JUNE 15.2021

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AVEVA EMEA Advisory Group Meeting - DAY 2: AVEVA Thermodynamics

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AVEVA

Agenda

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- Welcome and Introductions Day 2
- AVEVA Thermodynamic Updates
- AVEVA Thermodynamic Roadmap
- Break
- Presentation from Advisor (Dr.Westhaus of DECHEMA)
- Status of advisors' ideas on Aha Portal
- Enhancement Requests
- Meeting wrap-up

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Roadmap Overview of AVEVA™ Thermodynamics

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Customer Benefits

Primarily Goals	*Key highlights*
High Accuracy and Wide Range of Applicable Substances	• Chen's Electrolyte-NRTL (done), HF Thermo method (done) • Electrolyte enhancements and amine • gE-type mixing rules for high-press. ,non-ideal mix. • Improve data libraries (bio, hydrogen,…) • Refinery features on AVEVA™ Simulation • Update interface with external thermo like REFPROP • Solid enhancements, hydrate • (Long term) polymer (including Elec.PC-SAFT)
Ready for EO and Dynamic	• Equilibrium algorithm improvements • Fast and robust VLLE for dynamic (on-going)
Easy of use	• Thermo Access Interface with DPP of DECHEMA (1st phase was done) • User-Added Thermodynamics (1st phase was done) • Interface with external databanks such as DIPPR (done) • Flexible utilities/diagrams • Thermo Over-ride on AVEVA Process Simulation • User data manage for UNIFAC (done), Fill Options enhancements

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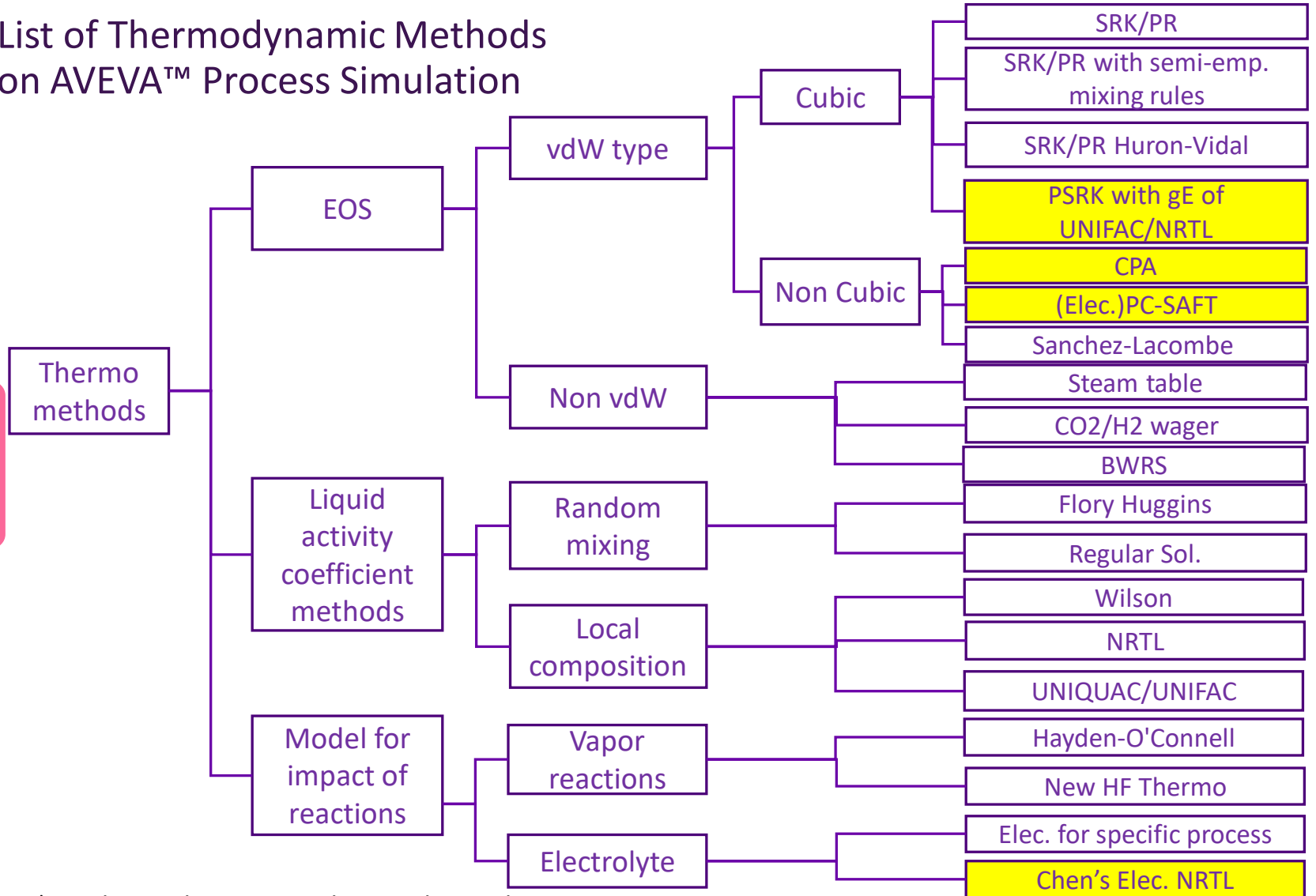
List of Thermodynamic Methods on AVEVA™ Process Simulation



*:can be used in gamma-phi, together with Henry

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Plans on Thermodynamic features on AVEVA™ Simulation: Chen's Electrolyte NRTL on AVEVA™ Simulation

- Objective and background
  - Chemical users need to simulate processes such as sulfuric acid production
  - Chen's elec-NRTL has been widely accepted by Chemical Users
- Solutions
  - Implement e-NRTL on AVEVA™ Simulation
  - Enable to apply e-NRTL to activity coefficient of species
  - At the first version, databank (scalable) should have a small set of parameters
  - In the future, REGRESS should have access to not only Pitzer parameters but also reaction constants
- Delivery
  - Implemented on AVEVA™ Simulation in 2020
  - Data/flash-algorithms are being updated

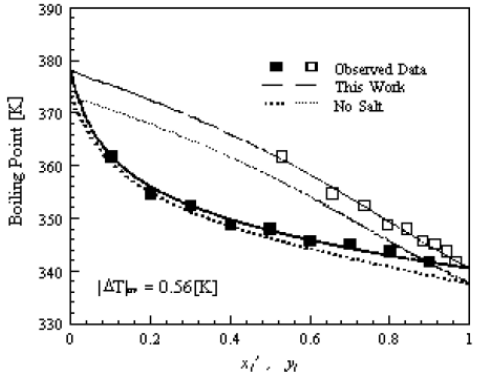
$$\ln\gamma_m = \frac{\sum_j X_j G_{jm}\tau_{jm}}{\sum_k X_k G_{km}} + \sum_{m'} \frac{X_{m'} G_{mm'}}{\sum_k X_k G_{km'}} \left(\tau_{mm'} - \frac{\sum_k X_k G_{km'}\tau_{km'}}{\sum_k X_k G_{km'}} \right)$$

$$+ \sum_c \sum_{a'} \frac{X_{a'}}{\sum_{a''} X_{a''}} \frac{X_c G_{mc,a'c}}{\sum_k X_k G_{kc,a'c}} \left(\tau_{mc,a'c} - \frac{\sum_k X_k G_{kc,a'c}\tau_{kc,a'c}}{\sum_k X_k G_{kc,a'c}} \right)$$

$$+ \sum_a \sum_{c'} \frac{X_{c'}}{\sum_{c''} X_{c''}} \frac{X_a G_{ma,c'a}}{\sum_k X_k G_{ka,c'a}} \left(\tau_{ma,c'a} - \frac{\sum_k X_k G_{ka,c'a}\tau_{ka,c'a}}{\sum_k X_k G_{ka,c'a}} \right)$$

Non-electrolyte term

Electrolyte terms



Methanol-water-$CaCl_2$ system at 101.3kPa

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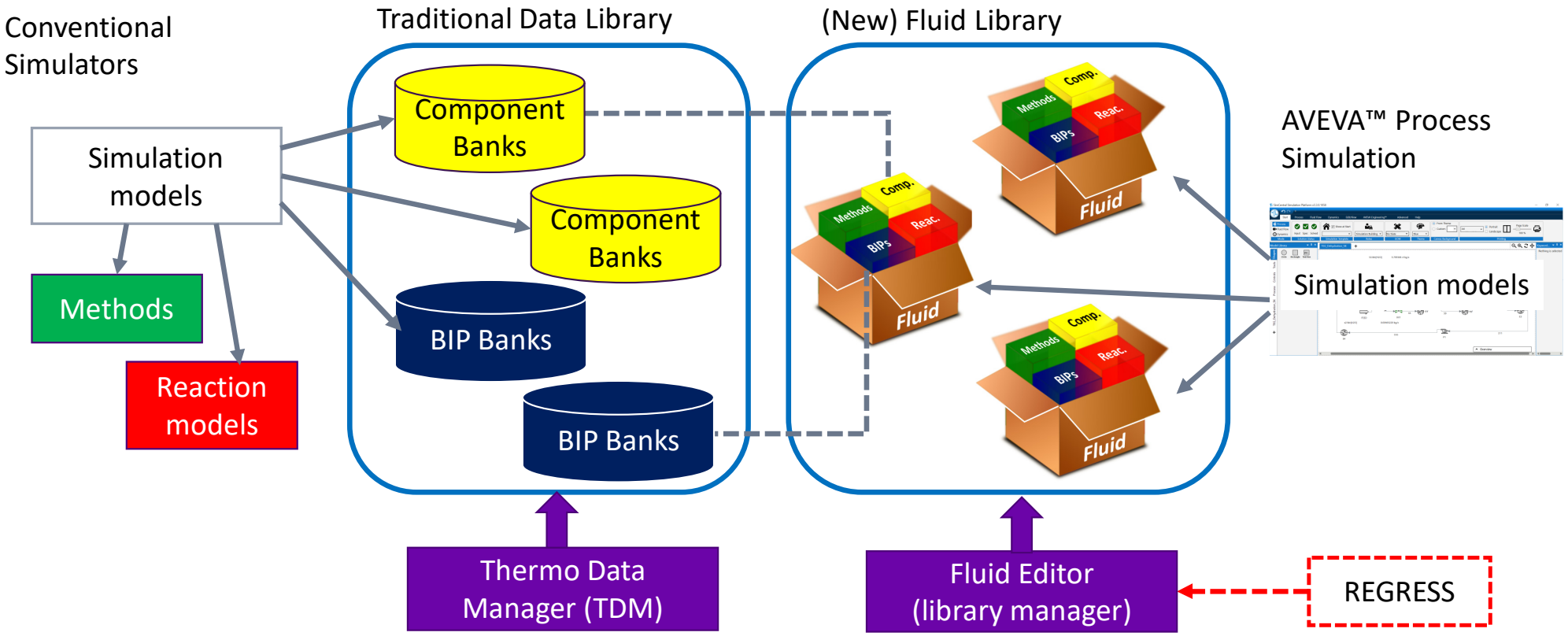
“Fluid” Concept on AVEVA Process Simulation (SimCentral)



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Interface of DPP with AVEVA™ Process Simulation

Objective and Background

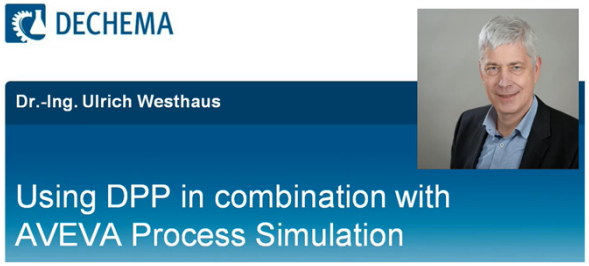
- DECHEMA's Data Preparation Package (DPP) has been widely used by major chemical companies for regression of thermophysical property models, which has seamless interface with DETHERM (database).
- Enables users to manage/ determine parameters of thermodynamic methods in AVEVA Process Simulation, utilizing excellent regression capability of DPP and huge number of experimental data in DETHERM.

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

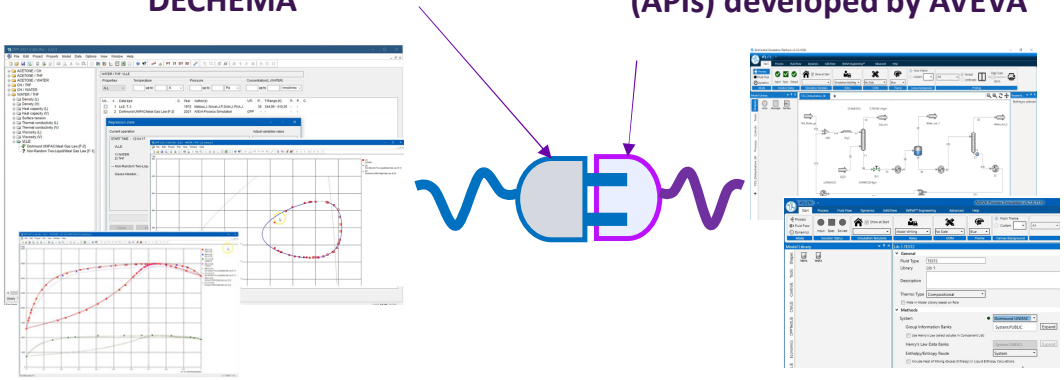
Delivery

- DPP 2021 "Preview Release" available now and works with AVEVA Process Simulation version 5.2 for data regressions of Pure Component Data, Ideal, Henry, and NRTL for VLE and VLLE.
- More thermo methods are being available in subsequent versions



Interface developed by DECHEMA

Thermo Access Interface (APIs) developed by AVEVA



DPP of DECHEMA

AVEVA Process Simulation

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DIPPR LITE on AVEVA™ Process Simulation

Objectives/Background

- DIPPR's published databank have been widely applied to process simulations by chemical companies.
- Enable users to apply DIPPR LITE databank to simulations in AVEVA Process Simulation and AVEVA PRO/II Simulation

Challenges

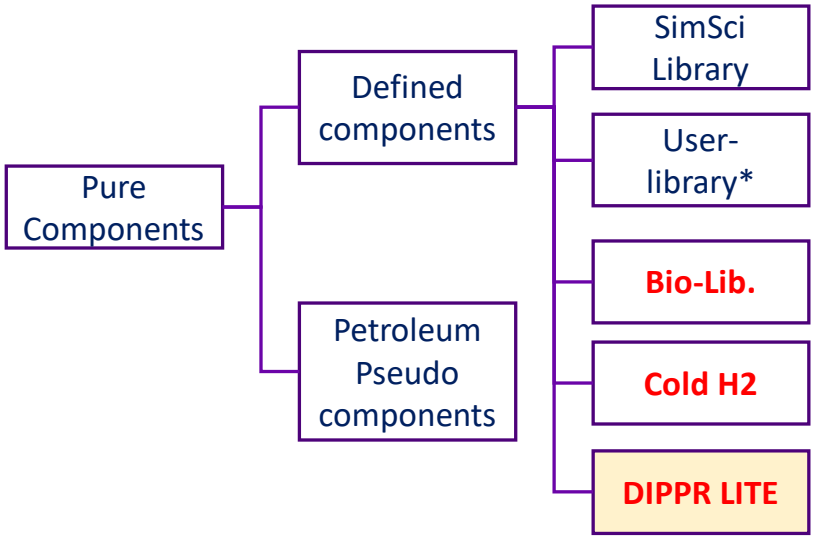
- Users sometimes need parameters (such as those for alpha formula for CEOS) which are not covered by DIPPR LITE databank even when applying it to major part of the simulations

Solutions

- With legal arrangement, AVEVA redistributes DIPPR LITE
- Parameters for alpha formula for cubic EOS are added by AVEVA when DIPPR bank is redistributed with permission of DIPPR
- AVEVA distributes UNIQAC pure component parameter bank which work with DIPPR in UNIQAC thermo procedure

Delivery

- AVEVA PRO/II Simulation installer already has DIPPR LITE
- AVEVA Process Simulation starts to be equipped with DPPR LITE from version 5.3



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Bio-Library on AVEVA™ Process Simulation

Objectives/Background

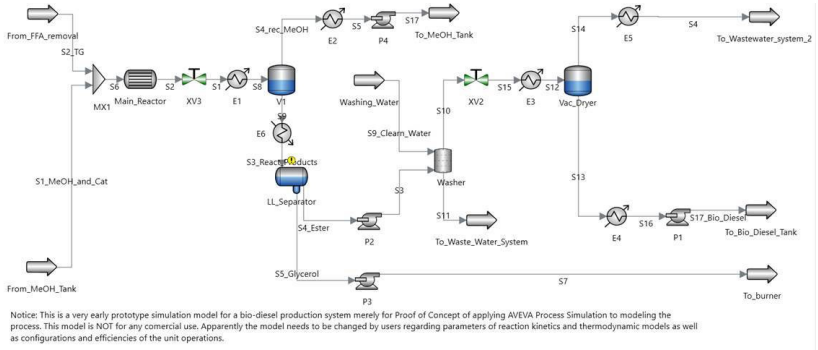
- Modeling production processes for the following bio-diesels and bio-ethanol
  - Hydrogenated vegetable oil (HVO)
  - Fatty acid methyl esters
  - Fermentation ethanol

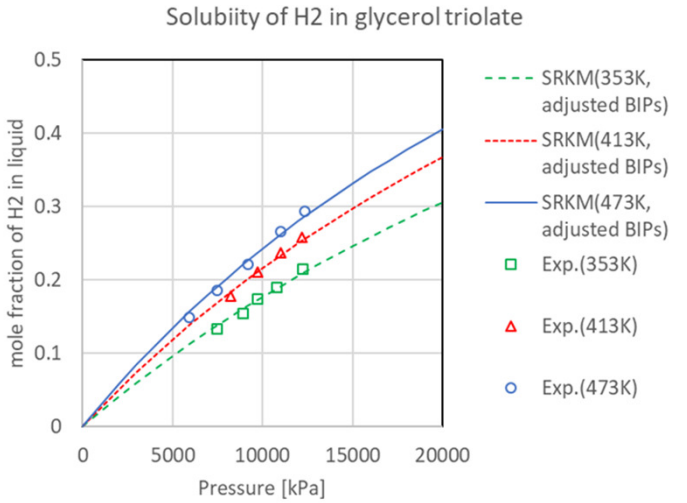
Solutions

- Provide the following two databanks
  - Bio-diesel: triglycerides, monoglycerides, diglycerides, fatty acids and methyl esters
  - Bio-ethanol: polysaccharide
- BIPs for SRKM for hydrogen solubility in triglycerides (required for modeling HVO production)

Delivery

- Databanks: AVEVA PRO/II Simulation and AVEVA Dynamic Simulation have been equipped from around 2008. AVEVA Process Simulation is equipped with them from 5.3
- BIPs for SRKM for hydrogen solubility in triglycerides will be incorporated to databanks in 2021





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Cold Hydrogen Library

Coming soon

Objectives/Background

- Model cryogenic processes of mixtures of hydrogen with other components

Challenge:

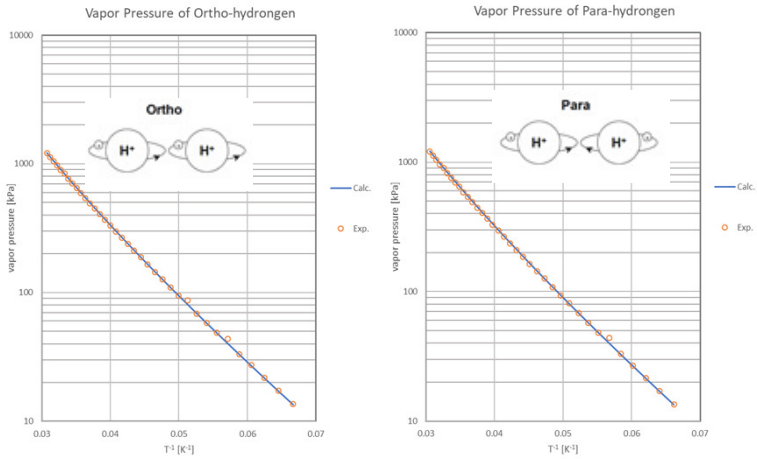
- Conventional data were for usage of hydrogen at ambient or high temperatures and are not ready for cryogenic usage.
- Especially heat capacity of hydrogens show strongly non-linear behavior at cryogenic conditions.
- Spin isotherms (ortho and para) need to be considered.
- Hydrogen can be mixed with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

Solutions:

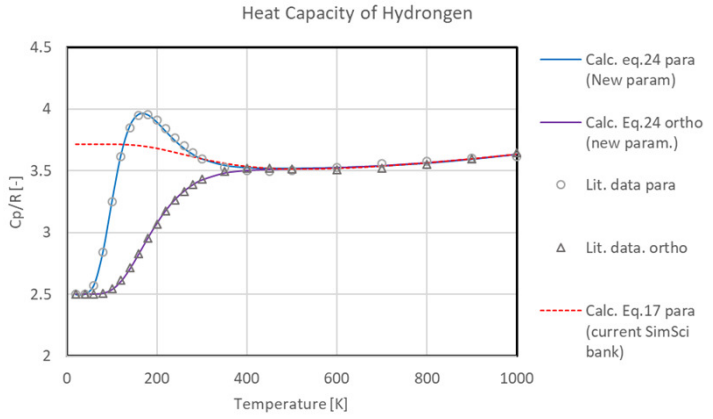
- Create a new databank which covers ortho- and para-hydrogens.
- Adjust parameters (especially ideal gas cp) with the newest experimental data.
- Provide example simulation models

Delivery

- Beta version is available
- Will be incorporated into installers of AVEVA Process Simulation, AVEVA PRO/II Simulation, and AVEVA Dynamic Simulation in 2021



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



Ideal gas heat Capacity of ortho and para-hydrogens

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Wilson Equation with Inclusive Temp. Dependence Form

In Progress

Objectives
- Enable users to utilize existing assets of binary interaction parameters of Wilson Equation

Challenges
- There have been several forms of temperature dependency equation for $\lambda_{i,j}$

Solution
- Create an "inclusive" equation which "contains" the existing form (or the parameters of existing form can be easily converted, just switching order or sign)

Delivery
- AVEVA Process Simulation 5.3
- Other products: subsequent versions

$$\ln \gamma_i = 1 - \ln \sum_{j=1}^{N} x_j A_{ij} - \sum_{k=1}^{N} \frac{x_k A_{ki}}{\sum_{j=1}^{N} x_j A_{kj}}$$

$$\Lambda_{i,j} = \Theta_{i,j} \exp\left(\frac{\lambda_{i,j}}{RT}\right)$$

where: $\lambda_{i,j} = a_{i,j} + b_{i,j}T + c_{i,j}T^2 + d_{i,j}T \ln T + e_{i,j}T^3 + \frac{f_{i,j}}{T}$

and: $\Theta_{i.j} = \begin{cases} 1, & \text{for NOVOL} \\ \frac{V_j^L}{V_i^L}, & \text{for STD25C, RACKETT} \end{cases}$

and: $R = \begin{cases} 1.98720425864083, & \text{for KCAL} \\ 8.31446261815324, & \text{for KJ} \\ 1, & \text{for K} \end{cases}$

$$\Lambda_{i,j} = a_{i,j}$$

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Extended Temperature Dependency

Enable customers in the chemical industry to readily start using AVEVA Products

- UNIQUAC (done): All the products
  - -Uij/RT = aji + bji/T + cji*ln(T) + dji*T
- Extended Antoine (done ad Correlation **28**): AVEVA Process Simulation
  - $\ln(P)=c_1+ c_2/(c_3+T)+ c_4*T+ c_5*\ln(T)+ c_6*T^{c7}$
- kij for SRKM: Done for AVEVA Process Simulation, on-going for other products
  - Kij=kijA+kijB/T+kijC/T^2+ kijD*T
- Henry (done) : Done for AVEVA Process Simulation
  - Ln(H)= a+b/T+c*ln(T)+d*P+e*T
- Wilson: Will be done for all the products
  - Equation (previous slide)

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Robust and fast VLLE and VLWE

In Progress

Objectives/Background

- Design of CDU and azeotropic distillation requires robustly solving VLWE and VLLE respectively on AVEVA Process Simulation
- OTS of CDU and azeotropic distillation requires robustly solving VLWE and VLLE respectively on AVEVA Dynamic Simulation. VLWE and VLLE may occur at anywhere in the columns.

Challenges

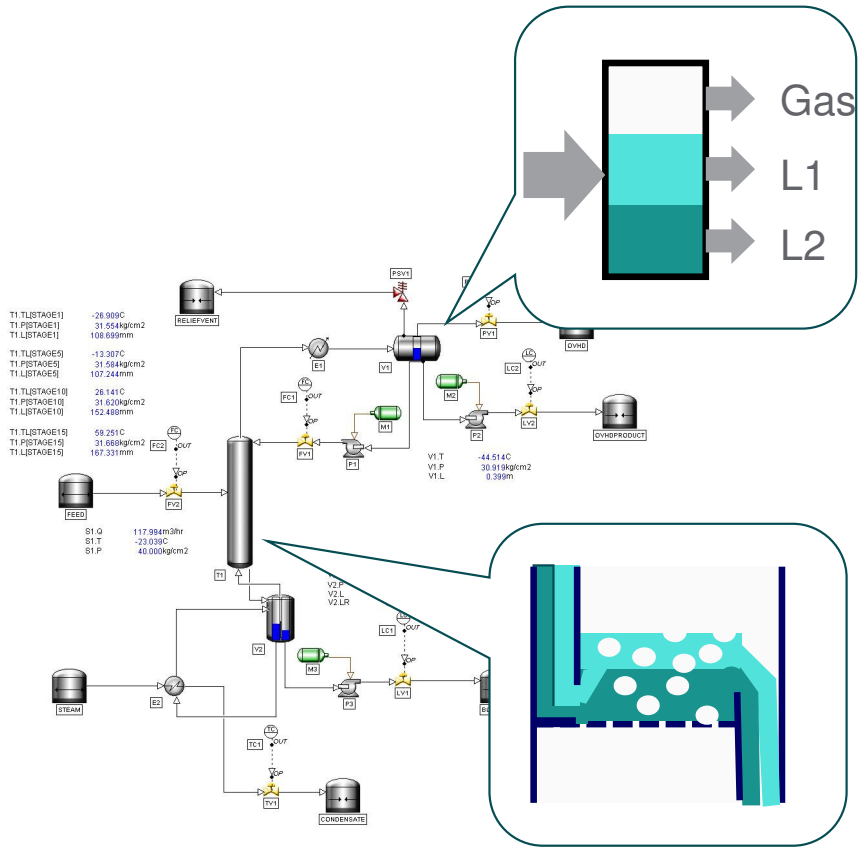
- Each phase may appear and disappear depending on conditions

Solution

- Develop new flash algorithms.

Status and plan

- VLLE on AVEVA Process Simulation is being improved. Multiple initiatives are in progress. (Improvement of VLWE will follow.)
- AVEVA Dynamic Simulation will be also equipped with an improved VLLE algorithm which is currently being tested. (Improved VLWE is already available on AVEVA Dynamic Simulation)



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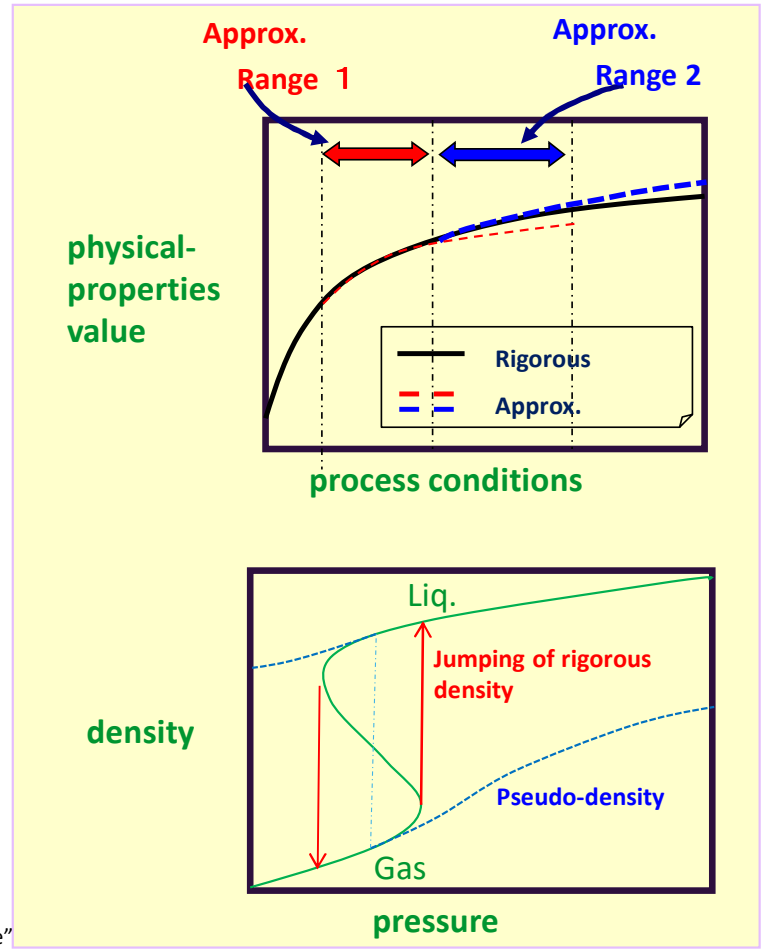
Fast and Robust Mathematical Platform

- Local Models
  - Taylor expansion to predict physical properties.
  - The values of coefficients are automatically updated by the patented logic.

$$X(a) = X(a_0) + (a - a_0)\frac{\partial X}{\partial a_0} + \frac{(a - a_0)^2}{2}\frac{\partial^2 X}{\partial a_0^2} + \ldots$$

  - US Patent 7676352 B1 by Gang,Xu et al.
  - Further improvement was done in 2015 (patent has been issued)

- Pseudo-Density Root*,**:
  - Prevent sudden jump of density root by pseudo density, but eventually converge to the true solution for phase equilibrium.
  - The pseudo-density curve is automatically created by the patented algorithm.
  - US Patent 8165860 B2 by Gang,Xu et al.



*Gang Xu and Nevin Gerek Inse: "Tangent Point Approach in Reliably Solving the Density Roots for PC-SAFT Equation of State" accepted by J.Chem.Eng. Data

**Xu, G. Pseudo-Extrapolation Algorithm for General Equation of State Model. AIChE Annual Meeting, October 19, 2011.

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Thermo Methods for HF-Mixtures

Reaction model combined with EOS and Activity Coefficient Method (when needed)

Objectives

- Modeling processes which uses HF at elevated pressures, such as HF alkylation in refineries

Solutions

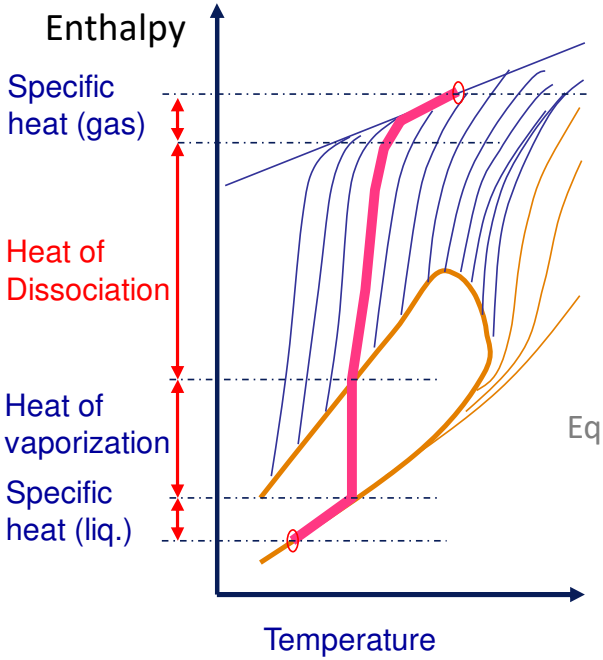
- (AVEVA PRO/II Simulation) Implement HEXAMER model of Twu, which is a combination of reaction equilibrium with SRKS EOS
- (AVEVA Process Simulation) Enable SRKM to work with reaction equilibrium
- Both work with activity coeff. (gamma-phi) with a term ($y_{HFm,sat,o,1}$) related to reaction in gas phase

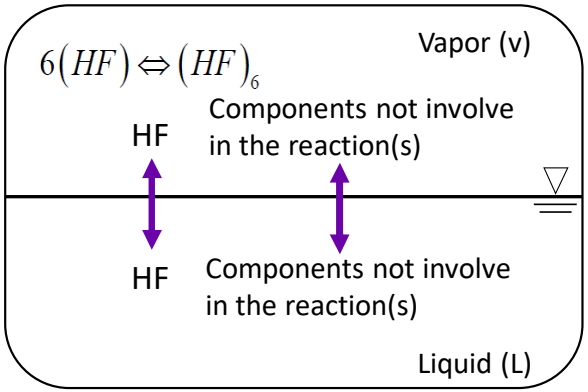
Reaction considered

$$6(HF) \Leftrightarrow (HF)_6$$

Delivery

- Hexamer has been available in AVEVA PRO/II Simulation and AVEVA Dynamic Simulation
- AVEVA PRO/II Simulation 2020.1 was equipped with the Hexamer-gamma-phi model
- AVEVA Process Simulation 5.1 was equipped with the Hexamer-gamma-phi model





Equilibrium conditions

- Pressure: $P^L = P^V$
- Temperature: $T^L = T^V$
- Physical (phase)equil.: $f_i^L = f_i^V$
- Chemical (reaction) equilibrium

$$K(T) = \frac{\phi_6}{\phi_1^6}\frac{z_6}{z_1^6}\frac{1}{P^5}$$

Equation for gamma-phi

$$y_1 \emptyset_{V,1} P = x_1 \gamma_1 P_{sat,o,1} \emptyset_{L,sat,o,1} y_{HFm,sat,o,1} (Poynting)$$

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Interface of AVEVA PRO/II Simulation with REFPROP 10

New Features of REFPROP Version 10

1. **Infrastructure**
   - Increased calculation speed.
2. **Addition of new components/physical properties**
   - The addition of the following fluids: 1-propanol, isopropanol, 1-butanol, 1-hexanol, chlorine, dichloroethane, ethylene glycol, ethylene oxide, hexadecane, docosane, R30, R40, R1233zd(E), R1243zf, R1336mzz(Z), and vinyl chloride.
   - Transport equations have been added or modified for acetone, benzene, 1-butene, carbon dioxide, carbonyl sulfide, cis-butene, cyclohexane, cyclopentane, cyclopentane, D4, D5, D6, dichloroethane, diethyl ether, dimethyl carbonate, docosane, ethylene, ethylene oxide, heptane, hydrogen chloride, isobutene, isohexane, isooctane, isopentane, m-xylene, MD2M, MD3M, MD4M, MDM, MM, neon, neopentane, Novec-649, o-xylene, p-xylene, pentane, propylene, R114, R161, R1233zd(E), R1234yf, R1234ze(Z), R1243zf, R245fa, RE143a, RE347mcc, R40, trans-butene, toluene, undecane, and vinyl chloride.
3. **Increase in accuracy/ update of parameters**
   - The equations of state have been revised for cyclopentane, D4, heptane, hexane, hydrogen chloride, hydrogen sulfide, isopentane, MDM, MM, octane, pentane, R161, R245fa, R32, RE347mcc (HFE-7000), sulfur dioxide, and xenon.
   - Mixture parameters were fitted (or refitted) for the following binary mixtures: R1234yf with R32, R125, R134a, and R1234ze(E), R1234ze(E) with R125 and R134a, and CO2/R1216
   - New mixture models with improved accuracy for ammonia/water and ethylene glycol/water.
   - New reference equations of state for ammonia, helium, heavy water, and oxygen.
   - New estimation scheme for selected families of binary mixtures (n-alkane + n-alkane mixtures, mixtures with CO2) to obtain estimated interaction parameters for mixtures that have not been fitted.
   - Most surface tension

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Roadmap Overview - AVEVA™ Thermodynamics

	Today (delivered)	Tomorrow (FY 22)	Future (FY 23-25)
Goals	**AVEVA Process Simulation** • **Chemical Process** Simulation Improvements • Committed key items **AVEVA Dynamic Simulation** • Key items for OTS projects **AVEVA PRO/II Simulation** • Committed key items	**AVEVA Process Simulation** • **Chemical Process** Simulation Improvements • **Downstream, Upstream Process** Simulation **AVEVA Dynamic Simulation** • Key items for OTS projects **AVEVA PRO/II Simulation** • Committed key items	**AVEVA Process Simulation** • **Chemical Process Simulation Improvements** • **Downstream, Upstream Process Simulation** **AVEVA Dynamic Simulation** • Key items for OTS projects **AVEVA PRO/II Simulation** • Committed key items

Initiatives	**AVEVA Process Simulation**
	• **Thermo Methods**: **SRK Huron-Vidal (SRKH)**, **LK**, **e-NRTL**, HF-Thermo, Transport prop. mixing rules, IF97 Transport prop.
	• **Thermo Diagrams**
	  • Liquid-Liquid Diagrams, Ternary Diagrams
	• **Thermo Data Override (**NRTL, Pure Comp. and Henry**)**
	• **Integration/Interface**
	  • User Added Thermo Interface
	  • Thermo Access Interface
	  • Improve PPDX import/export
	  • Data export for HTRI
	• **Thermo Architecture and Flash**
	  • VLLE Update
	  • Non-Equilibrium Solids
	  • Electrolyte Precipitates
	AVEVA Dynamic Simulation
	• Project supports
	AVEVA PRO/II Simulation
	• HF-Thermo
		AVEVA Process Simulation
		• **Thermo Methods**
		  • EOS: PSRK , CPA, GERG-2008
		  • Amine/Sour Methods
		• **Thermo Diagrams**
		  • Thermo Diagrams for a Given Composition
		• **Integration/Interface**
		  • Thermo Access Interface (**Phase1**,Phase2, Phase3)
		• **Thermo Data**
		  • Electrolyte Species and Reaction Data
		  • FILL options
		  • Water and gas Solubility, new API methods
		• **Thermo Architecture and Flash**
		  • Updated hydrate (Phase-1), Solid features Phase-2
		  • Improve flash algorithms
		AVEVA Dynamic Simulation
		• Open form VLLE flash calculation
		• Super-linear Local Model for performance
		• Project Support
		AVEVA PRO/II Simulation
		• REFPROP 10 interface
		• Project Support
		• Update TDM regress
			AVEVA Process Simulation
			• **Thermo Methods**
			  • EOS: Elec. PC-SAFT, BWRS
			  • Refinery Inspection Properties
			  • Wax and asphaltene model
			• **Thermo Diagrams**
			  • Native REGRESS
			• **Integration/Interface**
			  • Interface with Spiral Crude database
			  • Assay/feed data import from external sources
			• **Thermo Data**
			  • More Electrolyte Species and Reaction Data
			  • More FILL options
			  • Heavy Oil
			• **Thermo Architecture and Flash**
			  • Distillation curves, Crude Assay Characterization
			  • Polymer
			  • Updated hydrate (Phase-2)
			  • Enhance solid feature(Phase-3)
			AVEVA Dynamic Simulation
			• Usage of new computer architecture and technologies
			AVEVA PRO/II Simulation
			• Committed key items

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Roadmap Overview of AVEVA™ Thermodynamics

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Customer Benefits

Primarily Goals	*Key highlights*
High Accuracy and Wide Range of Applicable Substances	• Chen's Electrolyte-NRTL (done), HF Thermo method (done) • Electrolyte enhancements and amine • gE-type mixing rules for high-press. ,non-ideal mix. • Improve data libraries (bio, hydrogen,…) • Refinery features on AVEVA™ Simulation • Update interface with external thermo like REFPROP • Solid enhancements, hydrate • (Long term) polymer(including Elec.PC-SAFT)
Ready for EO and Dynamic	• Equilibrium algorithm improvements • Fast and robust VLLE for dynamic (on-going)
Easy of use	• Thermo Access Interface with DPP of DECHEMA (1st phase was done) • User-added Thermodynamics (1st phase was done) • Interface with external databanks such as DIPPR (done) • Flexible utilities/diagrams • Thermo Over-ride on AVEVA Process Simulation • User data manage for UNIFAC (done), Fill Options enhancements

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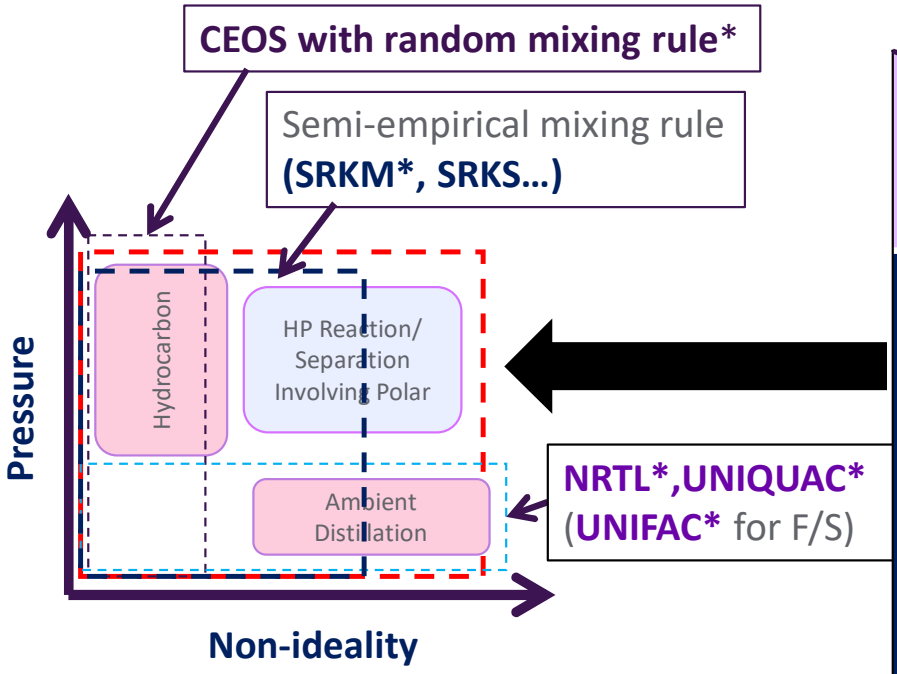
Thermo Methods for Non-Ideal Mixtures



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**(MHV-1), VTPR****, MHV-2, Wang-Sandler Twu-Bluck-Coon	(none)
	Association	Cubic Plus Association (CPA)***	PC-SAFT***

*:Already implemented in AVEVA Process Simulation
**:Discussed in the next slide
***:In the roadmap
****:To be discussed

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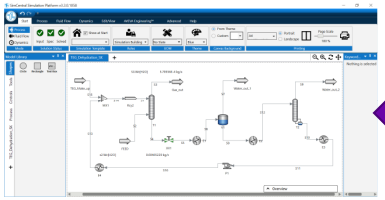
Use of SRK+ Holderbaum-Gmehling Mixing Rule (SRK-HG)

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

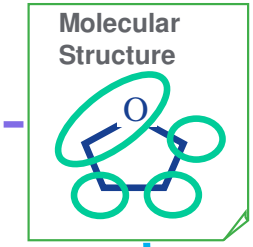
Process Simulations



Holderbaum-Gmehling (HG) Mixing Rule*

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

g^E of UNIFAC



UNIFAC FILL

g^E of NRTL**

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

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

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

NRTL Bank

Experimental data

PSRK (SRK-HG + UNIFAC g^E)

SRK-HG + g^E of NRTL

- **AVEVA implemented PSRK (g^E of UNIFAC) in AVEVA PRO/II Simulation and AVEVA Dynamic Simulation**
- **Will be implementing SRK-HG + g^E of NRTL also in 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

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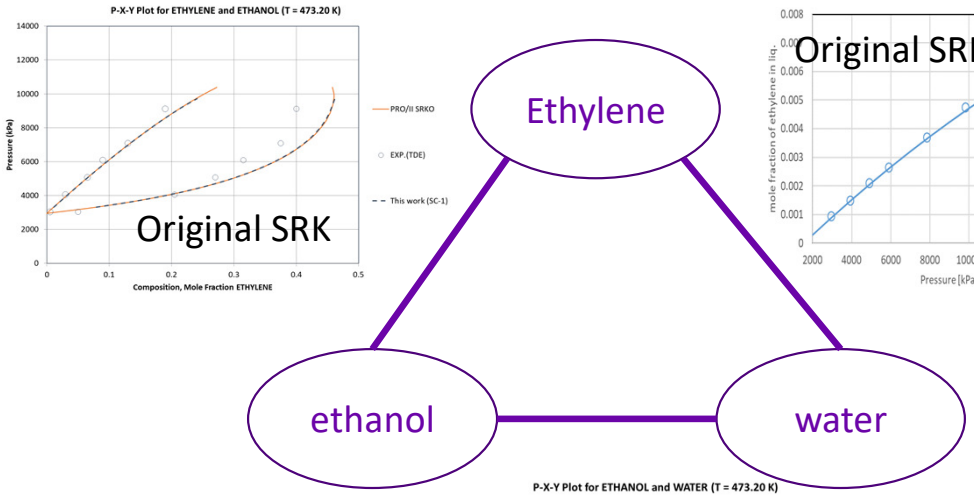
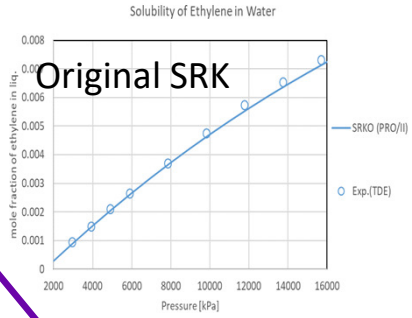
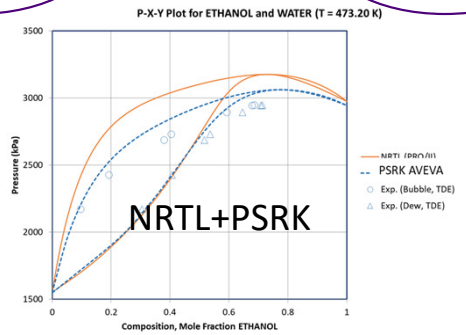
(Just POC was completed)

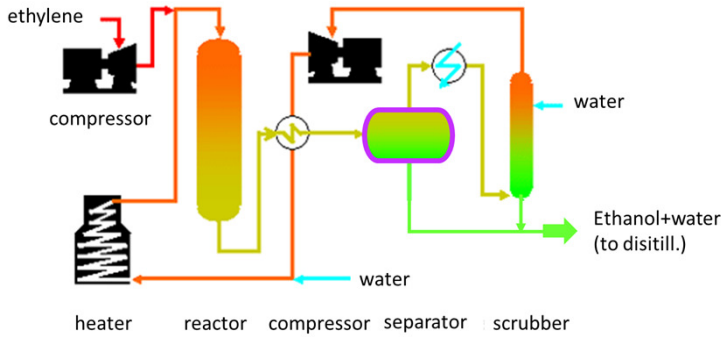
Simultaneous Mixed Usage of Multiple Type of Binary Parameters

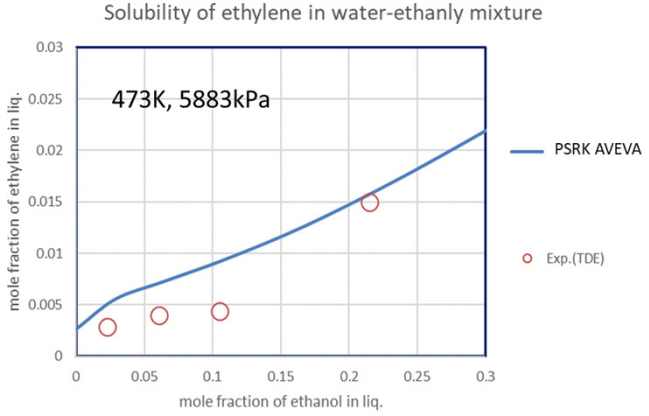
Example: Ethylene-Ethanol-Water System











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(Just POC was completed)

Relax Constraints for NRTL g^E to Include Quadratic Mixing Rule

$$a_m = \frac{b_m}{c}\sum_i x_i \frac{\sum_j x_j G_{ji}\tau_{ji}}{\sum_k x_k G_{ki}} + \frac{RTb_m}{C}\sum_i x_i \ln\left(\frac{b_m}{b_i}\right) + b_m \sum_i^{Nc} \frac{a_i}{b_i} x_i$$

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

Relax NRTL: Allow τ_{ji} to depend on composition

$\alpha_{ji} = 0$

$$\tau_{ji} = \frac{c}{RTb_m}\left\{\sqrt{a_i a_j}(1-k_{ji}) - a_i\left(\frac{b_j}{b_i}\right)\right\} + ln\left(\frac{b_m}{b_i}\right)\left(\frac{b_j}{b_m} - \frac{b_i}{b_m}\cdot\frac{x_i}{1-x_i}\right)$$

$\tau_{ji} = f(T)$

Should work together

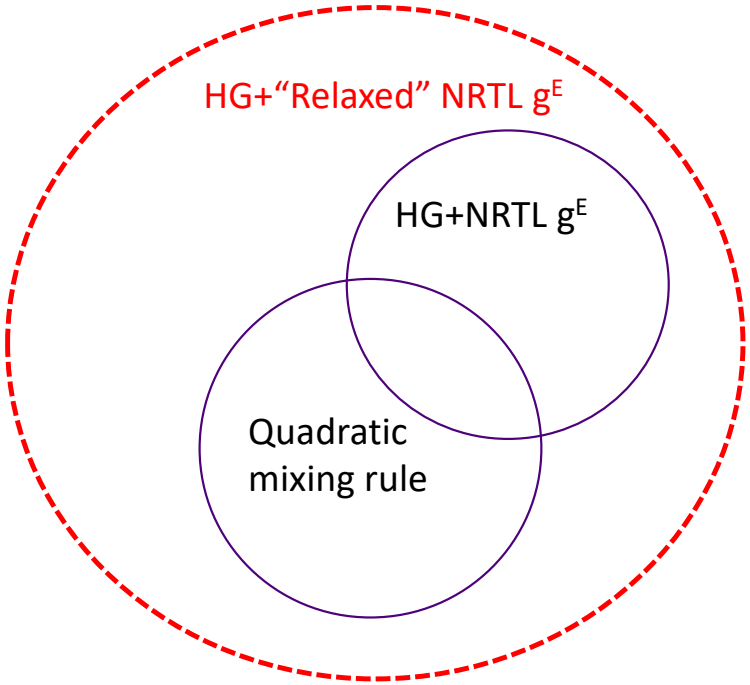
For some pairs

$$a_m = \sum_i \sum_j \sqrt{a_i a_j}(1-k_{ij})$$

Quadratic Mixing Rule

For some pairs

HG+NRTL g^E



*Detail will be presented at ESAT2021

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Fill Options for BIPs on AVEVA Process Simulation

FILL OPTION	Target pairs	Methods	Industry	Implementation timing
Water Correlation	water-hydrocarbon (or petro) pairs	CEOS	Common	Phase-1
MW Correlation	light gas-hydrocarbon(or petro) pairs	CEOS	Common	Phase-1
H2 Correlation	hydrogen-hydrocarbon(or petro) n pairs	CEOS	Common	Phase-1
Sulfur Correlation	Sulfur components-hydrocarbon(or petro) pairs	CEOS	Oil/gas	Phase-2
Glycol Correlation	glycol-petro pairs (invented by AVEVA)	CEOS	Oil/gas	Phase-2
Methanol Correlation	methanol-hydrocarbon(or petro) pairs	CEOS	Oil/gas	Phase-2
Azeotrope Fill	all component pairs which has azeotrope	NRTL, UNIQUAC	Chemical	done
Fill from infinite dilute activiy coefficient	component pairs which has infinite dilution activity coeff.	NRTL, UNIQUAC	Chemical	at the timing of REGRESS
Fill from mutual solubility	component pairs which has mutual solubility	NRTL, UNIQUAC	Chemical	at the timing of REGRESS
UNIFAC Fill for LACT	Paris of components covered by UNIFAC, including petroleum comp (DDBST UNIFAC Consortium members should be able to apply Consortium databank)	NRTL, UNIQUAC	Chemical	Phase-1
FILL from RS and FH		NRTL, UNIQUAC	Chemical	(non, scarcely used)
C1/C2 GOR	C1/C2-other hydrocarbons(or petro) pairs	CEOS	Oil/gas	(non, PPR78 is better)
Modified Gao	C1/C2/C3-other hydrocarbons(or petro) pairs	CEOS	Oil/gas	(non, PPR78 is better)
Modified Chueh-Prausnitz	hydrocarbon(or petro) -hydrocarbon(or petro)	CEOS	Oil/gas	Phase-1
PPR78 Fill Option	hydrocarbon(or petro) -hydrocarbon(or petro)	CEOS	Oil/gas	Phase-2
UNIFAC FILL for EOS	Paris of components covered by UNIFAC	SRKM, SRKH	Chemical	(after PSRK)

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Coverage of Each Electrolyte Method for Expected Applications

Bosen and Engels (Done)

Pitzer

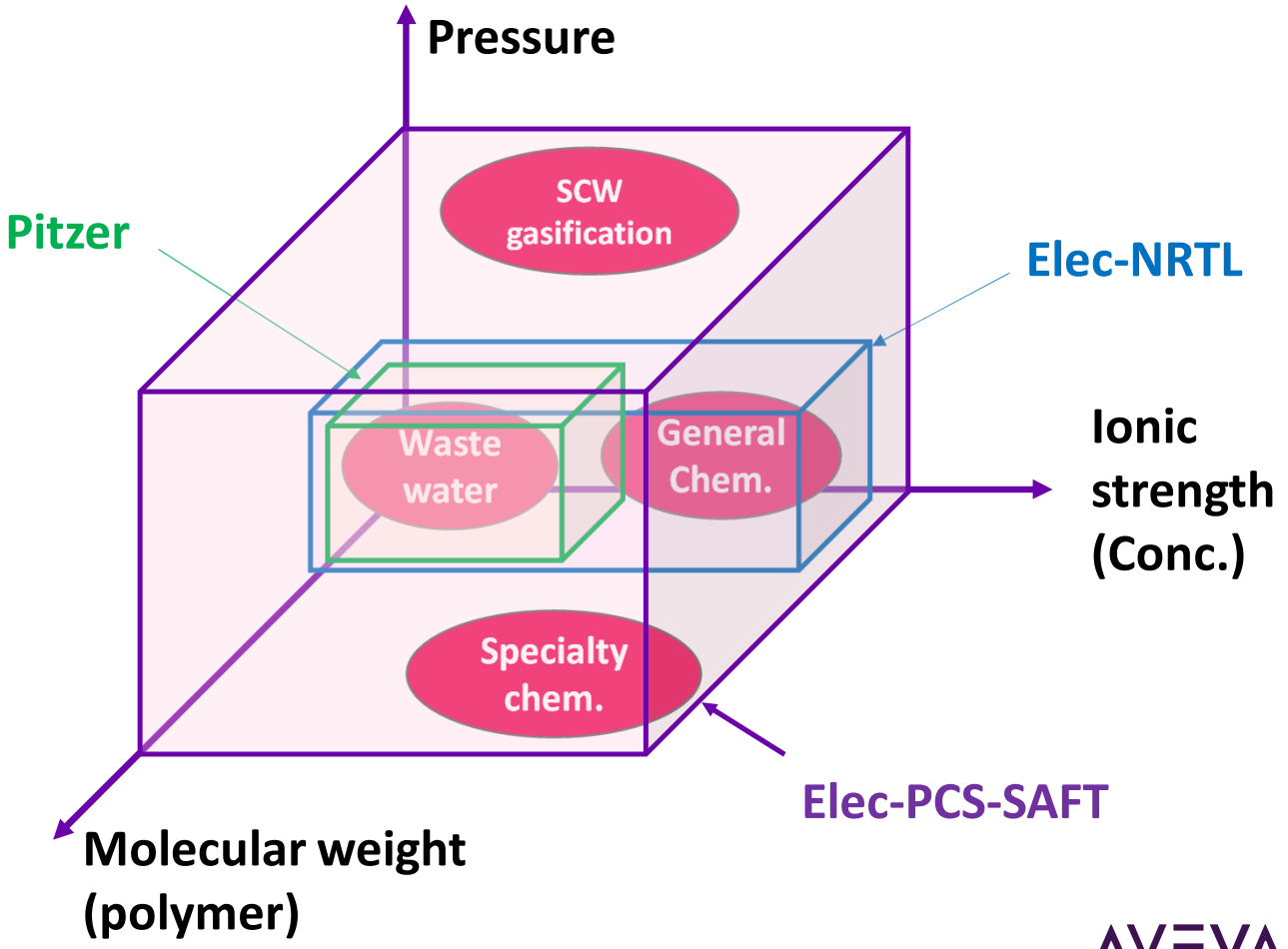
- Ionic strength: up to 10
- Aqueous electrolyte
- Low to medium press.
- Monomer

Elec. NRTL (done)

- Covers very high ionic strength
- Mixed solvent
- Low to medium press.
- Monomer

Elec.PC-SAFT(proposed)

- Covers very high ionic strength
- Mixed solvent
- Covers high pressure
- Covers elec. polymers



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Three Phase Electrolyte Plan

Phase 1 – Proof of Approach
(Complete)

Feature	Status
Prove Fluid Reaction Model approach.	*Complete*
Deliver H2SO4 components and reaction fluid.	*Complete*
Allow customers to extend to their own systems	*Complete*

Prove

Objective is to demonstrate that electrolytes can be solved in a rapid solution using an EO approach and deliver a typical system such as H2SO4.

Phase 2 – Functional Expert Use
(Almost completed)

Feature	Status
Develop Pitzer Method	*Code completed*
Create typical Reaction Model	*Underway*
Create e-NRTL Method	*Complete*
Solids/Precipitation Handling	*Complete*

Functional

Get 80% of most users functionality although there is a burden on users to supply data and reactions if is not one of the typical ones we deliver.

Pitzer is a common reference system that requires many of the same features as e-NRTL so we decided to do it first.

We chose e-NRTL since many customers already have data for it so that regression for a new method is not required.

Phase 3 – Generalized Use
(2021+)

Feature	Status
Extended Literature Component Data	*proposed*
Create framework to automatically populate species and reactions	*proposed*
Add Regression Capability	*proposed*
Consider e-PCSAFT	*Research phase (collaboration with University)*

Generalized

Extend to be a generalized electrolyte system with many built in component data and reaction data so that less expertise is required to construct the Fluid Reaction Model.

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AVEVA Invests in Improving Electrolyte PC-SAFT of TU Dortmund

Confirming applicability of ePC-SAFT to simulating acid gas removal using hybrid solvent*

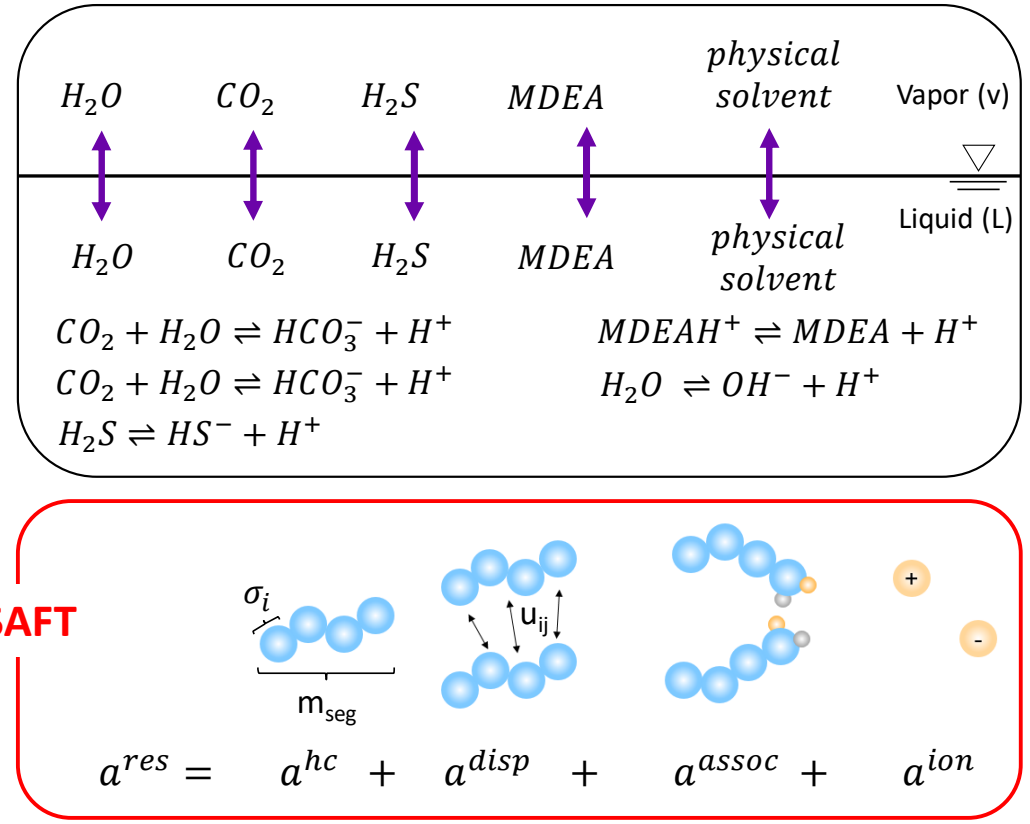
- Equilibrium conditions
  - Pressure: $P^L = P^V$
  - Temperature: $T^L = T^V$
  - Physical (phase)equilibrium:

$$x_i^L \cdot \varphi_i^L = x_i^V \cdot \varphi_i^V$$

  - Chemical (reaction) equilibrium for A+B=C+D:

$$K_{th} = \prod_i a_i^{\nu_i} = \frac{a_C * a_D}{a_A * a_B}$$

$$a_i = x_i \cdot \gamma_i$$



*Mark Bülow, Nevin Gerek Ince, Seiya Hirohama, Gabriele Sadowski, Christoph Held. Predicting Vapor–Liquid Equilibria for Sour-Gas Absorption in Aqueous Mixtures of Chemical and Physical Solvents or Ionic Liquids with ePC-SAFT. *Industrial & Engineering Chemistry Research* **2021,** *60* (17) ,

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Elec.PC-SAFT Update

Objectives

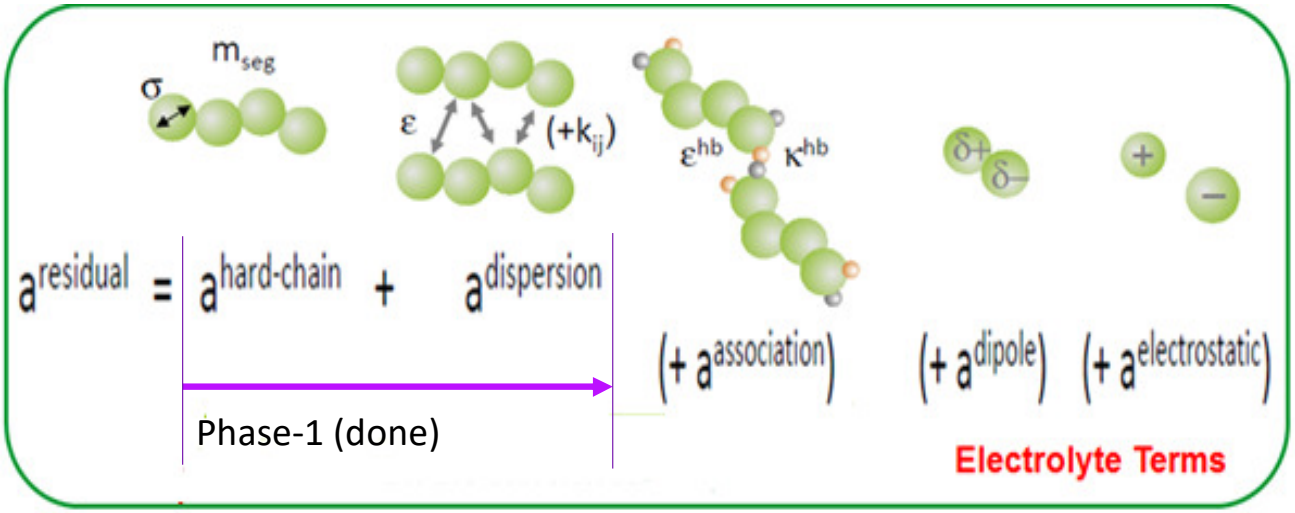
- Establish reliable thermo model to cover mixtures with polar and/or electrolyte polymer at elevated pressures

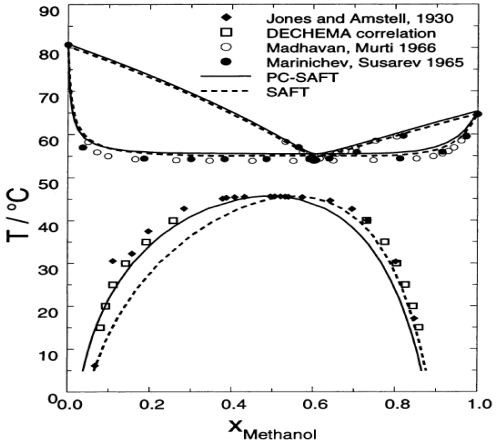
Solution

- Implement Electrolyte PC-SAFT on AVEVA Process Simulation which has;
  - Association term for chemical application
  - Add electrolyte terms for ions
  - Mixing rule for copolymers

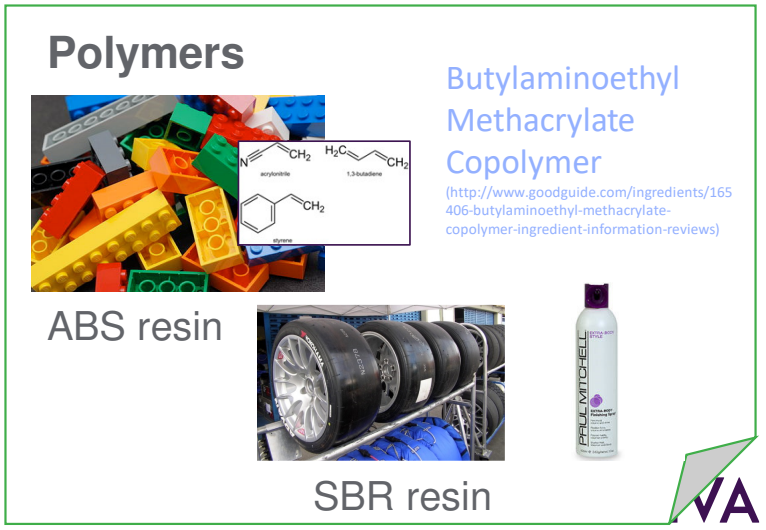
Status and plan

- Collaboration with Dortmund Technical University (almost finished)
- Implementation on AVEVA Process Simulation is being discussed





Methanol-Cyclohexane system



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Carbon Capture Simulation

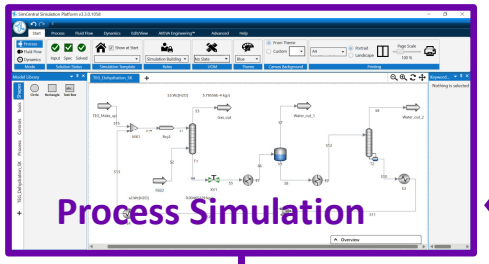
Objectives

- Support customers all through the life-cycle of carbon capture technologies which use amine/hybrid solvents;
  - Research phase: **Select optimal solvent**
  - Basic engineering: optimal design based on **customers' proprietary solvents**
  - Detail design: rating/sizing of equipment. Final checks of performance/ controls based on 3D data

Solution

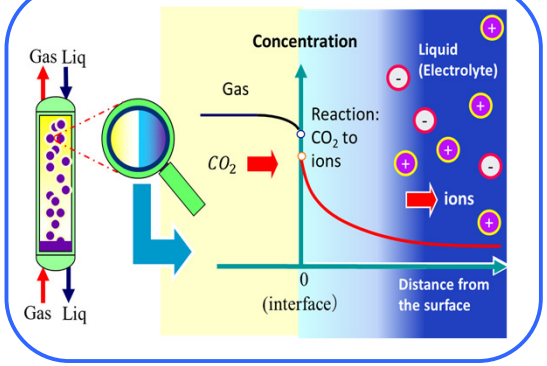
- Equip AVEVA Process Simulation with the following features
  - Mass-transfer model considering reactions at VL boundary layer
  - Rigorous and **flexible** thermo model for amines
  - **Data regression** covering reaction parameters

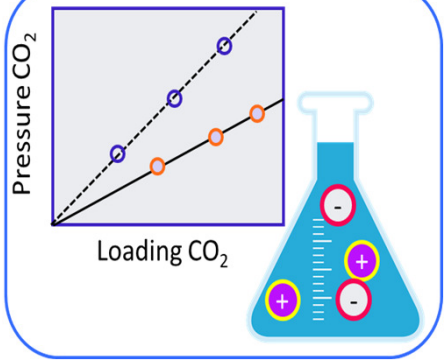
- Laboratory data
- Pilot plant data
- Solvent selection (combinatorial approach)



- Basic/detail design
- 3D data
- Equipment information

Autonomous adjustment of parameters using customers' proprietary data





Data regression covering reaction parameters

Mass-transfer model considering reactions at VL boundary layer

Rigorous and flexible thermo model for amines

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3Phase Plan for Amine on AVEVA Process Simulation

Phase-1:POC

Because the fluid contents can be modified by users, the “green box” partially reaches “carbon capture” from the very 1st phase.

Phase-2: Minimum core feature

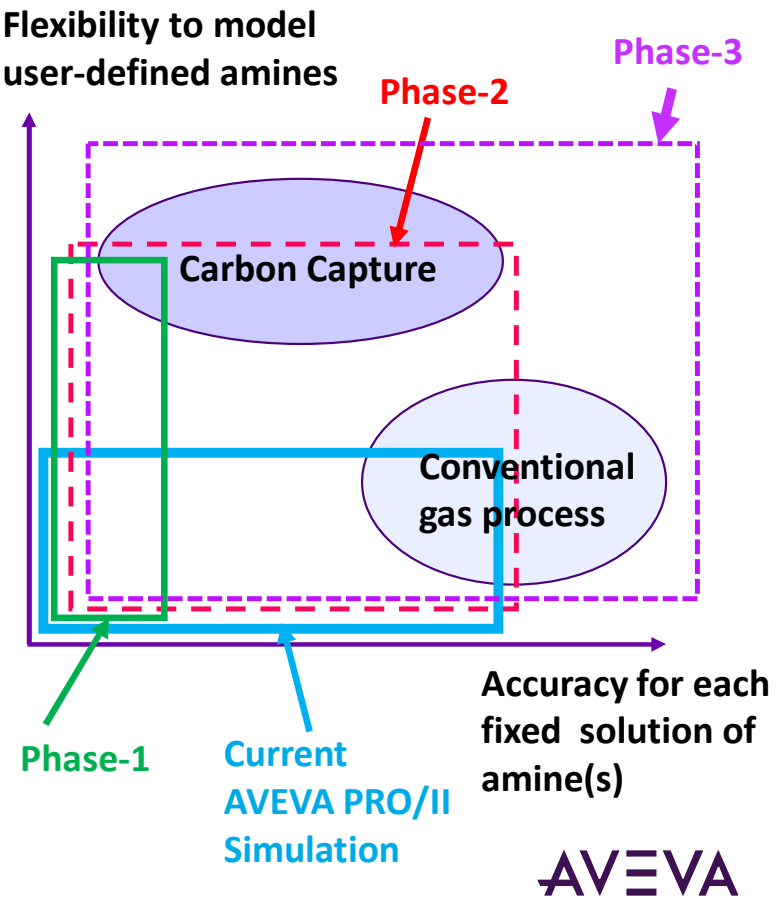
Extends our coverage to horizontal direction (accuracy) to the same extend with that of AVEVA PRO/II Simulation;

- Enhance default reaction set to cover some typical amines solutions, which are covered by AVEVA PRO/II Simulation
- Incorporate eNRTL to calculate activity coefficients of species in the above defined solutions

Phase-3: Extensions

To have some additional data and method to cover more types of amines and further flexibility

- Enhance default reaction set and data to cover some more defined amines + additives (including K2CO3) + hybrid solvents
- Regress for eNRTL (discussed in another front)
- ePC-SAFT (in electrolyte 3phase plan)



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Possible 3 Phases Plan for Solid for Chemicals

AVEVA Process Simulation

Phases	Phase-1	Phase-2	Phase-3
Timeframe	Completed	To be completed in 2022+ (**Partially in 2021**)	To be decided (long term)
Targets/ Objectives	• Committed Features • Defining minimum market requirements	Minimum market requirements	Advanced
Equilibrium	• Non-equilibrium solid • Electrolyte (solubility product) • Simple SLE for non-electrolyte	• **SLE based on activity coefficient methods (such as NRTL)** • **Detection of solid occurrence applying EOS to fluid phase**	• **General Fluid-Solid Equilibrium (SLE, SVE, SFE)**
Solid properties	• Enthalpy, entropy, density	• Fugacity	• **Particle size distribution for each component** • Slurry property (non-Newtonian viscosity behavior)
Unit Operation	• Simple equilibrium flash unit • Reactors	• Crystallizer and mechanical Separation • **Solid warning**	• Predict particle size • **Enhance solid warning (types of solid)**

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Solid Warning Needed for Flow Assurance and Avoiding Fouling

Category	Components	Typical location	Remarks on simulation	Applicable theories
Pure solids	CO2 and H2S, 20 hydrocarbons	Cryogenic in gas process	Not hydrate (may happen without water) JIP Project extensively covers the class of components	Solve $f_{each\ comp.,\ gas/liq} = f_{each\ comp.,\ solid}$ • $f_{each\ comp.,\ gas/liq}$: fugacity of each solid comp. in gas/liq using EOS • $f_{each\ comp.,\ solid}$: fugacity in each solid (pure comp.) using correlation
	water (ice)	pipe-line (gas)		
	sulfur	pipe-line (gas)	Need to model the reaction; H2S+(1/2)O2->H2O+S	Kinetic reaction model (looking for data for data regression)
Hydrates	Hydrate of gas mixtures (mainly methane, ethane, CO2….)	pipe-line(gas)/ cryogenic	Water is needed for hydrate to occur. Need to predict effect of gas dryer/inhibitor	Solve $f_{water,\ gas/liq} = f_{water,\ hydrate}$ • $f_{water,\ gas/liq}$:fugacity of water in gas/liq calculated using EOS • $f_{water,\ hydrate}$: fugacity of water in hydrate using Solid Solution Theory
Salts	ammonium hydrosulfide	Hydrotreater HX	precipitate from gas containing NH3 and H2S	Electrolyte
	ammonium chloride	VDU condenser	precipitate from gas containing NH3 and HCl	Electrolyte
Heavy oil	Asphaltene (crude)	pipe-line (oil)	(Many authors model asphaltene as liquid)	CEOS, RS,PC-SAFT, sac-NRTL
	Asphaltene (cracked oil)	thermal crackers	Kinetic model need to be combined	Dr.Takatsuka's theory (modified RS + kinetic model)

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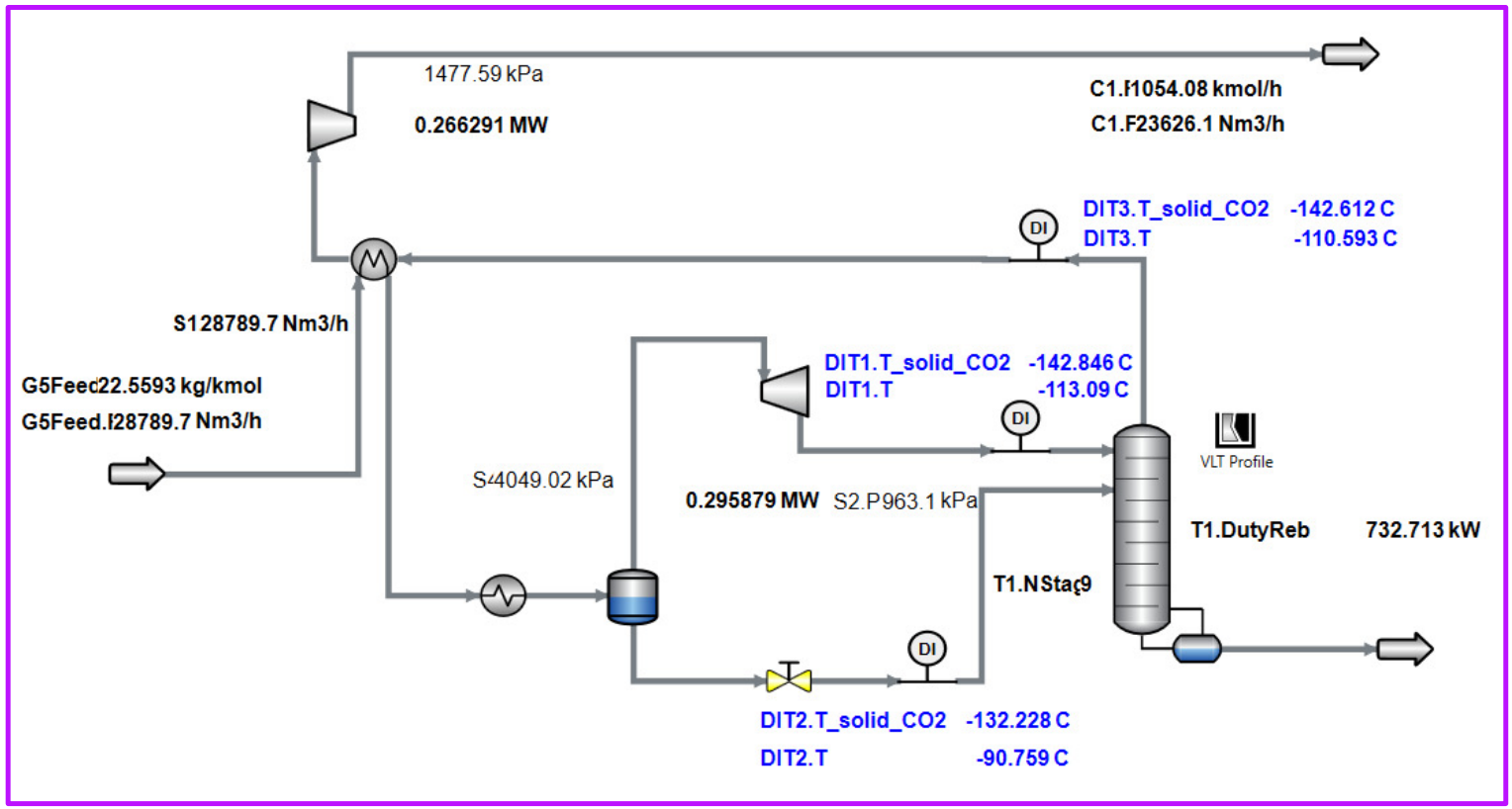
Quick Demo of POC: Solid Warning (Dry Ice)



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Joint Industrial Project (JIP) for Solid in LNG

Objective

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

Project members: AVEVA, TOTAL, and TechipFMC

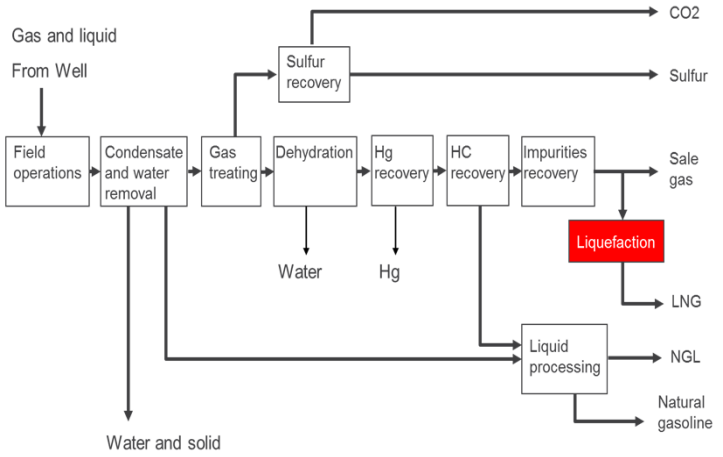
Scope of the works:

- Model: CEOS (SRK/PR) for fluid side. Currently 25 components (scalable)
- Update correlation for solid fugacity, alpha param., BIPs
- Establish flash algorithms: AVEVA PRO/II Simulation: VLL-multi. S
- Physical Properties: Fluid: enthalpy, entropy, and density, solid: enthalpy and density
- Technical detail was presented by Total at AWC Europe 2019, some additional work will be presented at ESAT2021

Status and plan:

- Already implemented in special versions of AVEVA PRO/II Simulation for TOTAL, and TechipFMC
- Will be available on general version of AVEVA PRO/II Simulation after exclusivity period.
- Equations and data will be utilized in AVEVA Process Simulation and AVEVA Dynamic Simulation





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Hydrates Prediction Feature on AVEVA™ Process Simulation

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

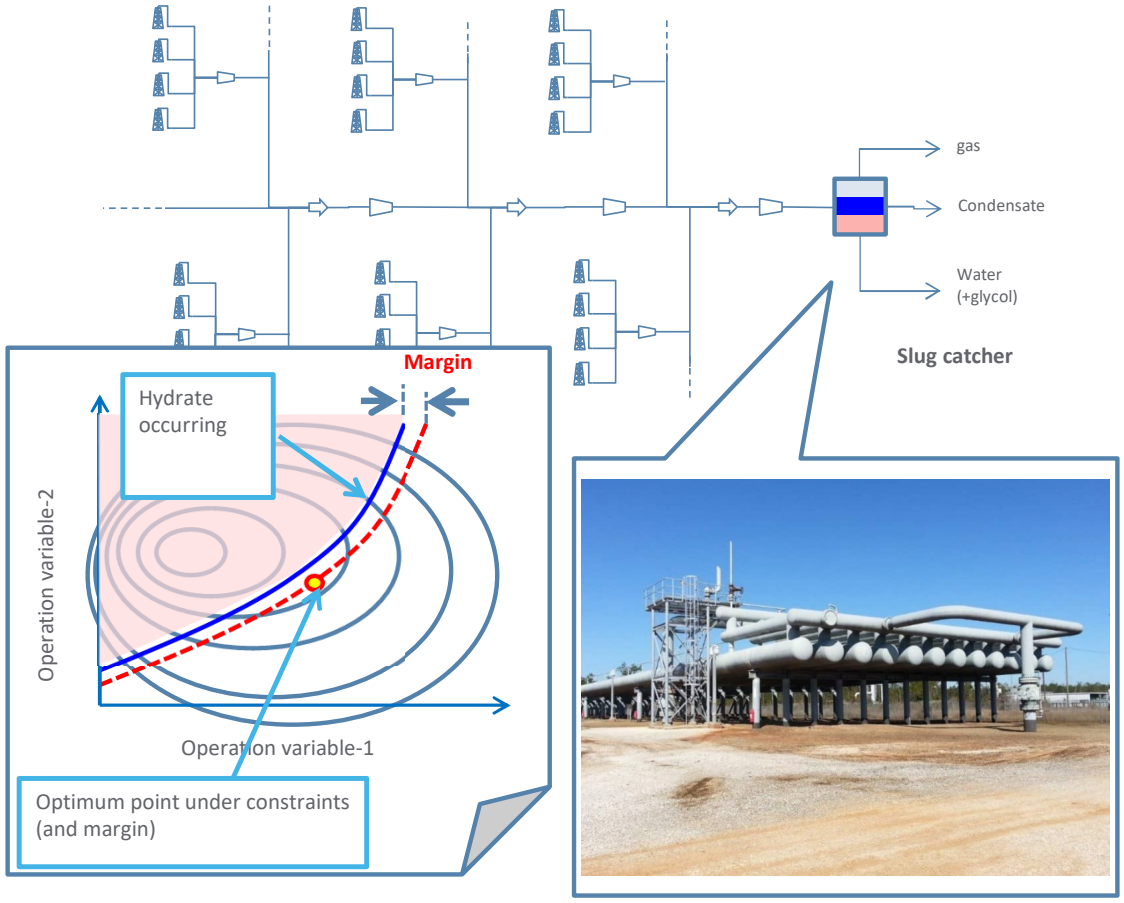
- Plural types hydrates need to be considered, including newly discovered ones
- Hydrate features on AVEVA PRO/II Simulation is 30+ years old

Solutions

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

Status and plan

- Phase-1 (natural gas): 2021
- Phase-2 (general): 2022+



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Plan for Hydrate Prediction

Capabilities		Conventional on AVEVA PRO/II Simulation	Phase-1 (Simple) on AVEVA Process Simulation(2021)	Phase-2 (Ultimate) on AVEVA Process Simulation (2022+)
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)

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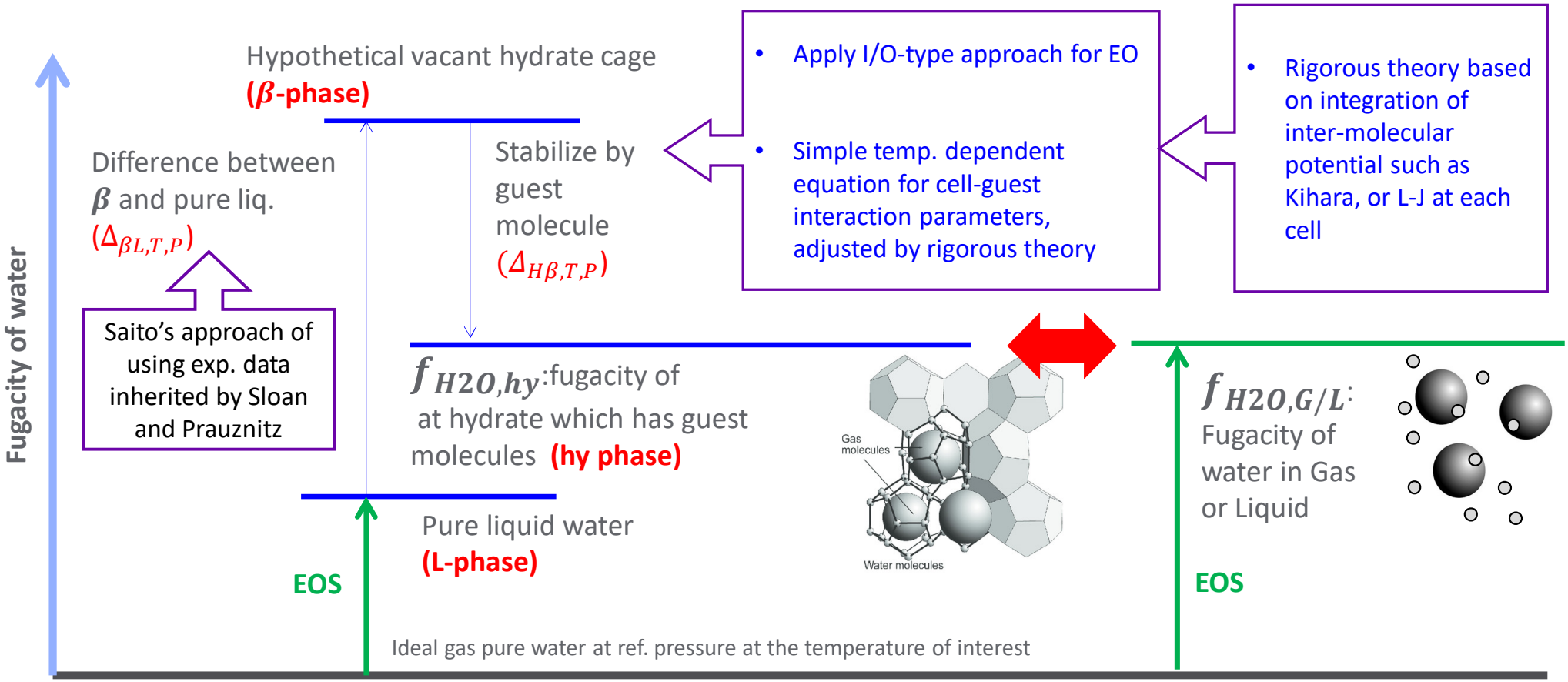
Usage of Solid Solution Theory on EO Architecture for Hydrate Prediction



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Agenda

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- Welcome and Introductions Day 2
- AVEVA Thermodynamic Updates
- AVEVA Thermodynamic Roadmap
- Break
- Presentation from Advisor (Dr.Westhaus of DECHEMA)
- Status of advisors' ideas on Aha Portal
- Enhancement Requests
- Meeting wrap-up

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DECHEMA

Dr.-Ing. Ulrich Westhaus



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Enhancement Requests on Aha Idea

Top 11 items as of June 10. 2021

Number of voting	Items	Status
9	Implement CPA (Cubic Plus Association) EOS	In roadmap
8	Phase envelope including all the phases equilibrium	In roadmap
7	Implementation of new activity coefficient models based on new concepts	In roadmap
7	Binary parameter converter (Hirohama-Bluck-Sasaki method)	In roadmap
7 (recently increased)	Add/expand the thermodynamic function to handle CO2 capture (amine)	In roadmap
6	Interface with external thermodynamic databases such as NIST, DETHERM	In progress (DETHERM)
6	Automatic conversion function of correlation equation on TDM	To be discussed
5	Extension of maximum available temperature of liquid enthalpy curve of SimSci DB	Partially done
3	PSRK with adjustable parameters (with NSTL gE)	In roadmap
3	Regress/Plot Update	In roadmap

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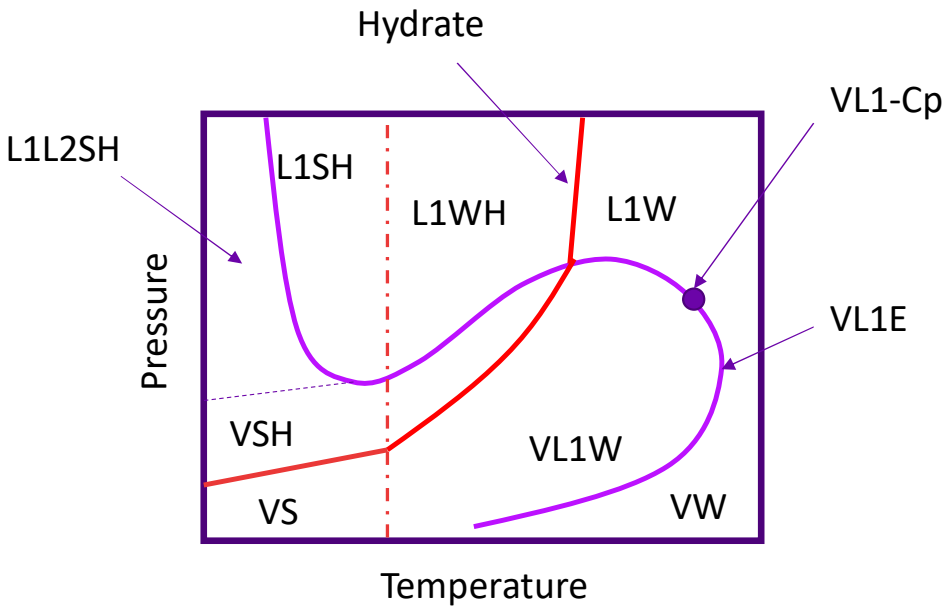
Phase Envelope Update

Objectives
- Accurately understand the behavior of oil and gas flows

Challenges
- Current Phase Envelope considers only VLE

Solutions
- Incorporate all the phase equilibria
  - LLE
  - Solid
  - Hydrate

Plan
- Will be planned after hydrate update
- Platform would be AVEVA Process Simulation



Schematic phase envelope
of hydrocarbon-water mixture

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FILL from UNIFAC to CEOS

Direct Conversion of Parameters using gE

Objective and Background

- Model chemical processes with non-ideal mixture at elevated pressure for which some BIPs are missing for EOS
- Some clients like to keep using SRKM which is fairly accurate and very robust

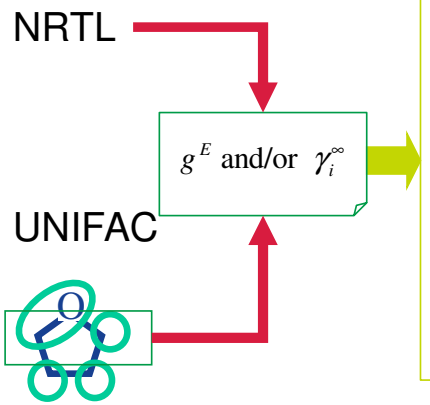
Solutions

- Develop Fill Option for SRKM, which fills BIPs using UNIFAC (The procedure has been already established*)

Delivery

- Being discussed

*Seiya Hirohama, David Bluck, and Masakazu Sasaki; "Direct prediction of the binary parameters of a cubic equation of state from those of a low-pressure gE model", Fluid Phase Equilibria 302 (2011) 305–309



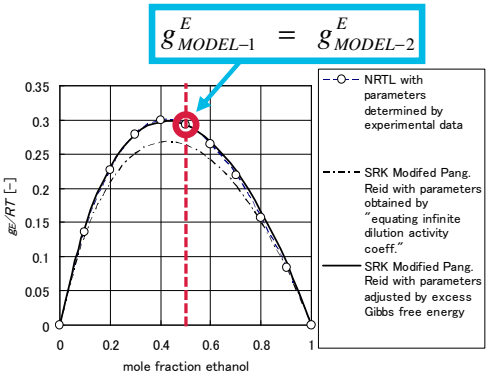
Modified Pang.-Reid mixing rule with SRK

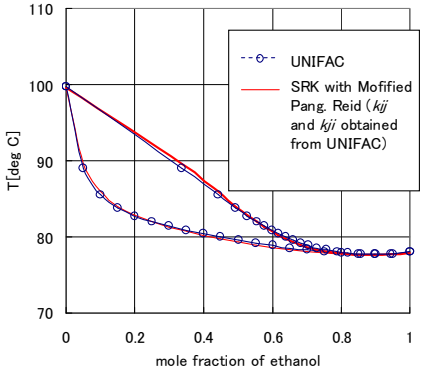
$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)}$$

$$a = \sum\sum x_i x_j a_{ij}$$

$$a_{ij} = \sqrt{a_i a_i}\left\{(1-k_{ij}) + (k_{ij}-k_{ji})\frac{x_i}{x_i+x_j}\right\}$$

$$b = \sum x_i b_i$$





Vapor-liquid equilibria for ethanol-water system

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Data Update

Temperature Range of Liquid Enthalpy for Some Components (Urgently Requested by Advisory Group in 2020)

Objective and Background

- Accurate simulation for chemical process

Challenge

- Some components have very narrow temperature ranges (especially very low Tmax) for liquid enthalpy

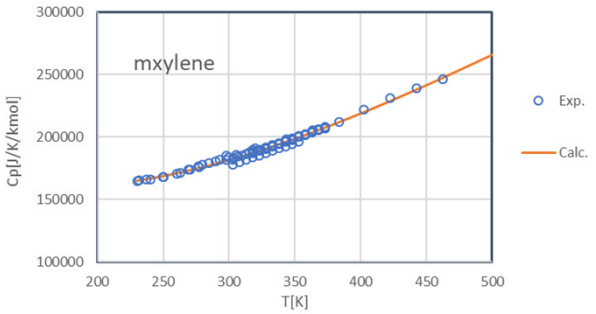
Solution

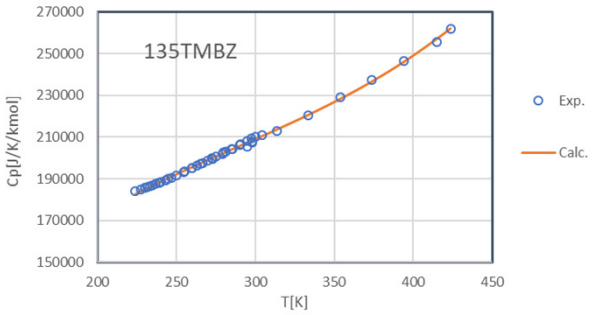
- Enhance the temperature coverage using the newest data

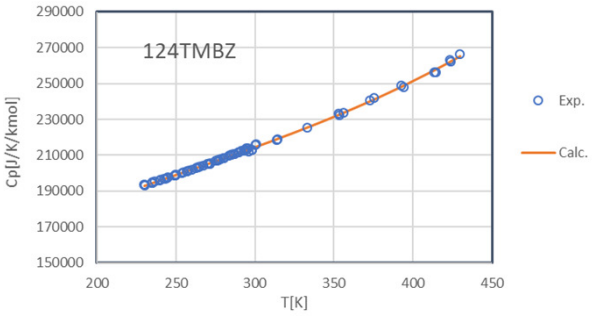
Delivery

- Regression was completed
- Coming in 2021 for all the products (SimSci bank)

Full name		m-xylene	Mesitylene	1,2,4-trimethylbenzene
Alias		MXYLENE	135MBENZ	124MBENZ
CAS#		108-38-3	108-67-8	95-63-6
Temperature range[K]	Tmin	230	224	224
	Tmax	540	430	430
FYI: Tmax [K] in the old databank		360	350	350







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Agenda

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- Welcome and Introductions Day 2
- AVEVA Thermodynamic Updates
- AVEVA Thermodynamic Roadmap
- Break
- Presentation from Advisor (Dr.Westhaus of DECHEMA)
- Status of advisors' ideas on Aha Portal
- Enhancement Requests
- Meeting wrap-up

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Usage of AI in Thermodynamics

Brainstorming

- Type of Uses
  - Intelligence in simulation tool: suggestions using knowledgebase
  - Autonomous selection of thermo methods/ algorithms (e.g. proactive prediction of existing phases)
  - Property estimation based on molecular structure (often combined with quantum chemistry or group-contribution/QSPR)

- Type of methodologies
  - Machine (deep) learning
  - Relational database
  - Combination with 1st principle type methods



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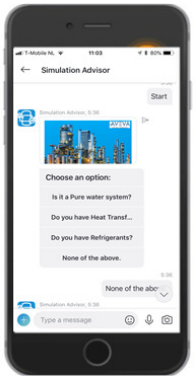
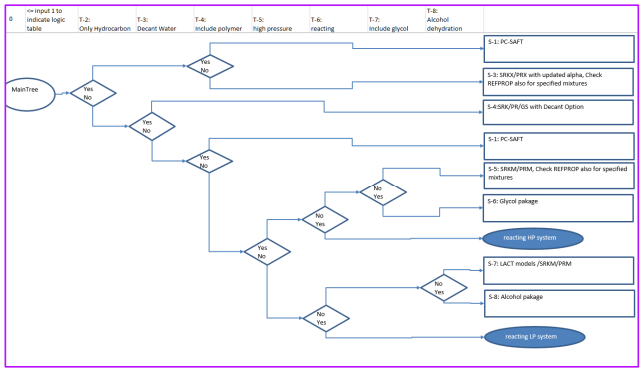
Use of AI for Advising Thermo Method and Data





Objectives

- Make suggestion to customers on thermo configurations such as methods and data

Solution

- Use of autonomous SNS tools (like BOTs) which enable users to have “structured conversation” with an expert system based on “decision tree” using popular platforms like smart phones
- Human interventions are recorded in data storage. Machine-learning is applied to improve the decision tree
- Helps for education/training (joyful contents)

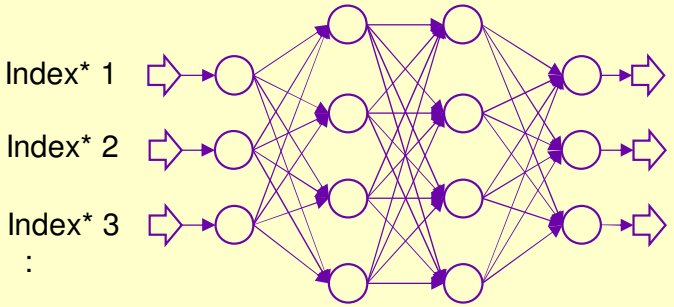
Plan

- Timeframe: being discussed
- Phase-1:Suggest methods and data sets based on a fixed decision tree and data availability maps.
- Phase-2:(Long term) Dragonize simulation file. Machine-learning to autonomously improve the decision learning from human interventions

Partial Update of Decision Tree Using Machine-learning

In input parameters
(demands, scalable)

Output parameters
(simulation configurations, scalable)



*Example of index: “robustness required”, performance (speed), outcome of other decision trees, accuracy for specific systems….
**Recommendation could be thermo sets, databanks, configurations for unit operations, and their combinations.

(A patent was submitted)

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Thank You !

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The company's engineering, planning and operations, asset performance, and monitoring and control solutions deliver proven results to over 16,000 customers across the globe. Its customers are supported by the largest industrial software ecosystem, including 4,200 partners and 5,700 certified developers. AVEVA is headquartered in Cambridge, UK, with over 4,400 employees at 80 locations in over 40 countries.

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