



# ADVANCED PROCESS MODELLING FORUM 2017

London 25–26 April

## gSAFT

Advances in thermodynamic modelling

Thomas Lafitte – Principal Scientist



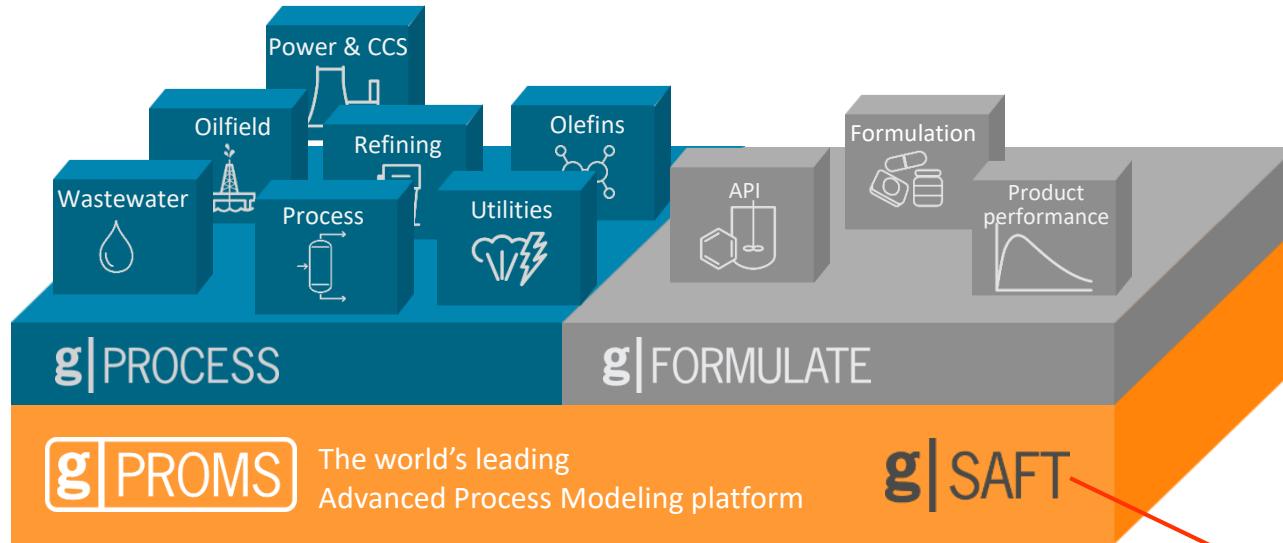
# Introduction to gSAFT



# The gPROMS software suite – 2017



Platform Environments Libraries



## “Simple” products gPROMS ProcessBuilder

## Formulated products gPROMS FormulatedProducts

## Platform functionality

### Process modelling

- Equation-oriented solution power
- Custom model construction
- Steady-state and dynamic simulation and optimisation
- Advanced parameter estimation
- Powerful dynamic and mixed-integer optimisation
- Global system analysis
- High-performance computing

### Materials modelling

- Molecular & ionic species
- Complex species & mixtures
- Gas, liquid, solid phases
- Phase & reaction equilibrium

A single powerful software platform  
Effective & efficient  
software development & maintenance



ADVANCED PROCESS MODELLING FORUM 2017

Molecular representation



Functional group representation

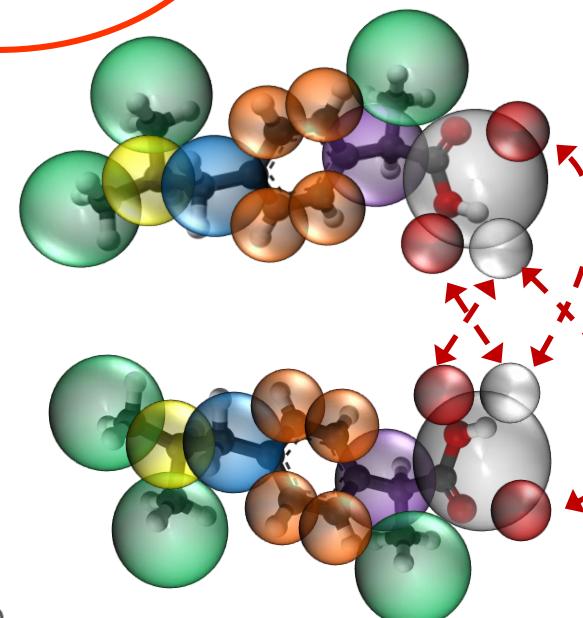
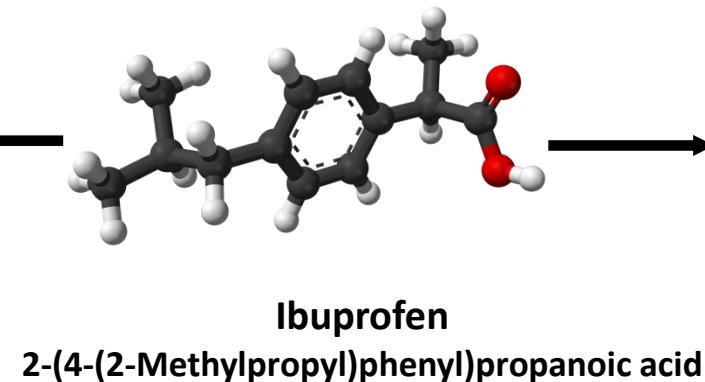
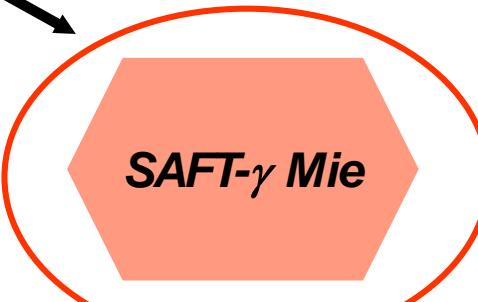
**SAFT-VR SW**



**PC-SAFT**



**SAFT- $\gamma$  Mie**



# SAFT- $\gamma$ Mie equation of state

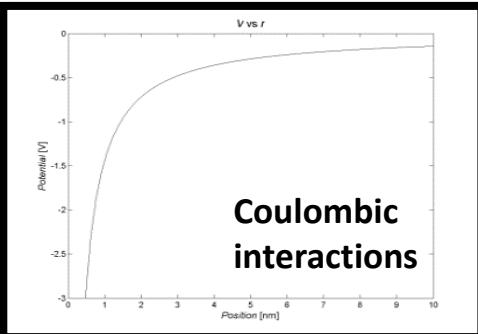
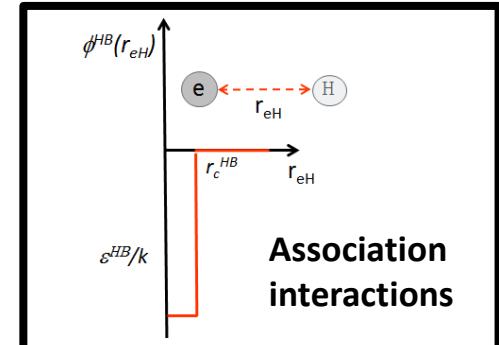
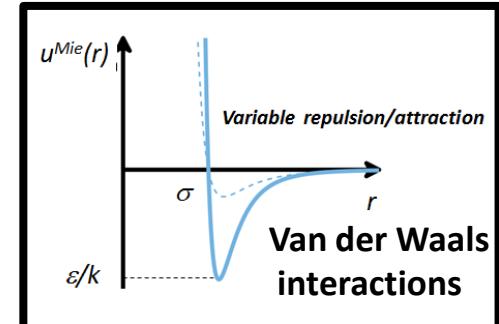
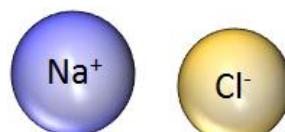
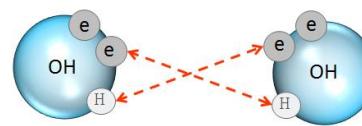
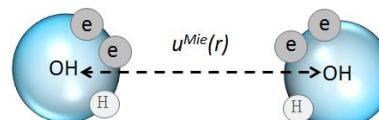
## Molecular models

### ■ Example mixture:



### ■ Groups interact via

- dispersion/repulsion (van der Waals) forces
- hydrogen bonding via off-centre electron donor/acceptor (“association”) sites
- ionic (coulombic) forces



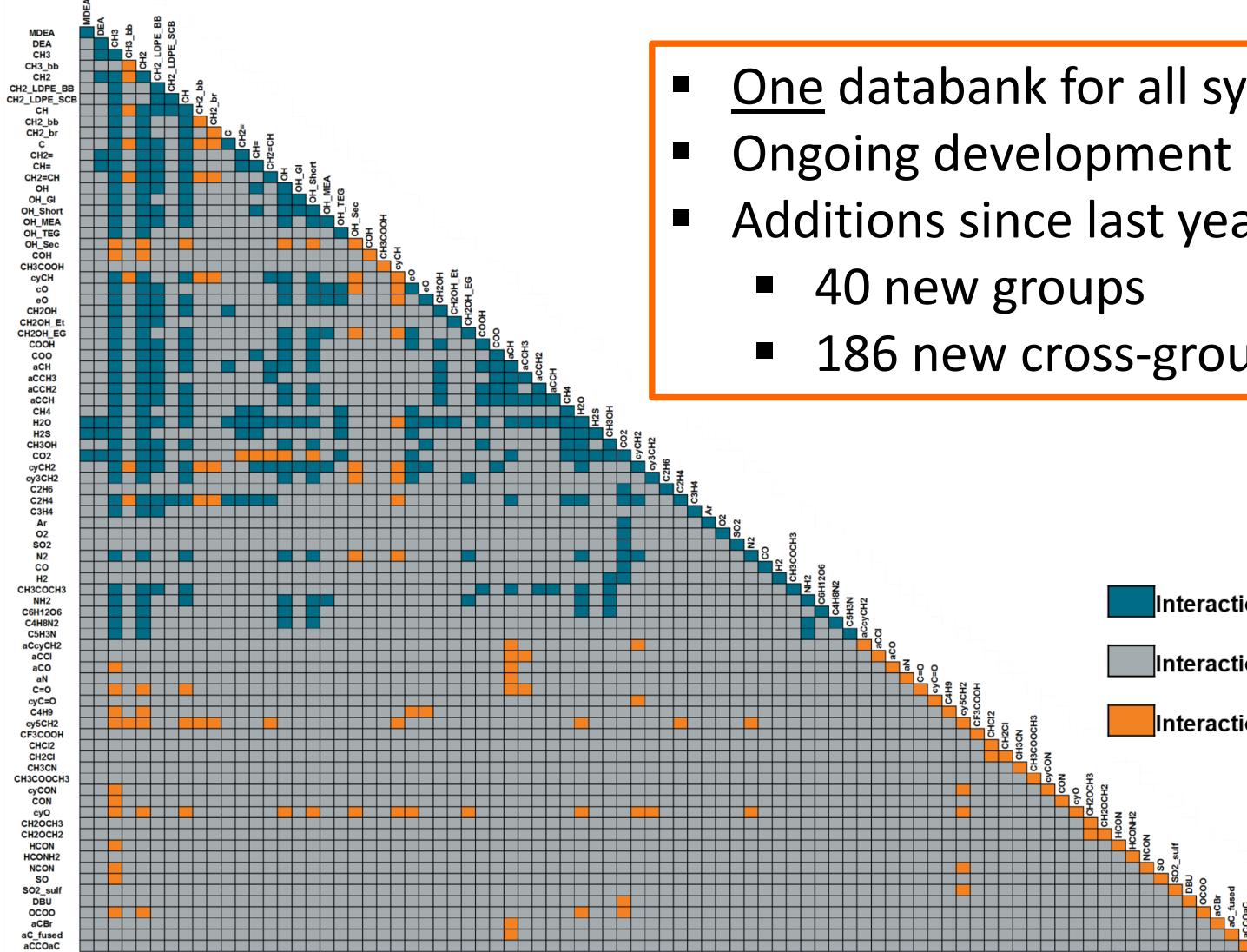
- Advantages over activity coefficient models
  - applicable to both **pure compounds** and **mixtures**
  - consistent modelling of gas and liquid phases (necessary for **near critical region**)
  - accurate predictions at **high pressure**
  - **all thermodynamic** properties can be computed with a single set of parameters
- Advantages of over cubic EOSs and activity coefficient models
  - can be applied **consistently** to small molecules, polymers and electrolytes
  - accurate computation of both phase equilibrium and **second derivative properties** (heat capacity, speed of sound etc...)

**Simple workflow  
for modelling of  
complex systems**

**Easier/more reliable  
configuration of  
physical properties**

**Single  
universally-applicable  
parameter databank**

## Group parameter databank – April 2017



- One databank for all systems
- Ongoing development effort
- Additions since last year's APMF
  - 40 new groups
  - 186 new cross-group interactions

# gSAFT for polymer systems

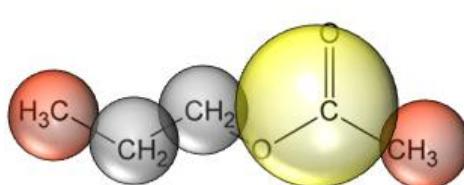


## Highlights

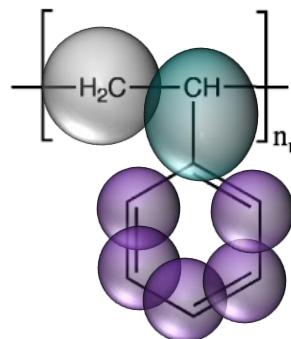
- Robust solution of phase equilibrium of systems involving polymers
- Single predictive tool for VLE, LLE and VLLE
- Natural handling of polydispersity

# gSAFT for polymer systems

## VLE predictions - I

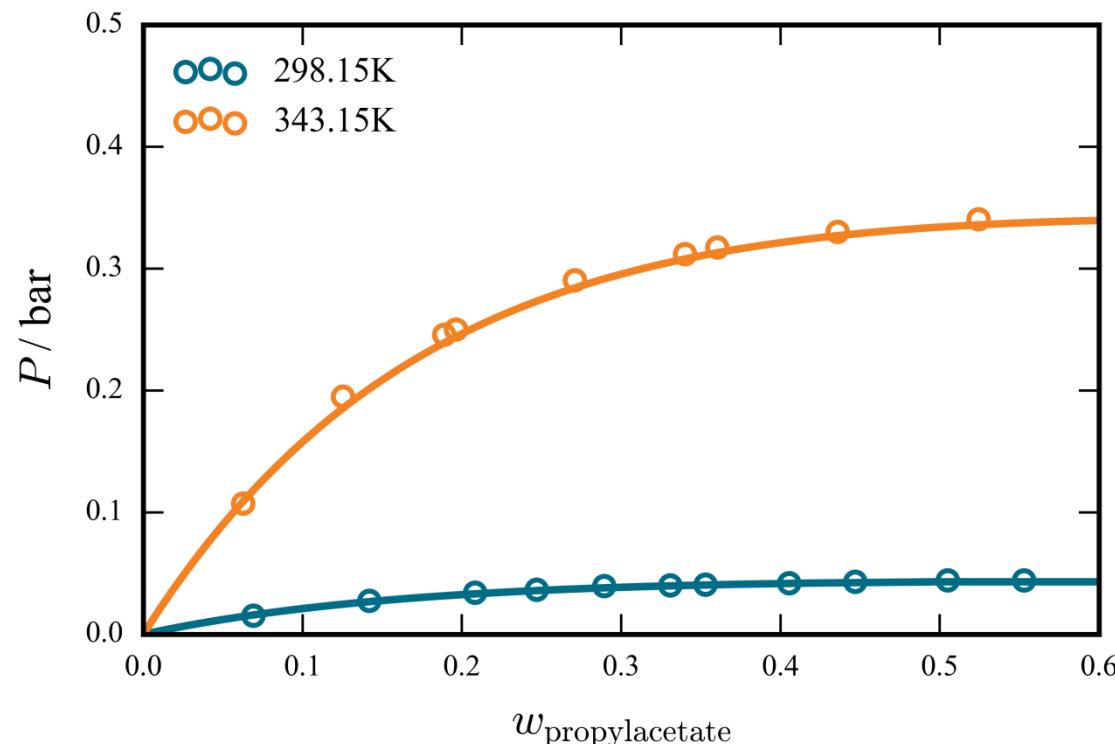


Propyl acetate



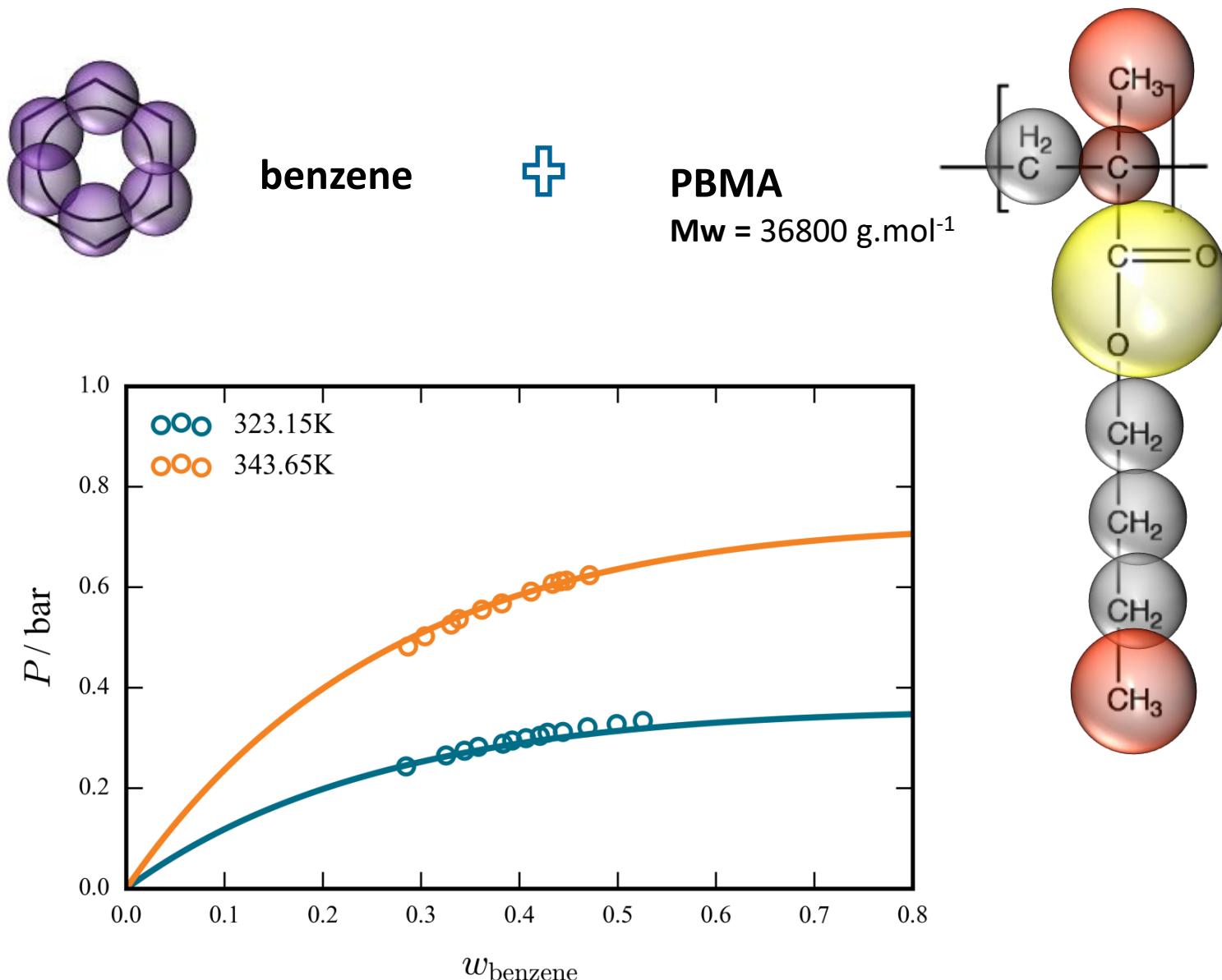
Polystyrene

Mw = 290000 g.mol<sup>-1</sup>

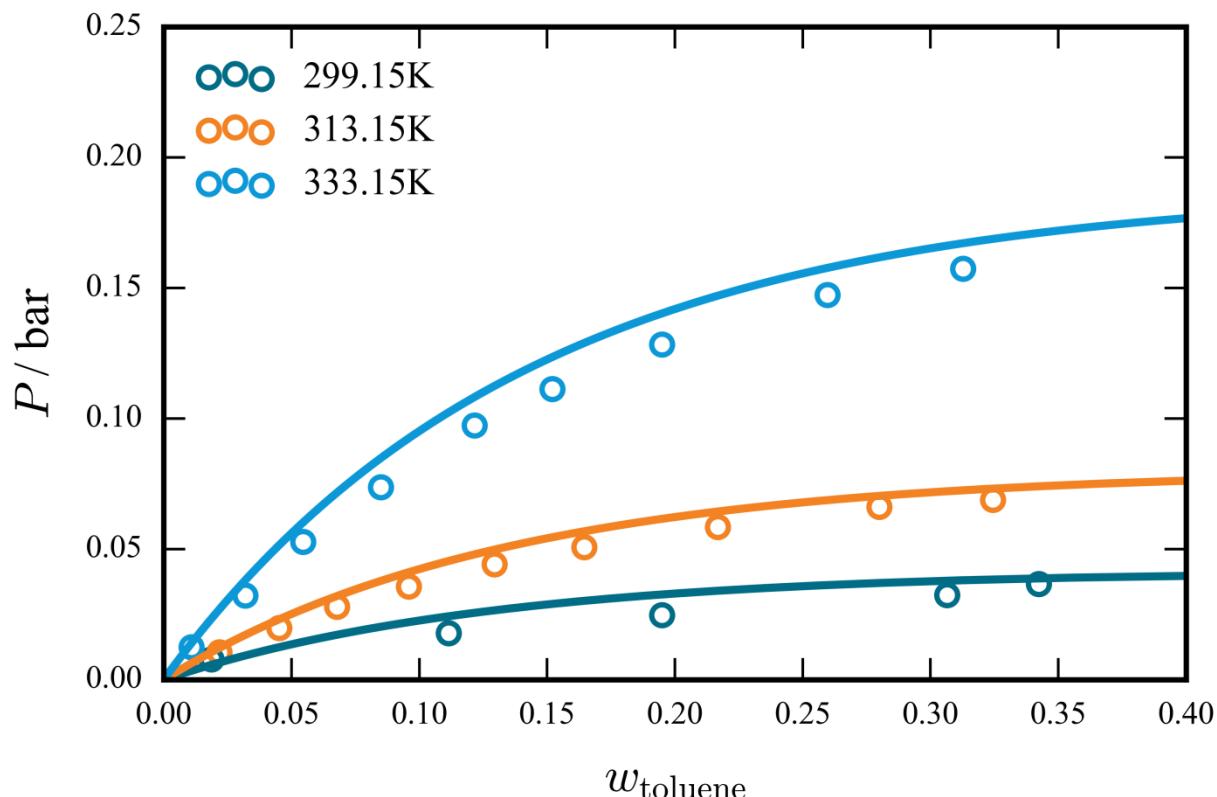
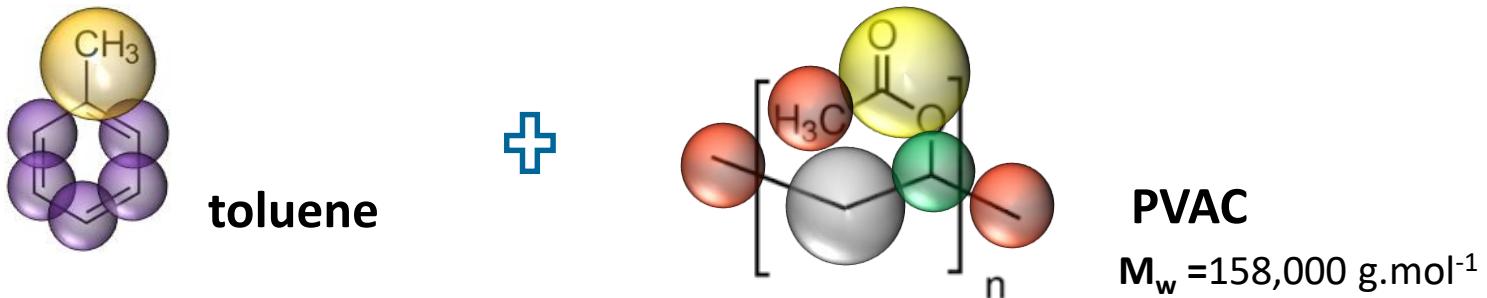


# gSAFT for polymer systems

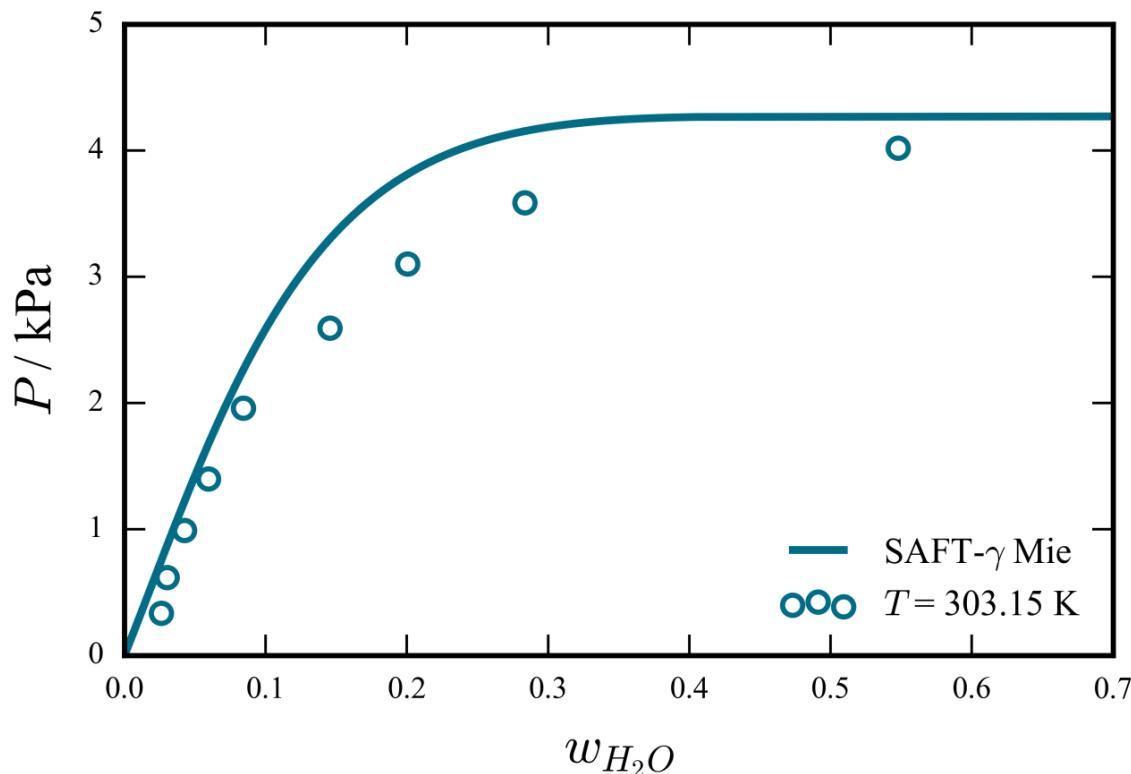
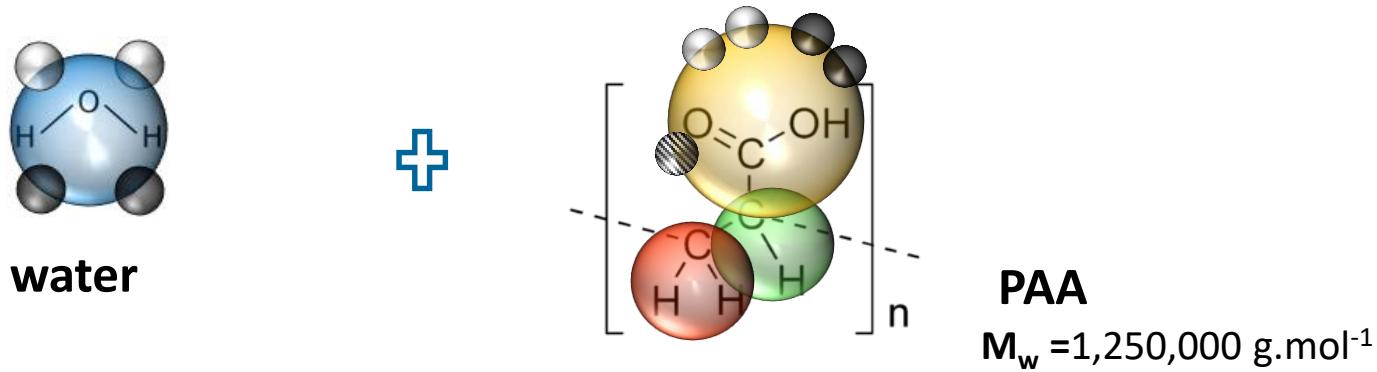
## VLE predictions - II

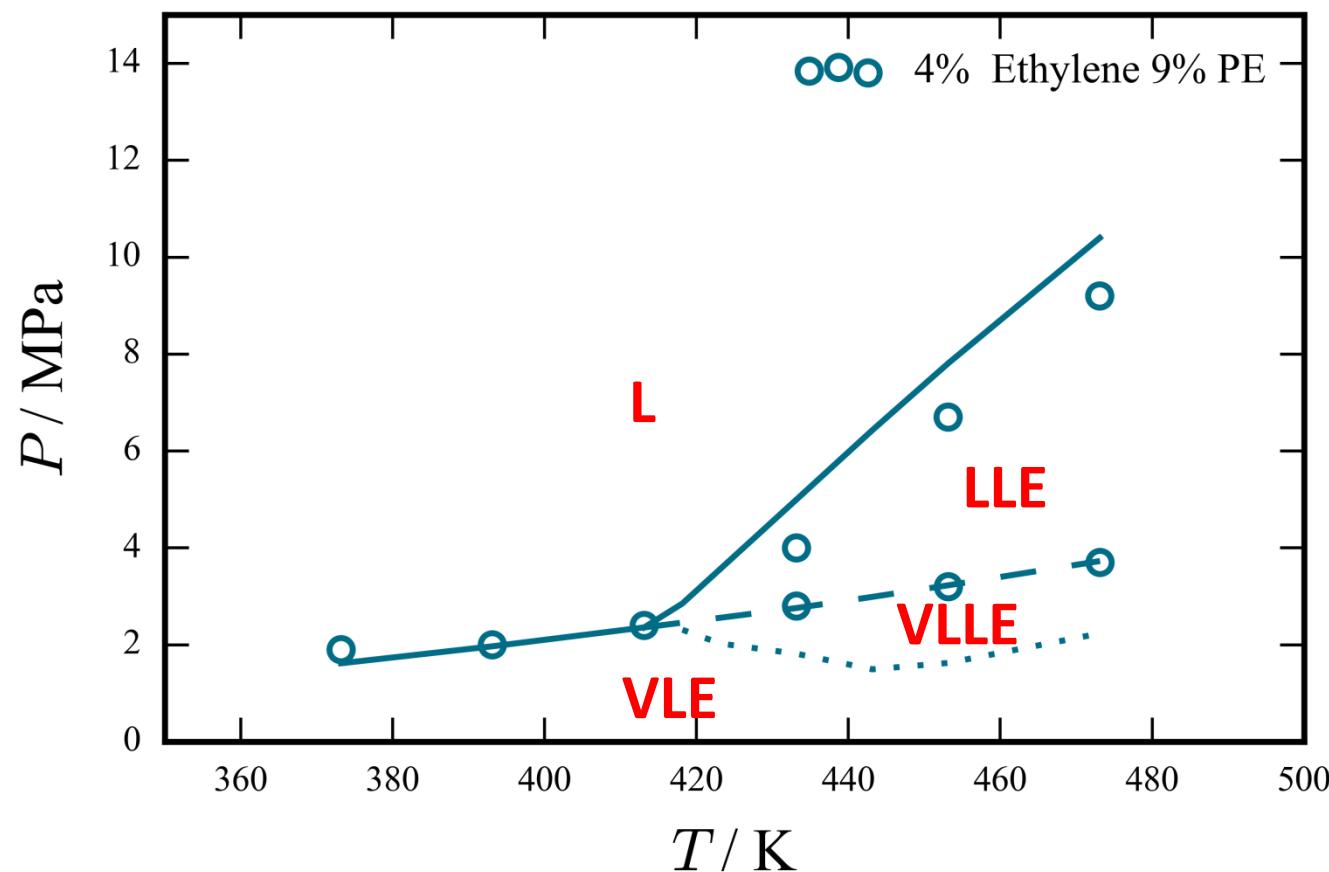
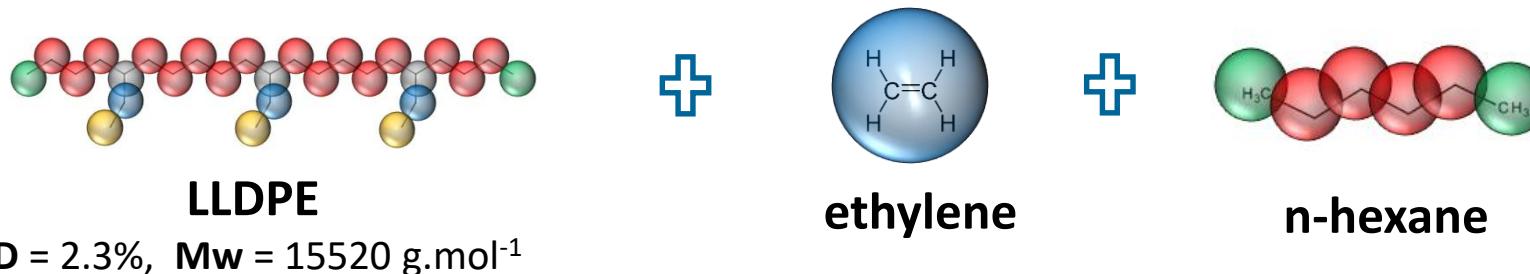


# gSAFT for polymer systems VLE predictions - III



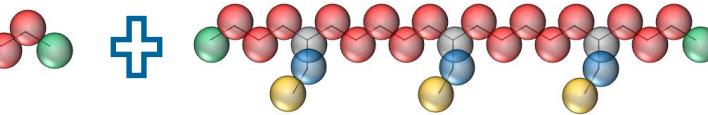
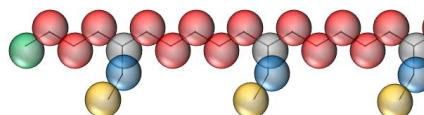
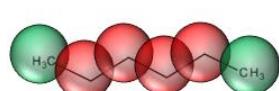
# gSAFT for polymer systems VLE predictions - IV



Expt data: X. Chen et al., *Fluid Phase Equilibria*, 215 (2004) 105

# gSAFT for polymer systems

## Polymer blends



n-hexane

LLDPE

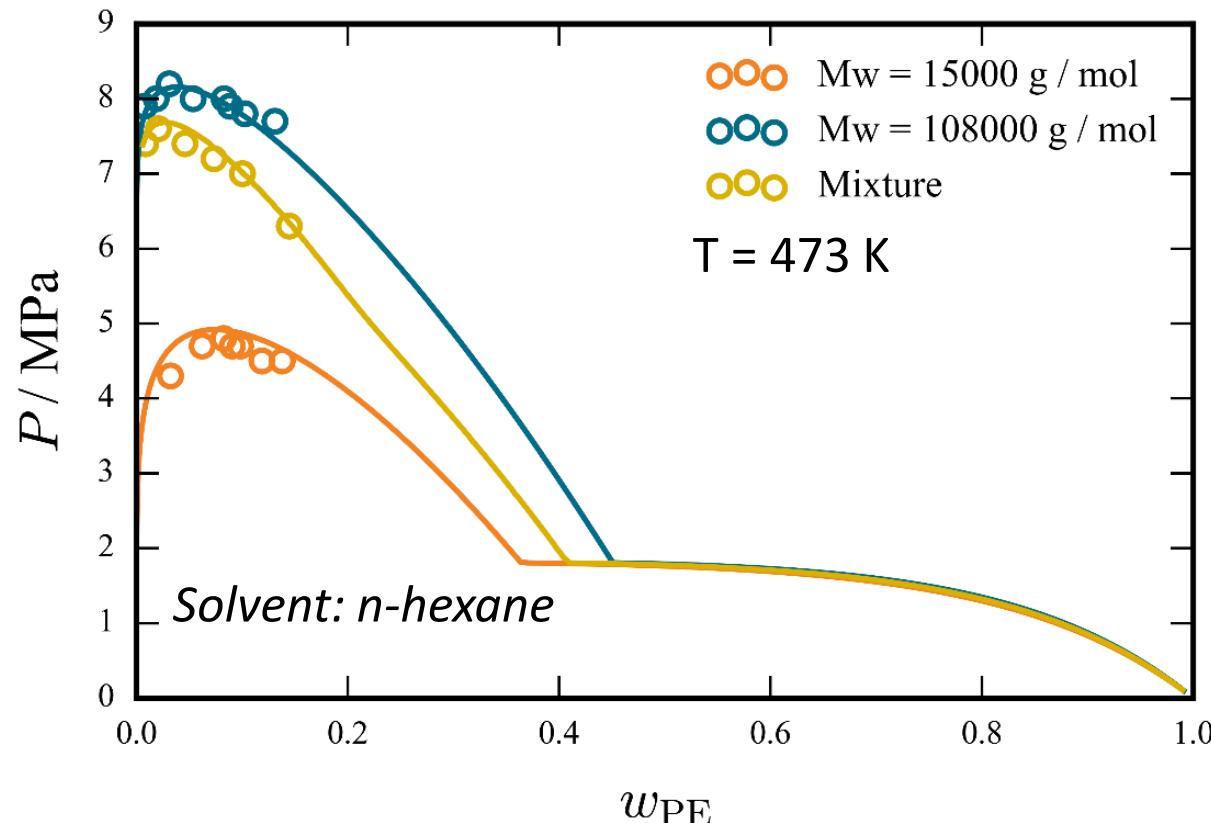
BD = 2.3%

$M_w = 15,520 \text{ g} \cdot \text{mol}^{-1}$

LLDPE

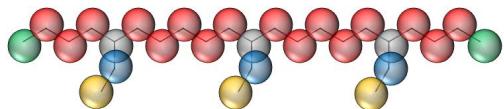
BD = 1.9%

$M_w = 108,000 \text{ g} \cdot \text{mol}^{-1}$

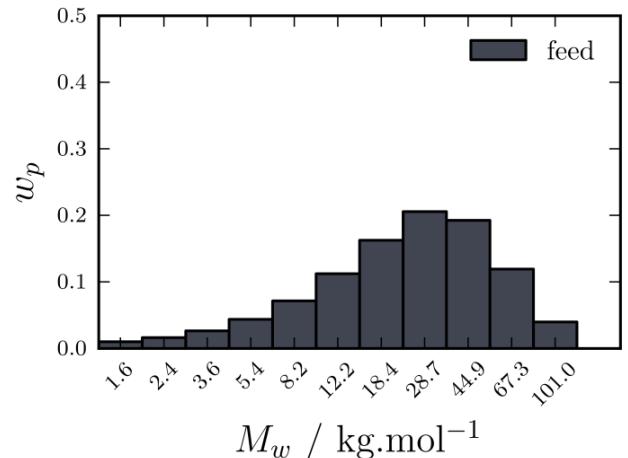
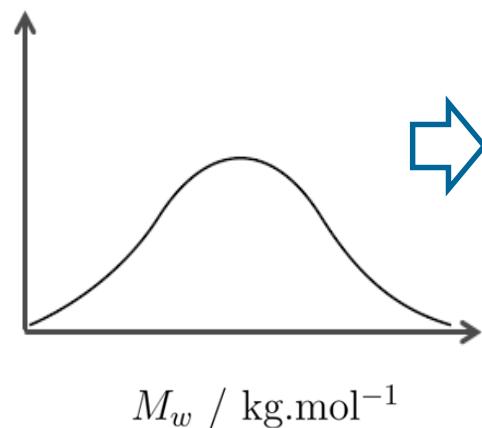


# gSAFT for polymer systems

## Handling of polydispersity



Continuous distribution      Discretised distribution



### gSAFT configuration file

```
<gsaft>
<databank name = "GC_Mie_databank.dtb"/>
<compounds>
  <compound name = "ethylene"/>
  <compound name = "LLDPE-1600">
    <group name = "CH3" multiplicity="2"/>
    <group name = "CH2_bb" multiplicity="93"/>
    <group name = "CH_bb" multiplicity="4"/>
    <group name = "CH3_br" multiplicity="4"/>
    <group name = "CH2_br" multiplicity="12"/>
  </compound>
  <compound name = "LLDPE-2400">
    <group name = "CH3" multiplicity="2"/>
    <group name = "CH2_bb" multiplicity="135"/>
    <group name = "CH_bb" multiplicity="7"/>
    <group name = "CH3_br" multiplicity="7"/>
    <group name = "CH2_br" multiplicity="21"/>
  </compound>
  <compound name = "LLDPE-3600">
    <group name = "CH3" multiplicity="2"/>
    <group name = "CH2_bb" multiplicity="199"/>
    <group name = "CH_bb" multiplicity="12"/>
    <group name = "CH3_br" multiplicity="12"/>
    <group name = "CH2_br" multiplicity="35"/>
  </compound>
  <compound name = "LLDPE-5400">
    <group name = "CH3" multiplicity="2"/>
    <group name = "CH2_bb" multiplicity="437"/>
    <group name = "CH_bb" multiplicity="29"/>
    <group name = "CH3_br" multiplicity="29"/>
    <group name = "CH2_br" multiplicity="87"/>
  </compound>
</compounds>
.....
</gsaft>
```

# gSAFT for polymer systems

## gSAFT configuration file



gPROMS ProcessBuilder 1.2.0 (dev)

File Edit View Entity Activities Tools Window Help

28 library projects hidden

- demo\_LLDPE
  - Variable Types
  - Stream Types
  - Connection Types
- Models
- Tasks
- Processes
- Experiments
  - Experiment Designs
  - Parameter Estimations
  - Optimisations
  - Global System Analysis
  - Saved Variable Sets
- Miscellaneous Files
  - gsaft\_config.xml

gSAFT configuration file

LLDPE\_hexane\_ethylene (demo\_LLDPE)

```
graph LR; Feed((Feed)) --> Sep[Separator_3_phase]; Sep --> Vapour((vapour)); Sep --> liquidI((liquidI)); Sep --> LiquidII((LiquidII));
```

gML Flow Transportation

gML Heat Exchange

gML Mass Balance

gML Reaction

gML Separations - Adsorption

Projects

Interface | Interface language | Topology | gPROMS language | Properties

Palette

146.3 / 354.3 MB

# Using gSAFT in gPROMS ProcessBuilder

gPROMS ProcessBuilder 1.2.0 (dev)

File Edit View Entity Activities Tools Window Help

LLDPE\_hexane\_ethylene (demo\_LLDPE)

Feed (Source\_material\_gML)

Thermal specification: Temperature

Component specification: Component fractions and overall flowrate

Composition specification: Mass

Flowrate specification: Mass

Main

Dynamics

Initial guesses

Reporting

Numerics

Material: gSAFT::gsaft\_config.xml -mass

Pressure: 2 MPa

Temperature: 453.15 K

Mass fraction: Uniform for entire array

Components	Mass fraction
ethylene	0.95
LLDPE-1600	4.75153E-5
LLDPE-2400	9.65322E-5
LLDPE-3600	0.000198938
LLDPE-5400	0.000420322
LLDPE-8200	0.0021138
LLDPE-12200	0.004917335
LLDPE-18400	0.010498631
LLDPE-28700	0.016463112
LLDPE-44900	0.012336147
LLDPE-67300	0.0019372
LLDPE-101000	1.26831E-5

kg/kg

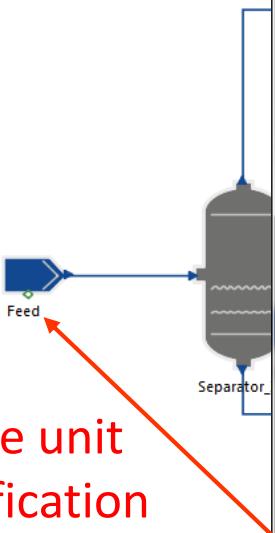
Mass flowrate: 10.0 kg/s

OK Cancel Reset all Help

Projects

Interface Interface language Topology gPROMS language

Source unit specification



The screenshot shows the gPROMS ProcessBuilder interface. A process diagram on the left features a 'Feed' source connected to a 'Separator' unit. A red arrow points from the text 'Source unit specification' to the 'Feed' source in the diagram. On the right, a configuration dialog box is open for the 'Feed' source. It contains tabs for Main, Dynamics, Initial guesses, Reporting, and Numerics. Under the Main tab, various specifications are set: Thermal specification (Temperature), Component specification (Component fractions and overall flowrate), Composition specification (Mass), and Flowrate specification (Mass). A detailed table lists component mass fractions for a gSAFT model. The table includes columns for Components and Mass fraction, with values for ethylene, LLDPE-1600, LLDPE-2400, LLDPE-3600, LLDPE-5400, LLDPE-8200, LLDPE-12200, LLDPE-18400, LLDPE-28700, LLDPE-44900, LLDPE-67300, and LLDPE-101000.

# Using gSAFT in gPROMS ProcessBuilder

The screenshot shows the gPROMS ProcessBuilder interface version 1.2.0 (dev). The main window displays the 'Feed (Source\_material\_gML)' dialog. This dialog is used to specify feed conditions for a process stream. It includes sections for Thermal specification (Temperature), Component specification (Component fractions and overall flowrate), Composition specification (Mass), and Flowrate specification (Mass).

A red box highlights the 'Material' section, which contains a dropdown menu set to 'gSAFT::gsaft\_config.xml -mass'. A red arrow points from the 'gsaft\_config.xml' file in the project tree on the left to this dropdown.

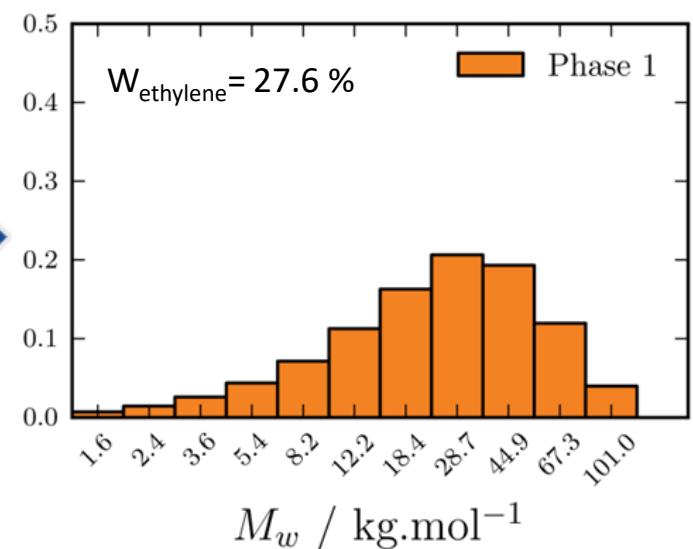
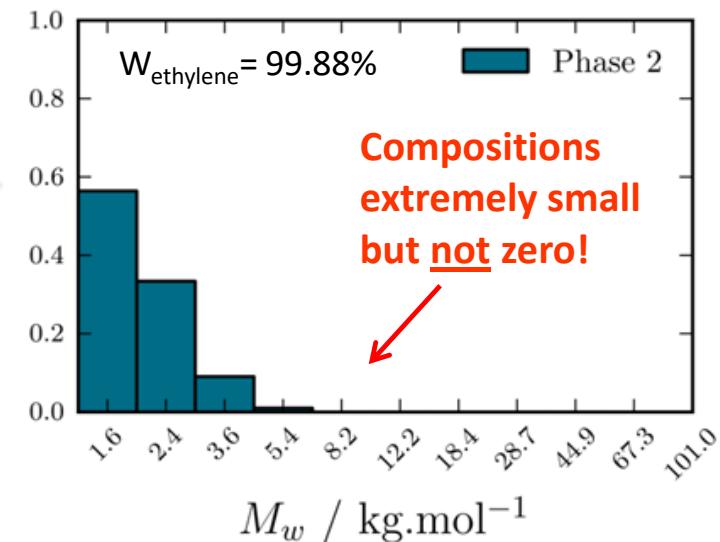
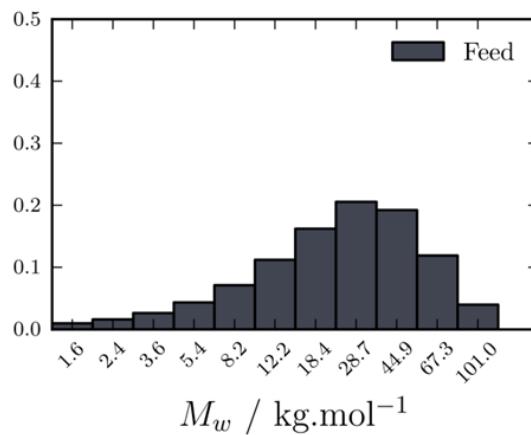
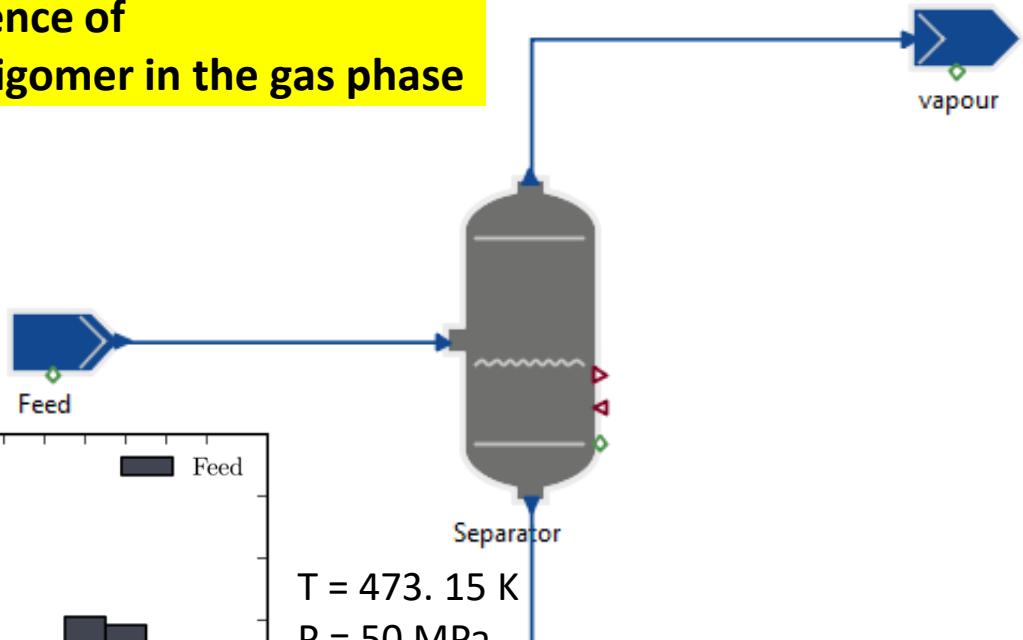
The 'Material' section also includes checkboxes for Pressure (set to 2 MPa) and Temperature (set to 453.15 K). There are two radio button options for Mass fraction: 'Uniform for entire array' (selected) and 'Per element'.

Below these settings is a table titled 'Components' showing mass fractions for various components:

Component	Mass Fraction
ethylene	0.95
LLDPE-1600	4.75153E-5
LLDPE-2400	9.65322E-5
LLDPE-3600	0.000198938
LLDPE-5400	0.000420322
LLDPE-8200	0.0021138
LLDPE-12200	0.004917335
LLDPE-18400	0.010498631
LLDPE-28700	0.016463112
LLDPE-44900	0.012336147
LLDPE-67300	0.0019372
LLDPE-101000	1.26831E-5

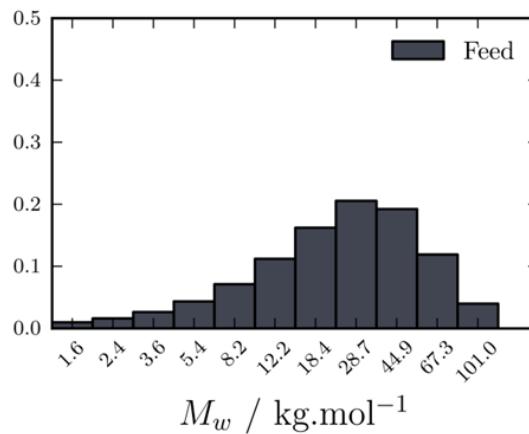
At the bottom of the dialog are buttons for 'OK', 'Cancel', 'Reset all', and 'Help'. The project tree on the left shows a folder named 'demo\_LLDPE' containing various types and models, with 'gsaft\_config.xml' highlighted by a red box and an arrow pointing to it from the dialog.

- Robust numerics in gSAFT phase equilibrium calculations
- Allow presence of polymer/oligomer in the gas phase

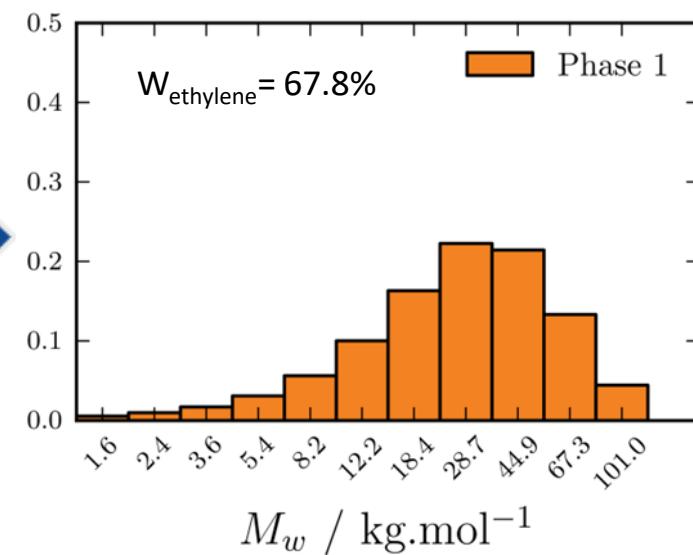
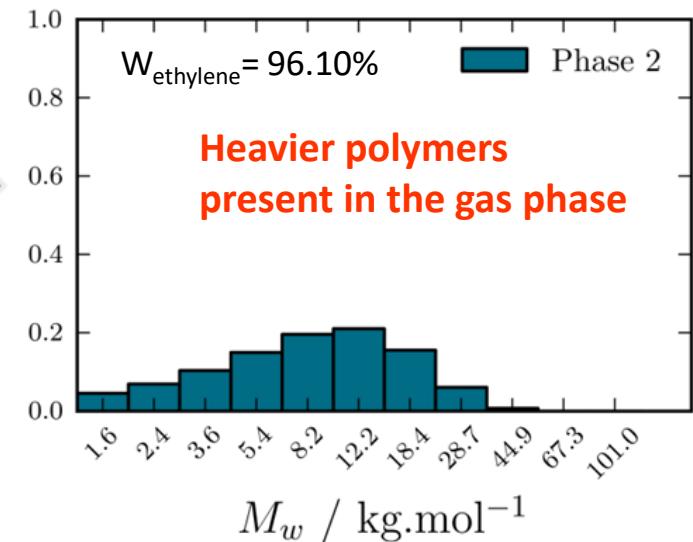
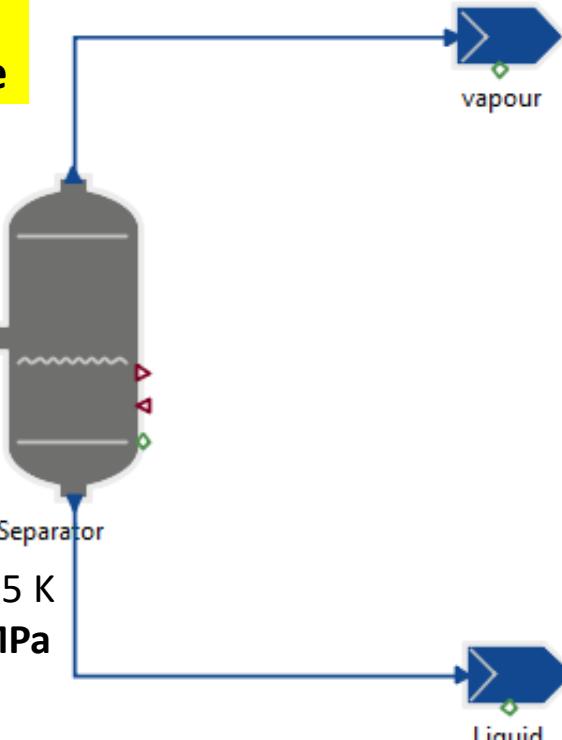


- Robust numerics in gSAFT phase equilibrium calculations
- Account for presence of polymer/oligomer in the gas phase

Increasing pressure...



T = 473.15 K  
P = 100 MPa



# gSAFT for reactive systems



## Highlights

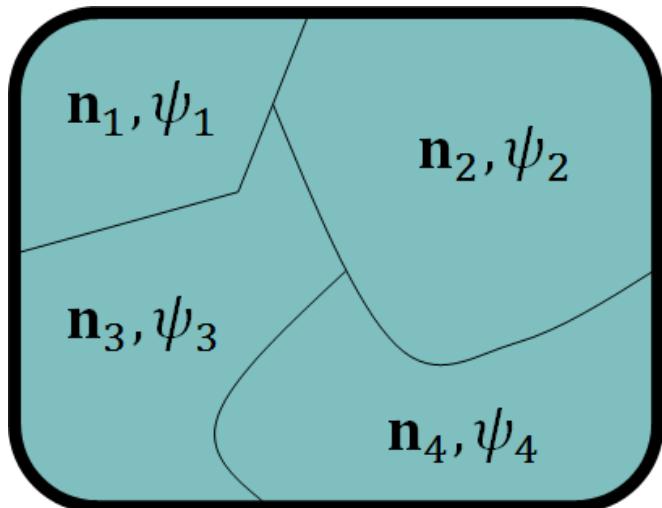
- Robust algorithm – can handle species present in extremely small amounts
- General for any type of system (charged or neutral)
- Handles multiple phases

# Fundamental equations - I

Equilibrium: minimise free energy of system

$$G = \sum_{k=1}^{NP} \sum_{i=1}^{NC} n_{ik} (\mu_i^{[k]} + F \psi_k q_i)$$

Multiphase system @ uniform  $T, P$



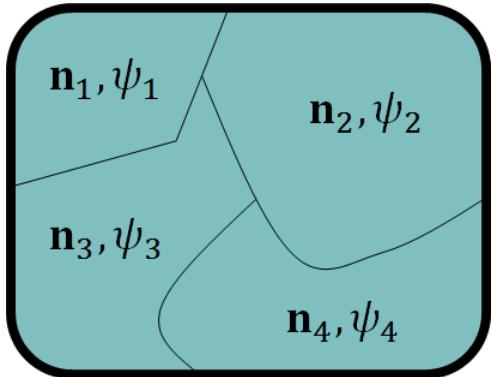
with respect to:

- $n_{ik}$ = amount of species  $i$  in phase  $k$
- $\psi_k$ = electrical potential of phase  $k$
- $\xi_j$ = extent of reaction  $j$

subject to:

$$\sum_{k=1}^{NP} n_{ik} = n_i^o + \sum_{j=1}^{NR} v_{ij} \xi_j, \quad \forall i = 1, \dots, NC$$

## Fundamental equations - II



$$\min_{n_{ik}, \psi_k, \xi_j} G = \sum_{k=1}^{NP} \sum_{i=1}^{NC} n_{ik} (\mu_i^{[k]} + F \psi_k q_i)$$

subject to:

$$\sum_{k=1}^{NP} n_{ik} = n_i^o + \sum_{j=1}^{NR} v_{ij} \xi_j, \forall i = 1, \dots, NC$$

**$NC \times NP + NR + NP - 1$**   
**equations in**  
 $n_{ik}, \xi_j, (\psi_k - \psi_{NP})$

**"Reaction equilibrium"**

$$\sum_{i=1}^{NC} v_{ij} \mu_i^{[NP]} = 0, \quad \forall j = 1, \dots, NR$$

**"Phase equilibrium"**

$$\left. \begin{aligned} \mu_i^{[k]}(T, P, \mathbf{n}_k) - \mu_i^{[NP]}(T, P, \mathbf{n}_k) + F(\psi_k - \psi_{NP})q_i &= 0 \quad \forall i \\ \sum_{i=1}^{NC} q_i n_{ik} &= 0 \end{aligned} \right\} k = 1, \dots, NP - 1$$

**"Electroneutrality"**

## ■ TPFlash equilibrium method:

**EQUATION**

```
...  
FlashResults = physprops.TPflash(T, P, n0) ;  
...
```



Initial composition of the system  
(reaction will not necessarily conserve the initial molar amounts)

**Usage identical to standard, non-reactive TPflash calculation**

→ Handling of simultaneous phase/reaction equilibrium  
is transparent to the model developer

## ■ Output vector FlashResults contains

- Mole fractions of each compounds in each phase
- Enthalpy of each phase
- Amount of each phase
- Volume of each phase



*identical to standard TPFlash method*

# gSAFT for reactive systems

## gSAFT configuration file

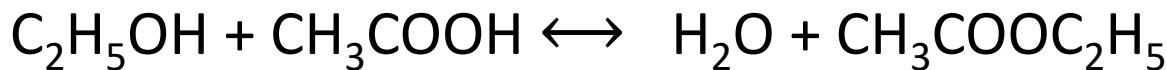
The screenshot shows the gPROMS ProcessBuilder 1.1.0 software interface. On the left, the project tree shows a folder named 'gSAFT\_demo' containing various types like Variable Types, Stream Types, and Models. A red box highlights the 'Miscellaneous Files' folder, which contains a file named 'gsaft\_config.xml'. A red arrow points from the text 'gSAFT configuration file' to this folder. The main workspace displays the XML code for the gSAFT configuration file. An orange box highlights the reaction section, specifically the 'esterification' reaction. To the right, a palette window is open, showing various icons categorized under 'gML Basics', 'gML Connectivity', 'gML Control', 'gML Flow Transportation', 'gML Heat Exchange', and 'gML Signal'. A red box highlights the 'Reaction stoichiometry' section of the XML code.

```
<gsaft>
    <databank name = "GC_Mie_databank.dtb"/>
    <compounds>
        <compound name = "ethanol"/>
        <compound name = "acetic_acid"/>
        <compound name = "water"/>
        <compound name = "ethyl_acetate"/>
        <compound name = "acetone"/>
        .....
    </compounds>
    <reactions>
        <reaction name="esterification">
            <compound ref="acetic_acid" stoich="-1"/>
            <compound ref="ethanol" stoich="-1"/>
            <compound ref="water" stoich="1"/>
            <compound ref="ethyl_acetate" stoich="1"/>
        </reaction>
        .....
    </reactions>
</gsaft>
```

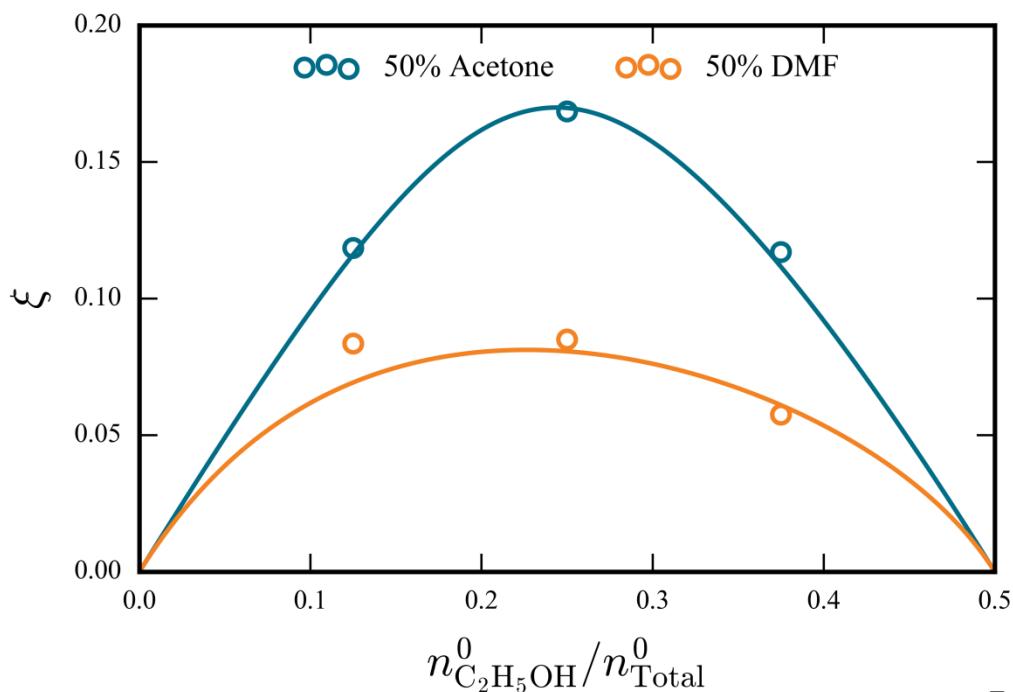
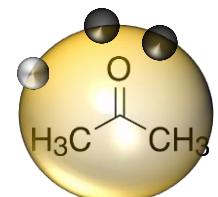
gSAFT configuration file

Reaction stoichiometry

## Example #1: ethanol/acetic acid esterification



Solvent:

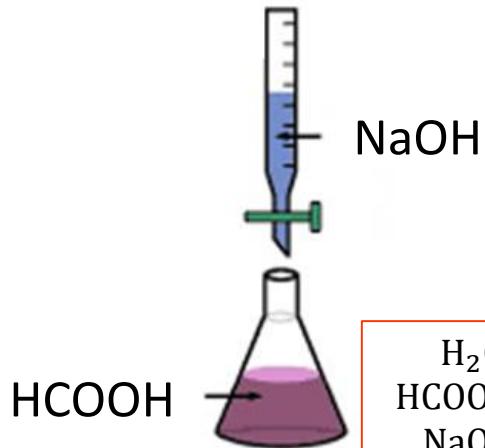


→ Accurate predictions for all input compositions

→ Predicts effect of solvent on reaction extent

Expt data: Riechert et al., *AIChE J.*, **61**, 3000-3011 (2015)

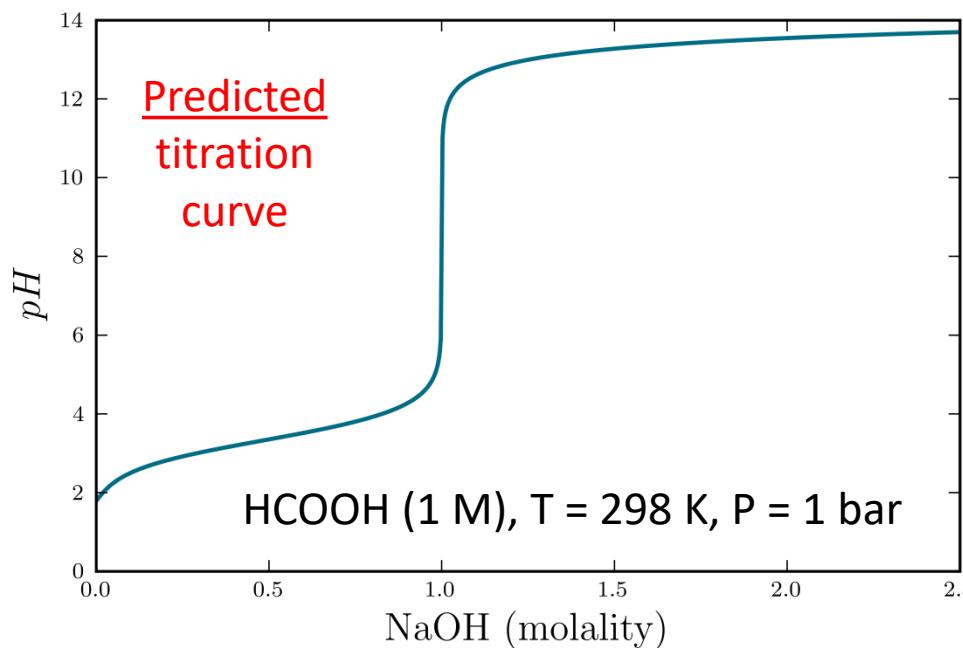
## Example #2: formic acid titration with sodium hydroxide

**EQUATION**

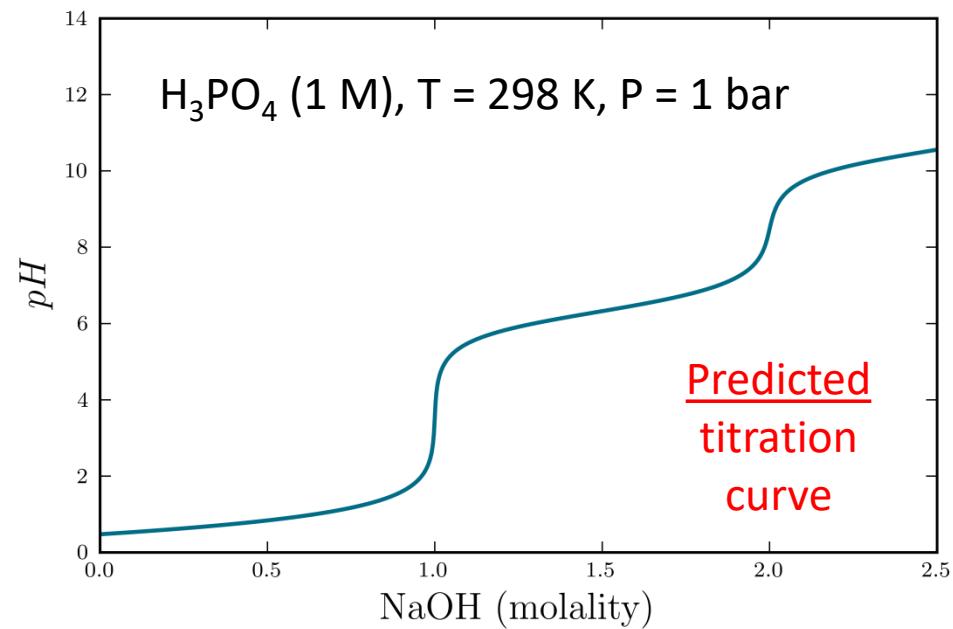
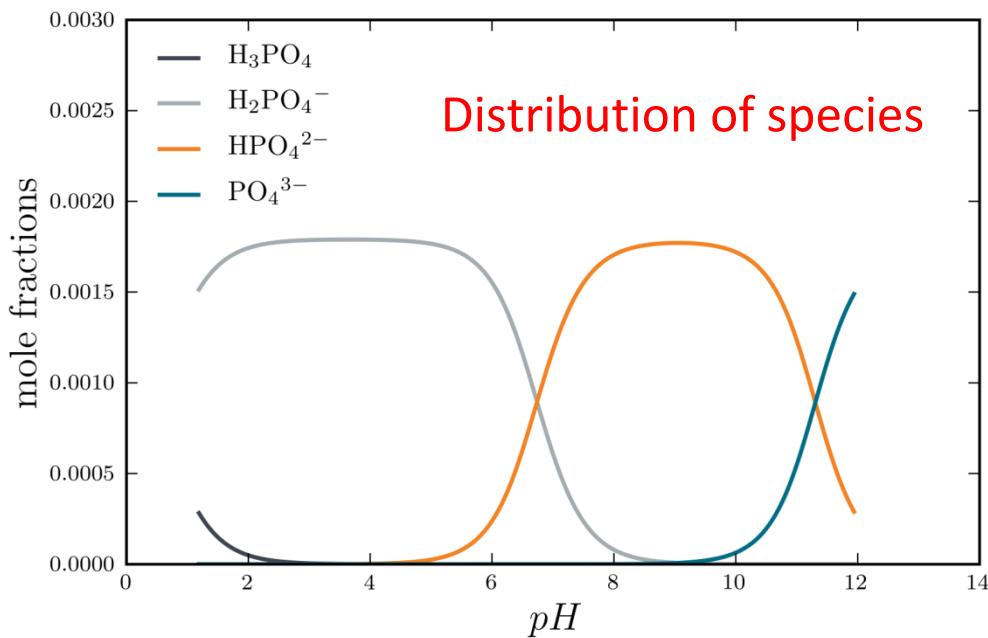
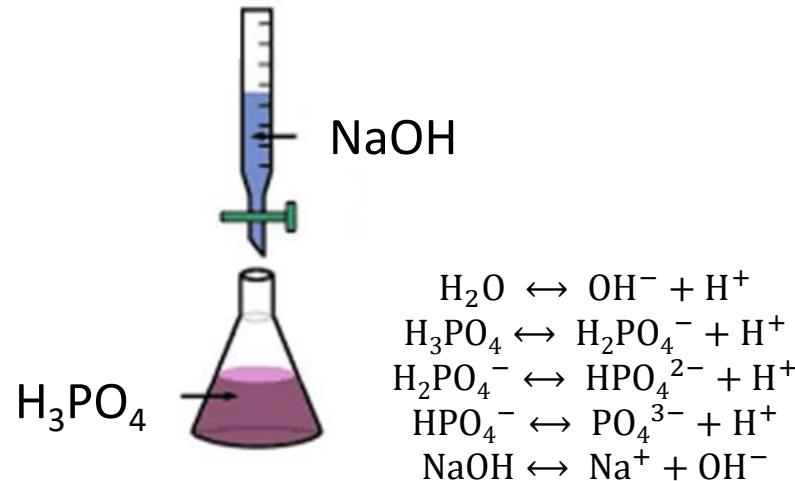
```
pH = physprops.LiquidpH(T, P, n);
```

...

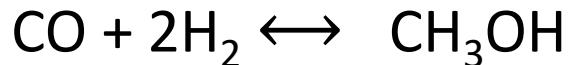
Equilibrium composition of the phase of interest  
(as determined by the TPFlash method)



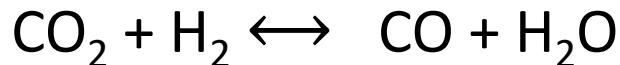
## Example #3: phosphoric acid titration with sodium hydroxide



## Example #4: Methanol synthesis in methane solvent



*Solvent: CH<sub>4</sub>*



## ■ Configuration file

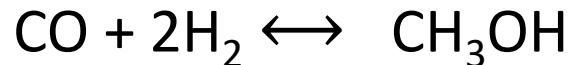
```
<gsaft>
  <databank name = "GC_Mie_databank.dtb"/>
  <compounds>
    <compound name = "methane"/>
    <compound name = "hydrogen"/>
    <compound name = "methanol"/>
    <compound name = "carbon_monoxide"/>
    <compound name = "carbon_dioxide"/>
    <compound name = "water"/>
  </compounds>
  <reactions>
    <reaction name="reaction1">
      <compound ref="carbon_monoxide" stoich="-1"/>
      <compound ref="hydrogen" stoich="-2"/>
      <compound ref="methanol" stoich="1"/>
    </reaction>
    <reaction name="reaction2">
      <compound ref="carbon_dioxide" stoich="-1"/>
      <compound ref="hydrogen" stoich="-1"/>
      <compound ref="carbon_monoxide" stoich="1"/>
      <compound ref="water" stoich="1"/>
    </reaction>
  </reactions>
</gsaft>
```

- Same usage as single phase case



- All complexity handled internally

## Example #4: Methanol synthesis in methane solvent



*Solvent: CH<sub>4</sub>*



T = 473.15 K, P = 300 bar

**Initial state (moles):**

$$n_{\text{CO}}^0 = 15 \quad n_{\text{H}_2}^0 = 74 \quad n_{\text{CO}_2}^0 = 8 \quad n_{\text{CH}_3\text{OH}}^0 = 0 \quad n_{\text{H}_2\text{O}}^0 = 0 \quad n_{\text{CH}_4}^0 = 3$$

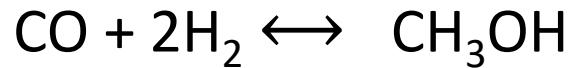
**Equilibrium**

Composition [mole fractions]

	CO	CO <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub> O	CH <sub>3</sub> OH	CH <sub>4</sub>	Total moles
<b>Phase I (Liquid)</b>	4.47E-06	3.02E-04	0.057833	0.261706	0.665527	0.01462678	28.38529
<b>Phase II (Vapour)</b>	5.78E-05	8.88E-04	0.653611	0.044693	0.208591	0.09215885	25.64612

Two phases (VLE) present at equilibrium

## Example #4: Methanol synthesis in mixed solvent



*Solvent: CH<sub>4</sub>, nC<sub>18</sub>*



*Addition of n-octadecane as solvent*

*Initial state (moles):*

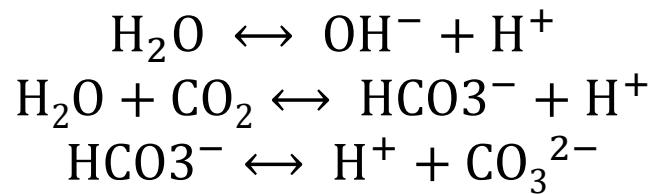
$$n_{\text{CO}}^0 = 15 \quad n_{\text{H}_2}^0 = 74 \quad n_{\text{CO}_2}^0 = 8 \quad n_{\text{CH}_3\text{OH}}^0 = 0 \quad n_{\text{H}_2\text{O}}^0 = 30 \quad n_{\text{CH}_4}^0 = 3 \quad n_{\text{C18}}^0 = 10$$

*TPFlash calculation*

Three phases (VLLE) are formed

Composition [mole fractions]

	CO	CO <sub>2</sub>	H <sub>2</sub>	H <sub>2</sub> O	CH <sub>3</sub> OH	CH <sub>4</sub>	nC <sub>18</sub>	Total moles
<b>Phase I (Vapour)</b>	0.001163	0.093993	0.561118	0.177271	0.128593	0.036983	0.000876	48.841
<b>Phase II (Liquid)</b>	0.000162	0.037529	0.054879	0.087432	0.146021	0.012634	0.661339	16.167
<b>Phase III (Liquid)</b>	7.346e-6	0.003135	0.003088	0.822784	0.170680	0.000303	9.595e-8	34.472

Example #5: pH of water + CO<sub>2</sub>

**Initial state (moles):** n<sub>H<sub>2</sub>O</sub><sup>0</sup> = 55.5      n<sub>CO<sub>2</sub></sub><sup>0</sup> = 1.6597 (composition close to phase boundary)

**Equilibrium predictions:**

Composition [mole fractions]

T = 308 K, P = 15 MPa

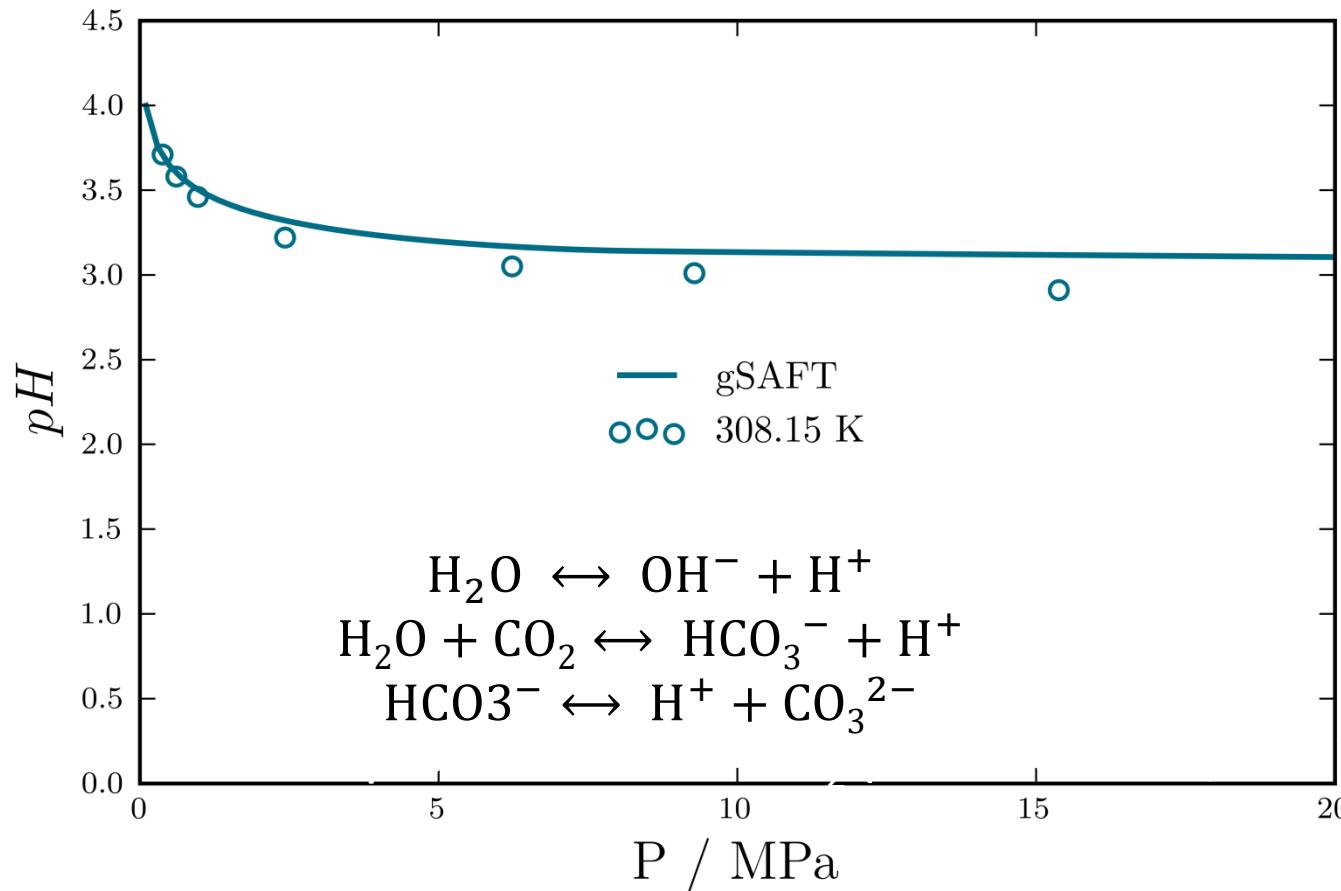
	H <sub>2</sub> O	CO <sub>2</sub>	HCO <sub>3</sub> <sup>-</sup>	CO <sub>3</sub> <sup>2-</sup>	OH <sup>-</sup>	H <sup>+</sup>	Total moles	pH
<b>Phase I (Liquid)</b>	0.973731	0.026239	1.48E-5	6.90E-13	4.28E-13	1.48E-5	57.004	3.099
<b>Phase II (Vapour)</b>	0.004746	0.99525	0	0	0	0	0.16391	N/A

**Experimental value: pH = 2.97**

C. Peng, J. P. Crawshaw, G. Maitland, and J. P. M. Trusler,

"The pH of CO<sub>2</sub>-saturated water at temperature between 308 K and 423 K at pressures up to 15 MPa"

J. Supercritical Fluids, **82**, 129 (2013)

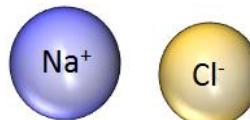
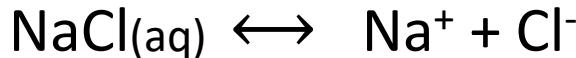
Example #5: pH of water + CO<sub>2</sub>

C. Peng, J. P. Crawshaw, G. Maitland, and J. P. M. Trusler,

*"The pH of CO<sub>2</sub>-saturated water at temperature between 308 K and 423 K at pressures up to 15 MPa"*

*J. Supercritical Fluids*, **82**, 129 (2013)

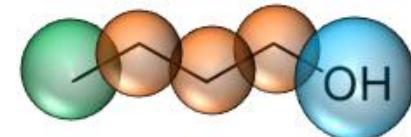
■ Reaction:



water



1-butanol



■ Example calculation:

**Initial amount**

$$n_{\text{H}_2\text{O}}^0 = 0.5$$

$$n_{\text{butanol}}^0 = 0.5$$

$$n_{\text{NaCl}}^0 = 0.05$$

**Equilibrium**

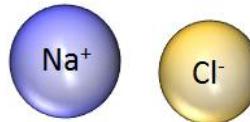
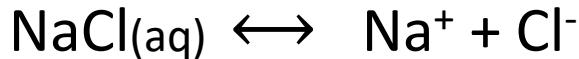
Composition [mole fractions]

T = 298 K, P = 0.1 MPa

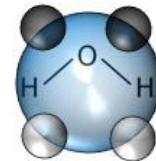
	water	1-butanol	NaCl	Na <sup>+</sup>	Cl <sup>-</sup>	Total moles
<b>Phase I (Liquid)</b>	0.7424	5.438E-4	0	0.1285	0.1285	0.3884
<b>Phase II (Liquid)</b>	0.2974	0.7023	0	1.315E-4	1.315E-4	0.16391

Ions present in  
both liquid phases

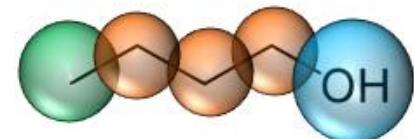
■ Reaction:



water

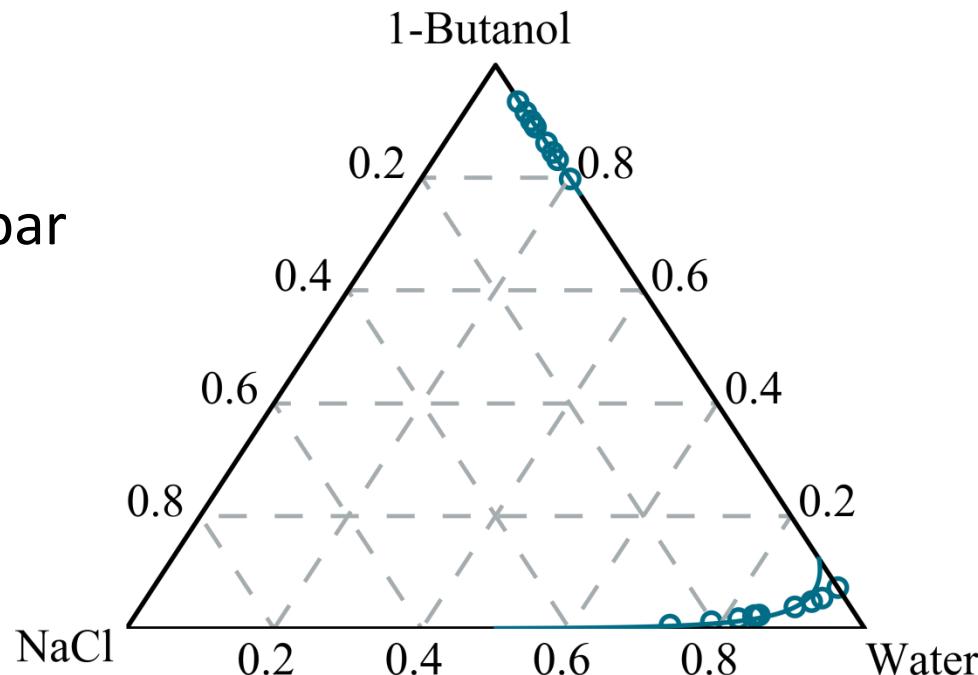


1-butanol



■ Ternary diagram:

$T = 298.15 \text{ K}$ ,  $P = 1 \text{ bar}$



# Handling of solid phases in gSAFT



# Handling of solid phases in gSAFT

## Solubility of non-dissociating solids

### ■ Solid-liquid equilibrium condition

$$\mu_i^s(T, P) = \mu_i^l(T, P, x)$$

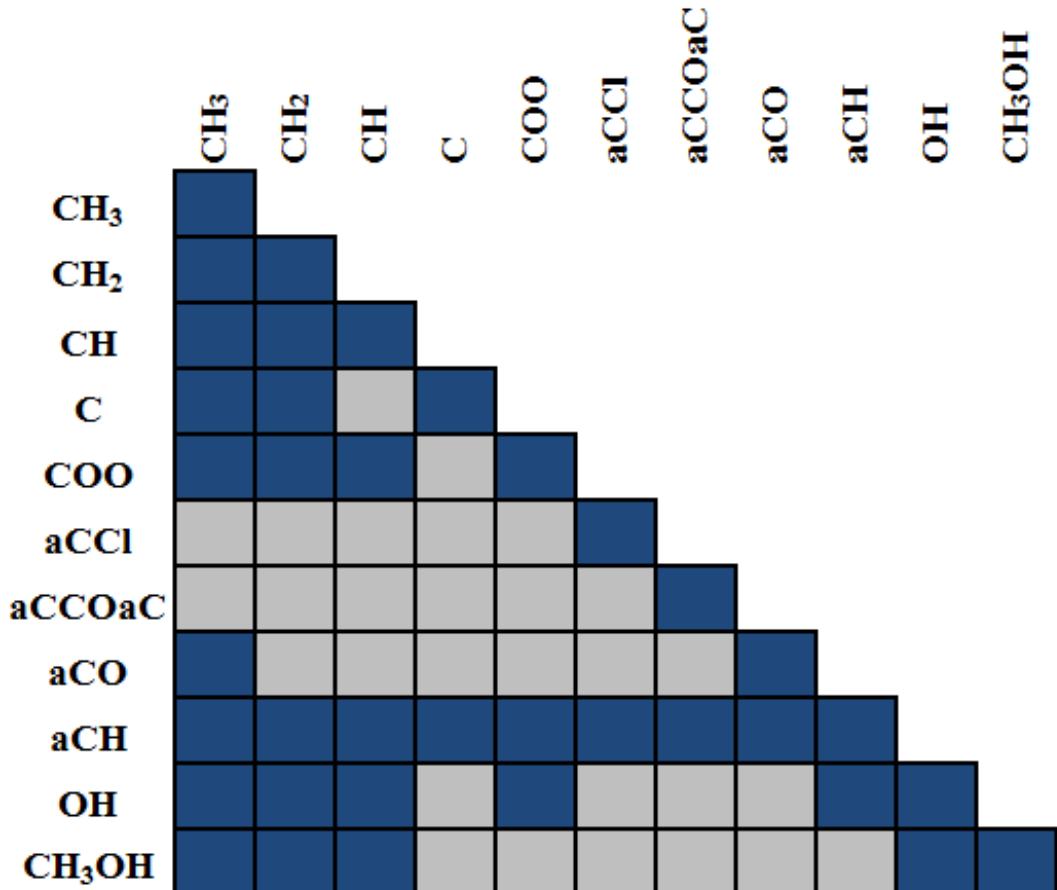
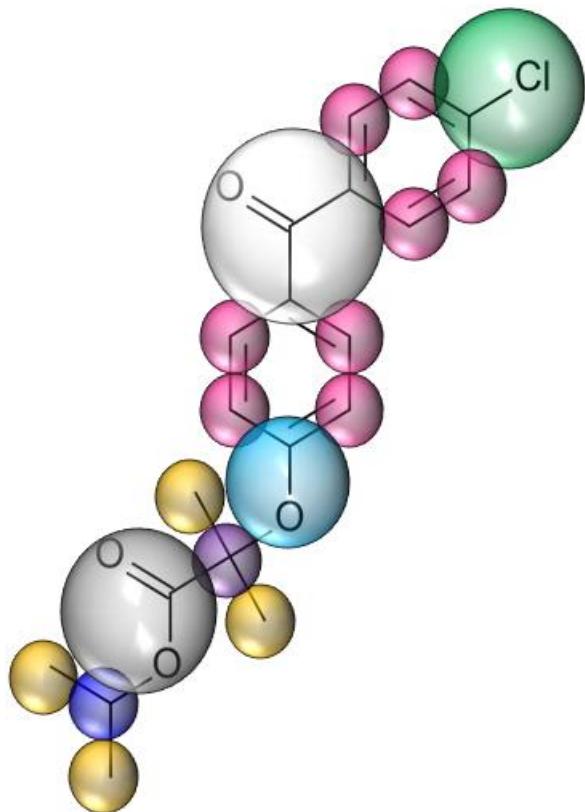


**Amorphous solid**  
*Treat as liquid*  
→ use gSAFT

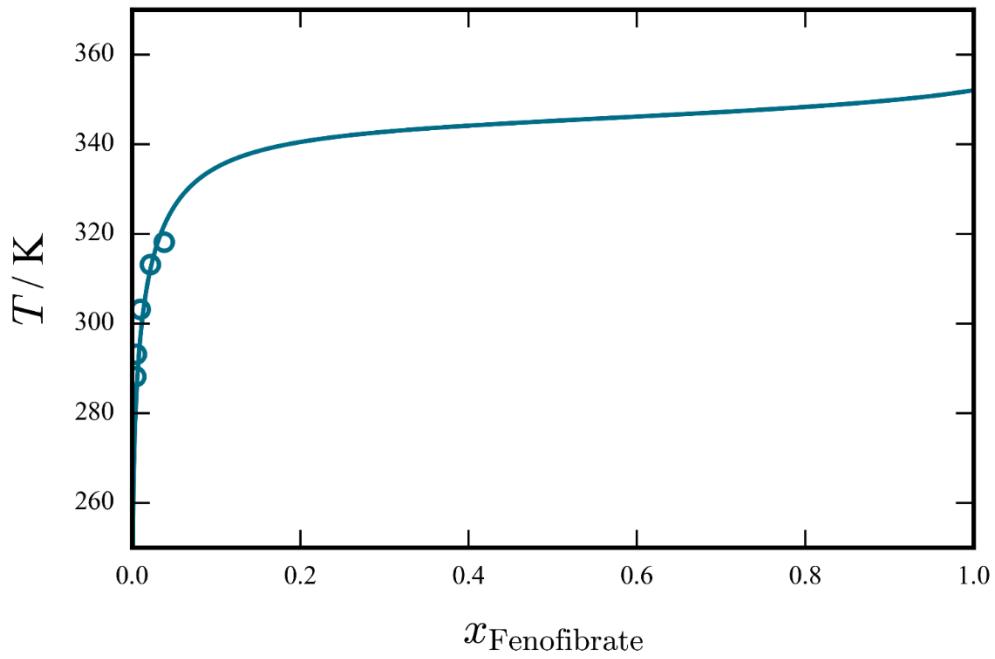
**Crystalline solid**  
*Use appropriate expression for chemical potential (several options)*

**Liquid**  
*Use gSAFT*

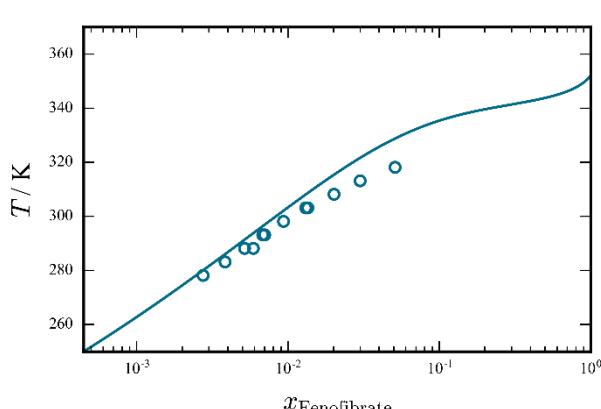
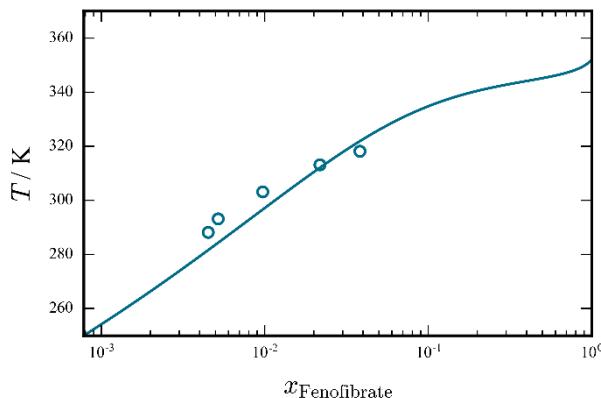
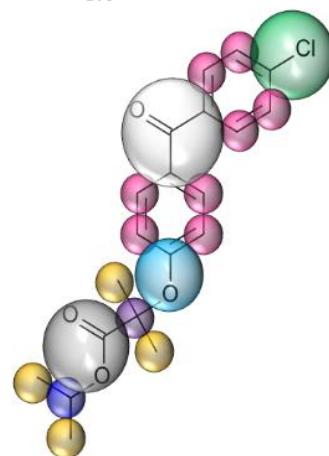
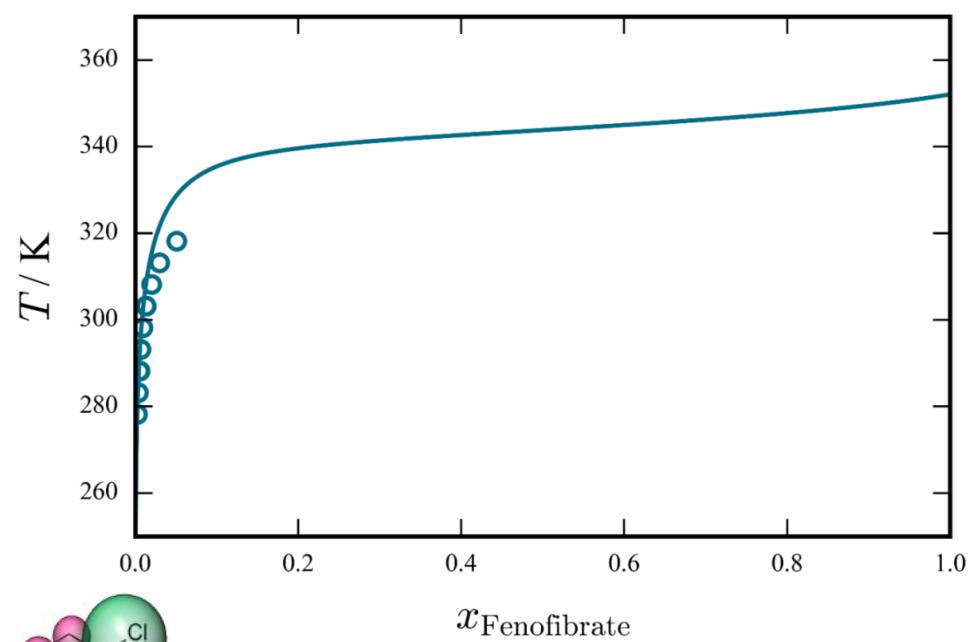
## Example: Fenofibrate in alcohols



## Solubility in methanol



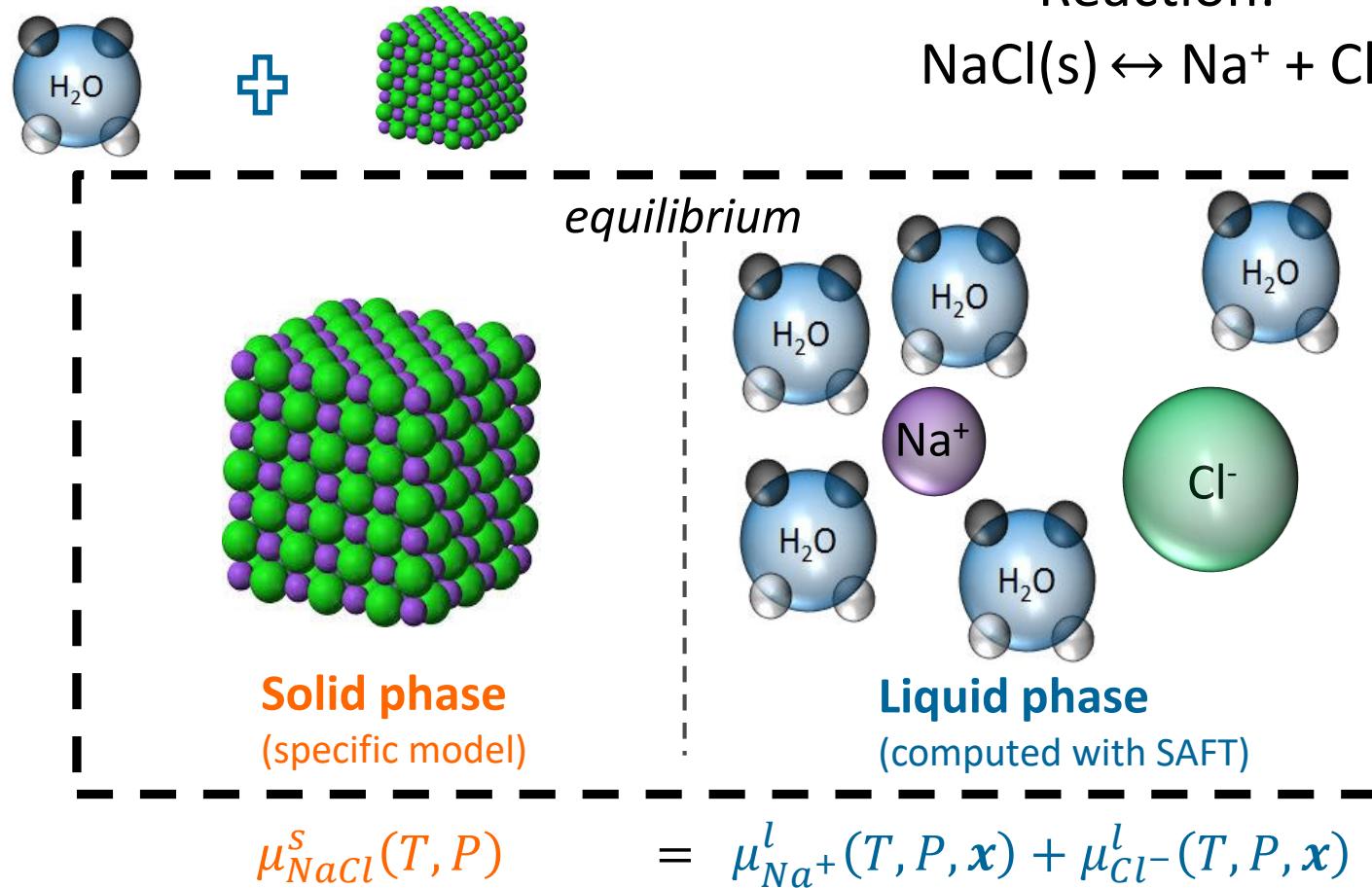
## Solubility in ethanol



# Handling of solid phases in gSAFT

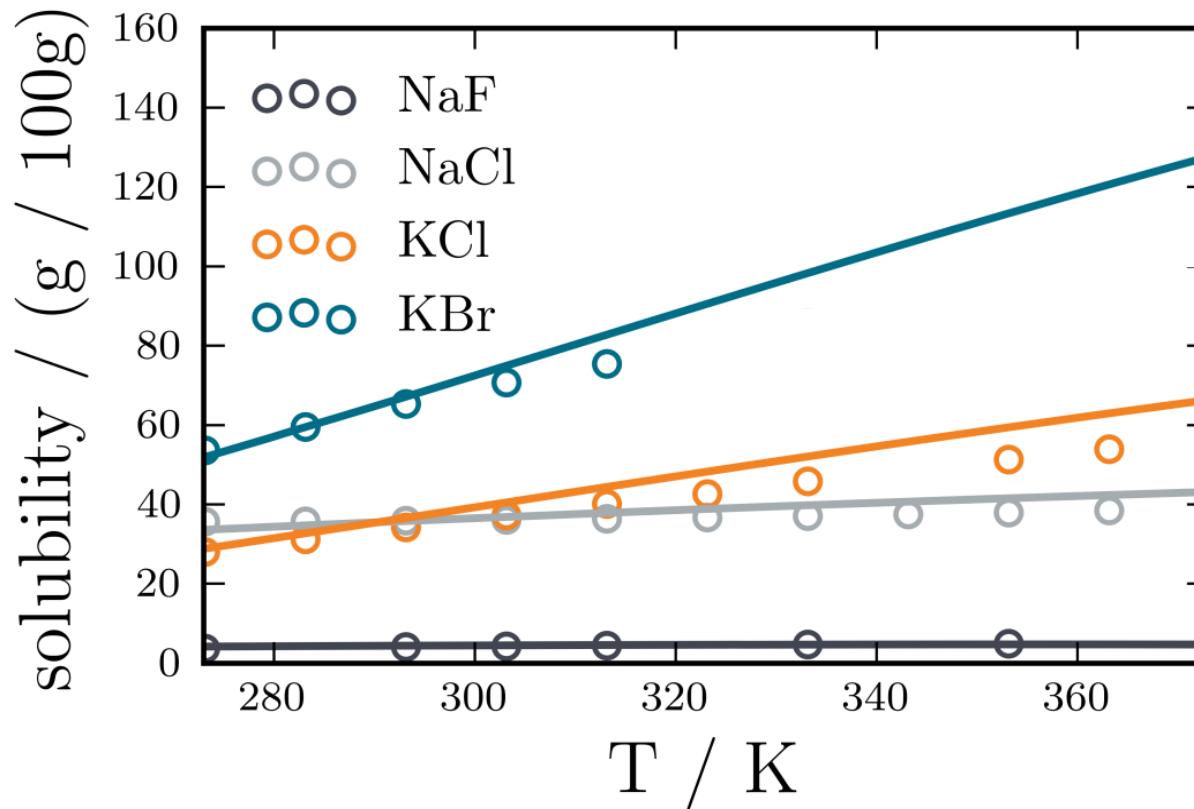
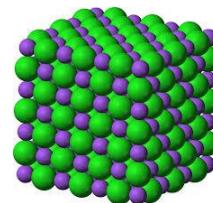
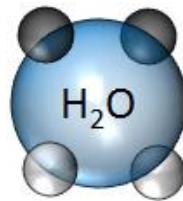
## Solubility of dissociating solids

Example system:



equations depend on dissociation reactions taking place

## Example: alkali halides in water



# Handling of solid phases in gSAFT

## Generalised fluid/solid equilibrium calculations



- gSAFT databank extended with
  - parameters required to characterise crystalline solid chemical potential
  - possible dissociation reactions
- User identifies possible solid phases in gSAFT configuration file
  - single compound each
- Extended TPFlash equilibrium method:

### EQUATION

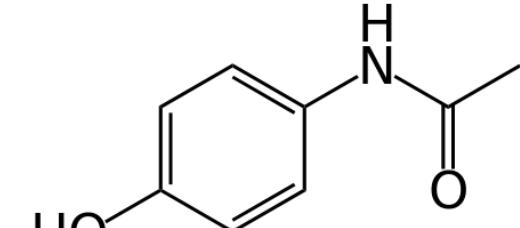
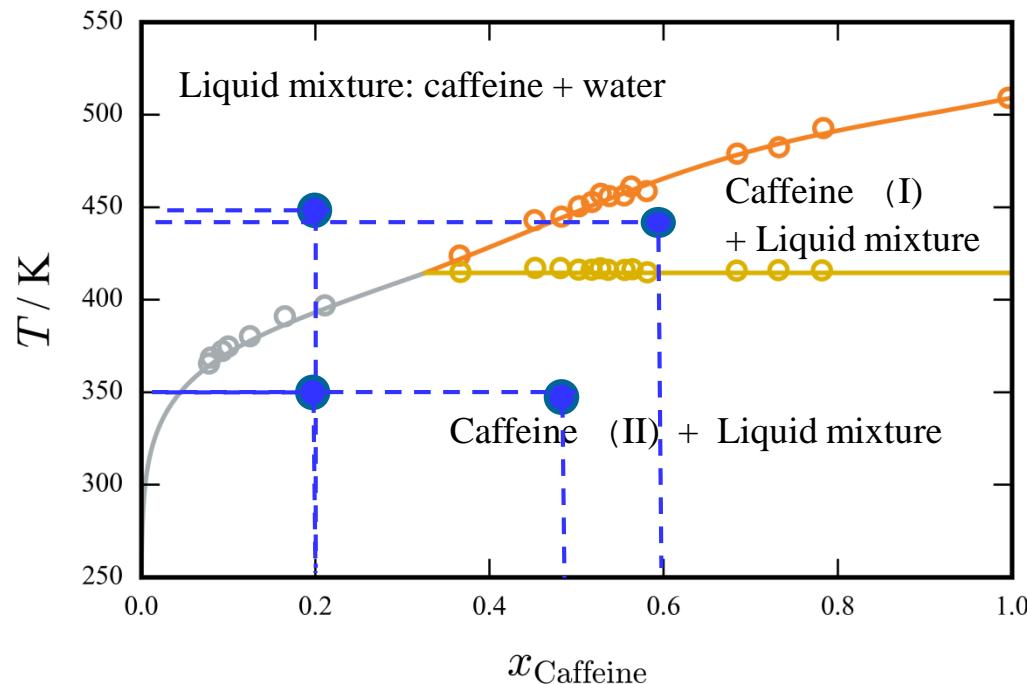
```
FlashResults = physprops.TPflash(T, P, n0) ;
```

- Output vector FlashResults contains
  - Mole fractions of each compounds in each **fluid** phase
  - Enthalpy of each **fluid** phase
  - Amount of each **fluid** phase
  - Volume of each **fluid** phase
  - **Amount of each possible solid phase**

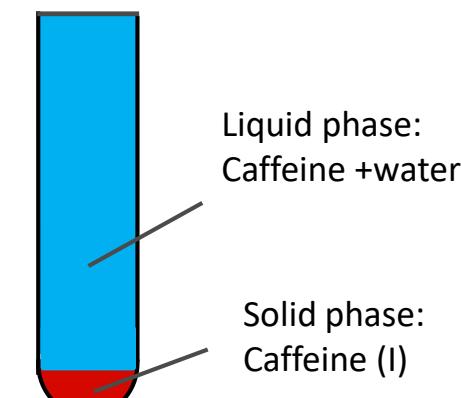
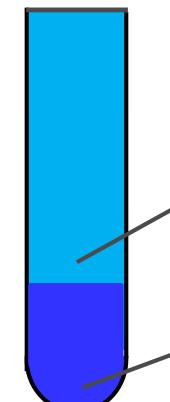
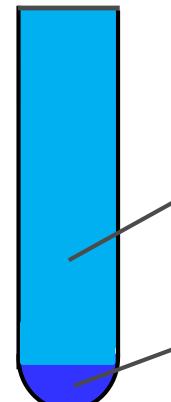
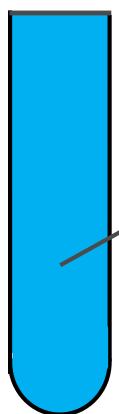
Ongoing development  
Estimated availability: 2017/Q3

# Handling of solid phases in gSAFT

Generalised fluid/solid equilibrium – caffeine + water example



**Caffeine exhibits polymorphic transitions**



# Custom databank management in gSAFT



# gSAFT custom databank management

## A new gSAFT software feature



### ■ Why you may want to have your own databank?

- You want to **refine existing parameters** using your own experimental data
- You want to **add new groups** that are not present in standard gSAFT databank

### ■ Custom databanks can be developed and used with standard databank

- Software handles “on-the-fly merging” of the databanks during execution

#### *Using standard gSAFT databank*

```
<gsaft>
  <databank name = "GC_Mie_databank.dtb"/>
    <compounds>
      <compound name = "methane"/>
      <compound name = "hydrogen"/>
      <compound name = "methanol"/>
      <compound name = "carbon_monodixe"/>
      <compound name = "carbon_dioxide"/>
      <compound name = "water"/>
    </compounds>
    <reactions>
      <reaction name="reaction1">
        <compound ref="carbon_monoxide" stoich="-1"/>
        <compound ref="hydrogen" stoich="-2"/>
        <compound ref="methanol" stoich="1"/>
      </reaction>
    </reactions>
  </gsaft>
```

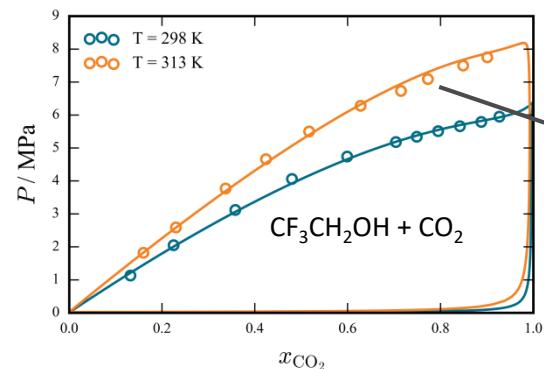
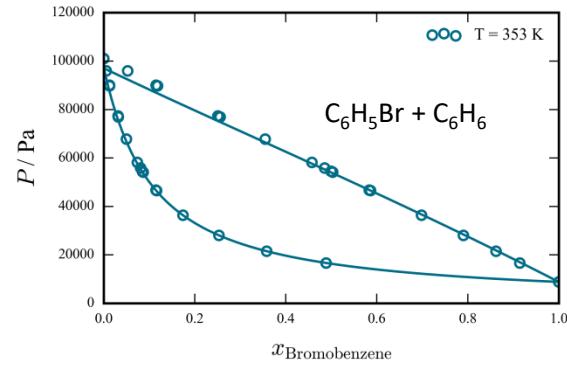
#### *Using a custom databank on top of the standard one*

```
<gsaft>
  <databank name = "GC_Mie_databank.dtb:Custom_databank.xml"/>
    <compounds>
      <compound name = "methane"/>
      <compound name = "hydrogen"/>
      <compound name = "methanol"/>
      <compound name = "carbon_monodixe"/>
      <compound name = "carbon_dioxide"/>
      <compound name = "water"/>
    </compounds>
    <reactions>
      <reaction name="reaction1">
        <compound ref="carbon_monoxide" stoich="-1"/>
        <compound ref="hydrogen" stoich="-2"/>
        <compound ref="methanol" stoich="1"/>
      </reaction>
    </reactions>
  </gsaft>
```

# gSAFT custom databank management Tool for estimating gSAFT parameters



## gSAFT Material Modeller (gSAFTmm)

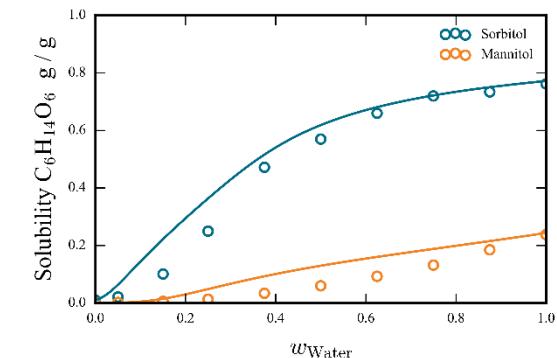
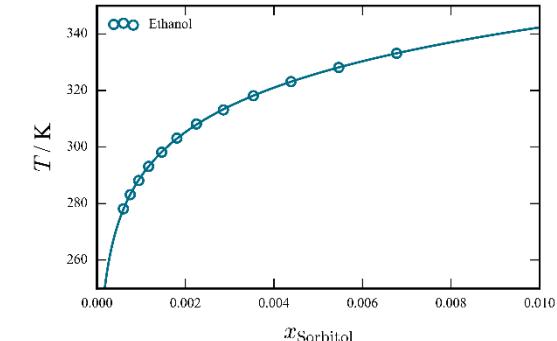


```
Python 2.7.11 Shell
File Edit Shell Debug Options Window Help
Python 2.7.11 (v2.7.11:6d1b6a68f775, Dec  5 2015, 20:40:30) [MSC v.1500 64 bit (AMD64)] on win32
Type "copyright", "credits" or "license()" for more information.

>>>
>>> from gSAFTmm import gSAFT
>>> S = gSAFT.System("GC_Mie_Databank.dtb<water,ethanol>")
>>> P = 101325.0
>>> z = [0.5,0.5]
>>> S.BubbleTemperature(P,z)
352.9308824915346
>>> S.BubbleTemperatureCompositions(P,z)
{'water': 0.33216841034237304, 'ethanol': 0.6678315896585177}
>>> T = 298.15
>>> S.VapourPressure(T)
{'water': 3213.369667081217, 'ethanol': 7781.798364149457}
>>> S.SinglePhaseDensity(T,P,z)
879.3909261514317
>>> S = gSAFT.System("GC_Mie_Databank.dtb<water,ethanol,methanol>")
>>> z = [0.3,0.4,0.3]
>>> S.BubbleTemperature(P,z)
348.806344398678744
>>> S.BubbleTemperatureCompositions('water': 0.1952498284071013628976483618)
>>> |
```

Standardised  
experimental data  
format

```
1 {
  "Compounds" :
    [ "trifluoroethanol", "carbon_dioxide" ],
  "BubblePressure" :
  [
    {
      "VarianceModel" : "Constant_Relative" ,
      "StdDeviation" : 0.01
    },
    "Data":
    [
      [ 298 , [ 0.868 , 0.132 ], 1130000 ],
      [ 298 , [ 0.775 , 0.225 ], 2050000 ],
      [ 298 , [ 0.642 , 0.358 ], 3120000 ],
      [ 298 , [ 0.52 , 0.48 ], 4060000 ],
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      [ 298 , [ 0.205 , 0.795 ], 5510000 ],
      [ 298 , [ 0.158 , 0.842 ], 5660000 ],
      [ 298 , [ 0.112 , 0.888 ], 5790000 ],
      [ 298 , [ 0.073 , 0.927 ], 5950000 ],
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      [ 313 , [ 0.372 , 0.628 ], 6280000 ],
      [ 313 , [ 0.285 , 0.718 ], 6730000 ],
      [ 313 , [ 0.227 , 0.773 ], 7090000 ],
      [ 313 , [ 0.151 , 0.849 ], 7500000 ],
      [ 313 , [ 0.099 , 0.901 ], 7750000 ]
    ]
  }
}
```

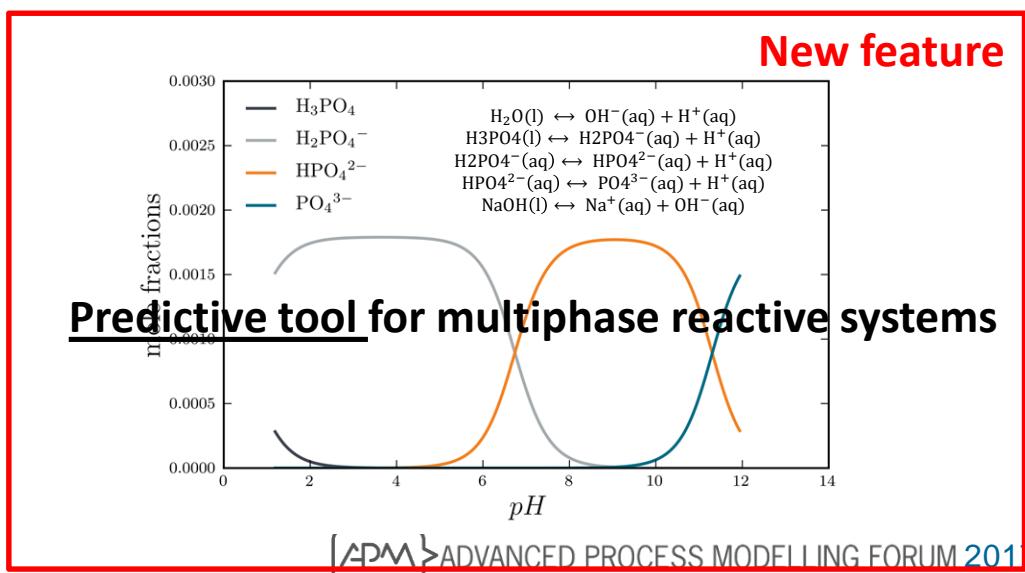
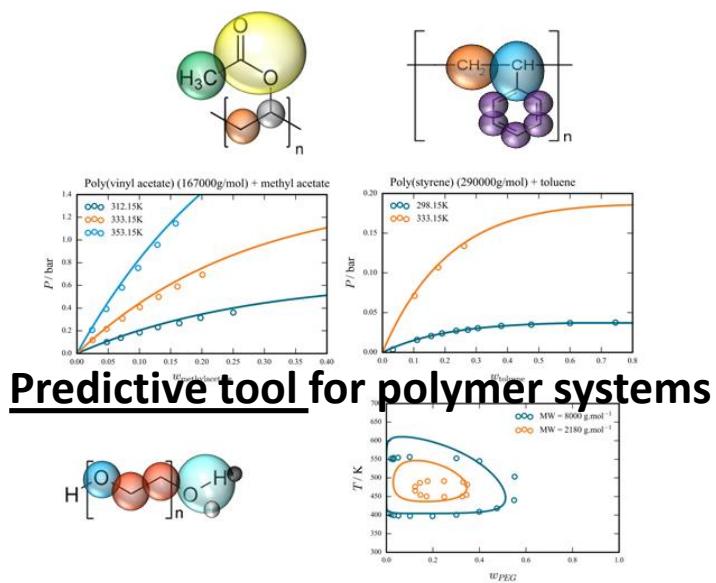
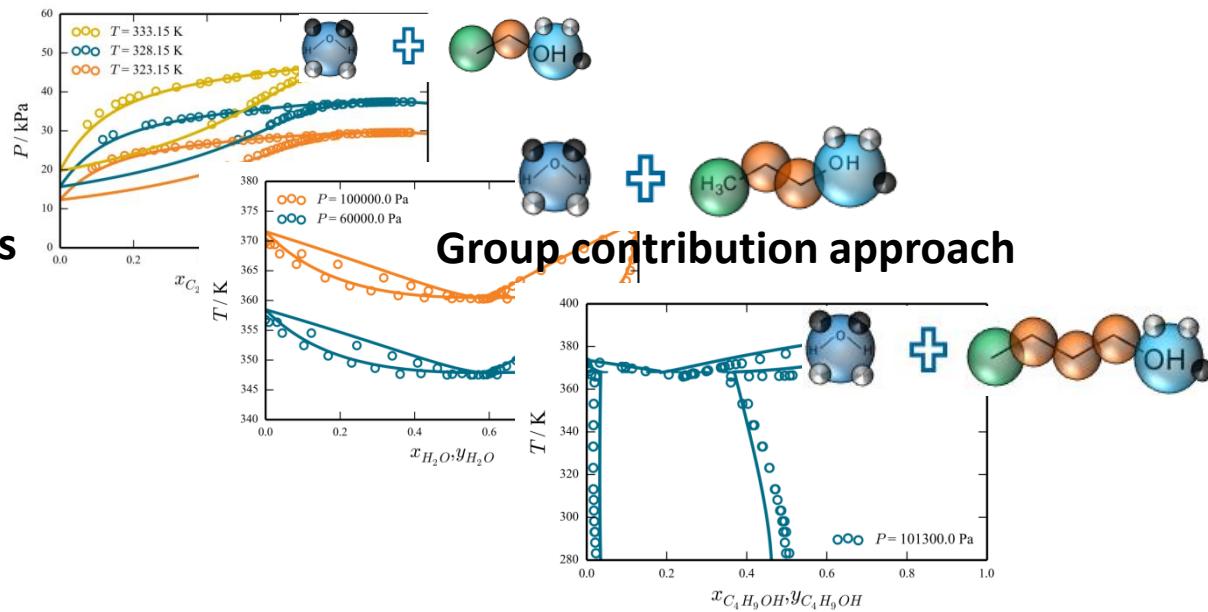
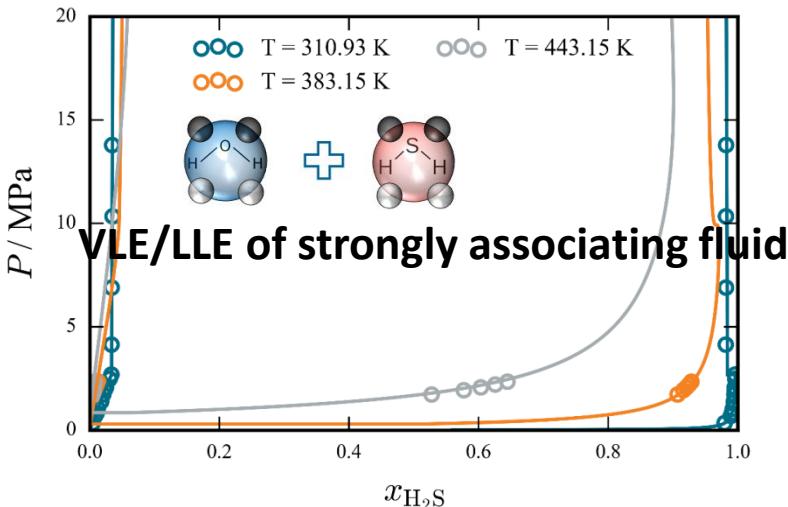


# Concluding remarks



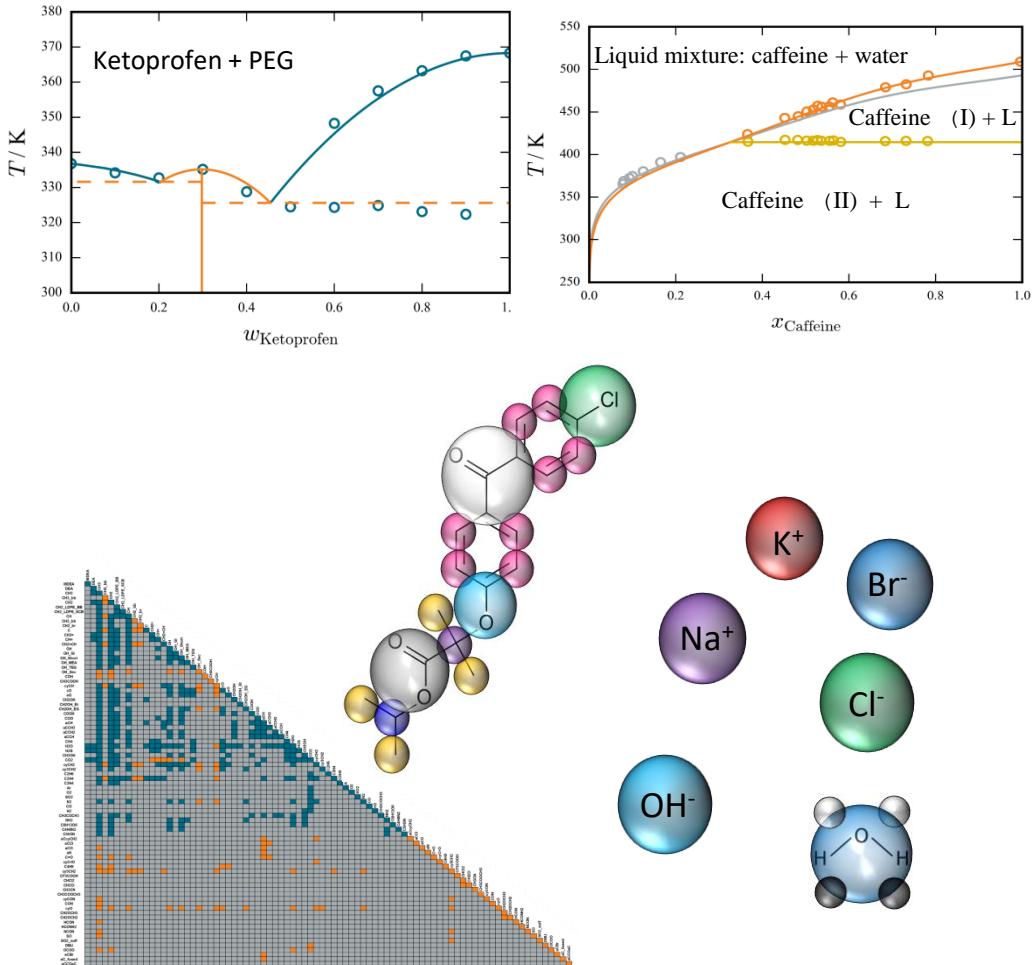
# gSAFT in gPROMS v5.0

General physical property engine based on rigorous thermodynamic framework



- General phase & reaction equilibrium including solid phases
  - Easy computation of complex fluid/solid phase diagrams (including polymorphs)

- Wider range of systems:
  - Extended database of group parameters
  - Focus on API(s) and ions



Thank you

[t.lafitte@psenterprise.com](mailto:t.lafitte@psenterprise.com)

