

Part 4. Calculation of activity coefficients in built-in functions of GEM-Selektor code

1. Individual aqueous species

The chemical potential of j -th aqueous ion or complex is approximated in the GEM IPM algorithm by the following expression in the uniform (mole fraction) scale [Karpov et al., 1997; 2001]:

$$v_j = \frac{\partial G(x)}{\partial x_j} = \frac{g_j}{RT} + \ln \frac{x_j}{X_w} - \ln \frac{x_{j_w}}{X_w} + \ln \gamma_j + \ln \frac{1000}{M_w} + 1 - \frac{x_{j_w}}{X_w} \quad (4-1),$$

where $G(x)$ is the total Gibbs energy of the system (in moles); g_j is the partial molal apparent Gibbs energy function of j -th aqueous species at T, P of interest in the molal scale; x_j is the mole quantity of j -th species and x_{j_w} - that of the water-solvent; X_w is the total mole quantity of the aqueous phase (including water-solvent); γ_j is the activity coefficient (in rational scale); and $M_w = 18.0153 \text{ g mol}^{-1}$ is the gram-formula mass of H_2O . The last three terms on the right side represent the conversion from the practical asymmetrical (i.e. molal) to the rational (i.e. mole fraction) concentration scale.

For the water-solvent (H_2O), the following approximation of chemical potential is used:

$$v_{j_w} = \frac{g_{j_w}}{RT} + \ln \frac{x_{j_w}}{X_w} + \ln \gamma_{j_w} + 2 - \frac{x_{j_w}}{X_w} - \frac{X_w}{x_{j_w}} \quad (4-2),$$

the activity coefficient of water γ_{j_w} is by default taken as unity because the mole quantity of

water x_{j_w} will be adjusted on GEM iterations, resulting in both activity $\exp\left(v_{j_w} - \frac{g_{j_w}}{RT}\right)$

and mole fraction of H_2O $\chi_{j_w} = \frac{x_{j_w}}{X_w}$ less than unity at non-zero concentration of dissolved salts. However, it is possible to write a Phase definition script for calculation of γ_{j_w} if needed.

Activity coefficients of aqueous species (γ_j in eqn 4-1) will be re-calculated on all iterations of the GEM algorithm because these values affect chemical potentials and depend on concentrations of dissolved ionic species, which are initially unknown. Equations for aqueous activity coefficients use the *effective ionic strength* I - a measure of a “concentration of charge”:

$$I = \frac{1}{2} \sum_j^{n(L_w)} m_j z_j^2 \quad (4-3),$$

where z_j is the formula charge of j -th species and m_j is its molality (in moles per 1 kg H_2O),

$$m_j = \frac{x_j}{x_{j_w}} \cdot \frac{1000}{M_w} = 55.508435 \frac{x_j}{x_{j_w}} \quad (4-4),$$

where $M_w = 18.0153$ is the gram-formula mass of H_2O . Note that in ion-association aqueous models, the effective ionic strength, which counts only charged aqueous species, is usually less than the formal ionic strength obtained from the bulk concentration of a dissolved salt.

The physical theory of Debye and Hückel (1923) relates the activity coefficient of aqueous ion to its charge and the ionic strength of the aqueous electrolyte. This is based on representing the ions as point charges in an ideal structureless dielectric solvent and considering long-range Coulombic forces between charges of opposite sign working against disorder caused by

thermal Brownian movement. Derivation of this theory is lengthy, but readily available from textbooks (e.g. [Robinson and Stokes, 1968]). The final result is called the Debye-Hückel equation:

$$\log \gamma_j = \frac{-A_\gamma z_j^2 \sqrt{I}}{1 + \dot{a} B_\gamma \sqrt{I}} \quad (4-5).$$

There, \dot{a} (in 10^{-8} cm) is an average distance of approach of two ions of opposite charge (or the ion-size Kielland's parameter for individual ions), and

$$A_\gamma = 1.82483 \cdot 10^6 \rho_0^{0.5} (\epsilon_0 \cdot T)^{-1.5} \quad (4-6),$$

$$B_\gamma = 50.2916 \rho_0^{0.5} (\epsilon_0 \cdot T)^{-0.5} \quad (4-7),$$

where ρ_0 is density ($\text{g} \cdot \text{cm}^{-3}$) and ϵ_0 is the dielectric constant of pure water at temperature T (K) and pressure P (bar) of interest. The latter two values are obtained internally from SUPCRT92 subroutines [Johnson et al., 1992] incorporated into the GEMS code. At $T_r = 25$ C and $P_r = 1$ bar, $A_\gamma \approx 0.5114$ and $B_\gamma \approx 0.3288$.

Equation (4-5) works well at relatively low ionic strength ($0.001 \leq I \leq 0.1$ m). At low ionic strength ($I < 0.001$ m), the denominator in eqn (4-5) approaches unity, converting it into the Debye-Hückel limiting law:

$$\log \gamma_j \approx -A_\gamma z_j^2 \sqrt{I} \quad (4-8).$$

Extension of the Debye-Hückel theory to account for the polarization of solvent molecules in the vicinity of ionic charges has added a linear term to the extended Debye-Hückel equation:

$$\log \gamma_j = \frac{-A_\gamma z_j^2 \sqrt{I}}{1 + \dot{a} B_\gamma \sqrt{I}} + b_\gamma \cdot I \quad (4-9),$$

where b_γ is a semi-empirical coefficient, either individual for a given electrolyte ion (in this case eqn (4-9) is also called the Truesdell-Jones equation), or common for all minor aqueous species [Helgeson et al., 1981] in the predominant (NaCl) electrolyte. The extended equation (4-9) is thought to be applicable up to 1-2 molal ionic strength using $b_\gamma = 0.064$ and it was implemented with common b_γ as a built-in function in GEM-Selektor. This function can be used either with individual Kielland ion-size parameters \dot{a}_j (collected from DComp or ReacDC records) as formerly suggested by Karpov, or with an average parameter $\dot{a} = 3.72$ (in 10^{-8} cm), the same for all ionic species, as proposed in [Helgeson et al., 1981]. The Kielland's (1936) table of effective ionic radii \dot{a}_j can be found in textbooks (e.g. [Nordstrom and Munoz, 1994; Langmuir, 1997]) with recommended default values for missing ionic species.

Usage of individual Kielland's parameters may be more appropriate at relatively low ionic strength. On the other hand, application of eqn (4-9) with the common ion-size parameter \dot{a} seems to be more warranted at higher ionic strength and/or elevated temperatures.

Another built-in function in the GEMS code implements the popular Davies equation:

$$\log \gamma_j = -A_\gamma z_j^2 \left(\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right) \quad (4-10).$$

This semi-empirical equation can be used at low temperatures and ionic strength between 0.1 and 0.7 molal; it is thought to be inaccurate at $I < 0.1$ m because it neglects the difference in ion approach parameters. The advantage of Davies equation is that it uses only the charge as

an individual species property; conversely, all ions of the same charge (e.g. +2 and -2) will have identical activity coefficients (note that this is also true for eqn 4-9 with common \dot{a} parameter).

Neutral aqueous species (dissolved gases and neutral complexes) require a simpler form of activity coefficient that can be assumed a linear function of ionic strength (the “salting-out” effect):

$$\log \gamma_j = b_g \cdot I \quad (4-11).$$

In the case of dissolved gases, the empirical b_g coefficient can be obtained from experimental values of the Setschenow coefficient, measured in electrolyte solutions under an assumption that the activity coefficient of a gas dissolved in pure water equals unity. Typical values of b_g lie between 0.02 and 0.2 [Langmuir, 1997], with an average 0.074 [Borisov and Shvarov, 1992]. In GEMS, the b_g values will be automatically collected from DComp or ReacDC records for neutral aqueous species, wherever provided.

Eqn (4-11) can also be obtained from eqn (4-9) at zero charge ($z_j=0$), suggesting that the common third parameter b_γ can be used as a generic salting-out coefficient of neutral aqueous complexes, for which the experimental Setschenow coefficient is not known. This option (or its alternative – to leave $\gamma_j = 1$ for neutral complexes) can be set in DComp or ReacDC records in the GEMS chemical thermodynamic database, according to the user’s preference.

Possible options for built-in calculation of aqueous activity coefficients in GEM-Selektor code are summarized in Appendix 4-1.

<SIT equations (to be implemented)>

2. Solid solutions, melts and liquid mixtures

Treatment of solid (and any condensed non-electrolyte) solutions in GEM-Selektor code is based on the following expression for the chemical potential of a j -th end member [Karpov et al., 1997; 2001]:

$$v_j = \frac{g_{j,T,P}}{RT} + \ln \chi_j + \ln \gamma_j \quad (4-12),$$

where $g_{j,T,P}$ is the molar apparent Gibbs energy function at T,P of interest; $\chi_j = \frac{x_j}{X_\alpha}$ is the mole fraction (x_j is the mole quantity of j -th species and $X_\alpha = \sum x_j$, $j \in L_\alpha$ is the total mole quantity in the α -th phase), and γ_j is an activity coefficient.

If all $\gamma_j = 1$ then eqn (4-12) reduces to the Raoult’s law of ideal mixing, where the activity of j -th end-member equals its mole fraction. This definition of ideal mixing is rather narrow because, in a broader sense, ideal solutions can be defined as having zero enthalpy and volume of dissolution [Oates, 1966; Anderson and Crerar, 1993]. Further complications include regular solutions (with non-zero enthalpy of dissolution) and non-ideal solutions where enthalpy, volume and entropy of dissolution are non-zero for an end-member. In general, one can write for the dissolution properties:

$$a_j = X_j \gamma_j, \quad \gamma_j \neq 1, \quad j \in L_\alpha;$$

$$\Delta S_d = -R \sum_j \chi_j \ln a_j;$$

$$\Delta V_d \neq 0; \quad \Delta H_d \neq 0;$$

$$\Delta G_d = \Delta H_d + RT \sum_j \chi_j \ln a_j$$

Here, a_j stands for the activity of j -th end-member and the subscript d refers to the difference of a particular property between a non-ideal solution and a mechanical mixture of its pure end-members [Anderson and Crerar, 1993]. In practice, the excess thermodynamic functions of mixed non-electrolyte phases are usually considered:

$$V_{EX} = V_{real} - \sum_j \chi_j V_j^o \quad (4-13),$$

$$H_{EX} = H_{real} - \sum_j \chi_j H_j^o \quad (4-14),$$

$$S_{EX} = S_{real} - \left(\sum_j \chi_j S_j^o - RT \sum_j \chi_j \ln \chi_j \right) \quad (4-15),$$

$$G_{EX} = G_{real} - \left(\sum_j \chi_j G_j^o - RT \sum_j \chi_j \ln \chi_j \right) \quad (4-16),$$

where the subscript *real* refers to an experimentally measurable property in the real system. Likewise, for one end-member, an excess partial property can be defined as a difference between the real and the ideal partial molar property. For instance, the excess partial Gibbs energy of j -th end-member (counted relative to Raoultian ideal mixing) is

$$\bar{G}_j^{EX} = \mu_{j,real} - \mu_{j,ideal} = \mu_j^o + RT \ln \chi_j \gamma_j - \mu_j^o - RT \ln \chi_j = RT \ln \gamma_j \quad (4-17).$$

The excess partial molar entropy, enthalpy, and volume can then be found by differentiating the \bar{G}_j^{EX} over temperature and pressure (see details in e.g. [Anderson and Crerar, 1993]):

$$\bar{S}_j^{EX} = -R \ln \gamma_j - RT \left(\frac{\partial \ln \gamma_j}{\partial T} \right)_{P, \chi} \quad (4-18);$$

$$\bar{H}_j^{EX} = -RT^2 \left(\frac{\partial \ln \gamma_j}{\partial T} \right)_{P, \chi} \quad (4-19);$$

$$\bar{V}_j^{EX} = -RT \left(\frac{\partial \ln \gamma_j}{\partial P} \right)_{T, \chi} \quad (4-20).$$

Thus, to describe real non-electrolyte solutions, it is sufficient to know (partial) molar properties of all end-members at T, P of interest plus functional dependencies of their activity coefficients on T, P and composition (i.e. on mole fractions χ_j of all end-members).

There is no general solution to this problem, though a great variety of semi-empirical models have been developed and parameterized for binary-, ternary-, ... symmetric and asymmetric systems. Some of the most frequently used mixing models are described below and implemented as built-in functions in the GEM-Selektor code (Appendix 4-2). In addition to those built-in mixing models, any arbitrary mixing model can be written by the user in a Phase definition script to calculate activity coefficients of end-members, which will be stored in the database and automatically executed on GEM iterations.

2.1. Margules model

The Margules binary mixing model is most frequently used (see e.g. [Anderson and Crerar, 1993]). It is based on the “subregular” expression for the excess Gibbs energy of mixture:

$$G_{EX} = \chi_1(W_2\chi_1\chi_2) + \chi_2(W_1\chi_1\chi_2) \quad (4-21),$$

where χ_1 and χ_2 are mole fractions of the first and second end member ($\chi_1 + \chi_2 = 1$) and W_1 , W_2 are Margules parameters (in J mol⁻¹), in general, functions of T and P but not of χ :

$$W_j = W_{U,j} - TW_{S,j} + PW_{V,j} \quad (4-22),$$

where W_U , W_S , and W_V are empirical parameters related to excess internal energy, entropy and volume of the mixture; they can be evaluated from experimental data. Next, the following expressions for partial excess Gibbs energies and activity coefficients can be obtained:

$$RT \ln \gamma_1 = \bar{G}_1^{EX} = (2W_2 - W_1)\chi_2^2 + 2(W_1 - W_2)\chi_2^3 \quad (4-23),$$

$$RT \ln \gamma_2 = \bar{G}_2^{EX} = (2W_1 - W_2)\chi_1^2 + 2(W_2 - W_1)\chi_1^3 \quad (4-24).$$

Eqns (4-23) and (4-24) comprise the so-called “subregular” or “asymmetric” Margules mixing model. Asymptotically (e.g. at $\chi_1 \rightarrow 1$ and $\chi_2 \rightarrow 0$), the activity coefficient of the “major” end-member $\ln \gamma_1 \rightarrow 0$ and that of the “trace” end-member $\ln \gamma_2 \rightarrow W_2/(RT)$. Likewise, at $\chi_1 \rightarrow 0$ and $\chi_2 \rightarrow 1$, $\ln \gamma_1 \rightarrow W_1/(RT)$ and $\ln \gamma_2 \rightarrow 0$. This asymptotic behavior simplifies modeling calculations when co-precipitation of trace components into host mineral is considered.

Eqns (4-23) and (4-24) are often used with dimensionless interaction parameters:

$$\ln \gamma_1 = (2a_2 - a_1)\chi_2^2 + 2(a_1 - a_2)\chi_2^3 \quad (4-25),$$

$$\ln \gamma_2 = (2a_1 - a_2)\chi_1^2 + 2(a_2 - a_1)\chi_1^3 \quad (4-26),$$

where $a_1 = W_1/RT$; $a_2 = W_2/RT$. If $a_1 = a_2 = a$ then eqns (4-25) and (4-26) reduce to the “regular” or “symmetric” Margules mixing model, typically used for carbonate or sulphate solid solutions [Lippmann, 1980; Glynn, 2000]:

$$\ln \gamma_1 = a\chi_2^2 \quad (4-27),$$

$$\ln \gamma_2 = a\chi_1^2 \quad (4-28).$$

In general, the binary interaction parameter $W = RT \cdot a$ is also a function of T, P but not χ :

$$W = W_U - TW_S + PW_V = W_H - TW_S \quad (4-29).$$

At $a > 2$, the binary mixture should exsolve into two co-existing phases of different composition along the *binodal solvus* curve [cf. Glynn, 2000]. The width of the miscibility gap depends on temperature; according to Lippmann [1980],

$$a_T \approx 2T_c/T \quad (4-30),$$

where T_c is the critical temperature (or the highest temperature of melting) for the ionic solid. At ambient temperatures, the values of a range from nearly zero to maximum 13-14 in various ionic binary mixtures, i.e. from complete miscibility to $\chi_1 \leq n \cdot 10^{-6}$ [Glynn, 2000].

If a miscibility gap is expected in the solid solution system then more than one mixed phase definition must be inserted into the GEMS chemical system definition (CSD), and a special

mode of automatic initial approximation has to be specified (Appendix 4-3) to ensure that the two-phase region is reproduced at appropriate bulk compositions.

The Margules model can be relatively easily expanded to ternary, quaternary, ... mixture systems. However, the number of interaction parameters increases drastically, making a much higher demand to experimental data needed for parameterization, and expressions for excess properties become very cumbersome. For instance, the ternary Margules model can be obtained from summation of G_{EX} for three binary models with common end-members:

$$G_{EX} = (W_{23}\chi_2^2\chi_3 + W_{32}\chi_3^2\chi_2) + (W_{13}\chi_1^2\chi_3 + W_{31}\chi_3^2\chi_1) + (W_{12}\chi_1^2\chi_2 + W_{21}\chi_2^2\chi_1) + W_{123}\chi_1\chi_2\chi_3 \quad (4-31).$$

The ternary interaction parameter W_{123} is often neglected [e.g. Anderson and Crerar, 1993]. Full theoretical expressions for sub-regular activity coefficients can be found in [Helffrich and Wood, 1989]. Assuming the regular mixing ($W_{ij} = W_{ji}$), one obtains for activity coefficients:

$$RT \ln \gamma_1 = W_{12}\chi_2(1 - \chi_1) + W_{13}\chi_3(1 - \chi_1) - W_{23}\chi_2\chi_3 + W_{123}\chi_2\chi_3(1 - 2\chi_1) \quad (4-32),$$

$$RT \ln \gamma_2 = W_{23}\chi_3(1 - \chi_2) + W_{12}\chi_1(1 - \chi_2) - W_{13}\chi_1\chi_3 + W_{123}\chi_1\chi_3(1 - 2\chi_2) \quad (4-33),$$

$$RT \ln \gamma_3 = W_{13}\chi_1(1 - \chi_3) + W_{23}\chi_2(1 - \chi_3) - W_{12}\chi_1\chi_2 + W_{123}\chi_1\chi_2(1 - 2\chi_3) \quad (4-34).$$

Thus, compared to the binary regular model (eqns 4-21 to 4-24), four Margules parameters are needed instead of one (or, including T, P dependence of mixing, 12 parameters are necessary instead of 3). In the quaternary case, six binary plus four ternary plus one quaternary Margules parameters (in total 11) would be necessary just for a regular approximation. This is why, in practice, full mixing models of the order above ternary are very seldomly used. Built-in Margules mixing models available in GEM-Selektor are limited to ternary case.

Various simplifications can be used to reduce the number of interaction parameters, for instance, it can be shown that some binaries in a multi-component mixture are ideal. One can also assume [Kulik et al., 2000] that in reality, two of six end-members together comprise more than 96% of the mixture (major end-members), and the remaining four are minor end-members, each less than 1% mole fraction ($\chi_j < 0.01$). Then activity coefficients of major end-members (1 and 2) can be considered as independent of mole fractions of minor end-members (indexed 3, 4, ...):

$$RT \ln \gamma_1 \approx W_0(1 - \chi_1)^2 \quad (4-35),$$

$$RT \ln \gamma_2 \approx W_0\chi_1^2 \quad (4-36).$$

For minor end-members, all minor-minor, ternary, quaternary, ... parameters can be neglected in the two major end-members (1 and 2) case:

$$RT \ln \gamma_3 \approx W_{31}\chi_1 + W_{32}\chi_2 - W_0\chi_1\chi_2 \quad (4-37)$$

$$RT \ln \gamma_4 \approx W_{41}\chi_1 + W_{42}\chi_2 - W_0\chi_1\chi_2 \quad (4-38)$$

and so on. Thus, in a regular mixture with two major and several minor end-members, one major binary parameter W_0 is needed, as well as two binary Margules parameters per minor

end-member (for both minor-major binaries). This simplified model appears to be practically useful for trace metal co-precipitation in host carbonates and sulfates.

2.2. Redlich-Kister model

The Redlich-Kister mixing model is a frequently used alternative to the Margules model, especially for binary mixtures. It is based on Guggenheim's expansion series for the excess Gibbs energy of mixing [cf. Glynn, 2000]:

$$G_{EX} = RT\chi_1\chi_2[a_0 + a_1(\chi_1 - \chi_2) + a_2(\chi_1 - \chi_2)^2 + \dots] \quad (4-39),$$

where $a_0, a_1, a_2 \dots$ are dimensionless fitting parameters (an equivalent form of eqn 4-39 uses $A_j = RTa_j$ parameters in $J \cdot mol^{-1}$). From the above equation, the following activity coefficients can be obtained:

$$\ln \gamma_1 = \chi_2^2[a_0 + a_1(3\chi_1 - \chi_2) + a_2(\chi_1 - \chi_2)(5\chi_1 - \chi_2) + \dots] \quad (4-40);$$

$$\ln \gamma_2 = \chi_1^2[a_0 - a_1(3\chi_2 - \chi_1) + a_2(\chi_2 - \chi_1)(5\chi_2 - \chi_1) + \dots] \quad (4-41).$$

The first two terms in eqns (4-39) to (4-41) are generally sufficient to represent experimental data. In this case, the last two equations calculate the same curves as the subregular Margules model (eqns 4-23 and 4-24), with the following relations between parameters:

$$W_{12} = RT(a_0 - a_1); \quad W_{21} = RT(a_0 + a_1) \quad (4-42).$$

Further reduction to the regular mixing model by setting $a_1=0$ and $a_2 = 0$ yields

$$W = RT \cdot a = RT \cdot a_0 \quad (4-43).$$

In GEM-Selektor, equations (4-40) and (4-41) with three parameters are implemented as a built-in function for the binary Redlich-Kister mixing model. Reduction to subregular and regular mixing models can be done easily by setting unnecessary coefficients to zero.

3. Fluids (under construction)

Ideal gas law $PV = xRT$; fluid as an ideal mixture of ideal gases (ambient T, P ; low P , high T).

Virial EoS to find (i) fugacities of pure gases at P, T ; (ii) fugacities of gases in the mixture at T, P, χ .

Van der Waals EoS and mixing models [cf. Anderson and Crerar, 1993, p.404-408].

CG EoS model [Churakov and Gottschalk, 2003a,b], third-party contribution (see **TPX-corrections-CG-EoS.pdf** document).

FGL module (Karpov et al. 199.) (corresponding states theory), in preparation.

MRK (for H_2O-CO_2 fluids) [Kerrick and Jakobs, 1981].

PREoS [Peng-Robinson, 1976] for H_2O -poor hydrocarbon mixtures. Modifications.

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Appendix 4-1. Built-in options for calculation of aqueous activity coefficients (GEMS v.2.1-PSI or later).

Code	Model	Equations	Input parameters
D	Davies	4-10	Ionic strength I (eqn 4-3, computed automatically on each GEM IPM iteration)
3	Extended Debye-Hückel / Kielland	4-9, 4-11	I ; individual ion-size parameter \bar{a} (Kielland, collected from DComp/ReacDC records); common b_γ (third) parameter (default 0.064)
H	Extended Debye-Hückel / Helgeson	4-9, 4-11	I ; common ion-size parameter $\bar{a} = 3.72$ (parameters from DComp/ReacDC records ignored); common b_γ parameter (default 0.064)
2	Debye-Hückel	4-5	I ; individual ion-size parameter \bar{a} (Kielland, collected from DComp/ReacDC records);
1	Debye-Hückel limiting law	4-8	I – ionic strength only (eqn 4-3)
S	SIT	<i>Under Construction</i>	

Note: Codes should be given in `p_solt[0,0]` field upon remake of Phase records or (for ion association aqueous models) selected during creation of a new modeling project.

Appendix 4-2. Built-in options for activity coefficients of solid-solution end members

Code	Model	Equations	Input parameters
R	Redlich-Kister binary	4-40, 4-41	a_0, a_1, a_2 coefficients for 1st end member; a_0, a_1, a_2 coefficients for 2nd end member.
M	Margules binary (sub)regular	4-23, 4-24	$W_{U,1}, W_{S,1}, W_{V,1}$ for 1 st end member; $W_{U,2}, W_{S,2}, W_{V,2}$ for 2 nd end member (eqn 4-22)
T	Margules ternary regular	4-32 to 4-34	$W_{U,12}, W_{S,12}, W_{V,12}; W_{U,23}, W_{S,23}, W_{V,23}; W_{U,13}, W_{S,13}, W_{V,13}; W_{U,123}, W_{S,123}, W_{V,123}$ (eqn 4-22).
U	User-defined		Must be provided as Phase scripts & parameters

Note: Codes should be given in `p_solt[0,0]` field upon remake of Phase records

Appendix 4-3. How to reproduce miscibility gaps in GEM-Selektor calculations
(to be provided soon)

Appendix 4-4. Built-in options for fluid mixtures (under construction)

Code	Model	Equations	Parameters
F	CG EoS 2003	Section 3	4 parameters, collected from DComp records
P	Peng-Robinson		

Note: Codes should be given in `p_soln[0,0]` field upon remake of Phase records or selected during creation of a new modeling project.