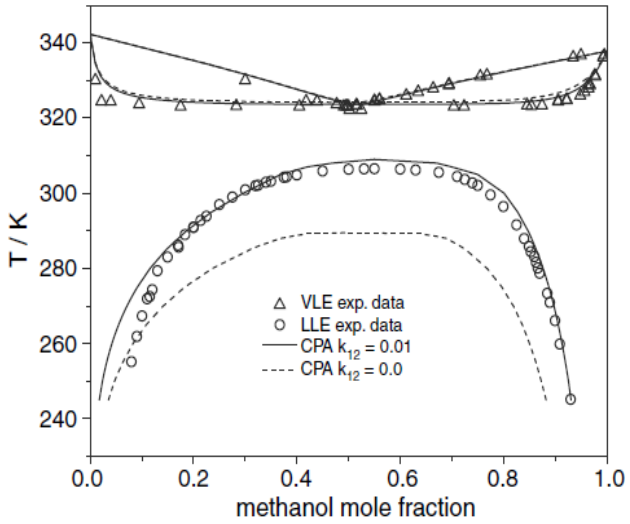
$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m(V_m + b)} - \frac{1}{2}\frac{RT}{V_m}\left(1 + \rho\frac{\partial \ln g}{\partial \rho}\right)\sum_i x_i \sum_{A_i}(1 - X_{A_i})$$

Association Term



$$X_{A_i} = \frac{1}{1 + \rho\sum_j x_j \sum_{B_j} X_{B_j}\Delta^{A_i B_j}}$$

Fraction of A-sites on molecule-I which are not bonded with other sites



For Internal Use Only. ©2021 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Done!

Wilson BIP Bank

Objectives and Background

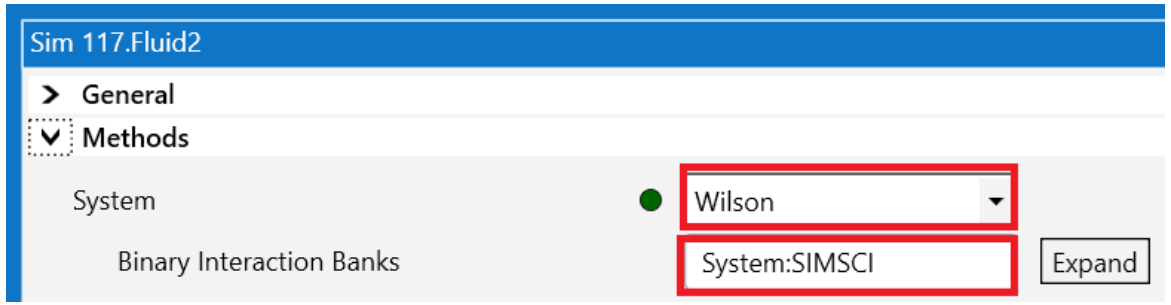
- In some fields of the chemical industry, Wilson is extensively used because physical meanings of parameters are clear.
- AVEVA's products did not have BIP databank for Wilson for some reason

Solutions

- Create Wilson databank
- For most of pairs, BIPs of NRTL were converted to BIPs of Wilson utilizing a theory that excess Gibbs energy of Wilson is equivalent with that of NRTL
- For selected around 20 pairs, data regression was conducted to determine BIPs after critically examining the source experimental data.

Delivery

- The Wilson BIP Bank is now available as "Syetem:SIMSCI" in AVEVA™ Process Simulation 2023
- The same bank will be available for all the AVEVA simulation products as soon as the products has the new temperature dependency form which has 13 parameters for each for each pair



$$\ln(\gamma_i) = 1 - \ln\left(\sum_j x_j \Lambda_{ij}\right) - \sum_k \frac{x_k \Lambda_{ki}}{\sum_j x_j \Lambda_{kj}}$$

$$\Lambda_{ij} = \Theta_{ij} \exp\left(\frac{\lambda_{ij}}{T}\right)$$

$$\lambda_{ij} = a_{ij} + b_{ij}T + c_{ij}T^2 + d_{ij}T\ln(T) + e_{ij}T^3 + \frac{f_{ij}}{T}$$

$$\Theta_{ij} = \begin{cases} 1 & when\ S_{ij} = 0\ (NOVOL) \\ \frac{V_j^L}{V_i^L} & when\ S_{ij} = 1\ (STD25C) \\ \frac{V_j^L}{V_i^L} & when\ S_{ij} = 2\ (RACKETT) \end{cases}$$

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

In progress!

Amine Thermo on AVEVA™ Process Simulation

Objectives/Background

- Simulation of CO2 capture by absorption using aqueous amine solutions (mixed with additives) as solvent requires rigorous thermo model which covers reaction equilibria and activity of species.

Solution

- For modeling reaction equilibria, the Fluid feature of AVEVA Process Simulation was applied.
- For modeling activity of species (including ions), Chens' electrolyte NRTL (eNRLT) on AVEVA Process Simulation was applied.
- Parameters of eNRTL were obtained from literatures
- Confirmed that simulations matches the loading curves

Delivery Plan

- MEA: Available on AVEVA Process Simulation 2023
- MDEA: Available on 2023.1 in January
- Customers can add their own Amines if they have their own data
- Regression of Amines and reactions and eNRTL expected around 2023.3 in July 2023.
- Other amines such as DEA, DGA, DIPA, TEA, AMP, PZ (Piperazine) and their mixtures, and Benfield (K2CO3) will be coming in the subsequent versions based on customer priorities

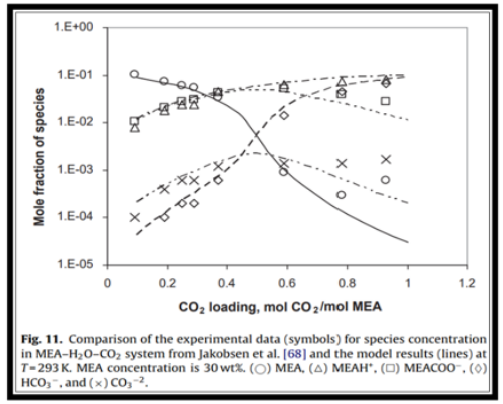


Fig. 11. Comparison of the experimental data (symbols) for species concentration in MEA–H_2O–CO_2 system from Jakobsen et al. [68] and the model results (lines) at T = 293 K. MEA concentration is 30 wt%. (○) MEA, (△) $MEAH^+$, (□) $MEACOO^-$, (◇) HCO_3^-, and (×) CO_3^{-2}.

Speciation

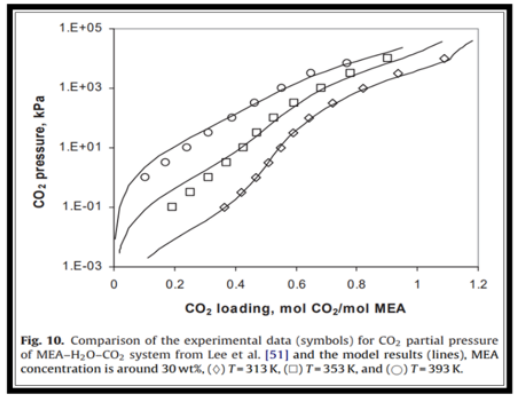
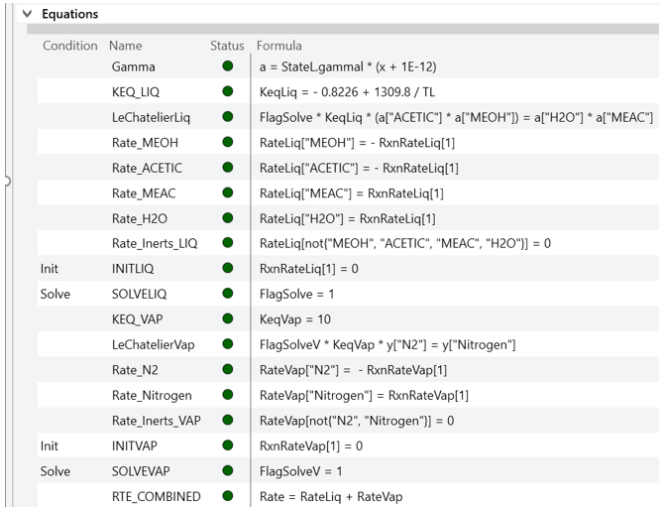


Fig. 10. Comparison of the experimental data (symbols) for CO_2 partial pressure of MEA–H_2O–CO_2 system from Lee et al. [51] and the model results (lines), MEA concentration is around 30 wt%, (◇) T = 313 K, (□) T = 353 K, and (○) T = 393 K.

Partial Pressure



Reaction Model

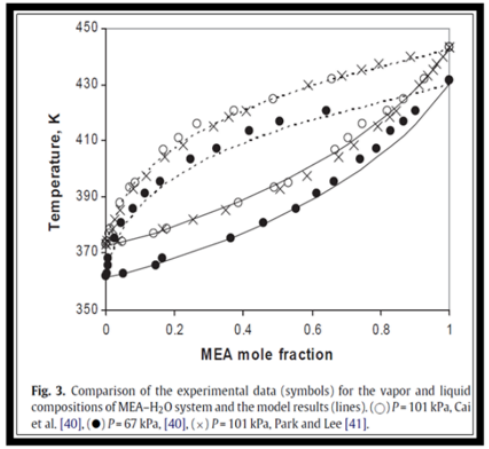


Fig. 3. Comparison of the experimental data (symbols) for the vapor and liquid compositions of MEA–H_2O system and the model results (lines). (○) P = 101 kPa, Cai et al. [40], (●) P = 67 kPa, [40], (×) P = 101 kPa, Park and Lee [41].

Binary Data

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

Ying Zhang and Chau-Chyun Chen. Industrial & Engineering Chemistry Research 2011 50 (1), 163-175

AVEVA ADVISORY GROUP MEETING

Thermodynamic updates/roadmap

1. **Overview of Roadmap of Therm. Features**
2. **Highlighted New Features/ Items in the Roadmap for;**
   - Design in Chemicals
   - Design in Oil&Gas
   - OTS
   - Commonly Utilized Items

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Background: Liquified Natural Gas (LNG) as a Key for Energy Security

Why LNG is important

- Natural gas has low C/H ratio: Low CO2 emission in comparison with other fossil fuels. Many countries incorporate natural gas into energy portfolio in transition to sustainable energy.
- LNG is “portable”: volume of LNG is 1/600th of natural gas. LNG enables transportation of natural gas to remote locations without pipeline. E.g. Currently huge amount of LNG is exported from the U.S. to Europe to which natural gas supply from Russia is not reliable.

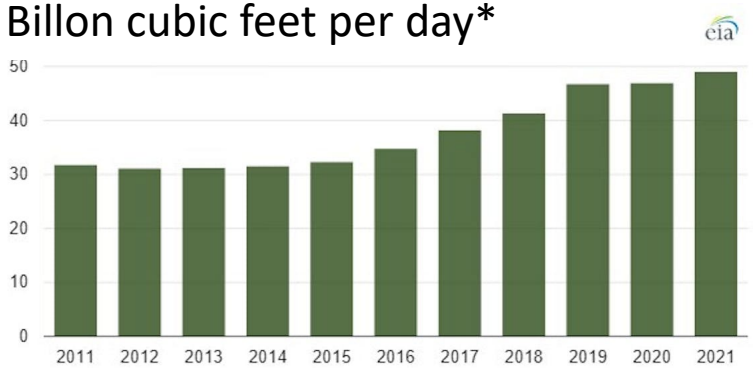
Problems to be solved

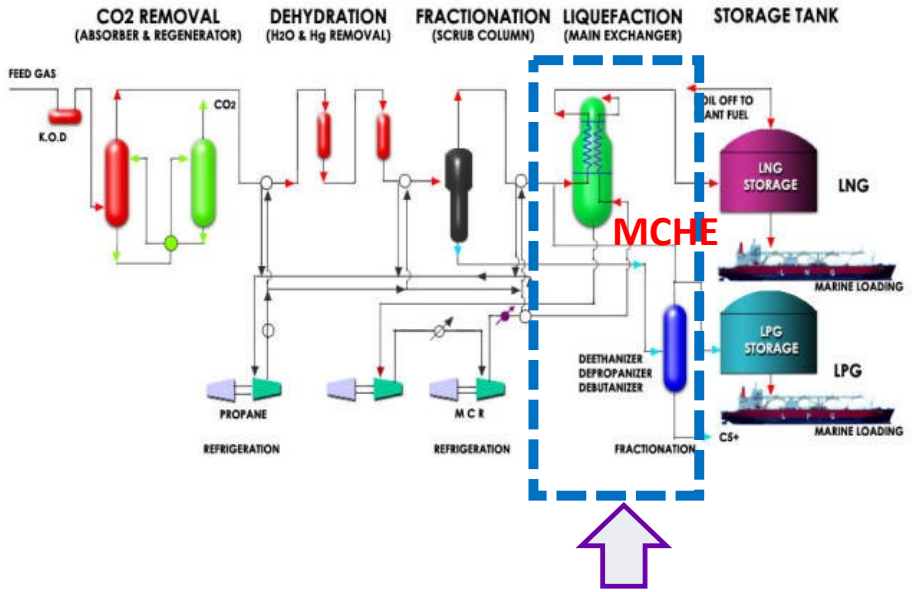
- In the cryogenic processing of natural gas mixtures, species such as CO_2 and the heavier hydrocarbons can form solids* which may lead a blockage/fouling of the equipment, process shutdown and/or costly repairs.
- Typically fouling requires costly maintenance of equipment – operating loss, cleaning cost (Typically $40,000 - $50,000 per heat exchanger)

Solution

- Develop a thermodynamic model that can predict reliable range of temperature and pressure where solid is not formed

Global annual LNG trade
Billon cubic feet per day*





A temperature of 110K is achieved after the natural gas is cooled in the Main Cryogenic Heat Exchanger (MCHE) at high pressure, usually higher than 50 bar

*Source: Oil & Gas Journal Jul.12.2022 (https://www.ogj.com/general-interest/economics-markets/article/14279418/giignl-global-lng-trade-grew-45-in-2021)

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Joint Industrial Project (JIP) for Solid in LNG

Objective

- Establish reliable thermodynamic base for LNG with focus on solid prediction

Project members:

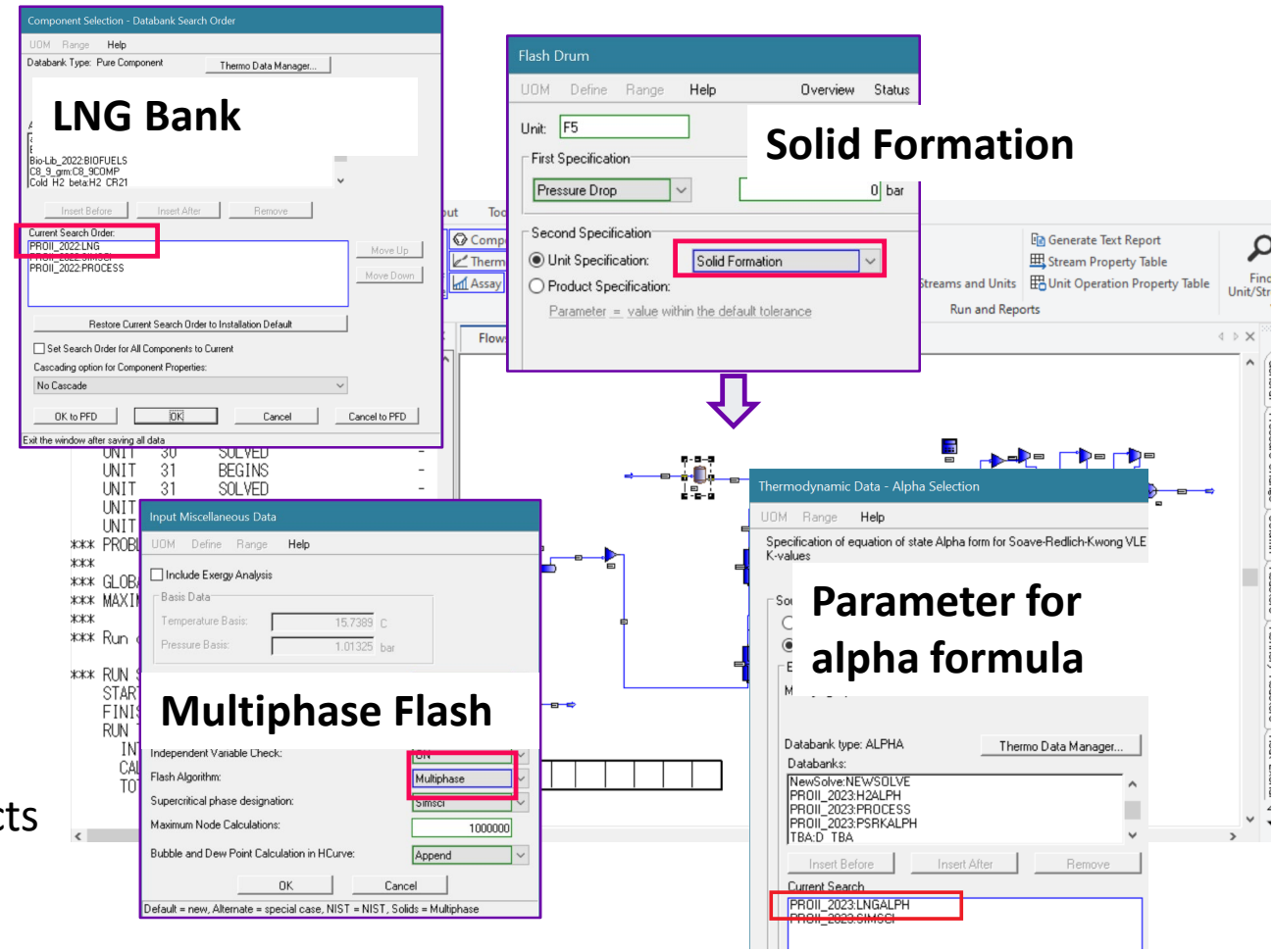
- TotalEnergies, Technip Energies, ARMINES, AVEVA

Scope of the works:

- Model: CEOS (SRK/PR) for fluid side. Currently 25 components (scalable)
- Update correlation for solid fugacity, alpha parameters, binary interaction parameters
- Establish flash algorithms: AVEVA™ PRO/II ™ Simulation
- Physical Properties: Fluid: enthalpy, entropy, and density, solid: enthalpy and density
- Technical detail was presented at ESAT2021 (some additional contents are being presented AIChE Annual Meeting on Nov.15.2022)

Status and plan:

- Had implemented in special versions of AVEVA PRO/II Simulation for TotalEnergies, and Technip Energies
- Became available on general version of AVEVA PRO/II Simulation after exclusivity period.
- Equations and data will be utilized in major AVEVA products



© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

Done!

Update of Ideal Gas Enthalpy of Ethane and Propane

Background/Objective

- Composition of LNG depends on gas source and type of the process (especially on whether the process has a demethanizer).
- Sum of ethane and propane can be around 15 mol% is some cases.
- Ideal gas enthalpy of ethane and propane gives impact on size of MCHE which is a huge device and gives cost impact.

Challenges

- Current parameter values in SimSci for ethane and propane covers limited portion of the expected temperature range of MCHE

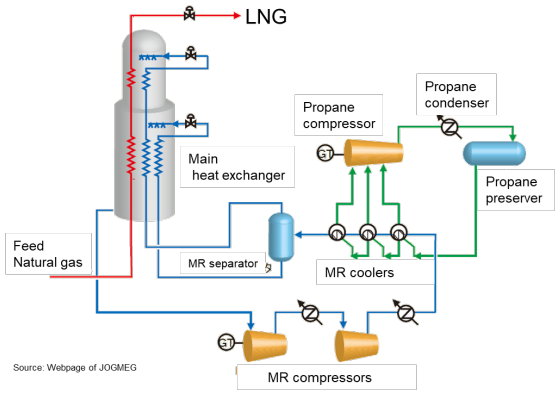
Solution

- Update parameters of ideal gas enthalpy correlation to cover the expected temperature range.

Results

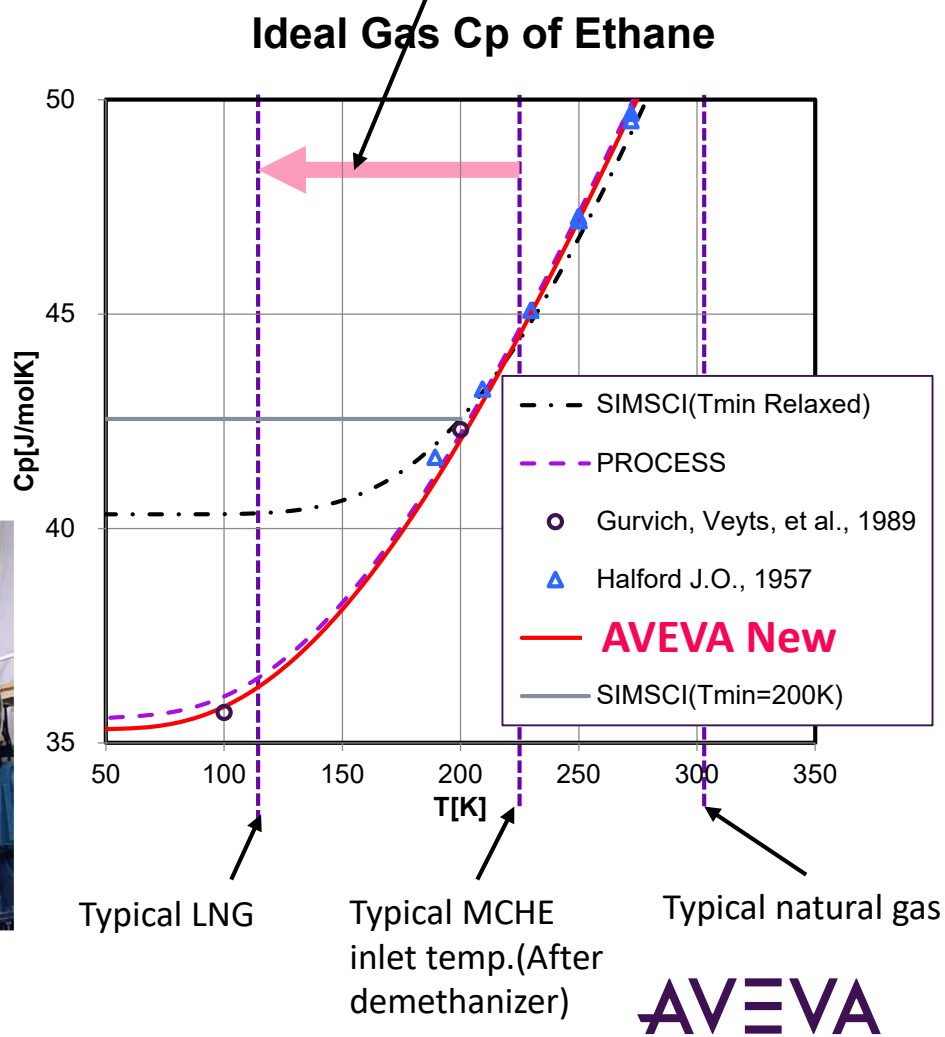
- Parameters of Eq.41 were determined using published data in the cryogenic region.
- LNG Bank equipped with the parameters will come with AVEVA products (2022)

MCHE





Temperature range of MCHE
(Cp gives impact on necessary area)



For Internal Use Only. ©2020 AVEVA Group plc and its subsidiaries. All rights reserved.

On the roadmap

Hydrates Prediction Feature

Objectives

- Predict hydrate occurrence as process constrain, considering effect of hydrate inhibitor and gas drier, and all the types of hydrates
- Design of upstream processes requires accurate prediction of hydrate occurring (warning) on AVEVA™ Simulation

Challenges

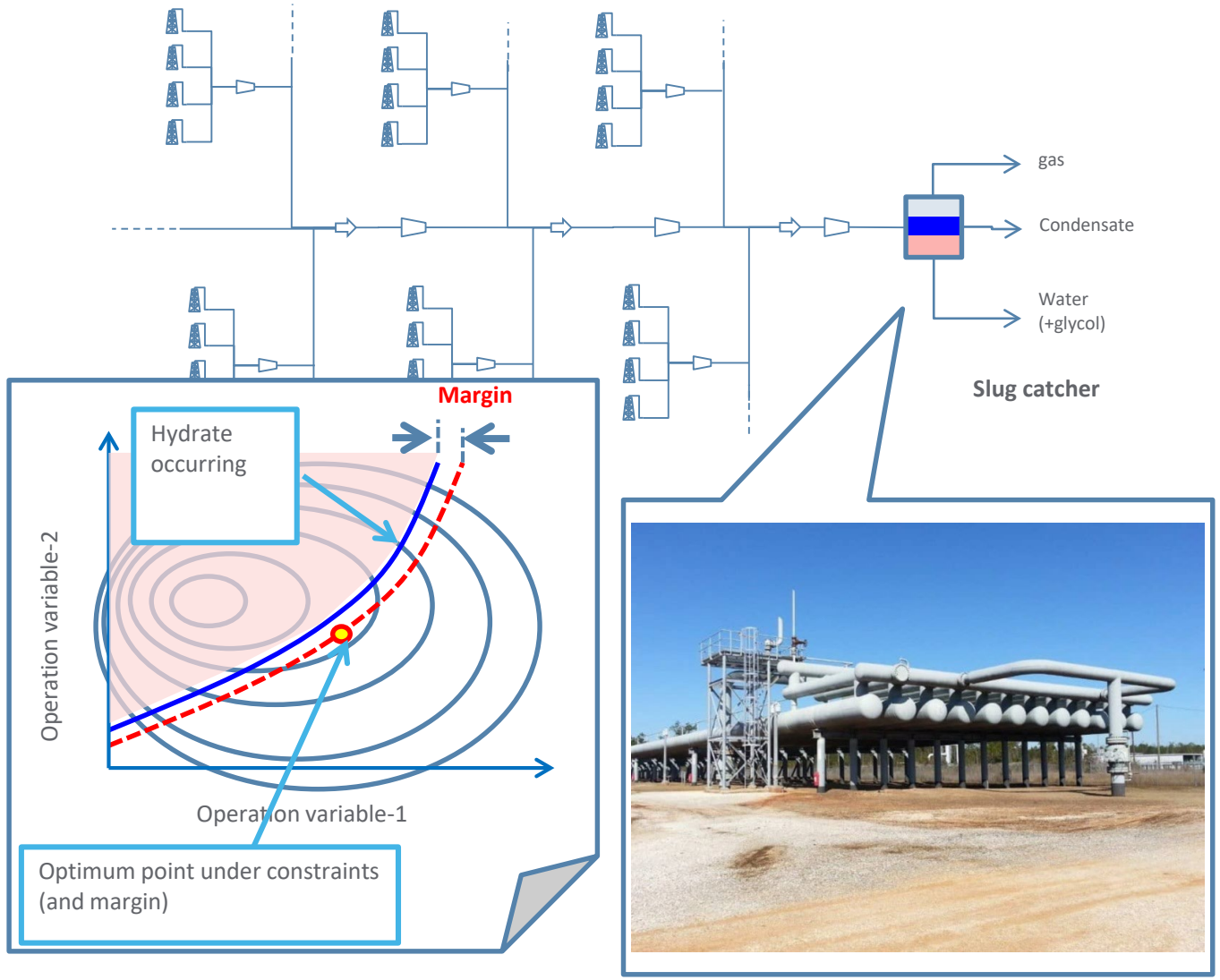
- Plural types hydrates need to be considered, including newly discovered ones
- Hydrate features on AVEVA PRO/II Simulation is 30+ years old

Solutions

- The latest knowledge of hydrate is utilized
- Room for process constraint can be defined by margin of water fugacity

Status and plan

- Implantation on AVEVA™ Process Simulation is planned in 2023 (design purpose)
- Discussing on implementing the same feature for AVEVA Process Optimization



© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

Plan for Hydrate Prediction

Capabilities		Conventional on AVEVA PRO/II Simulation	Phase-1 (Simple)	Phase-2 (Ultimate)
Predict effect of water content in gas stream		No	Yes	Yes
Predict effect of inhibitors	When only feed T,P,z are known	No	Yes	Yes
	When inhibitor fract. in liq. are known	Yes	Yes	Yes
Warning of hydrate occurrence	Give warning message hydrate	No	Yes	Yes
	Tell hydrate forming Tor P	No	Yes	Yes
	Draw plots of hydrate forming T-P	Yes	No (not needed)	Yes
Usage of hydrate as constraint for optimization	Tell how close to hydrate formation	No	Yes	Yes
	Solve hydrate module as a part of EO	No	Yes	Yes
	Use parameters for data-reconciliation	No	Yes	Yes
Flash calc. considering hydrate		No	No	Yes
Allow data regression for fitting to customer data		No	Yes (stand-alone tool)	Yes
Hydrate types considered	I (natural gas)	Yes	Yes	Yes
	II	Yes	no	Yes
	H	No	no	Yes
Hydrate guest component considered	Main components in natural gas	Yes	Yes	Yes
	Minor components in natural gas	Yes	No (can be added)	Yes
	Olefins: (ethylene, propylene)	Yes	no	Yes
	Heavier hydrocarbons	no	no	Yes
	For chemicals(refrigerants, noble gases)	Partially yes	no	Should cover a lot
Calculation method		Rigorous (direct)	Semi-Rigorous	Rigorous (I/O approach)

AVEVA

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA ADVISORY GROUP MEETING

Thermodynamic updates/roadmap

1. **Overview of Roadmap of Therm. Features**
2. **Highlighted New Features/ Items in the Roadmap for;**
   - Design in Chemicals
   - Design in Oil&Gas
   - OTS
   - Commonly Utilized Items

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Done!

Robust and Fast VLLE/VLWE on AVEVA™ Dynamic Simulation

Achieved by Open Form Flash and Super-Linear Local Model

Objectives and Background

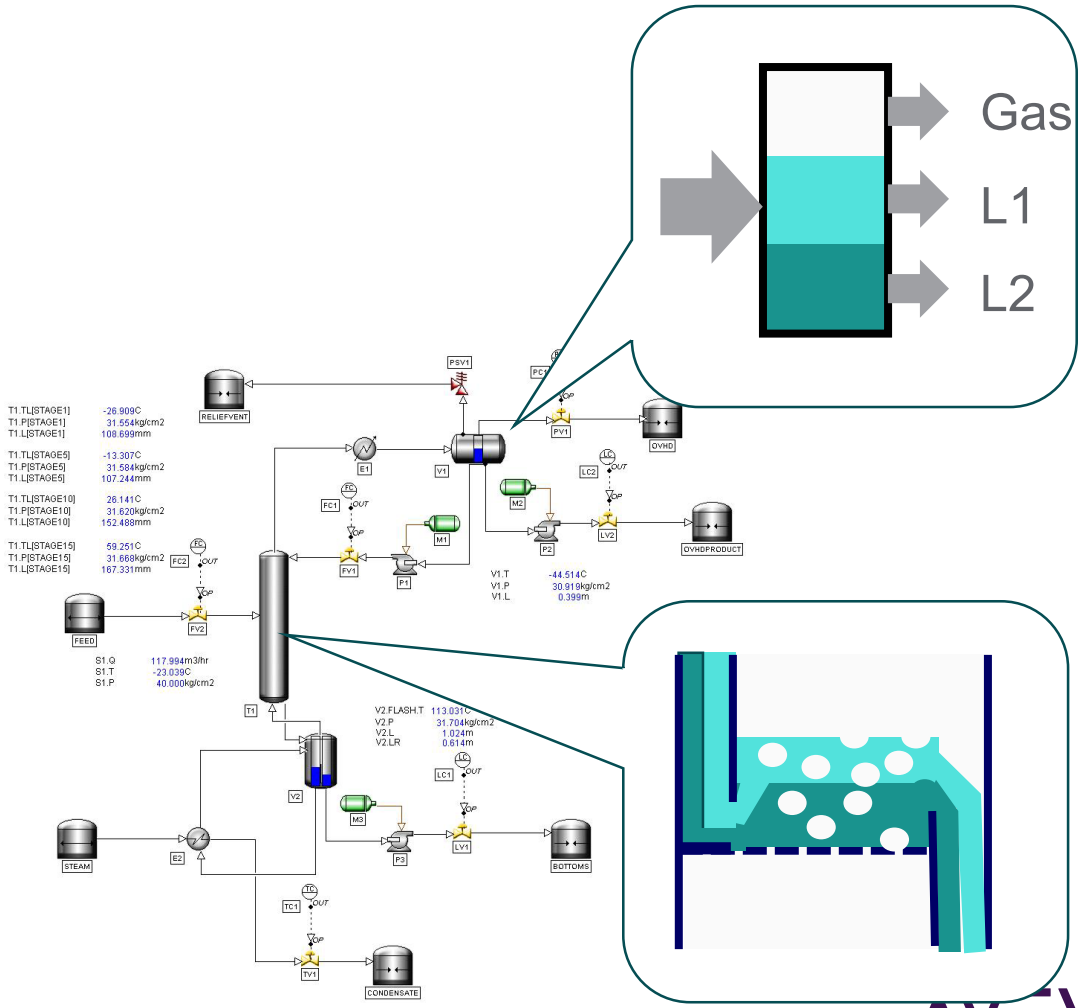
- OTS and engineering analysis of Chemical Processes often encounter VLLE in distillation columns.
- Traditional VLLE column faced difficulty in convergence for chemical systems

Solutions

- The following two technologies were successfully applied;
  - Open Form flash algorithm
  - Super-linear local model

Current Status

- The above two technologies are already available in the latest version of AVEVA™ Dynamic Simulation
- Performance and robustness are still being improved. Updates are coming in subsequent versions



©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA ADVISORY GROUP MEETING

Thermodynamic updates/roadmap

1. **Overview of Roadmap of Therm. Features**
2. **Highlighted New Features/ Items in the Roadmap for;**
   - Design in Chemicals
   - Design in Oil&Gas
   - OTS
   - Commonly Utilized Items

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

AVEVA

Cryogenic Hydrogen Library

Objectives/Background

- Model cryogenic processes of mixtures of hydrogen with other components

Challenge:

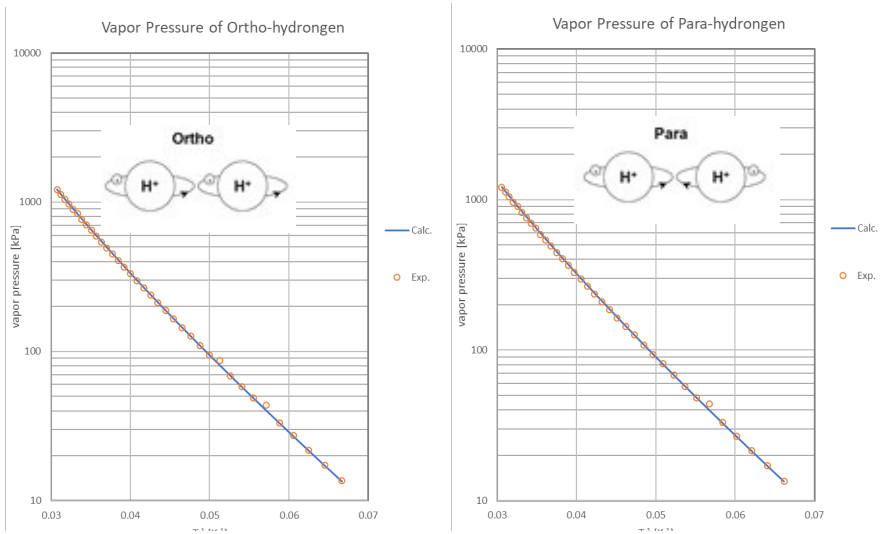
- Conventional data were for usage of hydrogen at ambient or high temperatures and are not ready for cryogenic usage.
- Especially heat capacity of hydrogens show strongly non-linear behavior at cryogenic conditions.
- Spin isotherms (ortho and para) need to be considered.
- Hydrogen can be mixed with other components (e.g. ethylene)

Solutions:

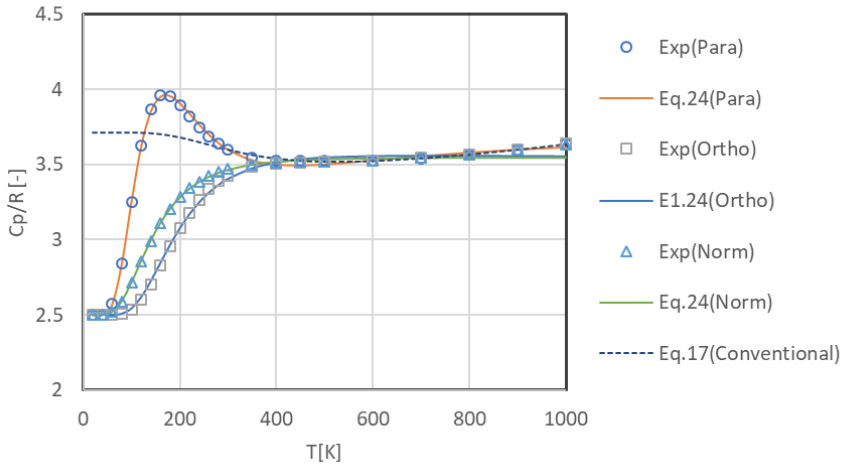
- Create a new databank which covers ortho- and para-hydrogens.
- Adjust parameters (especially ideal gas cp) with the newest experimental data.

Delivery

- Released with AVEVA PRO/II Simulation 2021.1
- All other products (early 2023)



Vapor pressure of ortho and para hydrogens (SRK with adjusted alpha parameters)



Ideal gas heat Capacity of ortho and para-hydrogens

Done!

Contents

Pure Component Databank: "H2_CR21"

- Components: Normal hydrogen, ortho hydrogen, and para hydrogen
- Updated properties
- Critical properties (Tc, Pc, Zc)
- Triple point (Tt, Pt)
- Ideal Gas Enthalpy correlation
- Temperature range: 2K-1000K
- Standard energies of formation
- **Standard enthalpy of formation**
- Standard Gibbs energy of formation
- Vapor pressure correlation
- Temperature range: from triple point to critical point
- (Other data stay the same with those in the conventical SimSci bank)

Databank for alpha parameter of SRK: "H2ALPHA"

- The coefficients allow SRK to match experimental data of vapor pressure of normal-H2, para-H2 and ortho-H2

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

Thermodynamic methodologies applicable to model cryogenic hydrogen on AVEVA products

Items		Available methodologies		
		IsomericHydrogen*	SRK or SRKM	NIST23 on REFPROP
Accuracy		Very high	Fair	Very high
Robustness		Excellent	Excellent	May need checks (pseudo-density root is not equipped)
Limitations		Hydrogen stream is only for hydrogens (no other component can be mixed). Other thermo methods (like SRK)are applied to He Brayton Cycle	Can be applied to hydrogen mixtures with other components	Hydrogen stream is only for hydrogens (no other component can be mixed). NIST23 can be separately applied to helium Brayton Cycle
Software products	AVEVA™ Process Simulation	✓	✓	(not applicable)
	AVEVA™ Process Optimization	(not applicable)	✓	(to be checked)
	AVEVA™ Dynamic Simulation AVEVA™ PRO/II™ Simulation	(not applicable)	✓	✓
Components	Ortho-H2	Registered in bank	Registered in bank	Registered in bank
	Para-H2	Registered in bank	Registered in bank	Registered in bank
	Normal-H2	Modeled (Fluid: Cryo_H2_ref)	Registered in bank	(will be available)
	Equilibrium H2	Modeled (Fluid: Cryo_H2)	Equilibrium reactor is needed	Equilibrium reactor is needed
Data banks	Component databank	SIMSCI	H2_CR21 (new)	Override (H2_CR21 in the future)
	Alpha databank	(not needed)	H2ALPH (new)	Override (H2ALPH in the future)
Applied methods	VLE (K-Val VLE)	Thermo Type:IsomericHydrogen	SRK or SRKM	SRK or SRKM
	Enthalpy, Entropy, Density	Thermo Type:IsomericHydrogen	SRK or SRKM	NIST 23
	Transport properties	IsomericHydrogen*(pure comp. ave.)	Pure component average	NIST 23
Reaction	Equilibrium	Can be calculated as a part of thermo. Readily model reaction in HX tubes.	Need to input equilibrium parameters	Need to input equilibrium parameters
	Heat of reactions from standard heat of formation	✓	✓	✓(currently a manual setting at each reactor is needed)
Remarks		Example simulation is available (AA2-hydrogen_liquifaction.simx)	New databanks (H2_CR21 and H2ALPH) will come soon	Currently modeled as mixtures of only normal-H2 and para-H2

© 2021 AVEVA Group plc and its subsidiaries. All rights reserved.

On the roadmap

Databank Enhancement

Objectives and Background

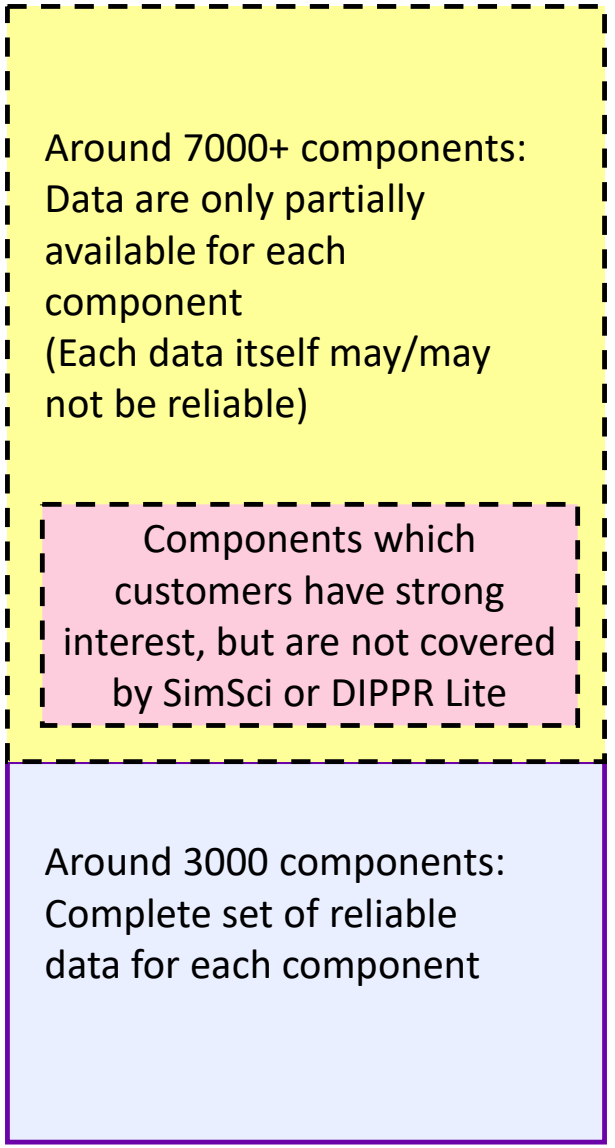
- More and more components are being needed in simulations even when data for each component is not complete, if the missing parts does not give significant impacts.
  - Chemicals: F/S of new processes
  - Refineries: 2DGC based characterization
- Traditional SimSci's conservative approach was employing only components which have complete and reliable data set based on experiments.

Solutions

- Create an options which enable customers to access component data even of components of which data are only partially available.

Delivery plan

- Timeframe is being discussed.
- Phased approach will be applied; Will start with components which customers have strong interest.
- Should be available for all the simulation products of AVEVA.



Phased approach is being discussed for covering this portion. (Of course, starting from the component which customers have strong interest.)

Covered by SimSci Bank + DIPPR Lite

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

Summary

What benefits AVEVA's new thermo. features bring to you…

- AVEVA is rapidly equipping AVEVA™ Process Simulation with new thermodynamic methods answering to requests of clients in the chemical industry. High pressure - nonideal mixtures are being covered… You can accurately model chemical processes making the most of your assets and know-how.

- AVEVA™ PRO/II™ Simulation is capable of predicting solid occurrence in LNG. AVEVA will be enabling clients to predict hydrate occurrence applying the latest theory…. You can correctly avoid solid occurring conditions without putting unnecessarily large margin on the design/operation.

- VLL-flash on AVEVA™ Dynamic Simulation is becoming more and more robust and fast. AVEVA's thermodynamic features for dynamic simulation will be thread-safe…. You can create rigorous OTS for large models, which should contribute to increasing availability of your plant.

- All of AVEVA's simulation software products are being equipped with new data sets for needs of emerging markets such as hydrogen, LNG. More data are coming for ammonia and bio-diesel. A phased approach for drastically enhancing databanks is being planned…. Using the data, you can swiftly conduct F/S of new processes. You can utilize data of new analytical devices (such as GCxGC) to model oils.

©2022 AVEVA Group plc and its subsidiaries. All rights reserved.

Thank you!

This presentation may include predictions, estimates, intentions, beliefs and other statements that are or may be construed as being forward-looking. While these forward-looking statements represent our current judgment on what the future holds, they are subject to risks and uncertainties that could result in actual outcomes differing materially from those projected in these statements. No statement contained herein constitutes a commitment by AVEVA to perform any particular action or to deliver any particular product or product features. Readers are cautioned not to place undue reliance on these forward-looking statements, which reflect our opinions only as of the date of this presentation.

The Company shall not be obliged to disclose any revision to these forward-looking statements to reflect events or circumstances occurring after the date on which they are made or to reflect the occurrence of future events.

For Internal Use Only. ©2022.AVEVA Group plc and its subsidiaries. All rights reserved.