

# Getting started with Simulis® Thermodynamics

Use Case 11: Management of electrolytic systems  
with the reactive models editor

Software & Services In Process Simulation

*We guide You to efficiency*



ProSim

# Introduction

This document presents the management of electrolytic thermodynamic models and the configuration tool of these reactive models

- Some definitions
- Use within Simulis Thermodynamics and visualization of parameters
- Presentation of the reactive models editor

# Some definitions

- Electrolyte:

- molecular or atomic species (gaseous, liquid or solid) which has some solubility in a solvent and react with it to form one or more ionic species (charged)

E. g.:  $\text{CO}_2$  (g),  $\text{NaCl}$  (s)

- Electrolyte equilibrium:

- Thermodynamic equilibrium involving species that are all in the solvent phase

E. g.:  $\text{CO}_2$  (aq) +  $\text{H}_2\text{O}$  (aq)  $\rightleftharpoons$   $\text{H}^+$  (aq) +  $\text{HCO}_3^-$  (aq)

# Some definitions

- Apparent species:

- molecule or atomic species defined by the user

E. g.:  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{NaCl}$

- True species:

- all species existing in the mixture, additional species with respect to the apparent species being created through electrolyte reactions (including apparent species)

E. g.:  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{NaCl}$ ,  $\text{HCl}$ ,  $\text{NaOH}$ ,  $\text{NaHCO}_3$ ,  $\text{Na}_2\text{CO}_3$ ,  $\text{Na}_2\text{CO}_3, \text{H}_2\text{O}$ ,  $\text{Na}_2\text{CO}_3, 7\text{H}_2\text{O}$ ,  $\text{Na}_2\text{CO}_3, 10\text{H}_2\text{O}$ ,  $\text{H}^+$ ,  $\text{OH}^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ,  $\text{Na}^+$ ,  $\text{Cl}^-$

# Some definitions

## ■ Global presentation of multiphase electrolyte systems

### • Systems with:

→ Water:  $H_2O$

→ Salts:  $NaCl$ ,  $KCl$ ,  $Na_2SO_4$  ...

→ Gas:  $CO_2$ ,  $NH_3$ ,  $CH_4$  ...

} Apparent species

### • Dissociation reactions:

→ Autoprotolysis of water:  $H_2O \rightleftharpoons H^+ + HO^-$

→ Salts:  $NaCl \rightleftharpoons Na^+ + Cl^-$

→ Gases:  $CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-$  ...

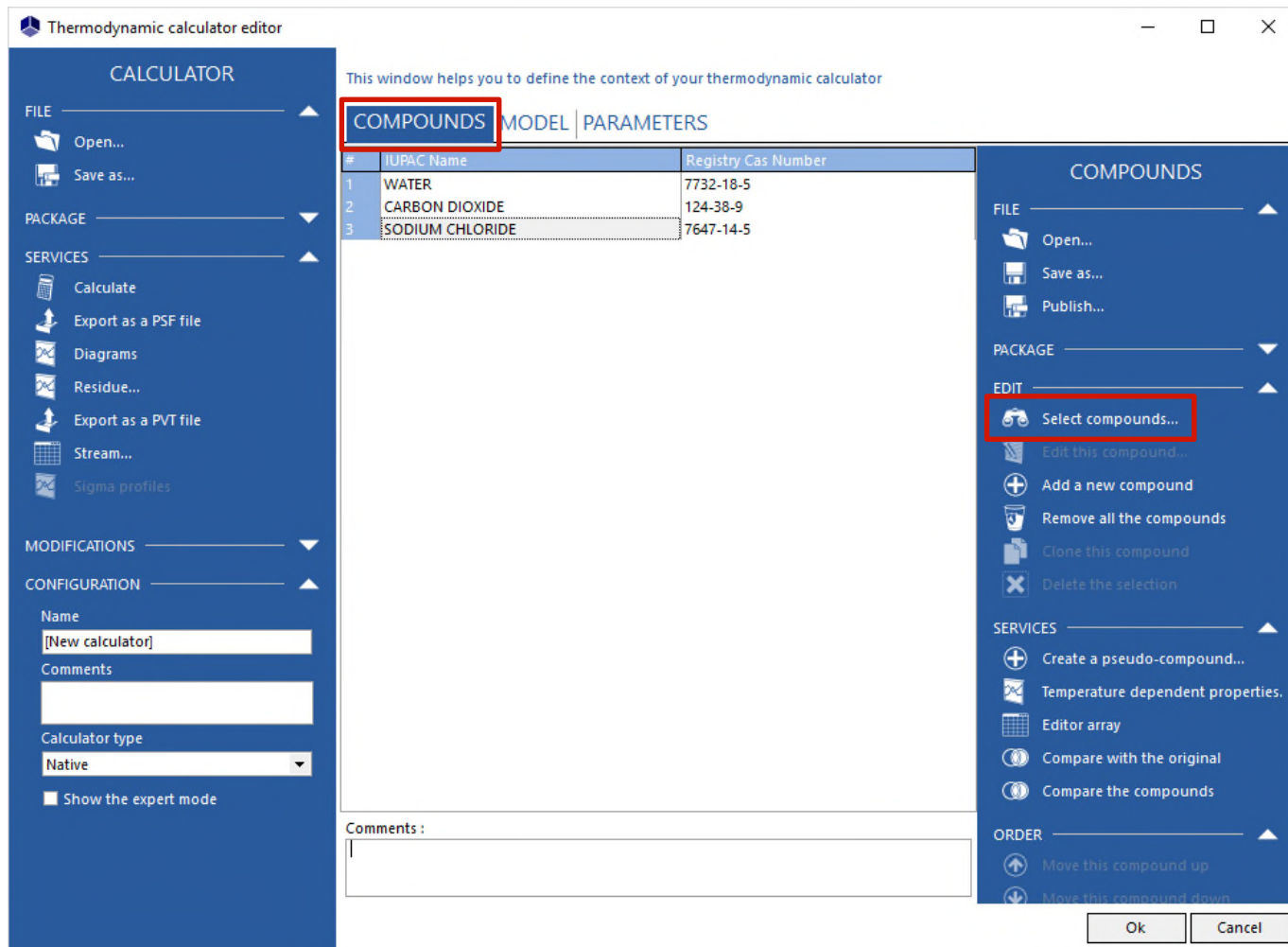
} True species

- Electrolyte solutions: strongly non ideal solutions (particles with electrically charged, electrostatic interactions)
- Use of specific thermodynamics to describe aqueous phase
- Liquid-solid, vapor-liquid, vapor-liquid-solid Equilibria

# Simulis Thermodynamics: Visualization of parameters

6

- Step 1: in the calculator, define apparent species of the system





# Simulis Thermodynamics: Visualization of parameters

7

- Step 2: choose an electrolyte thermodynamic model (in the category “Heterogeneous approach - Electrolytes”)

The screenshot shows the 'Thermodynamic calculator editor' window. The 'MODEL' tab is selected and highlighted with a red box. The 'Name' field is 'Sour water'. The 'Category' dropdown is set to 'Heterogeneous approach - Electrolyte', and the 'Profile' dropdown is set to 'Sour water', both highlighted with red boxes. Other settings include 'Approach type' as 'From activity coefficients', 'Equation of state' as 'Nakamura', 'Alpha function' as 'Not defined', 'Mixing rules' as 'Not defined', 'Activity coefficient model' as 'Edwards', 'Pure liquid fugacity standard state' as 'Henry's law with Poynting correction', 'Liquid molar volume' as 'Helgeson', 'Transport properties' as 'Mixed', 'Enthalpy calculation' as 'H\*=DH0f, ideal gas, 25°C, 1 atm', and 'User-defined thermodynamic model' as 'None'. The 'Model index' is set to 1. The 'Comments' field is empty. On the right, the 'THERMODYNAMIC MODEL' panel shows the 'CONFIGURATION' section with 'Parameters' selected. The 'Advanced' section is expanded, showing the 'Water-hydrocarbons model' with 'Sol A' at 6.25043 and 'Sol B' at 4015.3. Other options like 'The liquid phase splitting is taken into account', 'Predictive model parameters...', 'True species model', and 'Reactive model parameters...' are also visible. The 'Ok' and 'Cancel' buttons are at the bottom right.

Thermodynamic calculator editor

FILE

- Open...
- Save as...

PACKAGE

SERVICES

- Calculate
- Export as a PSF file
- Diagrams
- Residue...
- Export as a PVT file
- Stream...
- Sigma profiles

MODIFICATIONS

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

Native

☐ Show the expert mode

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS MODEL PARAMETERS

Name

Sour water

Category

Heterogeneous approach - Electrolyte

Profile

Sour water

Approach type

From activity coefficients

Equation of state

Nakamura

Alpha function

Not defined

Mixing rules

Not defined

Activity coefficient model

Edwards

Pure liquid fugacity standard state

Henry's law with Poynting correction

Liquid molar volume

Helgeson

Transport properties

Mixed

Enthalpy calculation

H\*=DH0f, ideal gas, 25°C, 1 atm

User-defined thermodynamic model

None

Model index

1

Comments :

THERMODYNAMIC MODEL

CONFIGURATION

Parameters

Thermodynamic assistant

Thermodynamic help

☐ Use a specific model for pure water

Advanced

☐ Water-hydrocarbons model

Sol A

6.25043

Sol B

4015.3

☐ The liquid phase splitting is taken into account

Predictive model parameters...

☐ True species model

Reactive model parameters...

Ok Cancel

# Simulis Thermodynamics: Visualization of parameters

- Simulis Thermodynamics (thermodynamic server of ProSim) offers several electrolyte or reactive thermodynamic models (cf. category of the models)
  - Sour Water
  - Pitzer
  - Amines and acid gases
  - e-NRTL
  - UNIQUAC electrolytes
  - ULPDHS
  - MSE
  - COSMO-UCAs
  - ...



# Simulis Thermodynamics: Visualization of parameters

9

- Step 2: case of a group contribution predictive electrolyte thermodynamic model, e. g. ULPDHS (in the category “Heterogeneous approach - Electrolytes - predictive models”)

The screenshot shows the 'Thermodynamic calculator editor' window. The 'MODEL' tab is selected and highlighted with a red box. The 'Name' field contains 'ULPDHS'. The 'Category' dropdown is set to 'All the profiles' and the 'Profile' dropdown is set to 'ULPDHS', both highlighted with red boxes. The 'Approach type' is 'From activity coefficients', 'Equation of state' is 'Nakamura', 'Alpha function' is 'Not defined', 'Mixing rules' is 'Not defined', 'Activity coefficient model' is 'ULPDHS', 'Pure liquid fugacity standard state' is 'Henry's law with Poynting correction', 'Liquid molar volume' is 'Helgeson', 'Transport properties' is 'Electrolytes', 'Enthalpy calculation' is 'H\*=DHof, ideal gas, 25°C, 1 atm', and 'User-defined thermodynamic model' is 'None'. The 'Model index' is set to 1. The 'Comments' field is empty. On the right sidebar, the 'THERMODYNAMIC MODEL' section is expanded, and the 'Predictive model parameters...' button is highlighted with a red box. A red arrow points from this button to the text 'Click on the button “Predictive model parameters...”’.

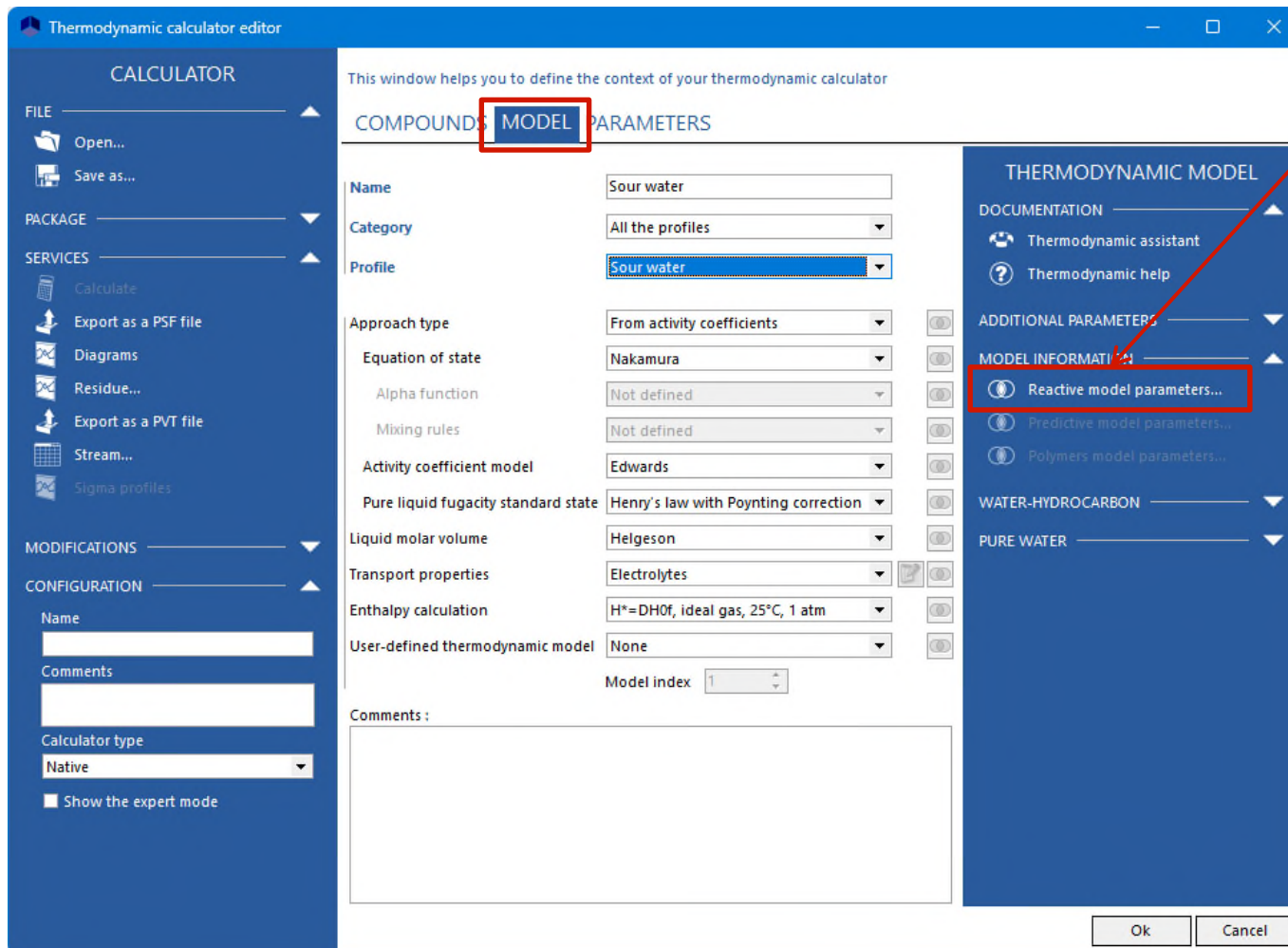
Click on the button  
“Predictive model  
parameters...”



Refer to “Getting started with Simulis Thermodynamics, Case 10”  
for more details concerning the use of group-contribution predictive models

# Simulis Thermodynamics: Visualization of parameters

- Step 3: visualization of parameters of the chosen model for the selected system



Click on the button  
“Reactive model  
parameters...”  
(enabled only if the model  
is an electrolyte model)

# Simulis Thermodynamics: Visualization of parameters

- Step 3a: list of true species that can exist in the system  
(apparent species + ionic species + salts  
+ other species that can be recombined)

Reactive models editor (ReadOnly)

HOME

About Predictive model parameters... Help Actions

COMPOUNDS REACTIONS BINARIES TERNARIES

COMPOUNDS

FILE

- Open...
- Save As...
- Publish...

PACKAGE

EDIT

- Import compounds...
- Edit this compound...
- Add a new compound
- Remove all the compounds
- Clone this compound
- Delete the selection

SERVICES

- Create a pseudo-compound...
- Temperature dependent properties.
- Editor array
- Compare with the original
- Compare the compounds

ORDER

- Move this compound up
- Move this compound down


| Compound name        | Chemical formula |
|----------------------|------------------|
| 1 WATER              | 7732-18-5        |
| 2 CARBON DIOXIDE     | 124-38-9         |
| 3 SODIUM CHLORIDE    | 7647-14-5        |
| 4 HYDROGEN CHLORIDE  | 7647-01-0        |
| 5 SODIUM HYDROXIDE   | 1310-73-2        |
| 6 SODIUM BICARBONATE | 144-55-8         |
| 7 SODIUM CARBONATE   | 497-19-8         |
| 8 Na2CO3, 7H2O       |                  |
| 9 Na2CO3, 10H2O      | 6132-02-1        |
| 10 Na2CO3, H2O       | 5968-11-6        |
| 11 Cl[-]             |                  |
| 12 Na[+]             |                  |
| 13 CO3[2-]           |                  |
| 14 HCO3[-]           |                  |
| 15 OH[-]             |                  |
| 16 H[+]              |                  |

Comments

Ok Cancel

List of apparent species  
(defined by the user)

List of true species  
(used by the  
electrolyte model)

 A double-click on a component allows to access its properties

# Simulis Thermodynamics: Visualization of parameters

- Step 3b: list of electrolyte reactions taken into account in the chosen reactive model for the selected system

Reactive models editor (ReadOnly)

HOME

About Predictive model parameters... Help Actions

COMPOUNDS REACTIONS BINARIES TERNARIES

REACTIONS

REACTIONS

- + Add a reaction
- Edit this reaction...
- Clone this reaction
- Delete this reaction
- Remove all the reactions
- Search...


ORDER

- Move up the reaction
- Move down the reaction

| #  | Name   |
|----|--|
| 1  | $\text{H}_2\text{O} \rightleftharpoons \text{H}^{+} + \text{OH}^{-}$   |
| 2  | $\text{H}_2\text{O} + \text{CO}_2 \rightleftharpoons \text{H}^{+} + \text{HCO}_3^{-}$  |
| 3  | $\text{HCO}_3^{-} \rightleftharpoons \text{H}^{+} + \text{CO}_3^{=}$   |
| 4  | $\text{NaCl} \rightleftharpoons \text{Na}^{+} + \text{Cl}^{-}$   |
| 5  | $\text{HCl} \rightleftharpoons \text{H}^{+} + \text{Cl}^{-}$   |
| 6  | $\text{NaOH} \rightleftharpoons \text{Na}^{+} + \text{OH}^{-}$   |
| 7  | $\text{NaHCO}_3 \rightleftharpoons \text{Na}^{+} + \text{HCO}_3^{-}$   |
| 8  | $\text{Na}_2\text{CO}_3 \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=}$   |
| 9  | $\text{Na}_2\text{CO}_3 \cdot 7\text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + 7\text{H}_2\text{O}$   |
| 10 | $\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + 10\text{H}_2\text{O}$ |
| 11 | $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + \text{H}_2\text{O}$     |

Comments:

Ok Cancel

 A double-click on a reaction allows to access to parameters of the selected equilibrium



# Simulis Thermodynamics: Visualization of parameters

- Step 3b: parameters of the selected electrolyte reaction (stoichiometry, speciation, possible precipitation)

Stoichiometry of the reaction

Parameters of the speciation (or dissociation)

Parameters of the precipitation (or solubility)

Correlation for speciation equilibrium constant (or for precipitation)

Parameters

Reaction (ReadOnly)

Unique ID: {91A07749-0919-4F5A-9A37-219293F24284}

Reaction name: H2O + CO2 <=> H[+] + HCO3[-]

| Compound       | Stoichiometry |
|----------------|---------------|
| WATER          | -1            |
| CARBON DIOXIDE | -1            |
| HCO3[-]        | 1             |
| H[+]           | 1             |

Speciation

Precipitation

☒ Configure the equilibrium constant

Correlation: Logarithmic

$$\ln(K_{eq}) = \frac{p_1}{T_K} + p_2 \cdot \ln(T_K) + p_3 \cdot T_K + p_4 + p_5 \cdot T_K^2 + p_6 \cdot T_K^3$$

Comments:

Parameters

| Parameter | Value     |
|-----------|-----------|
| p1        | -7742.6   |
| p2        | -14.506   |
| p3        | -0.028104 |
| p4        | 102.28    |
| p5        | 0         |
| p6        | 0         |

Ok Cancel



# Simulis Thermodynamics: Visualization of parameters

- Step 3c: interaction parameters of the chosen model between true species (binaries, possibly ternaries)

**Binaries**      **Ternaries**

The screenshot shows the 'Reactive models editor (ReadOnly)' window. The 'BINARIES' tab is selected in the top navigation bar. The central table lists interactions between compounds. The right panel shows the 'Parameter' dropdown set to 'Beta0' and the 'Correlation' dropdown set to 'Holmes'. Below these, the 'Value' is displayed as a function of  $p_1, p_2, p_3, p_4, p_5, p_6, p_7, p_8$ . At the bottom right, a 'Parameters' table lists the values for these parameters.

**List of parameters of the chosen model**

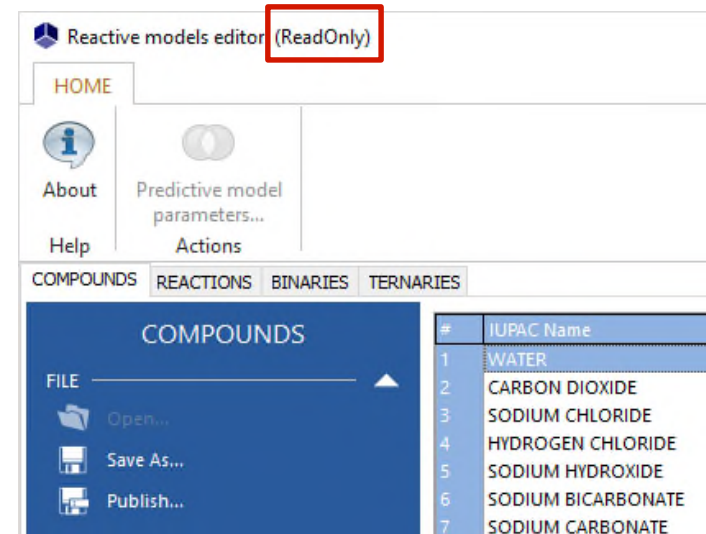
**Correlation for the selected binary (or ternary) interaction parameter**

**Parameters**

| Parameter | Value      |
|-----------|------------|
| p1        | 0.23159    |
| p2        | 0.00885495 |
| p3        | 0          |
| p4        | -0.0003152 |
| p5        | 0.000112   |
| p6        | 997        |
| p7        | 298.15     |
| p8        | 1          |

# Simulis Thermodynamics: Visualization of parameters

- Parameters of the chosen model for the selected system, accessible from the “Reactive model parameters...” button, are “Read Only” (no possible modification)



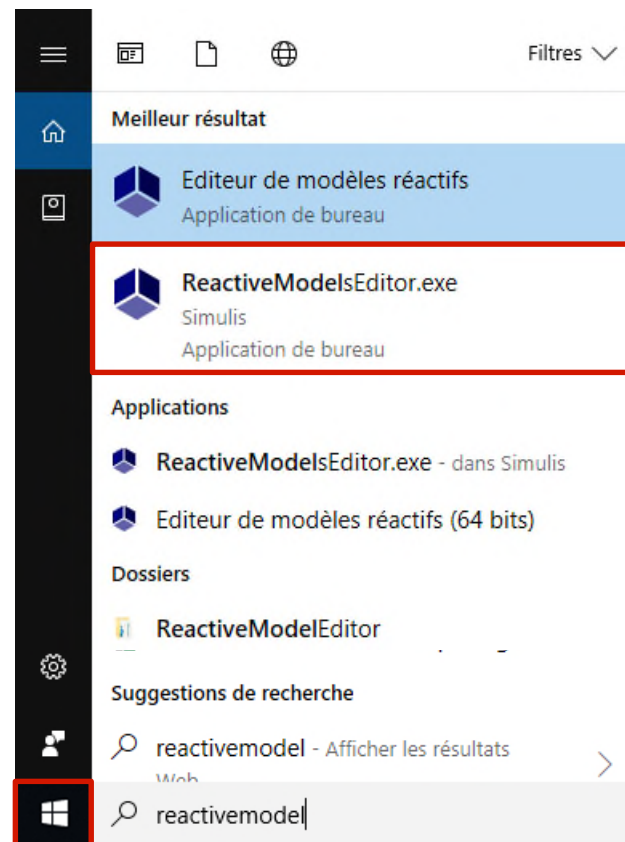
- Visualization of species, equilibrium reactions and interactions taken into account by the model
- Possibility to add systems or to modify parameters of existing systems



Use of the reactive models editor

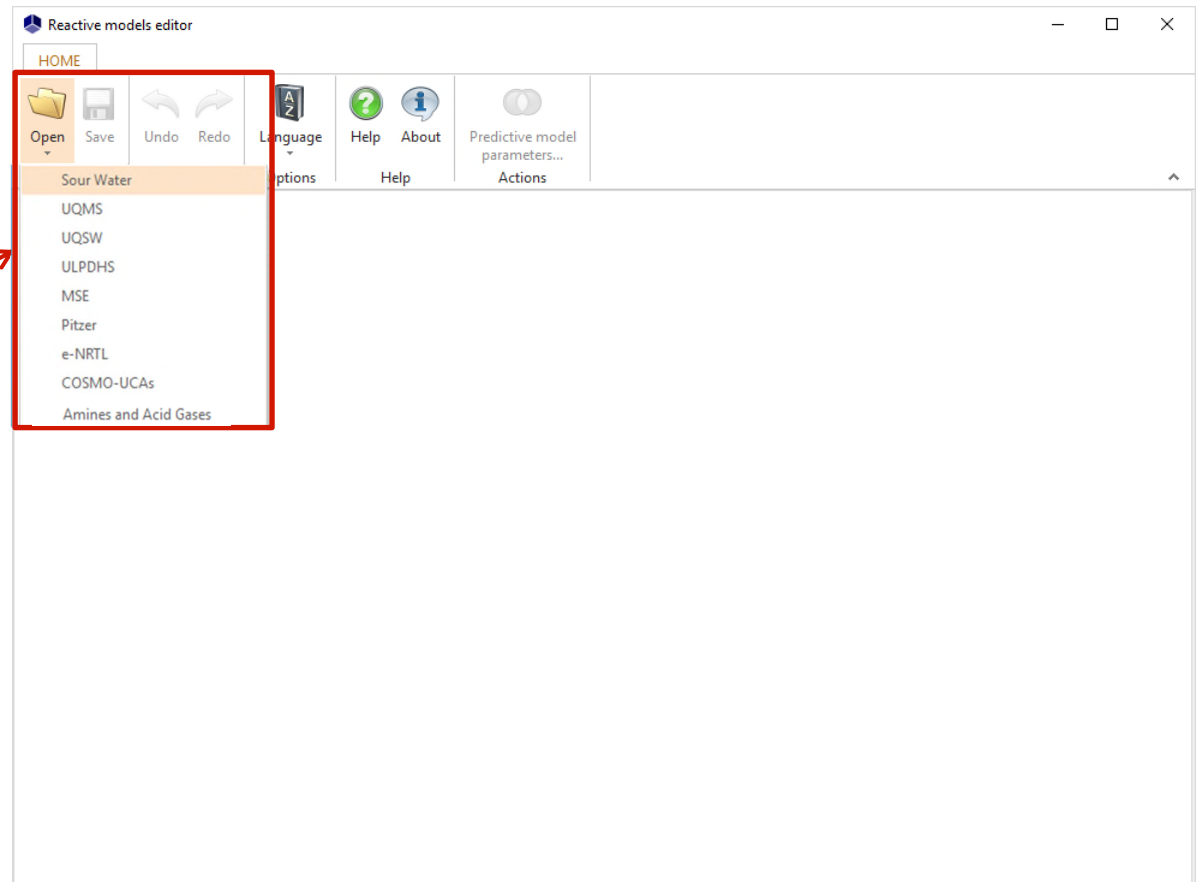
# Reactive Models Editor

- Reactive models editor: “**ReactiveModelsEditor.exe**”
  - Accessible from “Start” menu of WINDOWS
  - Or in directory: C:\Program Files (x86)\Simulis
  - Or in directory: C:\Program Files\Simulis



# Reactive Models Editor

- Reactive models editor: “ReactiveModelsEditor.exe”
  - Open a database associated to a model



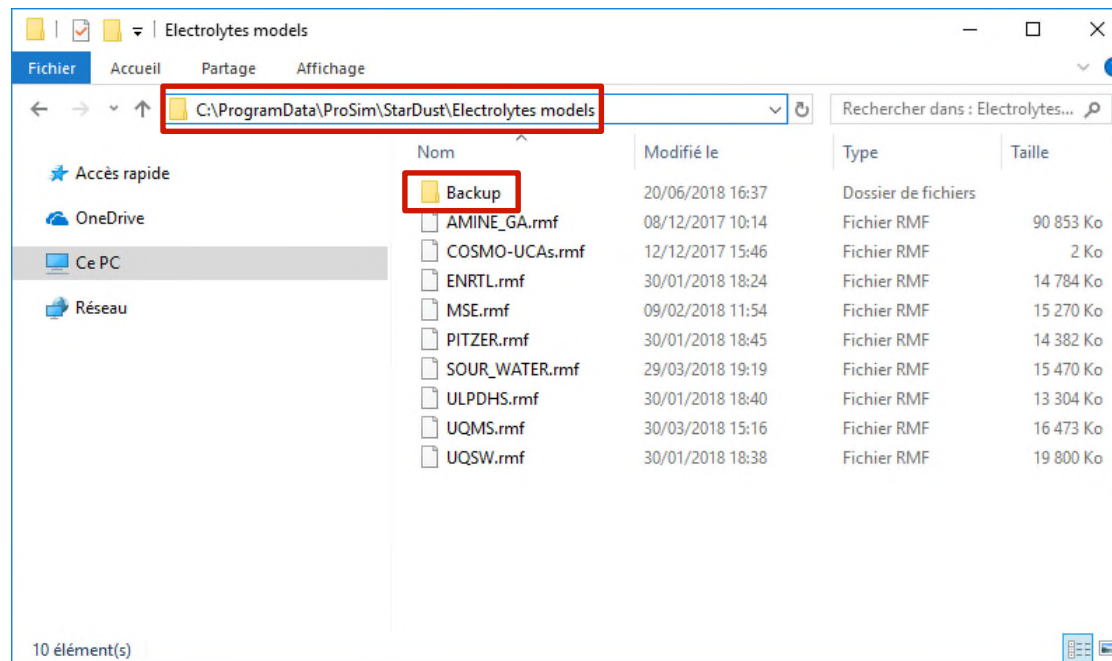
Access to databases  
of reactive model  
parameters

# Reactive Models Editor

- Data file of reactive model parameters (**rmf**)
  - In C:\ProgramData\Prosim\Stardust\Electrolytes models
  - 1 rmf file for each electrolyte model



It is strongly recommended to save original rmf files as well as the different versions created by the user





# Reactive Models Editor

List of compounds taken into account for the selected model (true species)

List of reactions taken into account for the selected model (access to speciation and precipitation constants)

Access to binary (possibly ternary) interaction parameters available for the selected model

The screenshot shows the 'Reactive models editor : Sour Water' window. The interface includes a ribbon with 'HOME' and 'Predictive model parameters...' tabs. The 'HOME' ribbon contains 'Open', 'Save', 'Undo', 'Redo', 'Language', 'Help', 'About', and 'Actions' buttons. The 'Predictive model parameters...' ribbon contains 'Edit', 'Modifications', 'Options', 'Help', and 'Actions' buttons. Below the ribbon are four tabs: 'COMPOUNDS', 'REACTIONS', 'BINARIES', and 'TERNARIES'. The 'COMPOUNDS' tab is active, showing a list of compounds with columns for '#', 'IUPAC Name', and 'Registry Cas Number'. A sidebar on the left contains a 'COMPOUNDS' section with a 'FILE' menu (Open..., Save As..., Publish...), a 'PACKAGE' dropdown, an 'EDIT' menu (Import compounds..., Edit this compound..., Add a new compound, Remove all the compounds, Clone this compound, Delete the selection), a 'SERVICES' section (Create a pseudo-compound..., Temperature dependent properties., Editor array, Compare with the original, Compare the compounds), and an 'ORDER' section (Move this compound up, Move this compound down). A 'Comments' text area is at the bottom.

| #  | IUPAC Name     | Registry Cas Number |
|----|----------------|---------------------|
| 1  | (NH4)2CO3      | 6721-33-1           |
| 2  | 1,3-BUTADIENE  | 106-99-0            |
| 3  | 1,4-PENTADIENE | 591-93-5            |
| 4  | 1,5-HEXADIENE  | 592-42-7            |
| 5  | 1-BUTENE       | 106-98-9            |
| 6  | 1-DECENE       | 872-05-9            |
| 7  | 1-DODECENE     | 1599-67-3           |
| 8  | 1-DODECENE     | 112-41-4            |
| 9  | 1-EICOSENE     | 3452-07-1           |
| 10 | 1-HEPTADECENE  | 6765-39-5           |
| 11 | 1-HEPTENE      | 592-76-7            |
| 12 | 1-HEPTYNE      | 628-71-7            |
| 13 | 1-HEXACOSENE   | 18835-33-1          |
| 14 | 1-HEXADECENE   | 629-73-2            |
| 15 | 1-HEXENE       | 592-41-6            |
| 16 | 1-HEXYNE       | 693-02-7            |
| 17 | 1-NONADECENE   | 18435-45-5          |
| 18 | 1-NONENE       | 124-11-8            |
| 19 | 1-NONYNE       | 3452-09-3           |
| 20 | 1-OCTACOSENE   | 18835-34-2          |
| 21 | 1-OCTADECENE   | 112-88-9            |
| 22 | 1-OCTENE       | 111-66-0            |
| 23 | 1-OCTYNE       | 629-05-0            |
| 24 | 1-PENTADECENE  | 13360-61-7          |
| 25 | 1-PENTENE      | 109-67-1            |
| 26 | 1-PENTYNE      | 627-19-0            |
| 27 | 1-TETRACONTENE | 61868-18-6          |
| 28 | 1-TETRACOSENE  | 10192-32-2          |
| 29 | 1-TETRADECENE  | 1120-36-1           |

# Reactive Models Editor

- Add a species

The screenshot shows the 'Reactive models editor : Sour Water' window. The 'COMPOUNDS' tab is selected, and the 'Add a new compound' button in the left sidebar is highlighted with a red box. A red arrow points from this button to the 'New compound' entry in the main table.

| #   | IUPAC Name                            | Registry Cas Number |
|-----|---------------------------------------|---------------------|
| 324 | SODIUM NITRATE                        | 7631-99-4           |
| 325 | SODIUM NITRITE                        | 7632-00-0           |
| 326 | SODIUM SILICATE                       | 6834-92-0           |
| 327 | SODIUM SULFATE                        | 7757-82-6           |
| 328 | SODIUM THIOSULFATE                    | 7772-98-7           |
| 329 | SQUALANE                              | 111-01-3            |
| 330 | SULFUR DIOXIDE                        | 7446-09-5           |
| 331 | SULFURIC ACID                         | 7664-93-9           |
| 332 | TETRASODIUM PYROPHOSPHATE             | 7722-88-5           |
| 333 | trans-2,2,4,6,6-PENTAMETHYL-3-HEPTENE | 27656-49-1          |
| 334 | trans-2-BUTENE                        | 624-64-6            |
| 335 | trans-2-DECENE                        | 20063-97-2          |
| 336 | trans-2-DODECENE                      | 7206-13-5           |
| 337 | trans-2-EICOSENE                      | 42448-85-1          |
| 338 | trans-2-HEPTENE                       | 14686-13-6          |
| 339 | trans-2-HEXENE                        | 4050-45-7           |
| 340 | trans-2-NONENE                        | 6434-78-2           |
| 341 | trans-2-OCTENE                        | 13389-42-9          |
| 342 | trans-2-PENTADECENE                   | 74392-36-2          |
| 343 | trans-2-PENTENE                       | 646-04-8            |
| 344 | trans-3-HEPTENE                       | 14686-14-7          |
| 345 | trans-3-HEXENE                        | 13269-52-8          |
| 346 | trans-3-OCTENE                        | 14919-01-8          |
| 347 | trans-4-OCTENE                        | 14850-23-8          |
| 348 | TRISODIUM PHOSPHATE                   | 7601-54-9           |
| 349 | VINYLACETYLENE                        | 689-97-4            |
| 350 | WATER                                 | 7732-18-5           |
| 351 | [New compound]                        |                     |

# Reactive Models Editor

- Add a ionic species: required properties
  - Name
  - CAS number or intrinsic number (negative value not used yet < -1000)
  - Molecular weight
  - Charge
  - Born constant
  - Thermal conductivity contribution (electrolyte solution)  
(only if the Jamieson-Thudope model is used)
  - Helgeson coefficients:  $A_1$ ,  $A_2$ ,  $A_3$ ,  $A_4$ ,  $C_1$ ,  $C_2$   
(only if the Helgeson model is used)
  - Standard entropy at 25°C - infinite dilution
  - Standard specific heat at 25°C - infinite dilution
  - Standard state enthalpy of formation - infinite dilution
  - Standard state Gibbs energy of formation - infinite dilution
  - Temperature dependent properties: those of water

# Reactive Models Editor

- Add a salt: required properties
  - Name
  - CAS number or intrinsic number (negative value not used yet < -1000)
  - Chemical formula
  - Molecular weight
  - Physical state at 25°C: solid
  - Physical state in aqueous solution at 25°C  
(must be different from “completely soluble”)
  - Solid standard state enthalpy of formation
  - Solid specific heat (temperature dependent)
  - Vapor pressure: non volatile (equation #101 with A=-30)
  - Enthalpy of vaporization: null (equation #100 with A=B=C=D=E=0)
  - Other temperature dependent properties: those of water

# Reactive Models Editor

- Add another component: required properties
  - Name
  - CAS number
  - Chemical formula
  - Molecular weight
  - Physical state at 25°C
  - Standard state enthalpy of formation at 25°C
  - Standard state Gibbs energy of formation at 25°C
  - Standard state absolute entropy at 25°C
  - Nakamura coefficients (A, B, C, D, A0, A1, B0, B1)  
(only if Nakamura equation of state is used)
  - All temperature dependent properties
  - Particularly Henry's law constant for solutes



# Reactive Models Editor

- Properties of the species



As part of the use of a reactive model, all properties of a component coming from the reactive models editor have priority compared to properties of a component selected in the calculator

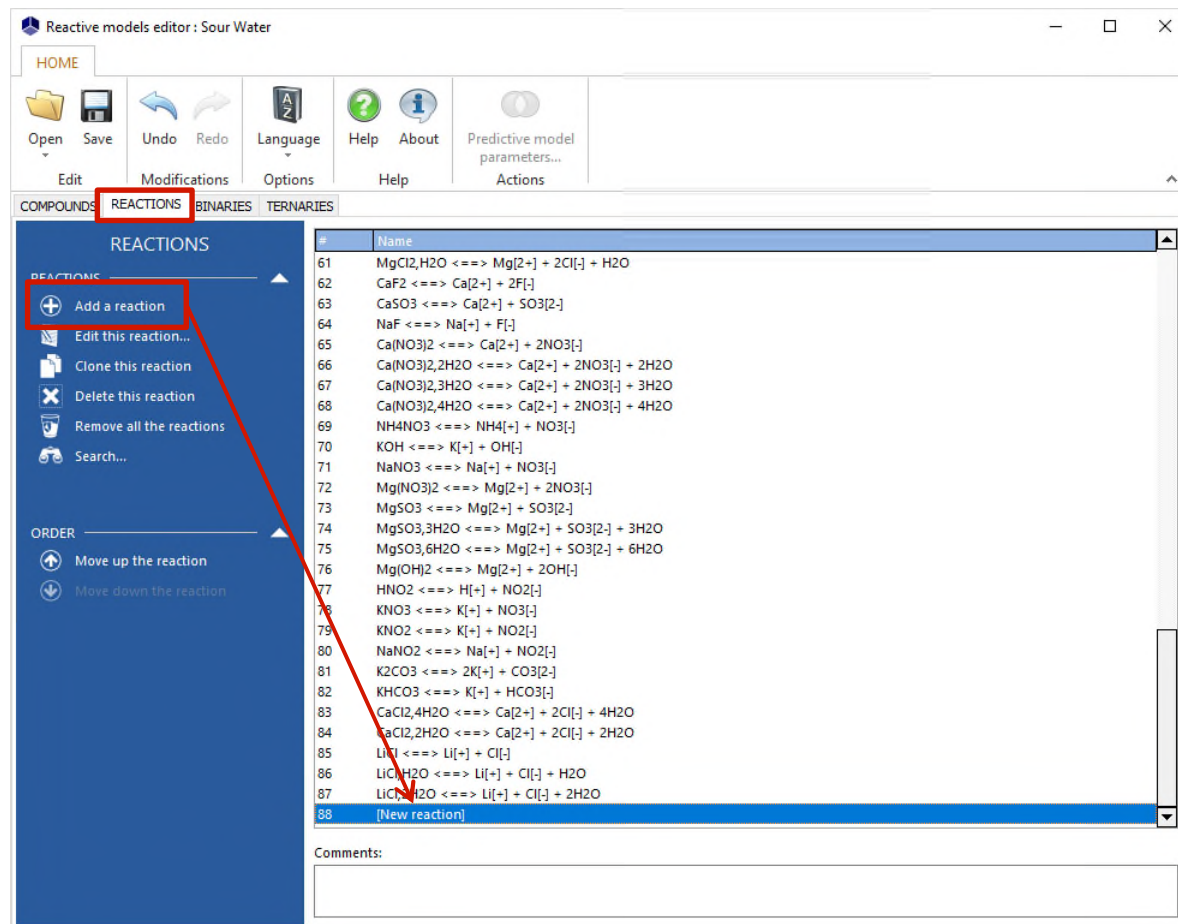
- Except for the following properties:

- Physical state at 25°C
- Physical state in aqueous solution at 25°C

(it allows to impose or not, directly in the components of the calculator, a possible precipitation for systems with many salts)

# Reactive Models Editor

- Add an electrolyte reaction



# Reactive Models Editor

## ■ Add an electrolyte reaction

1. Name of the reaction (e.g.  $A + B \rightleftharpoons C + D$ )
2. Add components of the reaction
3. Select each component concerned by the reaction from the dropdown list of species
4. Enter stoichiometric coefficients of the reaction

Reaction

Unique ID: {15427092-149A-40E4-AC8E-4FFB91E7D4-5}

Reaction name: [New reaction]

| Compound | Stoichiometry |
|----------|---------------|
|          | 0             |
|          | 0             |
|          | 0             |
|          | 0             |

Speciation | Precipitation

☐ Configure the equilibrium constant

Comments:

Ok Cancel

# Reactive Models Editor

- Add an electrolyte reaction (speciation constant)

1. Configure the equilibrium constant

2. Choice of the correlation

Reaction

Unique ID: {15427092-C49A-40E4-AC8E-4FFB91E7D4A5}

Reaction name: [New reaction]

| Compound | Stoichiometry |
|----------|---------------|
|          | 0             |
|          | 0             |
|          | 0             |
|          | 0             |

Speciation    Precipitation

☒ Configure the equilibrium constant

Correlation: Logarithmic

$$\ln(K_{eq}) = \frac{p_1}{T_K} + p_2 \cdot \ln(T_K) + p_3 \cdot T_K + p_4 + p_5 \cdot T_K^2 + p_6 \cdot T_K^3$$

Comments:

Parameters

| Parameter | Value |
|-----------|-------|
| p1        | 0     |
| p2        | 0     |
| p3        | 0     |
| p4        | 0     |
| p5        | 0     |
| p6        | 0     |

Comments:

Ok    Cancel

3. Parameters of the correlation



For a total dissociation

$$\ln(K_{eq}) = 35$$

(i. e.  $p_4 = 35$ )

# Reactive Models Editor

- Add an electrolyte reaction (precipitation constant, if necessary)

1. Configure the equilibrium constant

2. Choice of the correlation

3. Parameters of the correlation

The screenshot shows the 'Reaction' window in the Reactive Models Editor. The window is divided into several sections:

- Left Panel:** Contains a 'REACTION' header, 'COMPOUNDS' section with 'Add', 'Clone', 'Delete', and 'Clear' buttons, 'ORDER' section with 'Move up' and 'Move down' buttons, and 'MODIFICATIONS' section with 'Undo' and 'Redo' buttons.
- Top Section:** Displays the 'Unique ID: {15427092-C49A-40E4-AC8E-4FFB91E7D4A5}' and a 'Reaction name' field with the placeholder '[New reaction]'.
- Table:** A table with two columns: 'Compound' and 'Stoichiometry'. It contains four rows, all with a stoichiometry of 0.
- Speciation:** A dropdown menu set to 'Precipitation'.
- Configuration:** A checkbox labeled 'Configure the equilibrium constant' is checked. Below it, a 'Correlation' dropdown is set to 'Logarithmic'.
- Equation:** The logarithmic correlation equation is displayed:  $\ln(K_{eq}) = \frac{p_1}{T_K} + p_2 \cdot \ln(T_K) + p_3 \cdot T_K + p_4 + p_5 \cdot T_K^2 + p_6 \cdot T_K^3$ .
- Comments:** A text area for user comments.
- Parameters:** A table with two columns: 'Parameter' and 'Value'. It lists parameters p1 through p6, all with a value of 0.
- Buttons:** 'Ok' and 'Cancel' buttons are at the bottom right.

Red arrows point from the instructional text to specific elements: Arrow 1 points to the 'Stoichiometry' column, Arrow 2 points to the 'Correlation' dropdown, and Arrow 3 points to the 'Parameters' table.



# Reactive Models Editor

## ■ Add binary or ternary interaction parameters

1. Select the concerned species from the dropdown list of species

2. Select the interaction parameter of the model

3. Choice of the correlation

4. Parameters of the correlation

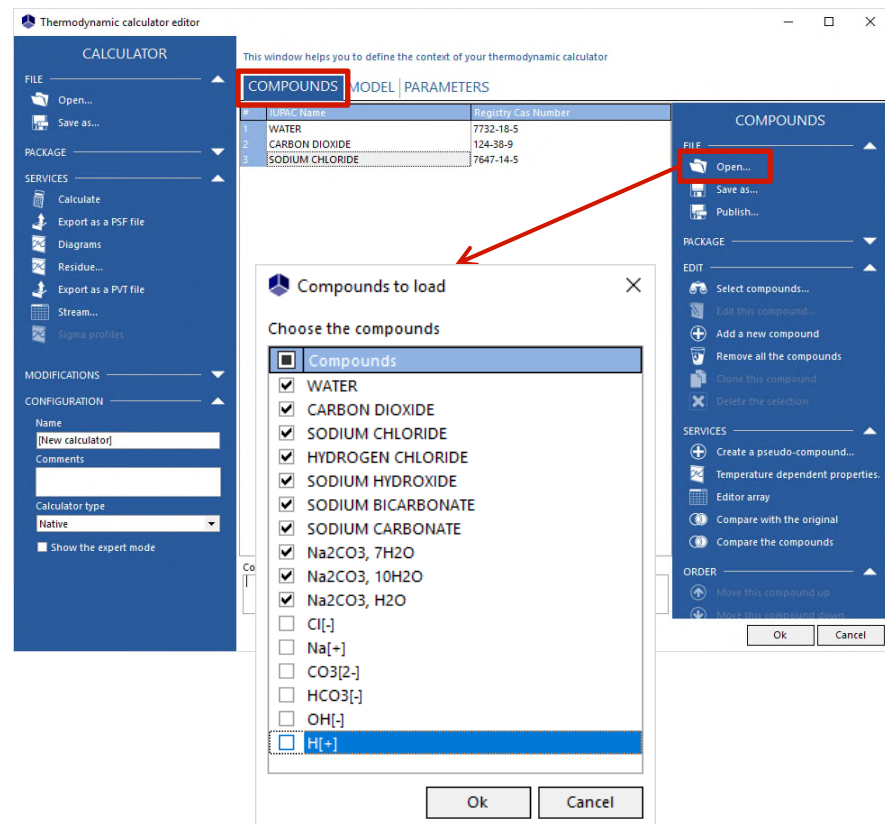
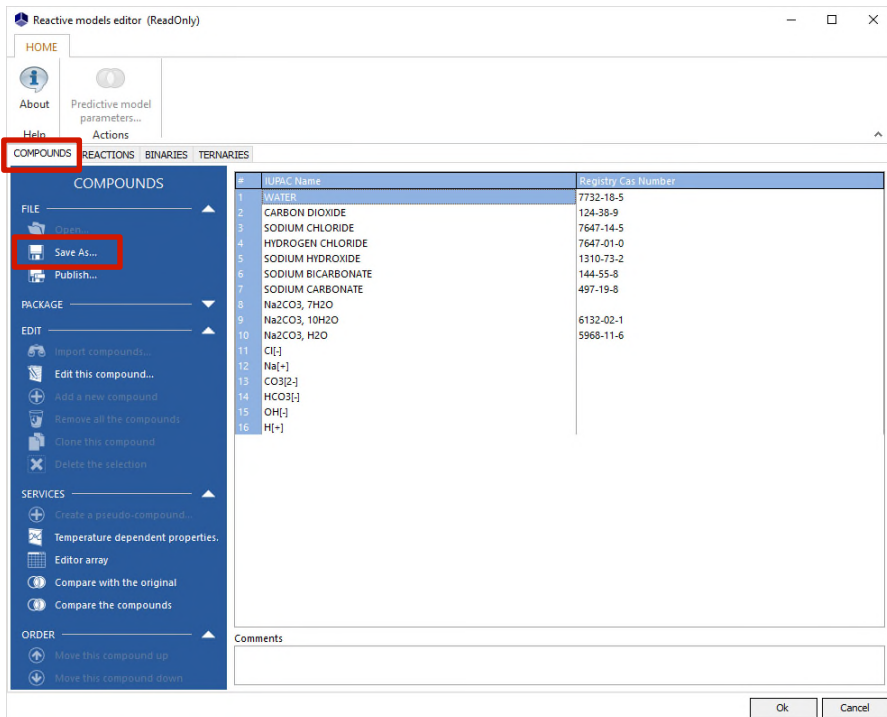
The screenshot shows the 'Reactive models editor : Sour Water' window. The 'BINARIES' tab is selected. On the left, the 'INTERACTIONS' panel has an 'Add' button highlighted with a red box. A red arrow points from this button to the 'Compound' column of a table. The table lists various chemical species, with 'Li[+]' and 'Cl[-]' highlighted at the bottom. Another red arrow points from the 'Li[+]' entry to the 'Parameter' dropdown menu, which is set to 'Beta0'. A third red arrow points from the 'Correlation' dropdown menu, which is set to 'Pitzer, de Lima and Moller'. A fourth red arrow points from the 'Parameters' table, which lists values for p1 through p10, all set to 0. The interface also includes a toolbar with 'Open', 'Save', 'Undo', 'Redo', 'Language', 'Help', 'About', and 'Predictive model parameters...' buttons, and a 'Comments' field at the bottom.

# Reactive Models Editor vs Calculator

- Add in the calculator all species that are able to precipitate or to be recombined

Visualization of parameters:  
Save all true species of the  
system as a \*.compounds file

Calculator:  
Open the \*.compounds file  
and choose non ionic species

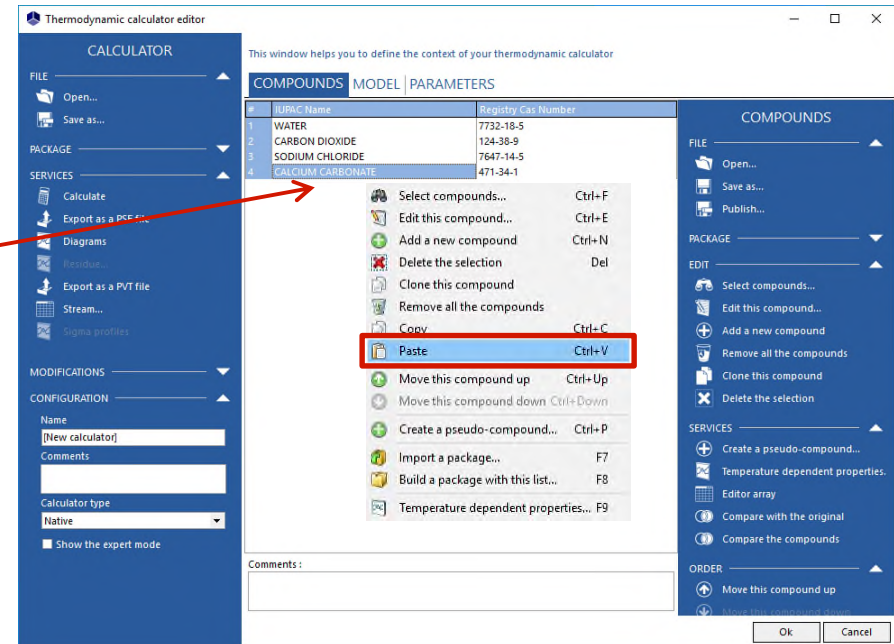
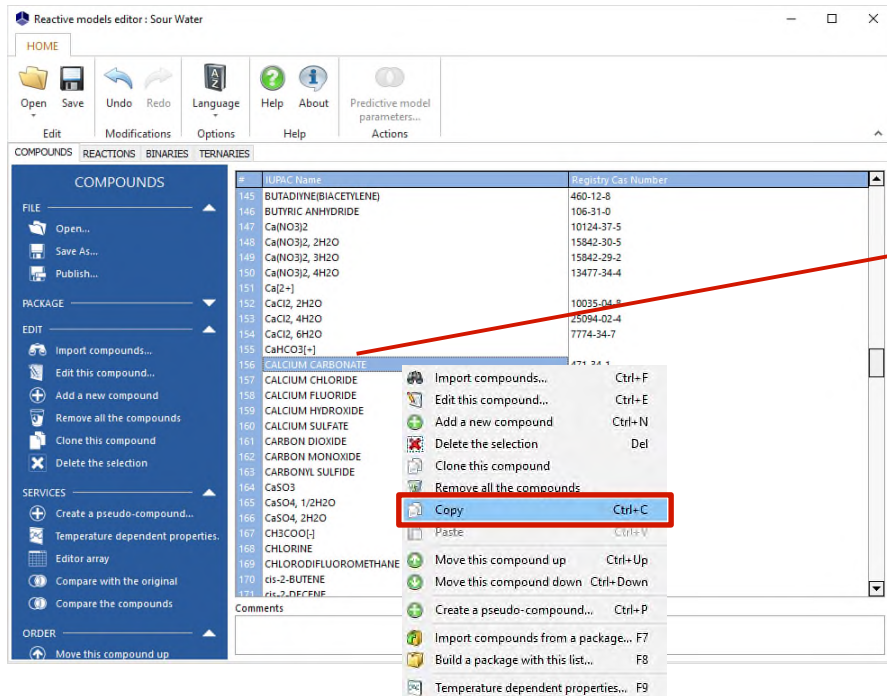


# Reactive Models Editor vs Calculator

- Add species of the reactive models editor to the calculator

Reactive models editor:  
Right click on a species,  
**Copy** (or CTRL + C)

Calculator:  
Right click in the component list,  
**Paste** (or CTRL + V)



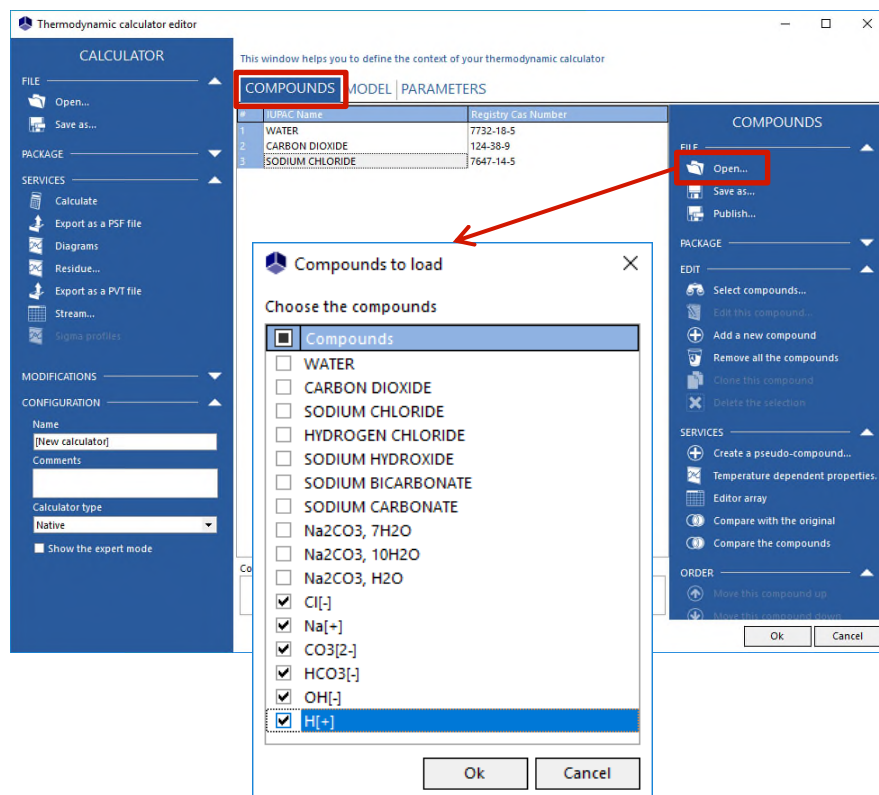


# Reactive Models Editor vs Calculator

## ■ Working directly with true species

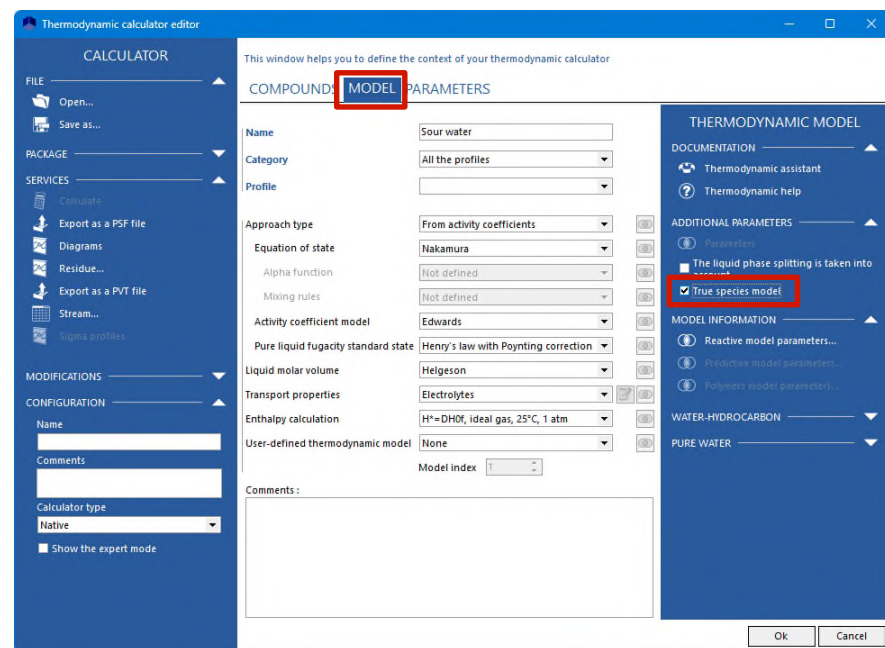
### Calculator - Compounds:

Open the \*.compounds file and choose ionic species in addition to apparent species defined by the user



### Calculator - Model:

Select the “true species model” option (no reaction taken into account)



Allows reaction description with controlled kinetics that are managed externally (e.g. ProSimPlus, Excel, Matlab...)



### ProSim SA

51, rue Ampère  
Immeuble Stratège A  
F-31670 Labège  
France

☎: +33 (0) 5 62 88 24 30



Software & Services In Process Simulation

[www.prosim.net](http://www.prosim.net)  
[info@prosim.net](mailto:info@prosim.net)



### ProSim, Inc.

325 Chestnut Street, Suite 800  
Philadelphia, PA 19106  
U.S.A.

☎: +1 215 600 3759