

Manual

Calculation of thermodynamic properties of aqueous electrolyte solutions

Exit Help About Notepad Calculator ELS_input.txt

Title Electrolyte activity coefficients Osmotic coefficients and Water activity Ionic activity coefficients

Calculation of
Thermodynamic properties
of aqueous electrolyte solutions:

using the
Pitzer-Mayorga and Lin-Tseng-Lee models for
Electrolyte activity coefficients,
Osmotic coefficients and water activity,

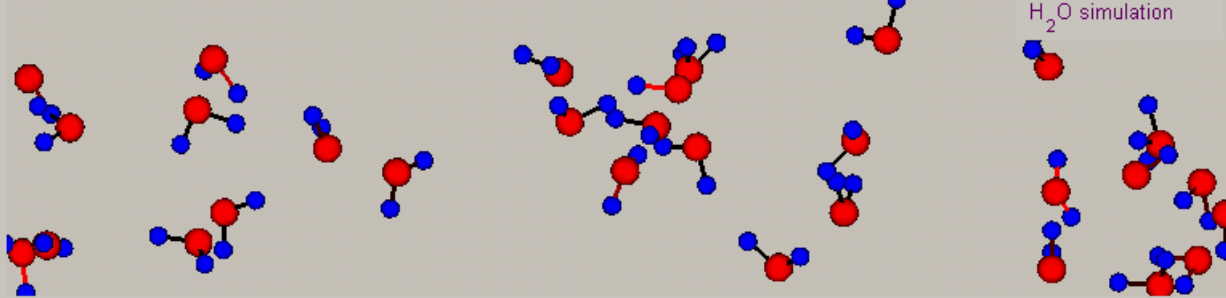
and the
Millero-Pitzer method for
Ionic activity coefficients

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H₂O simulation



The image shows a molecular simulation of water (H₂O). It features several water molecules, each consisting of one red sphere (oxygen) and two blue spheres (hydrogen) connected by lines. The molecules are arranged in a disordered, liquid-like structure. The background is a light gray. The text 'H₂O simulation' is written in purple in the upper right corner of the simulation area.

Introduction

The **Electrolytes program** is a program for calculating some thermodynamic properties of electrolyte solutions and ions. It employs three thermodynamic solution models to represent data in the most precise and convenient way. The **Electrolytes program** is oriented for the calculation of: **mean ionic electrolyte activity coefficients, electrolyte osmotic coefficients and corresponding water activities, and ionic activity coefficients.**

Electrolytes program has been developed under the Windows 9x, 2000 and Windows NT/XP operating systems. The 32-bit version was built by Borland Delphi 5.0. The first version program was released on December 5, 2003 as version 1.0.

Electrolytes program is composed of the following files:

- **electrolytes.exe** – the program exe-file
- **ELS_input.txt** – **input file**
- **ELS_help.chm** – the help file

If you have any suggestions, or know of any models and additional parameters that you would like to see added to the repertoire, please send us e-mail. We'll gladly attend to your comments since we wish to continue development and support of this program.

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Using Electrolytes.exe program

The **Electrolytes.exe** program has easy point-and-click interface which allows the user to:

- Choose from 2 built-in electrolyte solution thermodynamic properties models to calculate the activity electrolyte coefficients, the osmotic electrolyte coefficients and water activity in individual electrolyte solutions on two equations. Models are the Pitzer-Mayorga [6] and Lin-Tseng-Lee [22] models
- Calculate the ionic activity coefficients, using Millero-Pitzer equation [26]
- Inter-compare models
- Inter-compare electrolyte properties within a selected model
- Inter-compare ionic activity coefficients.
- Copy plots directly to the clipboard to use in another Windows application
- Save all calculation results in Rich Text Format file
- Read simple ASCII data files
- Use comments in input file and in final output
- Scale, translate, sort, remove, edited data set by hand similarly to a spreadsheet
- Receive and store calculated values in tabular and graphical formats

The **Electrolytes.exe** program has 3 main tabbed pages:

- ❑ **Electrolyte activity coefficients**
- ❑ **Osmotic coefficients and water activity**
- ❑ **Ionic activity coefficients**

Like all Windows applications, you can also select items off of the menu bar to accomplish certain tasks.

The toolbar gives access to frequently used commands

- ✓ **Exit**
- ✓ **Help**
- ✓ **About**
- ✓ **Notepad**
- ✓ **Calculator**

Background

It is necessary to know the activity coefficients and osmotic coefficients of electrolytes and the activity of water when studying the thermodynamics of electrolyte solutions, acid - basic equilibria or metal-ligand complex formation. These can present considerable problems since there are no complete and critically evaluated tables for such thermodynamic values for electrolyte solutions. Most of the tabular data which exist are out-of-date and, in addition, it is inconvenient to use tabulated values since approximation methods must be necessary to calculate interpolated values. As a result, it is preferable to use simple and adequate equations to calculate the concentration dependence of the values over as wide a concentration range as possible.

There are various models to describe the concentration dependence of activity electrolyte activity coefficients, ionic activity coefficients, osmotic coefficients and water activity.

Meissner and Kusik introduced the first model [1-2] to calculate activity and osmotic coefficients. This model was convenient for calculation but it has the large standard deviation of up to 10 %.

Bromley [3] modified the Debye-Huckel equation by including an additional term as a function of ionic strength. That allowed the calculation of activity and osmotic electrolyte coefficients for 1-1- electrolytes with an accuracy of about 5 % up to 6 mol/kg. However this model is only valid up to 1 mol/kg for higher orders of electrolytes.

Stokes and Robinson introduced a solvation model. They modified the Debye-Huckel equation by including effective hydration parameters [4]. This described 1-1- and 1-2- electrolytes with an accuracy of between 5 - 8 % up to 4 mol/kg.

Pitzer modified the Debye-Huckel equation by taking into account long-range and short-range electrostatic interactions. The short-range electrostatic interactions were considered as binary tabulated parameters [5-6]. This three-parametrical model described concentration dependences of activity and osmotic electrolyte coefficients for 1-1, 1-2, 2-1, 3-1, 4-1 and 5-1- electrolytes with accuracy about 5 % up to 3-6 mol/kg, but it did not adequately describe the concentration dependences for 2-2, 2-3 electrolytes. Another model was therefore considered which introduced additional coefficients in place of one of the Pitzer's parameter [7]. Later Pitzer and Simonson derived a new model based on mole-fractions to calculate activity coefficients in concentrated solutions up to fused salts [8].

The ASOG (Analytical Solution of Groups) group contribution method was used by Kawaguchi et al. [9] to calculate the activity coefficients for 1-1 and 1-2- electrolytes over a wide concentration range.

Cruz and Renon [10] used modified NRTL (Non-Random Two Liquid) equations (which were also used in reference [11]) to take account of short-range interactions. The equations derived allow the prediction of activity and osmotic coefficients of individual electrolytes up to 3-6 mol/kg. with an accuracy 0.56 % for 1-1 electrolytes and of 2.5-2.9 % for other types of electrolytes.

Chen et al. [12-13] used:

- 1) modified Pitzer equations, which take into account long-range interactions;
- 2) NRTL-type equations for short-range interactions.

They produced two-parametric equations that predict activity and osmotic electrolyte coefficients of individual and mixed electrolytes over a wide concentration range (up to 16-20 mol/kg) with an accuracy of 0.9 % for 1-1 -electrolytes and 3.0-7.0 % for other types of electrolytes.

Kim and Frederick [14-15] modified the Pitzer equation to be able to calculate the activity and osmotic coefficients over a wider concentration range than the original Pitzer equation.

Jaretun and Aly [16-17] used the original four- and three-parametric models to calculate activity and osmotic coefficients over a wide concentration range (up to 20 -25 mol/kg). Their models were based on application the "Local composition expressions" - the Percus - Yevick approximation to the Ornstein - Zernike equations. Model [16] predicts individual activity coefficients with an accuracy of 0.005 - 0.007 for 1-1, 1-2 and 3-1- electrolytes and 0.10-0.05 for 2-1, 2-2 and other electrolyte types. Osmotic coefficients are predicted with accuracy about 0.004 - 0.008 for 1-1, 1-2 and 3-1 electrolytes, and 0.05 for 2-1, 2-2 and other electrolyte types. However this model requires the use of 4 tabulated parameters. Model [17] allows the calculation of activity and osmotic coefficients of mixed electrolyte systems to a reasonable accuracy.

Narayanan and Ananth [18] produced a modified model, using the “Self-Consistent Composition Method” (SCCM) [19], to calculate coefficients of individual and mixed electrolyte solutions over a wide concentration range up to 20 mol/kg. Their model allows prediction with an accuracy of 0.5 % for 1-1-electrolyte, and 1.5-2.1 % for other electrolyte types in the concentration range up to 6 mol/kg. The activity coefficients of individual electrolytes are predicted with accuracies of about 0.01 for 1-1 electrolytes and 0.01- 0.06 for 2-1, 2-2 and other types. This SCCM model also allows the calculation of coefficients of mixed electrolyte systems with an accuracy of 1-5 %. The drawback of this model is the difficult formalism of the calculation of cross interactions, and it is also necessary to use 3 or more tabulated parameters in calculation of the thermodynamic properties of mixed electrolyte systems.

Correa et al. [20] derived a modified ASOG method with group contributions to calculate the water activity in individual and mixed electrolyte solutions. This method allows prediction of the water activity for individual electrolyte solutions with accuracy 0.02 - 0.70 %, and of mixed electrolyte solutions with an accuracy of 2 - 5 %.

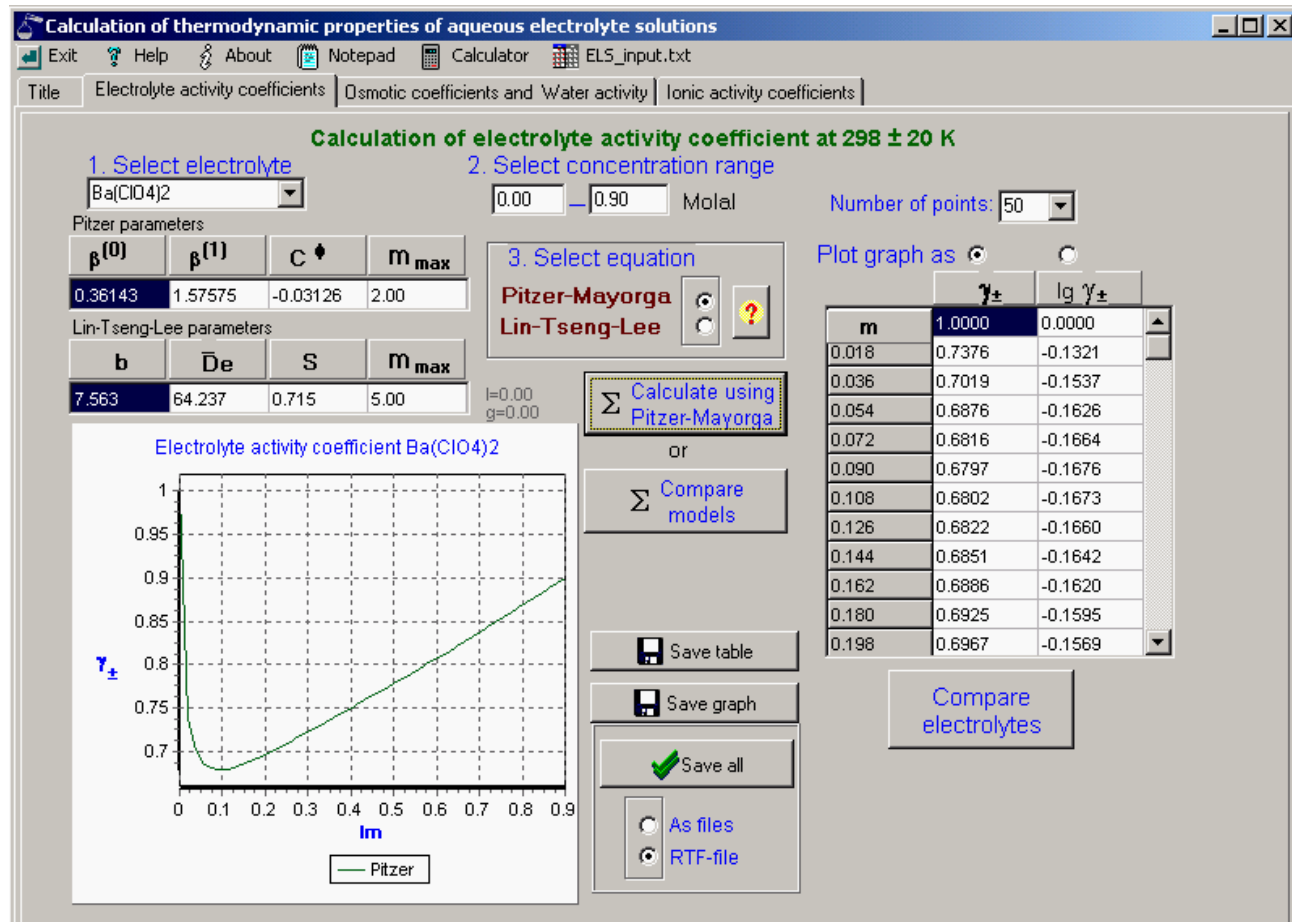
Chou and Tanioka [21] used the original one-parametrical equation to calculate the vapour pressure and water activity for single and mixed electrolyte systems over the temperature range of 298 - 374 K in a wide concentration range (up to 15 mol/kg). The model predicted water activity with an accuracy better than 0.17 % for 1-1- electrolytes (with Pitzer the accuracy is 0.25 %), 0.32 % for 2-1- electrolytes (Pitzer, 0.98 %), 0.26 % for 1-2- electrolytes (Pitzer, 0.45 %); 0.40 % for 2-2- electrolytes; 0.08 % for 3-1- electrolytes (Pitzer, 0.70 %), and 0.20 - 0.25 % for other electrolyte types.

Lin, Tseng and Lee [22] (in a further development and simplification of an earlier Lin, Lee, Tseng model [23]) used a three-parametrical model to calculate the activity and osmotic coefficients over a wider concentration range in comparison to the Pitzer equations. Many authors noticed that the overwhelming majority of researchers ignore the decrease of water dielectric constant as electrolyte concentration increased. This problem is discussed in details in reference [24]. Some authors have suggested using equivalent dielectric constants for a wide concentration range. This model allows the calculation of activity osmotic electrolyte coefficients with an accuracy 1.5 % - 6.0 % for all electrolyte types.

An analysis of the different models used to calculate activity and osmotic coefficients of electrolyte solutions shows (**Tables 1-4, Appendix**) that Pitzer-Mayorga model [5-6] and Lin-Tseng-Lee model [22] are the most convenient and consistent. These models are therefore used in this program. Noted it is recommended to use Pitzer-Mayorga model. In case of absence of Pitzer’s parameters it is necessary to use Lin-Tseng-Lee parameters.

Electrolyte activity coefficients

An 'Electrolyte activity coefficients' tabbed page is shown below



The Pitzer-Mayorga equation [6] used to calculate the electrolyte activity coefficients is:

$$\ln \gamma_{\pm} = -|Z_m Z_x| A_{\phi} \left[\frac{I^{1/2}}{1 + bI^{1/2}} + \frac{2}{b} \ln(1 + bI^{1/2}) \right] + m \left(\frac{2\nu_M \nu_X}{\nu} \right) B_{MX}^{\gamma} + m^2 \frac{2(\nu_M \nu_X)^{3/2}}{\nu} C_{MX}^{\gamma}$$

where

$$B_{MX}^{\gamma} = 2\beta_{MX}^{(0)} + \frac{2\beta_{MX}^{(1)}}{\alpha^2 I} \left[1 - e^{-\alpha I^{1/2}} (1 + \alpha I^{1/2} - (1/2)\alpha^2 I) \right]$$

$$C_{MX}^{\gamma} = (3/2)C_{MX}^{\phi}$$

$$A_{\phi} = (1/3)(2\pi N_0 d_w / 1000)^{1/2} (e^2 / D_e kT)^{3/2}$$

Critically selected Pitzer parameters [25] were used in most cases.

The Lin-Tseng-Lee equation [22], which is also used to calculate the electrolyte activity coefficients, is:

$$\ln \gamma_{\pm} = \ln \gamma_{\pm}^{\text{pdh}} + \ln \gamma_{\pm}^{\text{sv}}$$

where

the Debye-Huckel term $\ln \gamma_{\pm}^{\text{(pdh)}}$ represents the Pitzer term:

$$\ln \gamma_{\pm}^{\text{pdh}} = -zwA_{\phi} \left[\frac{I^{1/2}}{1 + bI^{1/2}} + \frac{2}{b} \ln(1 + bI^{1/2}) \right]$$

and short-range interactions $\ln \gamma_{\pm}^{\text{sv}}$ represent the term:

$$(\nu_+ + \nu_-) \ln \gamma_{\pm}^{\text{sv}} = S \cdot m^{2n}$$

b , \overline{D}_e , S , and n - individual parameters for each electrolyte.

Note also that $n=0.645$ for all the 144 systems studied by Lin-Tseng-Lee [22]. The \overline{D}_e parameter is used to calculate Debye-Huckel parameter A_ϕ :

$$A_\phi = (1/3)(2\pi N_0 d_w / 1000)^{1/2} (e^2 / D_e kT)^{3/2}$$

Calculate and save results

To calculate the concentration dependence of electrolyte activity coefficients

- ❖ Select electrolyte
- ❖ Select concentration (molal)
- ❖ Select equation type to calculate electrolyte activity coefficients
- ❖ Indicate the number of point
- ❖ Indicate desired type of "**Plot graph as**"
- ❖ Press the "**Calculate**" button

Graphs may be plotted using the coordinates

- ❖ $\ln \gamma_\pm$
- ❖ γ_\pm

You can save

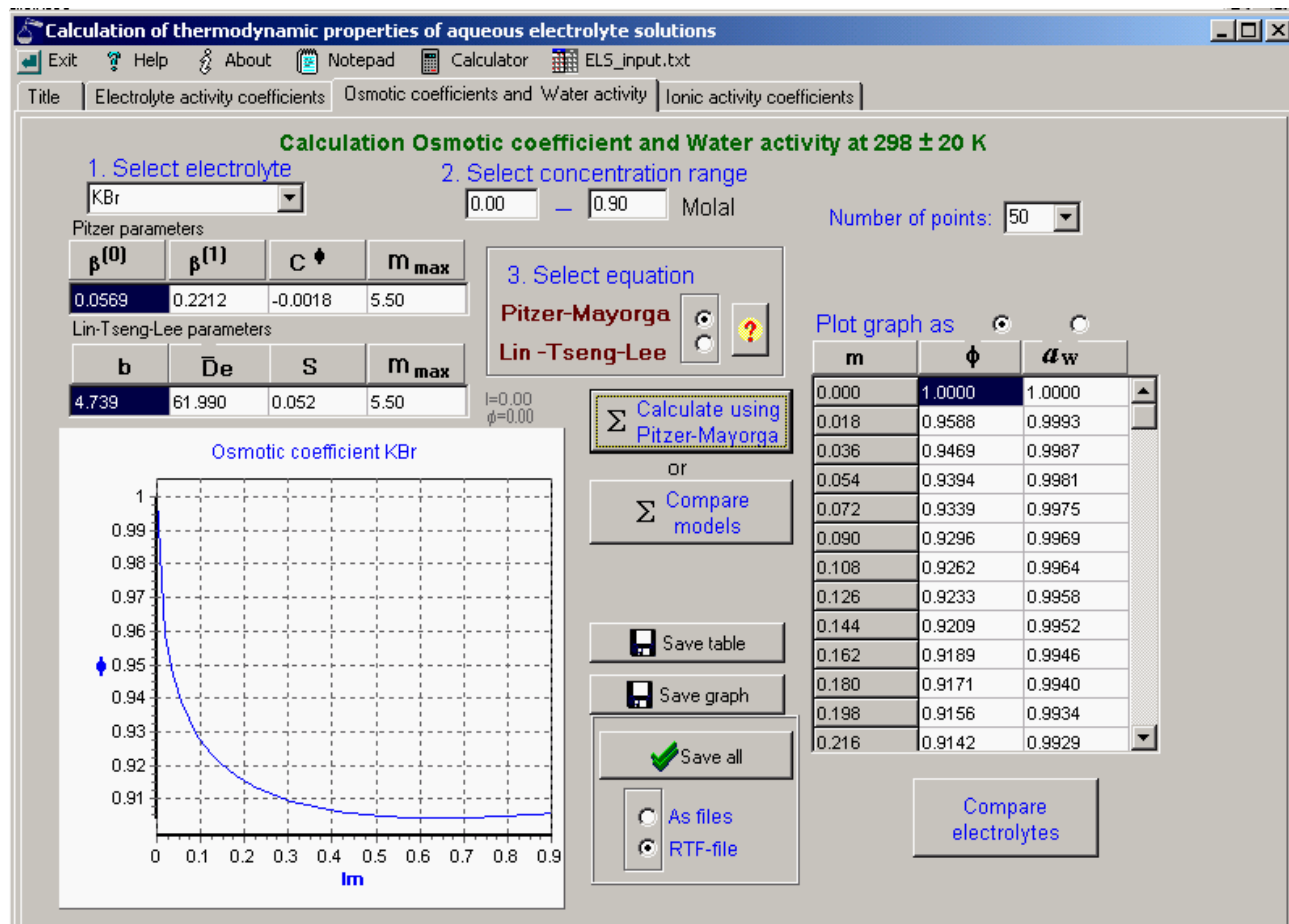
- ❖ the table of the calculated values as text file (*.txt) and to a clipboard simultaneously
- ❖ the plot as a graphic file (*.bmp) and to a clipboard simultaneously
- ❖ all results together (table, plot, comments) as a protocol in RTF format

You can also compare

- ❖ different models for a selected electrolyte "**Compare models**"
- ❖ different electrolytes for a selected equation "**Compare electrolytes**"

Osmotic electrolyte coefficients and water activity

An 'Osmotic electrolyte coefficients and water activity' tabbed page is shown below



The Pitzer-Mayorga equation [6] used to calculate osmotic electrolyte coefficients and water activity is:

$$\phi - 1 = |z_M z_X| f^\phi + m(2\nu_M \nu_X / \nu) B_{MX}^\phi + m^2 [2(\nu_M \nu_X)^{3/2} / \nu] C_{MX}^\phi,$$

where

$$f^\phi = -A_\phi I^{1/2} / (1 + bI^{1/2})$$

$$B_{MX}^\phi = \beta_{MX}^{(0)} + \beta_{MX}^{(1)} \exp(-\alpha I^{1/2})$$

The Lin-Tseng-Lee equation [22] is:

$$\phi = 1 - zwA_\phi \frac{I^{1/2}}{1 + bI^{1/2}} + \frac{S}{\nu_+ + \nu_-} \frac{2n}{2n + 1} m^{2n}$$

The water activity a_w is calculated using the well-known equation:

$$\phi = \frac{-1000}{\nu m M_w} \ln a_w.$$

Calculate and save results

To calculate the concentration dependence of osmotic coefficients and water activity

- ❖ Select electrolyte
- ❖ Select concentration (molal)
- ❖ Select equation type to calculate electrolyte activity coefficients

- ❖ Indicate the number of point
- ❖ Indicate desired type of "**Plot graph as**"
- ❖ Press the "**Calculate**" button

Graphs may be plotted using the coordinates

- ❖ ϕ
- ❖ a_w

You can save

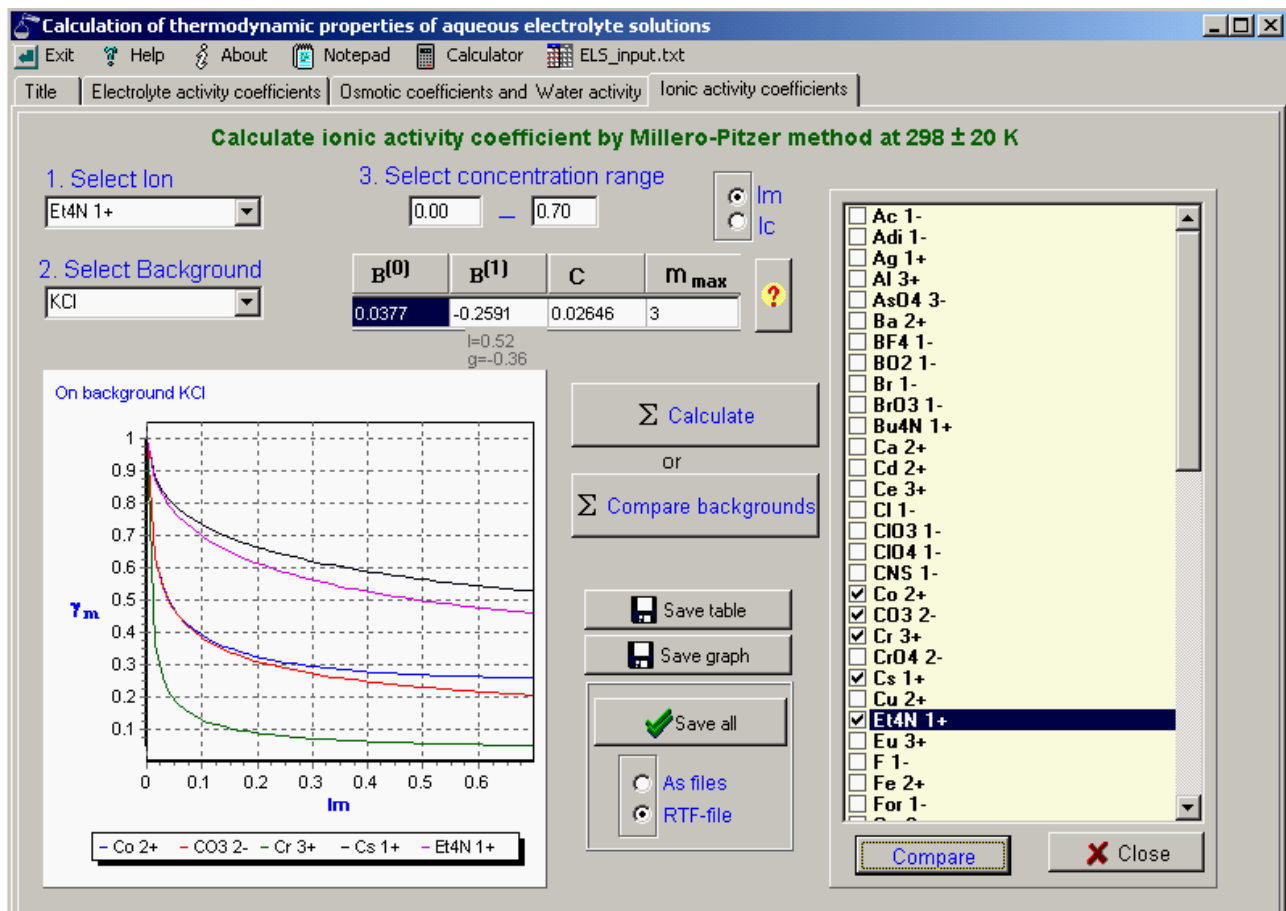
- ❖ the table of the calculated values as text file (*.txt) and to a clipboard simultaneously
- ❖ the plot as a graphic file (*.bmp) and to a clipboard simultaneously
- ❖ all results together (table, plot, comments) as a protocol in RTF format

You can also compare

- ❖ different models for a selected electrolyte "**Compare models**"
- ❖ different electrolytes for a selected equation "**Compare electrolytes**"

Ionic activity coefficients

The 'Ionic activity coefficients' tabbed page is shown below



A Pitzer-Millero type equation is used, based on a assumed ion pairing model [26]

$$\ln \gamma = Z_j^2 f^\gamma + IB_i^0 + B_i^1 f^1 + I^2 C_i$$

where f^γ and f^1 are functions of ionic strength I ,

B_i^0 , B_i^1 , and C_i are individual parameters determined from the coefficients of Pitzer and Mayorga [6]:

$$f^\gamma = -0.392 \cdot \left[\frac{I^{1/2}}{1 + 1.2I^{1/2}} + \frac{2}{1.2} \ln(1 + 1.2I^{1/2}) \right]$$

$$f^1 = 1 - \exp(-2I^{1/2})[1 + 2I^{1/2} - 2I].$$

All coefficients used are from [26].

Calculate and save results

To calculate the concentration dependence of ionic activity coefficients

- ❖ Select ion
- ❖ Select background
- ❖ Select concentration range (molal or molar)
- ❖ Indicate the number of point
- ❖ Indicate desired type of "Plot graph as"
- ❖ Press the "Calculate" button

Graphs may be plotted using the coordinates

- ❖ $\ln \gamma$
- ❖ γ

You can save

- ❖ the table of the calculated values as text file (*.txt) and to a clipboard simultaneously
- ❖ the plot as a graphic file (*.bmp) and to a clipboard simultaneously
- ❖ all results together (table, plot, comments) as a protocol in RTF format

You can also compare

- ❖ different backgrounds for selected ion "**Compare backgrounds**"
- ❖ different ions for selected background "**Compare ions**"

Input file

The **Electrolytes program** contains parameters for the thermodynamic equations, with references, in the file **ELS_input.txt**.

The first section of this file contains Lin-Tseng-Lee parameters (b,De,S) and Pitzer parameters (b(0),b(1),C(fi)) for each of 357 electrolytes. The Lin-Tseng-Lee's parameters used are from [22] and the Pitzer parameters are from [25].

Below is an example of this section:

```
-----
<electrolyte  <Lin-Tseng-Lee parameters>  <Pitzer parameters>
               b      De      S      mMAX      b(0)  b(1)  C(fi)  mMAX>
               {1-1 electrolyte}
CholineCl    0      0      0      0      0.0457 -0.196 0.00080      6.00
CholineBr    0      0      0      0      -0.0066 -0.227 0.0036 6.00
HCl          6.717  65.694 0.356  6.00  0.17750      0.2945 0.00080      6.00
HCl*         6.717  65.694 0.356  6.00  0.1801 0.2886 0.00015      6.00
<Mohamed El Guendouzi,a Abderrahim Dinane, Abdelfetah Mounir. Water activities, osmotic and activity
coefficients>
<in aqueous chloride solutions at T = 298.15 K by the hygrometric method. // J. Chem. Thermodynamics
2001, 33, 1-14>
HBr          7.059  64.202 0.490  3.00  0.2085 0.3477 0.00152      6.20
HI           9.633  63.821 0.558  3.00  0.2211 0.4907 0.00482      6.00
HClO4        6.662  64.527 0.419  6.00  0.17470      0.2931 0.00819      5.50
HNO3         5.882  63.078 0.220  3.00  0.1168 0.3546 -0.00539      6.00
-----
```

It should be noted that an asterisk (*) means data proposed by other authors with corresponding reference.

MMAX is the concentration limit applicable to the set of parameters.

The next section of the input file contains of Millero-Pitzer parameters (b(0),b(1),C(fi)) for different ions and backgrounds. These parameters are taken from [26]. An example is given below.

```
-----
<ion  charge b(0)  b(1)  C(fi)  mMAX>
      {NaClO4}
H      1+      0.6865 0.1779 0.03318      5.50
Na     1+      0.2093 0.1603 0.00507      6.00
K      1+      0.0967 0.1061 -0.00126 4.80
La     3+      1.5071 2.9211 0.02610      1.80
Ce     3+      1.4724 2.9211 0.02855      1.80
Pr     3+      1.4724 2.9211 0.02855      1.80
Nd     3+      1.4711 2.9211 0.02906      1.80
Pm     3+      1.4711 2.9211 0.02906      1.80
Sm     3+      1.4911 2.9211 0.02816      1.80
-----
```

The user can edit and add to the input file. Note that the columns need only be separated by tab (→).

Comments may be interspersed freely within the data files provided they are contained between angle brackets <>.

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Appendix

Table 1. Comparison of the accuracy (mean values from the same set of data) of models to predict the osmotic electrolyte coefficients in the average concentration range (up to 6 mol/kg)

Electrolyte	Cruz [10]	Chen [13]	modSCLC [18]	Pitzer [6]	LTL [22]	Jaretun-Aly [16-17]
1-1	0.56 %	0.91 %	0.48 %	0.50 %	2.00 %	0.96 %
2-1	3.10 %	6.60 %	1.90 %	2.10 %	4.94 %	2.95 %
1-2	2.05 %	1.50 %	0.94 %	0.95 %	2.75 %	1.63 %
3-1	2.50 %	6.45 %	3.75 %	1.25 %	2.35 %	0.71 %
Other	2.84 %	5.58 %	2.08 %	1.80 %	5.40 %	7.08 %
Rank of model*	2	2	2	3	3	4

* the number of adjustable parameters

Table 2. Comparison of the accuracy (mean values from the same set of data) of models to predict the osmotic electrolyte coefficients at high concentrations (above 6 mol/kg)

Electrolyte	Chen [13]	modSCLC [18]	Jaretun-Aly [16]
1-1	1.84 %	1.57 %	0.43 %
2-1	15.35 %	–	2.33 %
1-2	3.62 %	–	0.69 %
2-2	13.29 %	–	11.51 %
3-1	6.44 %	–	0.71 %
Other	19.93 %	–	7.08 %
Rank of model	2	2	4

Table 3. Comparison of the accuracy (mean values from the same set of data) of models to predict the activity electrolyte coefficients of individual electrolytes over the average concentration range (up to 6 mol/kg)

Electrolyte	Chen [13]	SCLC [19]	modSCLC [18]	LLT [23]	LTL [22]	Jaretun-Aly [16-17]
1-1	1.1 %	0.9 %	0.8 %	1.0 %	1.7 %	0.33 %
2-1	12.6 %	4.8 %	4.9 %	4.1 %	4.2 %	4.53 %
1-2	2.0 %	1.6 %	1.6 %	2.7 %	3.1 %	0.81 %
2-2	3.7 %	7.4 %	7.2 %	2.9 %	3.1 %	5.81 %
3-1	8.0 %	6.6 %	6.6 %	3.0 %	3.0 %	0.70 %
3-2	12.3 %	7.1 %	11.2 %	10.1 %	5.9 %	1.05 %
Rank of model	2	2	2	3	3	4

Table 4. Comparison of the accuracy (mean values from the same set of data) of models to predict the electrolyte activity coefficients of individual electrolytes at high concentrations (above 6 mol/kg)

Electrolyte	Chen [13]	modSCLC [18]	Jaretun-Aly [16]
1-1	3.83 %	3.32 %	0.33 %
2-1	29.90 %	–	4.53 %
1-2	4.67 %	–	0.81 %
2-2	6.84 %	–	5.81 %
3-1	7.86 %	–	0.70 %
Other	15.45 %	–	4.57 %
Rank of model	2	2	4