

# Getting started with Simulis® Thermodynamics

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

Software & Services In Process Simulation

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ProSim

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

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

The screenshot shows the 'Thermodynamic calculator editor' window. The 'COMPOUNDS' tab is selected and highlighted with a red box. The main area displays a table with three columns: '#', 'IUPAC Name', and 'Registry Gas Number'. The table contains three entries: 1. WATER (7732-18-5), 2. CARBON DIOXIDE (124-38-9), and 3. SODIUM CHLORIDE (7647-14-5). The 'COMPOUNDS' tab on the right sidebar is also highlighted with a red box, showing options like 'Select compounds...', 'Add a new compound', and 'Remove all the compounds'. The left sidebar contains various menu items like 'FILE', 'PACKAGE', 'SERVICES', 'MODIFICATIONS', and 'CONFIGURATION'. The bottom of the window has 'Ok' and 'Cancel' buttons.

#	IUPAC Name	Registry Gas Number
1	WATER	7732-18-5
2	CARBON DIOXIDE	124-38-9
3	SODIUM CHLORIDE	7647-14-5

# Simulis Thermodynamics: Visualization of parameters

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

The screenshot displays the 'Thermodynamic calculator editor' window. The 'MODEL' tab is selected and highlighted with a red box. The configuration is as follows:

- Name:** Sour water
- Category:** Heterogeneous approach - Electrolyte (highlighted with a red box)
- Profile:** Sour water (highlighted with a red box)
- 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:**  $H^* = DH_0^f$ , ideal gas, 25°C, 1 atm
- User-defined thermodynamic model:** None
- Model index:** 1

On the right side, the 'THERMODYNAMIC MODEL' configuration panel shows the 'Advanced' section with the following options:

- Use a specific model for pure water
- Water-hydrocarbons model
  - Sol A: 6.25043
  - Sol B: 4015.3
- The liquid phase splitting is taken into account
- True species model
- Reactive model parameters...

Buttons for 'Ok' and 'Cancel' are located at the bottom right of the window.

# 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

- 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 the 'Name' field is set to 'ULPDHS'. The 'Category' is set to 'All the profiles' and the 'Profile' is set to 'ULPDHS'. The 'Approach type' is 'From activity coefficients', the 'Equation of state' is 'Nakamura', and the 'Activity coefficient model' is 'ULPDHS'. The 'User-defined thermodynamic model' is set to 'None'. The 'Model index' is set to 1. The 'Predictive model parameters...' button in the 'MODEL INFORMATION' section is highlighted with a red box and an arrow pointing to it from the text on the right.

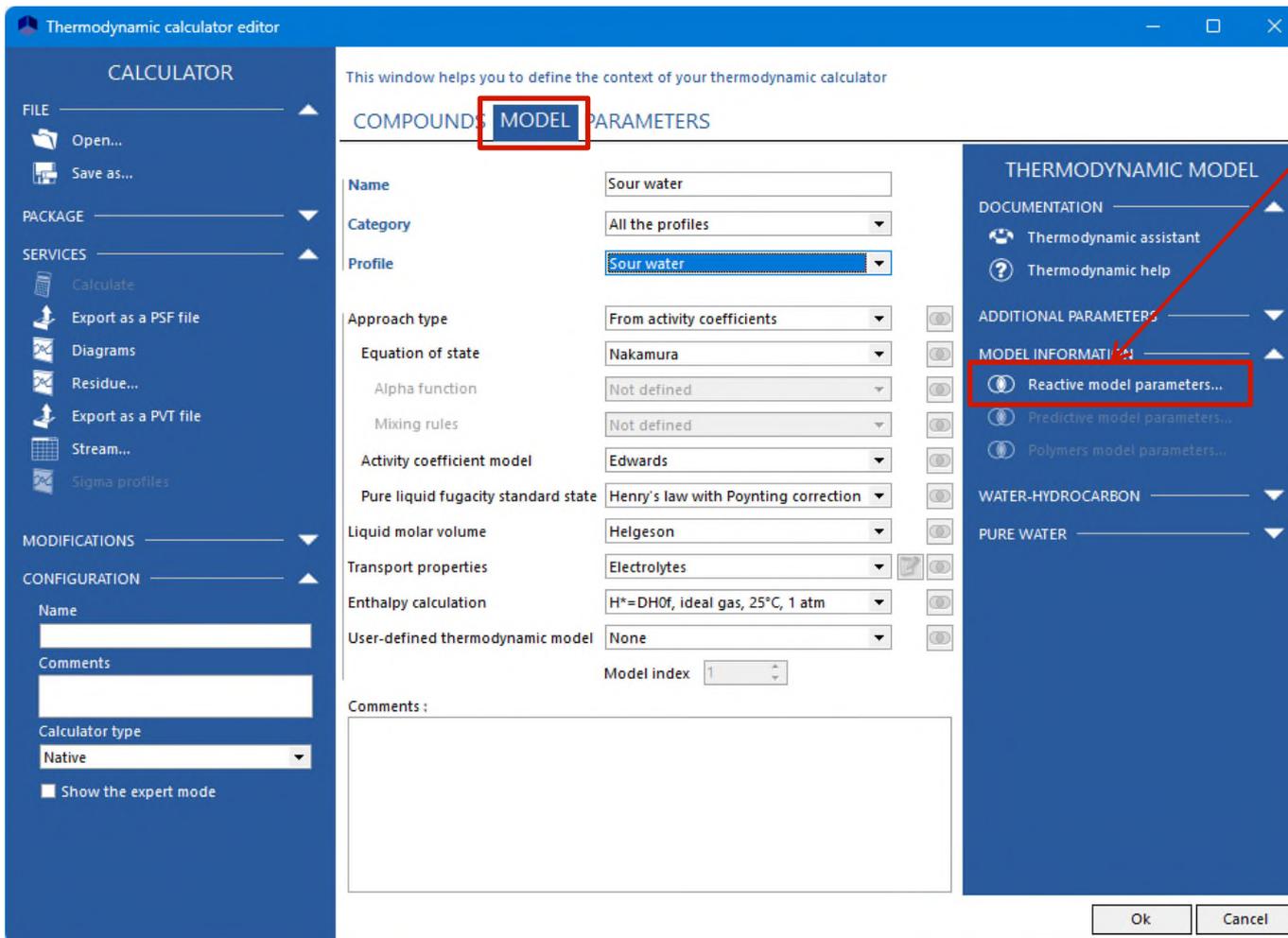
Click on the button  
“Predictive model  
parameters...”



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

Number	Compound name	CAS number
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	Na <sub>2</sub> CO <sub>3</sub> , 7H <sub>2</sub> O	
9	Na <sub>2</sub> CO <sub>3</sub> , 10H <sub>2</sub> O	6132-02-1
10	Na <sub>2</sub> CO <sub>3</sub> , H <sub>2</sub> O	5968-11-6
11	Cl[-]	
12	Na[+]	
13	CO <sub>3</sub> [2-]	
14	HCO <sub>3</sub> [-]	
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	$\text{Na}_2\text{CO}_3, 7\text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + 7\text{H}_2\text{O}$
10	$\text{Na}_2\text{CO}_3, 10\text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + 10\text{H}_2\text{O}$
11	$\text{Na}_2\text{CO}_3, \text{H}_2\text{O} \rightleftharpoons 2\text{Na}^{+} + \text{CO}_3^{=} + \text{H}_2\text{O}$

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

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:

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**

Reactive models editor (ReadOnly)

HOME

About Predictive model parameters... Help Actions

COMPOUNDS REACTIONS **BINARIES** TERNARIES

**INTERACTIONS**

INTERACTIONS

- Add
- Delete
- Remove all
- Search...

ORDER

- Move up
- Move down

The interactions are symmetric.

#	Compound	Compound
1	CARBON DIOXIDE	CARBON DIOXIDE
2	CARBON DIOXIDE	HCO3[-]
3	H[+]	Cl[-]
4	CARBON DIOXIDE	Na[+]
5	Cl[-]	Na[+]
6	OH[-]	Na[+]
7	CO3[2-]	Na[+]
8	HCO3[-]	Na[+]
9	CARBON DIOXIDE	Cl[-]

Parameter: Beta0

Correlation: Holmes

Value =  $p_1 + p_2 \cdot \ln\left(\frac{P_{\text{beta0}}}{P_0}\right) + p_3 \cdot (P_{\text{beta0}} - P_0) + p_4 \cdot (T_{\text{K}} - T_0) + p_5 \cdot (P_{\text{beta0}} - P_0)$

Parameters

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

Comments:

Ok Cancel

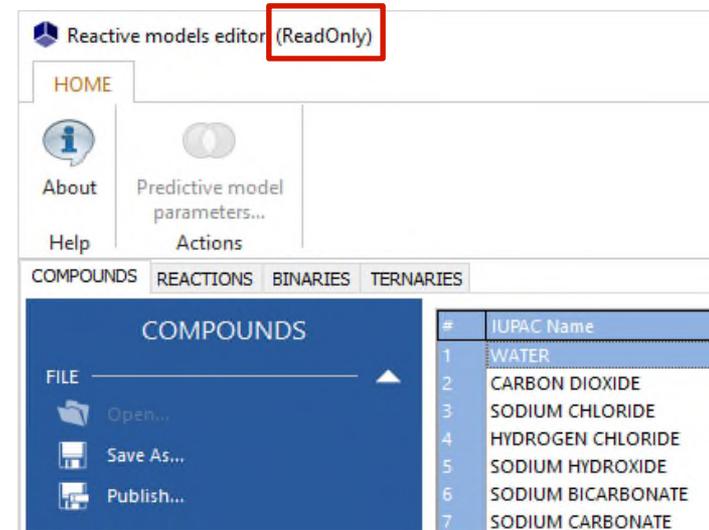
List of parameters of the chosen model

Correlation for the selected binary (or ternary) interaction parameter

Parameters

# 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)



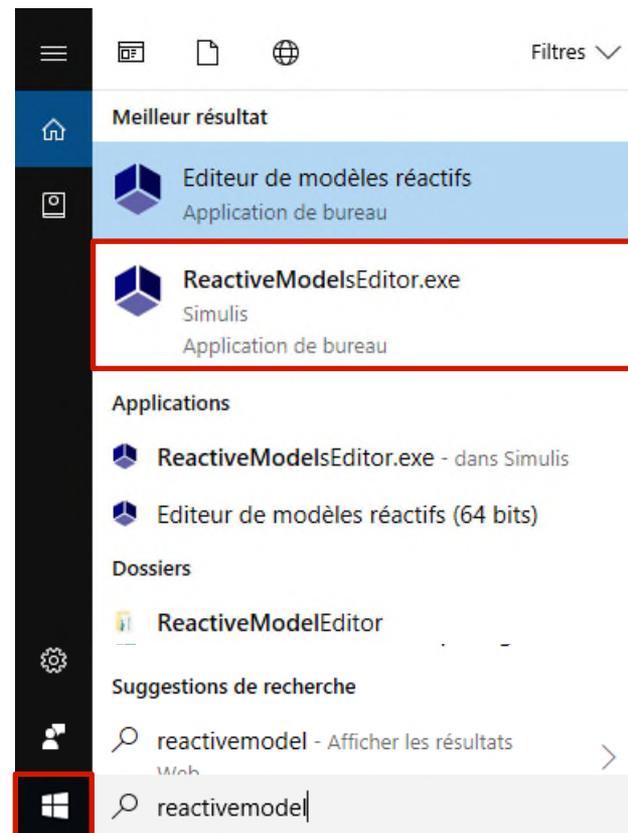
- Visualization of species, equilibrium reactions and interactions taken into account by the model
- Possibility to add systems or to modify parameters of existing systems



Use of the reactive models editor

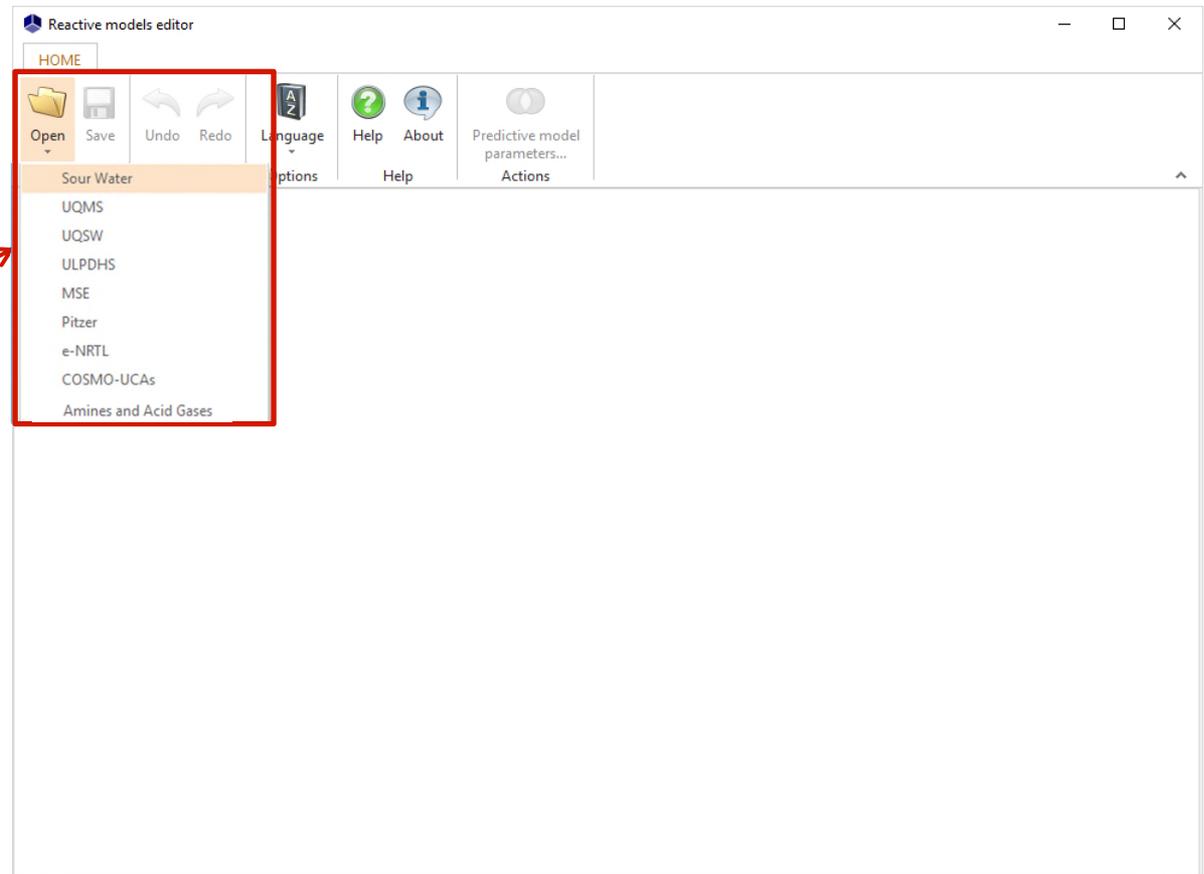
# Reactive Models Editor

- 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



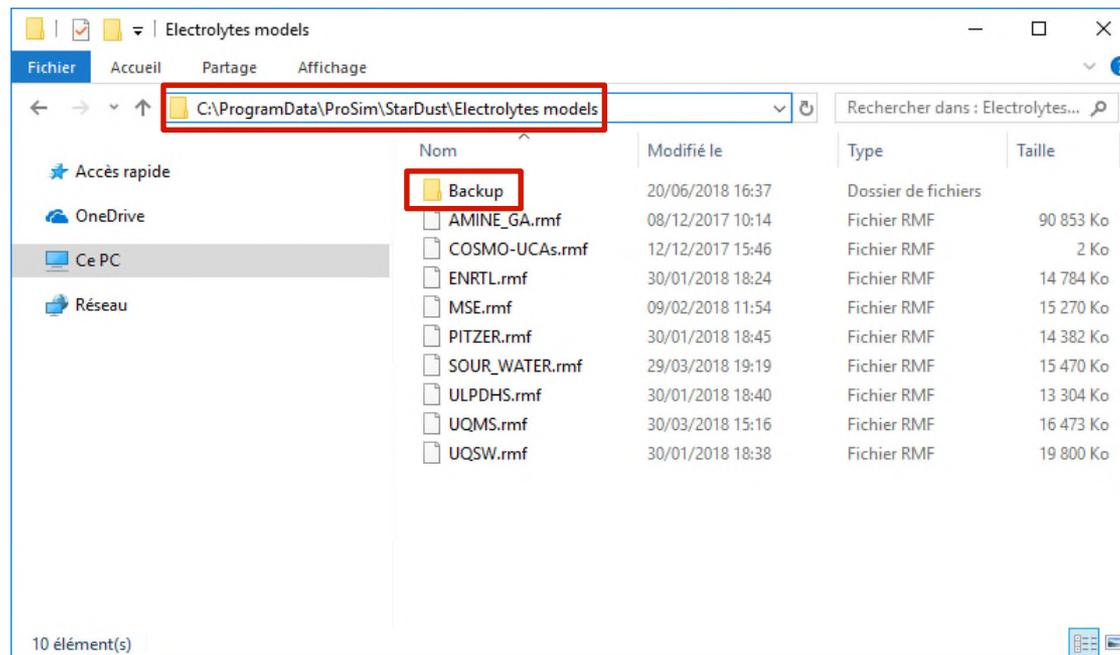
Access to databases  
of reactive model  
parameters

# 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

Reactive models editor : Sour Water

HOME

Open Save Undo Redo Language Help About Predictive model parameters...

Edit Modifications Options 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

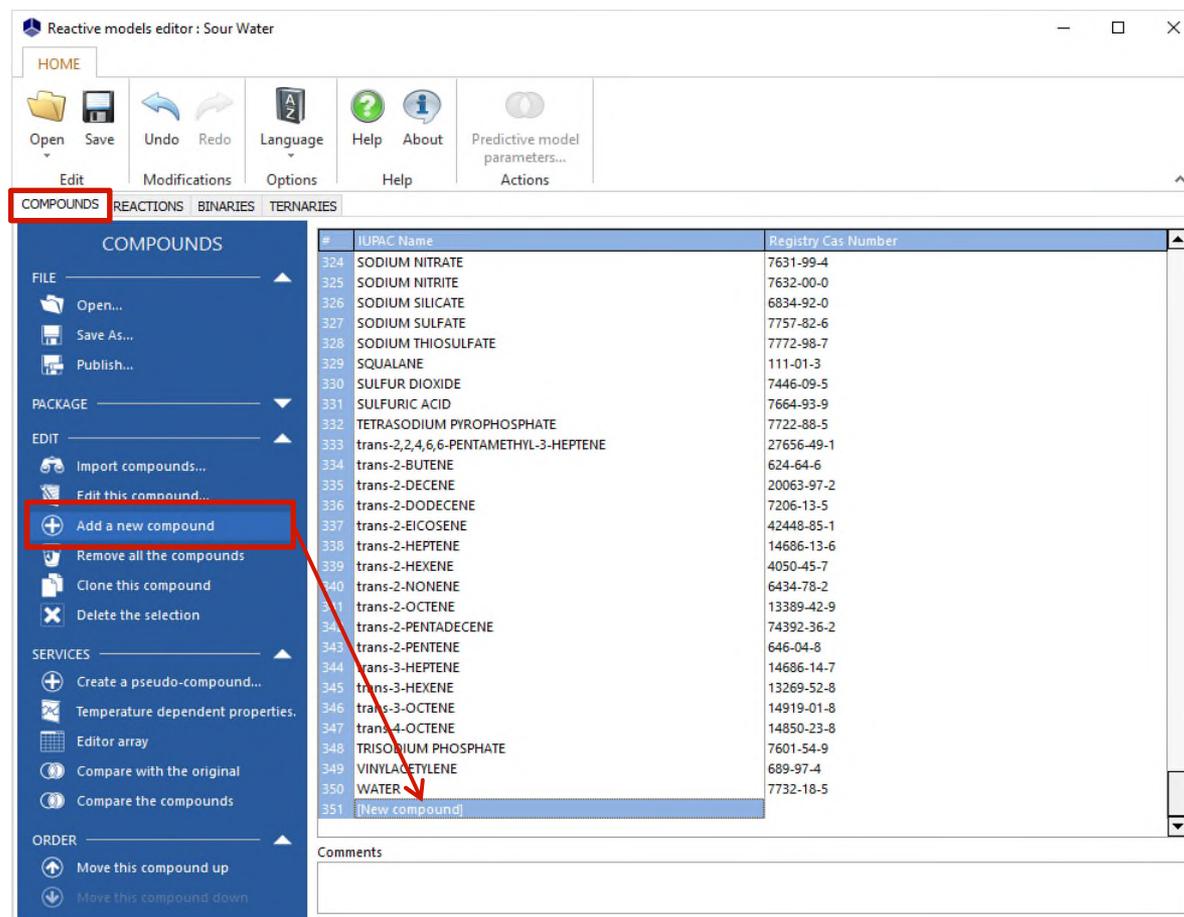
- Move this compound up
- Move this compound down

#	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

Comments

# Reactive Models Editor

- Add a species



Reactive models editor : Sour Water

HOME

Open Save Undo Redo Language Help About Predictive model parameters...

Edit Modifications Options 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

#	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	VINYLAETHYLENE	689-97-4
350	WATER	7732-18-5
351	[New compound]	

Comments

# 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 : Sour Water

HOME

Open Save Undo Redo Language Help About Predictive model parameters...

Edit Modifications Options 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
61	$\text{MgCl}_2, \text{H}_2\text{O} \rightleftharpoons \text{Mg}^{2+} + 2\text{Cl}^- + \text{H}_2\text{O}$
62	$\text{CaF}_2 \rightleftharpoons \text{Ca}^{2+} + 2\text{F}^-$
63	$\text{CaSO}_3 \rightleftharpoons \text{Ca}^{2+} + \text{SO}_3^{2-}$
64	$\text{NaF} \rightleftharpoons \text{Na}^+ + \text{F}^-$
65	$\text{Ca}(\text{NO}_3)_2 \rightleftharpoons \text{Ca}^{2+} + 2\text{NO}_3^-$
66	$\text{Ca}(\text{NO}_3)_2, 2\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{NO}_3^- + 2\text{H}_2\text{O}$
67	$\text{Ca}(\text{NO}_3)_2, 3\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{NO}_3^- + 3\text{H}_2\text{O}$
68	$\text{Ca}(\text{NO}_3)_2, 4\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{NO}_3^- + 4\text{H}_2\text{O}$
69	$\text{NH}_4\text{NO}_3 \rightleftharpoons \text{NH}_4^+ + \text{NO}_3^-$
70	$\text{KOH} \rightleftharpoons \text{K}^+ + \text{OH}^-$
71	$\text{NaNO}_3 \rightleftharpoons \text{Na}^+ + \text{NO}_3^-$
72	$\text{Mg}(\text{NO}_3)_2 \rightleftharpoons \text{Mg}^{2+} + 2\text{NO}_3^-$
73	$\text{MgSO}_3 \rightleftharpoons \text{Mg}^{2+} + \text{SO}_3^{2-}$
74	$\text{MgSO}_3, 3\text{H}_2\text{O} \rightleftharpoons \text{Mg}^{2+} + \text{SO}_3^{2-} + 3\text{H}_2\text{O}$
75	$\text{MgSO}_3, 6\text{H}_2\text{O} \rightleftharpoons \text{Mg}^{2+} + \text{SO}_3^{2-} + 6\text{H}_2\text{O}$
76	$\text{Mg}(\text{OH})_2 \rightleftharpoons \text{Mg}^{2+} + 2\text{OH}^-$
77	$\text{HNO}_2 \rightleftharpoons \text{H}^+ + \text{NO}_2^-$
78	$\text{KNO}_3 \rightleftharpoons \text{K}^+ + \text{NO}_3^-$
79	$\text{KNO}_2 \rightleftharpoons \text{K}^+ + \text{NO}_2^-$
80	$\text{NaNO}_2 \rightleftharpoons \text{Na}^+ + \text{NO}_2^-$
81	$\text{K}_2\text{CO}_3 \rightleftharpoons 2\text{K}^+ + \text{CO}_3^{2-}$
82	$\text{KHCO}_3 \rightleftharpoons \text{K}^+ + \text{HCO}_3^-$
83	$\text{CaCl}_2, 4\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{Cl}^- + 4\text{H}_2\text{O}$
84	$\text{CaCl}_2, 2\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + 2\text{Cl}^- + 2\text{H}_2\text{O}$
85	$\text{LiCl} \rightleftharpoons \text{Li}^+ + \text{Cl}^-$
86	$\text{LiCl}, \text{H}_2\text{O} \rightleftharpoons \text{Li}^+ + \text{Cl}^- + \text{H}_2\text{O}$
87	$\text{LiCl}, \text{H}_2\text{O} \rightleftharpoons \text{Li}^+ + \text{Cl}^- + 2\text{H}_2\text{O}$
88	[New reaction]

Comments:

# 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

Reaction

REACTION

COMPOUNDS

- Add
- Clone
- Delete
- Clear

ORDER

- Move up
- Move down

MODIFICATIONS

- Undo
- Redo

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

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

Comments:

Parameters

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

Comments:

Ok Cancel

# 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

The screenshot shows the 'Reactive models editor : Sour Water' window. The 'BINARIES' tab is selected, displaying a list of compounds in a table. The 'Add' button in the 'INTERACTIONS' panel is highlighted. The 'Parameter' dropdown is set to 'Beta0' and the 'Correlation' dropdown is set to 'Pitzer, de Lima and Moller'. The 'Parameters' table shows values for p1 through p10.

Compound	Compound
60	F[-]
61	HYDROGEN FLUORIDE
62	HYDROGEN FLUORIDE
63	HYDROGEN FLUORIDE
64	H[+]
65	Ca[2+]
66	Ca[2+]
67	Na[+]
68	Ca[2+]
69	NH4[+]
70	OH[-]
71	Na[+]
72	Mg[2+]
73	SO3[2-]
74	HSO3[-]
75	K[-]
76	K[+]
77	Na[+]
78	K[-]
79	K[+]
80	HYDROGEN SULFIDE
81	HYDROGEN SULFIDE
82	HYDROGEN SULFIDE
83	K[+]
84	Li[+]
85	Cl[-]

Parameter	Value
p1	0
p2	0
p3	0
p4	0
p5	0
p6	0
p7	0
p8	0
p9	0
p10	0

4. Parameters of the correlation

# 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 (ReadOnly)

COMPOUNDS

IUPAC Name	Registry Gas Number
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 Na <sub>2</sub> CO <sub>3</sub> , 7H <sub>2</sub> O	6132-02-1
9 Na <sub>2</sub> CO <sub>3</sub> , 10H <sub>2</sub> O	5969-11-6
10 Na <sub>2</sub> CO <sub>3</sub> , H <sub>2</sub> O	
11 Cl[-]	
12 Na[+]	
13 CO <sub>3</sub> [2-]	
14 HCO <sub>3</sub> [1-]	
15 OH[1-]	
16 H[+]	

Thermodynamic calculator editor

COMPOUNDS

IUPAC Name	Registry Gas Number
1 WATER	7732-18-5
2 CARBON DIOXIDE	124-38-9
3 SODIUM CHLORIDE	7647-14-5

Compounds to load

Choose the compounds

Compounds

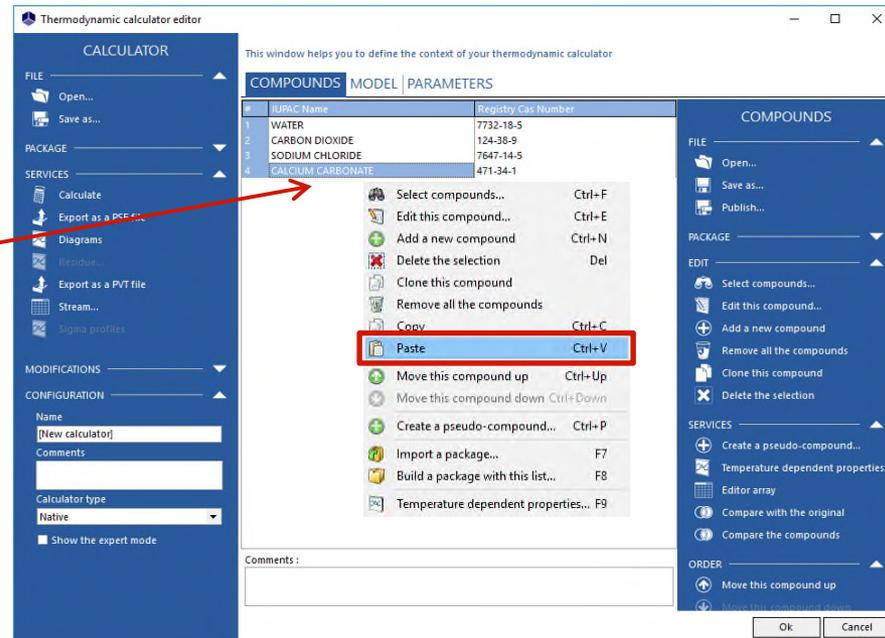
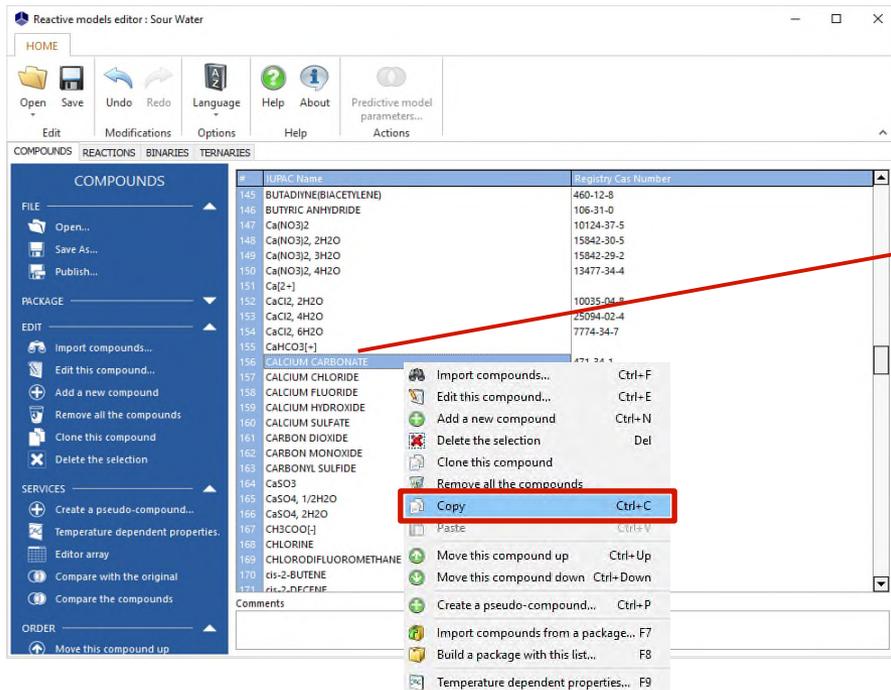
- WATER
- CARBON DIOXIDE
- SODIUM CHLORIDE
- HYDROGEN CHLORIDE
- SODIUM HYDROXIDE
- SODIUM BICARBONATE
- SODIUM CARBONATE
- Na<sub>2</sub>CO<sub>3</sub>, 7H<sub>2</sub>O
- Na<sub>2</sub>CO<sub>3</sub>, 10H<sub>2</sub>O
- Na<sub>2</sub>CO<sub>3</sub>, H<sub>2</sub>O
- Cl[-]
- Na[+]
- CO<sub>3</sub>[2-]
- HCO<sub>3</sub>[1-]
- OH[1-]
- H[+]

# 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)

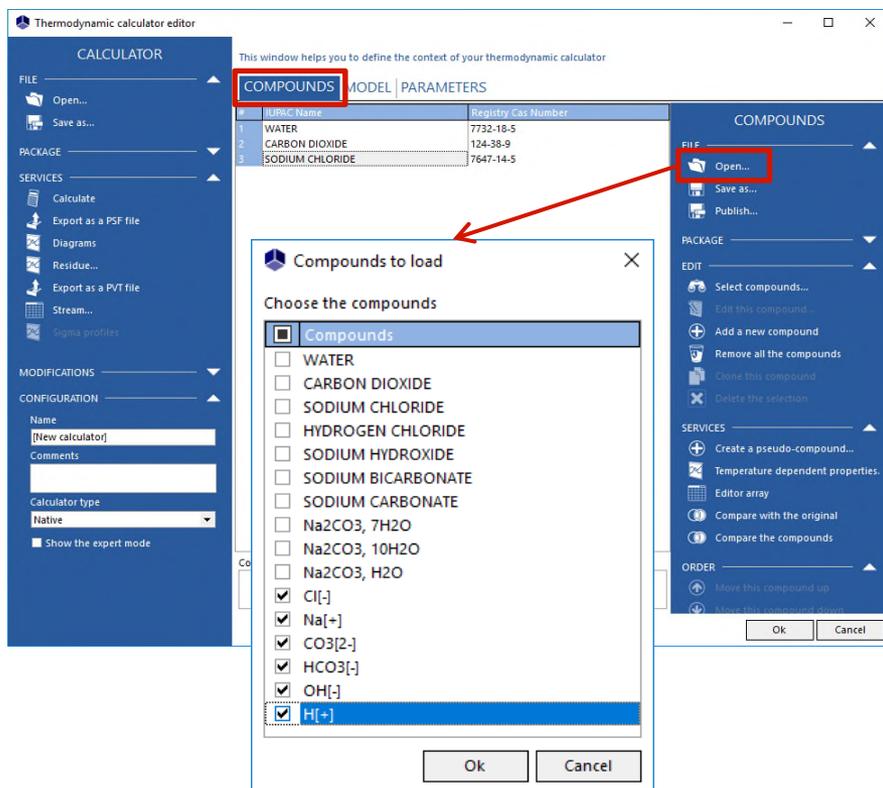
Calculator:  
Right click in the component list,  
**Paste** (or CTRL + V)



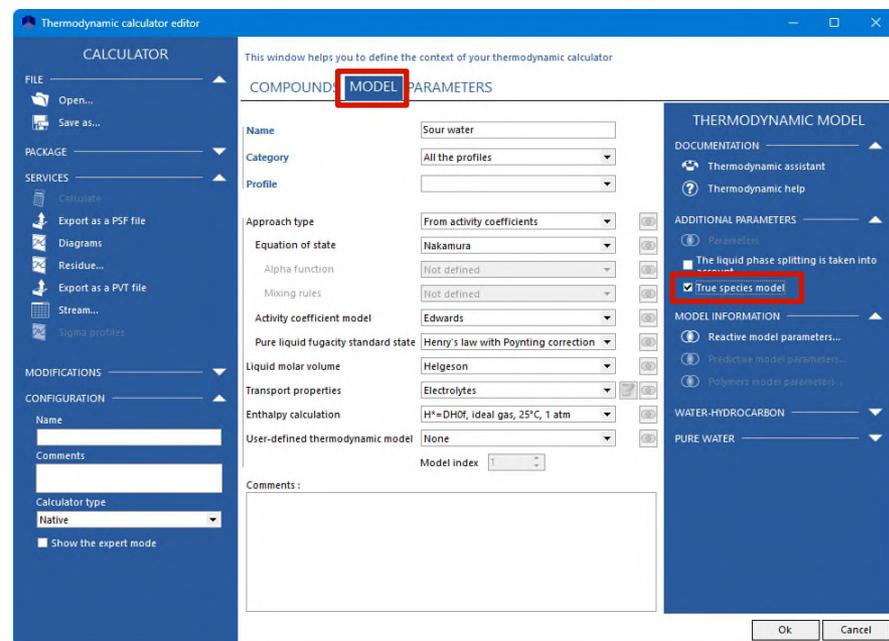
# Reactive Models Editor vs Calculator

## 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...)



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# ProSim

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