

Aqueous Electrolyte Modeling in Aspen Plus

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ABSTRACT: The presence of electrolytes in aqueous solutions has long been recognized as contributing to significant departures from thermodynamic ideality. The presence of ions in process streams can greatly add to the difficulty of predicting process behavior. The difficulties are increased as temperatures and pressures within a process are elevated. Because many chemical companies now model their processes with chemical process simulators it is important that such codes be able to accurately model electrolyte behavior under a variety of conditions. Here we examine the electrolyte modeling capability of ASPEN PLUS™, a widely used simulator. Specifically, we will present our efforts to model alkali metal halide and sulfate systems. We will show conditions for which the models within the code work adequately and how they might be improved for conditions where the simulator models fail.

INTRODUCTION

The demands on chemical plant designers and process engineers have never been greater. The burden of global economic competition requires that processes be operated at optimal efficiency. Increasingly stringent environmental and occupational safety regulations necessitate an accurate knowledge of the composition of process and waste streams. Such understanding, non-trivial under the best of circumstances, is often made much more difficult by the presence of electrolytes in these streams.

Processing difficulties encountered with electrolyte solutions are numerous. Ions in solution may react to form salts which may plug lines or otherwise foul or damage equipment. Additionally, the presence of electrolytes in solution may significantly affect the physical properties of the solution. The freezing and boiling points, gas solubility and phase behavior of a mixture may all be significantly altered by electrolytes. Chemical reaction equilibrium may also be effected by electrolytes. Electrolytes may form hazardous chemicals making their release into the environment tightly regulated. Any of these concerns may play prominent roles in how a chemical plant is designed and operated.

The difficulty in predicting the behavior of electrolyte solutions in chemical processes is increased at the elevated temperatures and pressures at which many of today's processes operate. Because data for electrolyte systems are often unavailable at high temperatures and pressures, engineers and chemists must rely on mathematical models to bridge the gap between available data and their particular conditions of interest. Much progress has been made in the past few decades in the development of models which provide reasonable predictions of behavior of concentrated electrolyte solutions including activity coefficient models and electrolyte equations of state. Computer codes have been developed, largely through the efforts of geochemists, which allow predictions of behavior of a large number of electrolyte systems. The status of such codes was recently reviewed by Bassett and Melchior. [1]

While such codes are certainly of value, the process engineer is frequently interested in a different set of questions than the geochemist. Questions concerning the sizing of equipment and the effects of operational changes on the chemistry of the process streams are often of primary importance. To address these questions many companies make use of process simulators. These computer codes are designed to allow companies to compute the material and energy balances of their process with mathematical models. As such, the simulators contain models of many unit operations common to the chemical industry, physical property models and databases containing physical properties and model parameters for a large number of compounds. Simulators provide a relatively inexpensive and rapid means of determining effects of process changes on equipment design and process stream behavior while providing a framework for optimizing process performance.

The value of a simulator is determined by the accuracy with which a particular process may be modeled. This is determined in great measure by the accuracy of its physical property models. Commercially available simulators are designed to be useful to as broad a base of customers as possible. For this reason, and because properties are most well understood at moderate conditions, models employed in the simulators tend to work best at these conditions. Provisions are often made within the code for a user to tailor the simulator to their particular needs.

In this paper we describe our efforts to extend the applicability of the electrolyte models in a common simulator, ASPEN PLUS™ (Aspen Technology, Inc.), to higher temperatures and pressures. Our experience indicates that the models within the simulator may be made to work reasonably well from ambient conditions to 250 to 300°C. Here, limitations of the code become apparent but may be minimized by use of user supplied models. Results obtained through the use of proprietary models will be shown which more accurately describe electrolyte behavior over a wider range of temperature. The work presented here is limited to aqueous systems and involves models for electrolyte solubilities. The results presented were computed with ASPEN PLUS™ Release 8.5-6. Aspen Technology has recently made available ASPEN PLUS™ Release 9. Our copy of this upgrade was obtained too late for use in this paper.

MODELING ELECTROLYTE SYSTEMS

Overview

Our interest has been in the successful implementation of aqueous electrolyte models into a process simulator for use with elevated temperatures and pressures. The use of water as a solvent offers peculiar challenges to such a task. Electrolyte properties are strongly influenced by the density and dielectric constant of the solvent. These properties, computed from the equations of Hill and Archer respectively, are shown as a function of temperature and pressure in Figure 1. [2,3] At temperatures below about 200° C, the dielectric constant remains relatively high and the density a weak function of temperature. The dielectric constant may be viewed as a rough indicator of a solvent's ability to solubilize electrolytes and at these relatively low temperatures, electrolytes are generally very soluble in water. As the critical point of water (374° C, 221 bar) is approached, both properties change

rapidly with temperature. In this region of rapid property change, simple temperature dependent models of electrolyte solubility often fail. Also note that the effects of pressure are magnified at the critical point.

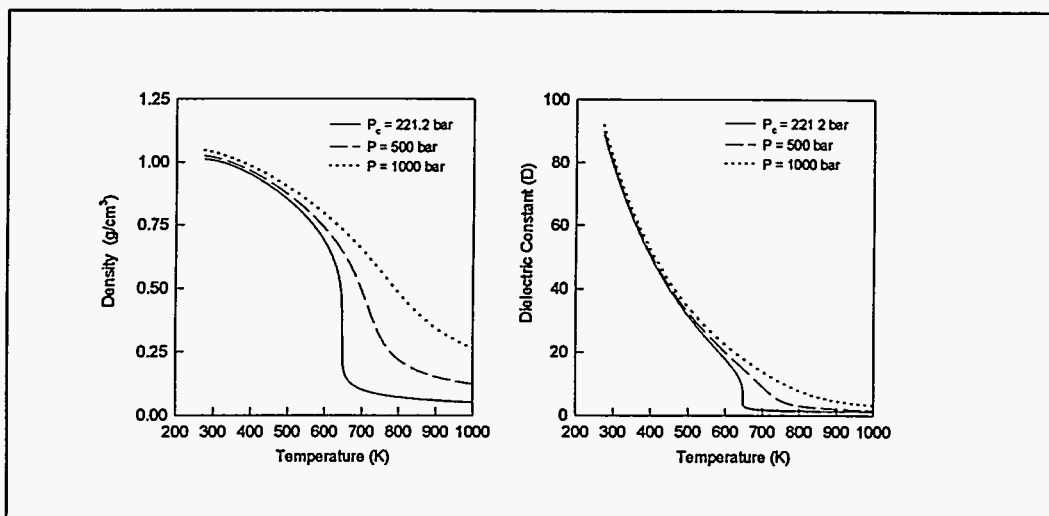


Figure 1. Properties of water as a function of temperature and pressure.

Until the ground-breaking work of Debye and Huckel, no real methods existed for modeling electrolyte behavior. [4] The model of Debye and Huckel described the long-range interactions between ions and has served as the foundation for our present day models. At higher electrolyte concentrations the assumptions of this model break down, limiting the model's effectiveness. Recently, two models describing electrolytes in terms of mean activity coefficients have gained widespread use which take into account short-range interactions encountered in concentrated solutions. Both are available in ASPEN PLUSTM and will be briefly described as they relate to our modeling efforts.

In 1973, Pitzer and his coworkers began publishing a series of papers introducing a model which allowed electrolyte systems to be accurately modeled to much higher concentrations than possible with the Debye-Huckel model alone. [5] In this model long-range interactions are described using the Debye-Huckel theory while short-range interactions are included through a virial expansion of the pressure equation. The resulting equation contains parameters describing binary interactions between ions and parameters which accounts for triple-ion interactions. Ions are assumed to be in a dielectric continuum. Pitzer has also published methods for introducing temperature dependency into his model. [6] While some work has been published describing extensions of the model for highly concentrated electrolyte solutions and mixed solvent systems, the model in its most common form is best suited for aqueous systems with electrolyte concentrations to approximately 6 molal. The Pitzer model is probably the most widely used model today and as such, possesses the larger database of model parameters to be found in the literature.

In 1982, Chen introduced an electrolyte activity coefficient model. [7] Like Pitzer, Chen utilized the Debye-Huckel model to describe long-range interactions between ions. To model the effects of short-range interactions, Chen modified the nonrandom two liquid (NRTL) theory of Renon and Prausnitz for use with electrolytes. [8] The Chen model is based on the assumptions of like-ion repulsion and local electroneutrality. The resulting model defines the mean activity coefficient of the ions in terms of binary interaction energy parameters, τ , which describe the excess Gibbs free energy resulting when the pure components are combined to form the electrolyte solution. These parameters may be defined for interactions between two ions, an ion and a solvent molecule or between two different solvent molecules. Thus for a given electrolyte system a number of binary

interaction parameters are used in the model of that system. Like Pitzer, Chen proposed methods to include temperature dependency in the τ parameter. [9]

While the Pitzer model has proven to be quite effective and has been used by researchers for a large number of systems, the Chen model offers several features which make its use attractive. Because interactions between ions and molecular species are accounted for in the Chen model, it is more naturally suited to describe electrolyte systems with mixed solvents and those containing weak electrolytes. The Pitzer model is developed using a virial expansion and in the form presented in this simulator is accurate only to concentrations of around 6 molal. Our experience indicates that the Chen model provides more stable extrapolation in concentration, particularly at elevated temperature. For these reasons the majority of our work has utilized the Chen model and unless otherwise indicated the results presented use that model. For regions where both models are applicable, our work indicates that similar accuracy may be obtained from the two models.

Implementation of Activity Coefficient Models in ASPEN PLUS

Activity Coefficient Models. Activity coefficient models are used in simulator to compute activity coefficients, enthalpies, and free energies. For a more detailed description of the implementation of these models in ASPEN PLUS the reader is referred to the manuals associated with the software. A brief description of the implementation is in order to provide a basis for the discussion of our modeling efforts.

The Pitzer model appears as it does in the original references with few exceptions. The temperature dependence of the binary B parameters is equivalent in form to that proposed by Pitzer. No temperature dependency is provided for the ternary parameters. ASPEN PLUSTM includes terms to describe ionic interactions with molecules for weak electrolyte systems though the model has not been used for modeling weak electrolytes in our research.

As with the Pitzer model, allowances are made in the Chen model to account for the often strong dependency of activity coefficients on temperature. The binary interaction parameters τ involving electrolyte interactions are given a temperature dependence through the following equation form

$$\tau = C + \frac{D}{T} + E \left[\left(\frac{T_R - T}{T} \right) + \ln \left(\frac{T}{T_R} \right) \right] \quad (1)$$

Here τ represents a binary interaction parameter, and C, D and E model parameters. For interaction parameters associated with two solvent molecules the E term is not included. While the binary interaction parameters as presented in the Chen model have some physical meaning they are typically used as fitting parameters and it is in that manner that they appear in ASPEN PLUSTM. For both the Pitzer and the Chen models, the model parameters are typically obtained from the literature or some combination of the parameters are regressed from experimental data.

Chemical Equilibrium Models. Salt solubility may be determined in ASPEN PLUSTM from either the reference state free energies of the reacting components or by use of chemical equilibrium constants. Chemical equilibrium coefficients are defined as

$$K = \frac{(\gamma_R[R])^r (\gamma_S[S])^s}{(\gamma_P[P])^p (\gamma_Q[Q])^q} \quad (2)$$

$$\ln K = A + \frac{B}{T} + C \ln T + DT \quad (3)$$

with

$$pP + qQ \approx rR + sS \quad (4)$$

Here [R] and [S] and [P] and [Q] represent the concentrations, on either a mole fraction or molality basis, of the products and reactants, respectively, of the reaction

The activity coefficients of the compounds are represented by γ_i , with A,B,C and D representing fitting parameters. In this paper, concentrations given in equation (2) are assumed to represent mole fractions.

User Input in Simulations. To be of value to the chemical processing industry, simulators must be sufficiently flexible to allow the user to adapt the modeling to their particular process. ASPEN PLUS™ provides a number of methods for such adaptation. First, the user may input model parameters from literature sources into the simulation. If no such parameters are available they may be regressed from experimental data. If more flexibility is needed, the user may enter Fortran code into the simulation input file. This provides a means of introducing calculations based on user defined models into the simulation. Finally user models may be written as Fortran subroutines to be called by the code during a simulation. The results presented today are produced from data regression and in-line Fortran code.

RESULTS

Three electrolyte systems have been chosen to demonstrate the strengths and weaknesses of the electrolyte models in ASPEN PLUS™. These systems, including NaCl, KCl and Na₂SO₄, were selected for their physical behavior and because of the availability of high temperature data.

Activity Coefficient Regressions

As an initial step in modeling, parameters for the activity coefficient models were regressed for the individual salts. Once regressed the activity coefficients are used to compute a number of properties including solution enthalpy, free energy and vapor pressure. Activity coefficient model parameters may be regressed from a number of sources including vapor liquid equilibrium data, mean activity or osmotic coefficient data, liquid enthalpy data or salt solubility data. Here we have chosen to regress parameters from the mean activity coefficient data. Values for NaCl were computed using

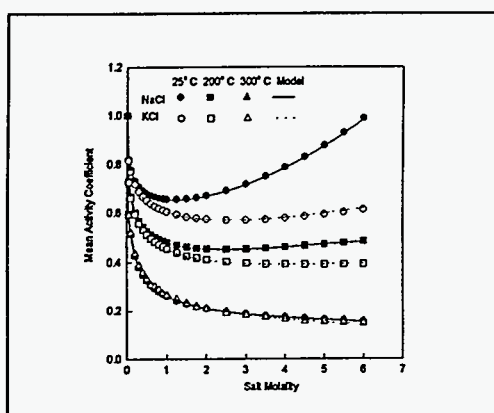


Figure 2: ASPEN PLUS Pitzer model of the mean activity coefficient of NaCl and KCl

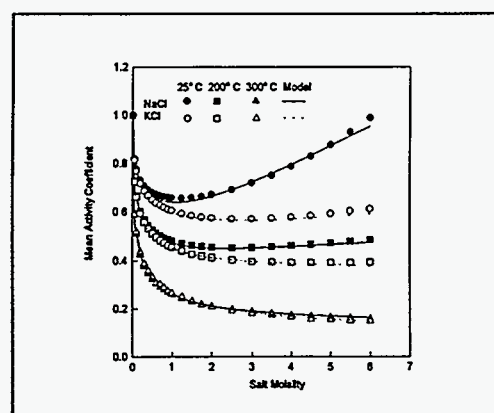


Figure 3: ASPEN PLUS Chen model of the mean activity coefficient of NaCl and KCl

the equation of Archer while those for KCl were taken from Holmes and Mesmer below 250°C and at 300°C those of Cobble. [10,11,12] The fits of these regressions are shown in Figures 2 and 3 for the Pitzer and Chen models respectively. The Pitzer model was found to provide a slightly better fit of the data than the Chen model though both gave good results.

Electrolyte Solubility

One method of modeling salt solubilities within ASPEN PLUS™ is through the use of chemical equilibrium constants. It is this approach that we explore here. Salt solubility data as a function of temperature and pressure is used in conjunction with the previously regressed activity coefficient model parameters to regress the coefficients of equation (3).

The salts of NaCl and KCl are each of a single form over a wide temperature range and thus provide a good test of polynomial form of the equilibrium constant given above. Figure 4 shows fits of solubility data for the salts obtained by regressing equilibrium constant parameters over the temperature range of 0 to 250°C at the saturation pressure of the electrolyte solution. For this range of temperature the fit obtained with the simulator model is excellent with errors not greater than 0.2 percent.

If the temperature range to be modeled is extended to include temperatures up to 350°C, it is found that the simple model does not adequately represent the data. The results obtained from a regression over this range of temperatures is shown in Figure 5. The parameters chosen for use in the simulator model were based on a least squares fit of the data. One could produce a less oscillatory curve with different model parameters but this would result in greater overall error in the fit of the data. Clearly the standard model is not suitable for describing the data over this range.

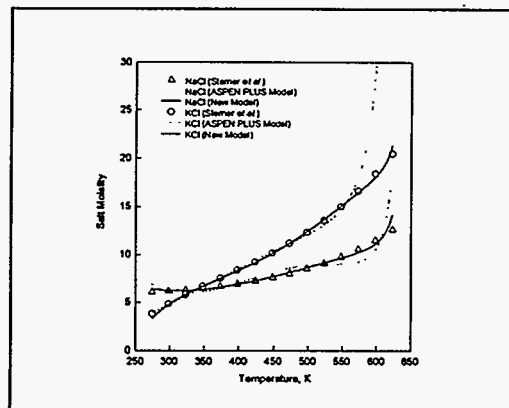
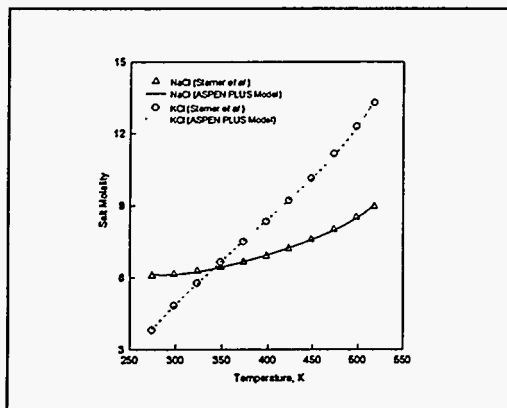


Figure 4: Solubility of NaCl and KCl from 0° C to 250° C at the saturation pressure. Figure 5: Solubility of NaCl and KCl from 0° C to 350° C at the saturation pressure.

Also shown in Figure 5 is a proprietary model which has been developed for use with electrolyte simulations in ASPEN PLUS™ at elevated temperatures and pressures. This improved model has proven effective at describing salt solubilities to the near critical region of the solution. The method by which the parameters for the new model are determined minimizes the effects of errors produced in other parts of the model such as the extrapolation of the activity coefficient models to higher temperatures and salt concentrations.

Representative of an electrolyte forming multiple solid phases is Na_2SO_4 . Here, the coefficients of equation (4) for each of the phases were regressed from the solubility data of Linke. [13] Activity

coefficient model parameters had been previously regressed. Because the temperature range covered by any of the individual salt forms was not large ($< 250^{\circ}\text{C}$), the polynomial equation for the equilibrium constant provided in the software package proved to model the solid phase equilibrium quite accurately. The fit is shown in Figure 6.

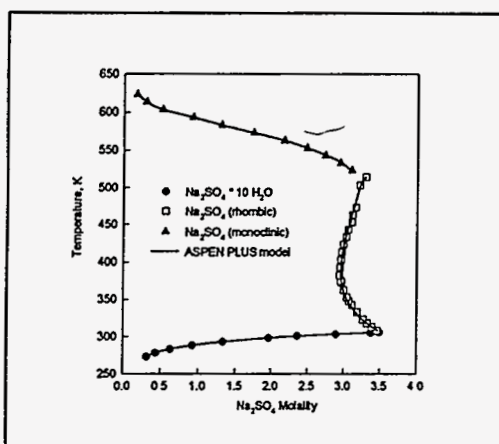


Figure 6: Solubility of Na_2SO_4 and its hydrates at saturation pressure.

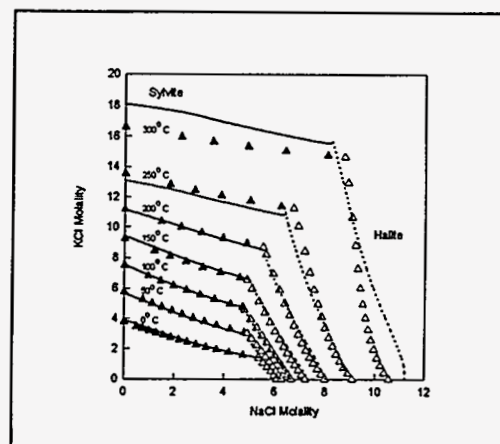


Figure 7: Solubilities in the $\text{NaCl(aq)}\text{-KCl(aq)}$ binary system from 0 to 300°C in increments of 50°C .

An interesting modeling challenge is the $\text{NaCl-KCl-H}_2\text{O}$ binary salt system. As was previously stated the Pitzer model is accurate only to concentrations of 6 molal. Above 300°C the molalities of NaCl and KCl at solid saturation are double and triple this concentration, respectively. The electrolyte concentrations in the binary solution approach 30 molal at these temperatures. For these reasons, the Chen electrolyte model is chosen to model the system.

As described, the Chen model contends with the short-range interionic and intermolecular interactions through the use of binary interaction parameters. Thus, for a binary salt system, interactions between the ions of the individual salts and the solvent and the interactions between the ions of the two salts should be accounted for. One procedure for determining these parameters is to first regress the interaction parameters for the individual salt systems and then to address the interactions between the ions of the two salts. Earlier, we presented results for both the $\text{NaCl-H}_2\text{O}$ and $\text{KCl-H}_2\text{O}$ systems from 0 to 250°C . Here we recalculate the parameters of equation (2) to include data to 300°C . The parameters for the individual electrolyte systems are then utilized in the regression of the interaction parameters between the ions of the two salts. To evaluate these binary salt interaction parameters, data are needed describing the solubility of NaCl in KCl(aq) , KCl in NaCl(aq) and data describing conditions in which both salts appear as solids. Sterner et al. have studied this binary system to temperatures in excess of 700°C and it is their data which was used for our regressions. [14]

The results of the regression are shown in Figure 7. The fit of the data is seen to be relatively good to approximately 250°C . At 300°C the fit is quite poor. As was demonstrated in the single salt systems, this is where the simple chemical equilibrium constant model supplied in $\text{ASPEN PLUS}^{\text{TM}}$ begins to fail. Pabalan and Pitzer have shown that it is possible to model this binary salt system with good accuracy to 350°C using a Margules expansion model for excess thermodynamic properties with appropriate expressions for the standard-state free-energy changes. [15] While it might be possible to include such a model into the Aspen code, this approach is nontrivial.

SUMMARY

Mean activity coefficients and salt solubility were modeled for a variety of electrolyte systems using the models available in a well known chemical process simulator, ASPEN PLUSTM. Both the Pitzer and Chen electrolyte activity coefficient models were found to give accurate representation of the experimental data. The solubility product model provided with the package were found to work well provided the parameters for those model are properly regressed and the range of temperatures kept relatively small. A proprietary user-supplied model was found to provide a more accurate means of describing the data above 300 °C. The ability to manipulate the property models is difficult for more complex aqueous systems, such as the binary salt NaCl-KCl system, because arbitrarily-chosen models may not be employed in the data regression system of the software package.

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**12th International Conference
on the
Properties of Water and Steam**

**Orlando, FL
September 14, 1994**

Seminar Outline

- **Introduction to chemical process simulators, discussion of their uses and our motivation for improving their electrolyte modeling capabilities**
- **Discussion of some of the challenges in modeling electrolyte systems**
- **Overview of ASPEN PLUS and a brief description of its electrolyte models**
- **Presentation of our efforts to improve and extend the applicability of these models to higher temperatures and pressures**

Chemical Process Simulators

- **Chemical process simulators are designed to perform material and energy balances on processes of interest to the chemical processing industry**
- **Simulators typically contain common unit operation models, physical property models and data banks containing information on a wide variety of chemical compounds**
- **Increasingly stringent environmental regulations have made the ability to accurately model streams containing electrolytes of vital economic interest to the chemical processing industry**
- **The physical property models within ASPEN PLUS include both the electrolyte models of both Pitzer and Chen.**

Electrolyte Modeling in ASPEN PLUS

- **Two activity coefficient models, those of Pitzer and Chen, are included in the simulator.**
- **Gas phase behavior may be modeled using the Redlich-Kwong-Soave or Peng-Robinson EOS or by using the ASME steam tables. Dissolved gases are modeled using Henry's Law.**
- **Chemical reaction equilibrium is modeled using a four parameter temperature dependent model for the equilibrium constant or by estimating solution composition from the free energy of the reaction components**
- **Models for computing thermodynamic properties such as enthalpy, free energy and heat capacities are contained in the code.**

User Input in ASPEN PLUS

Physical Property Data Input:

The user may enter physical property constants or model parameters.

Data Regression System (DRS):

The user may regress model parameters from experimental data.

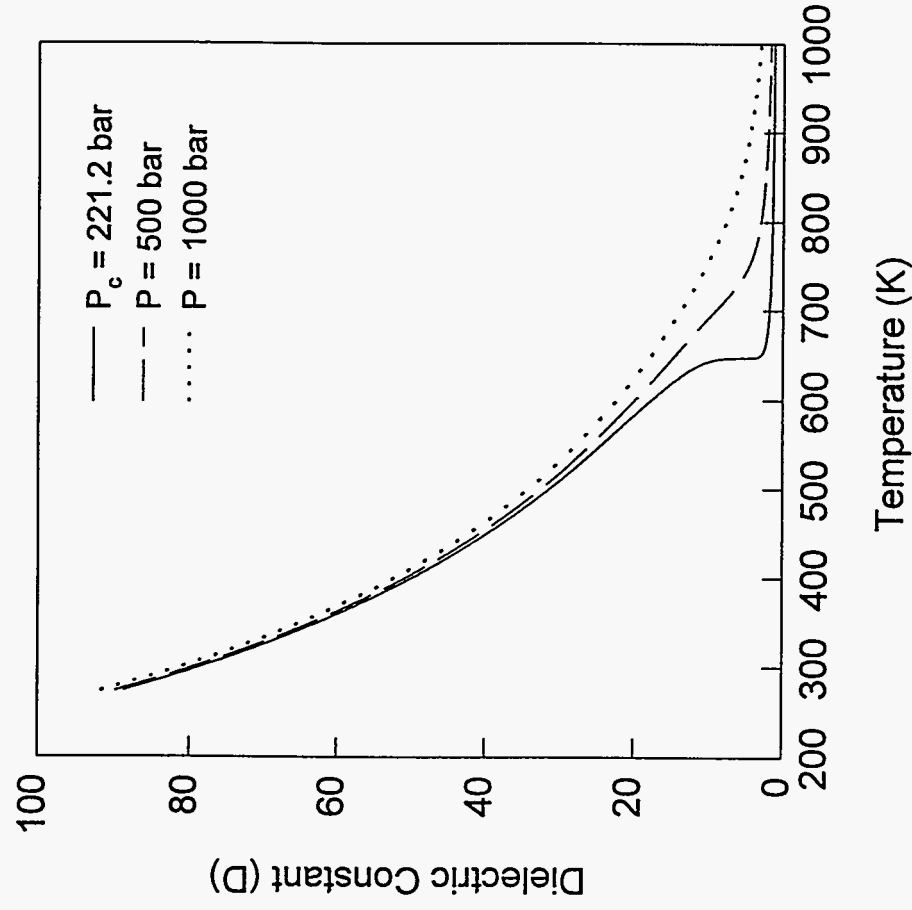
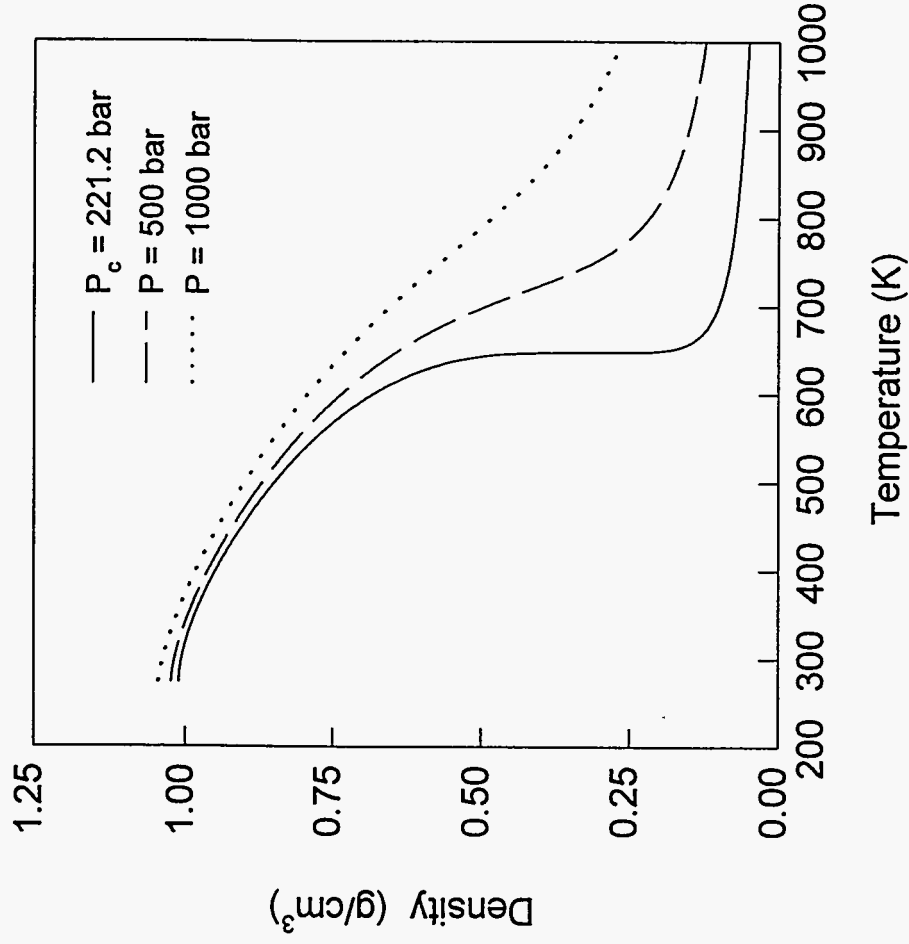
In-Line Fortran Code:

The user is able to add Fortran Code into the simulator input code.

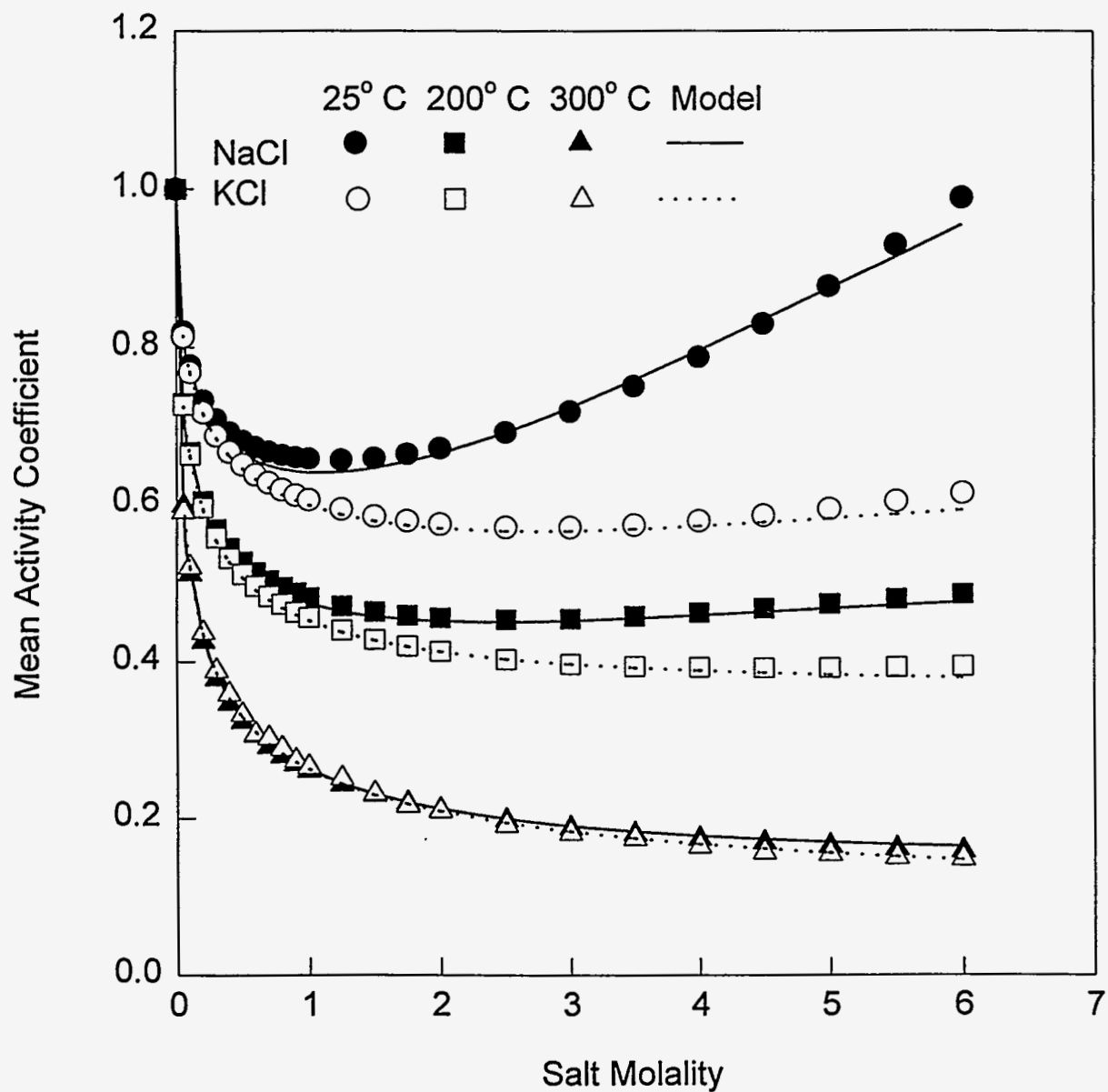
User Models:

User models are Fortran subroutines written according to specific rules with allow them to be called during a simulation.

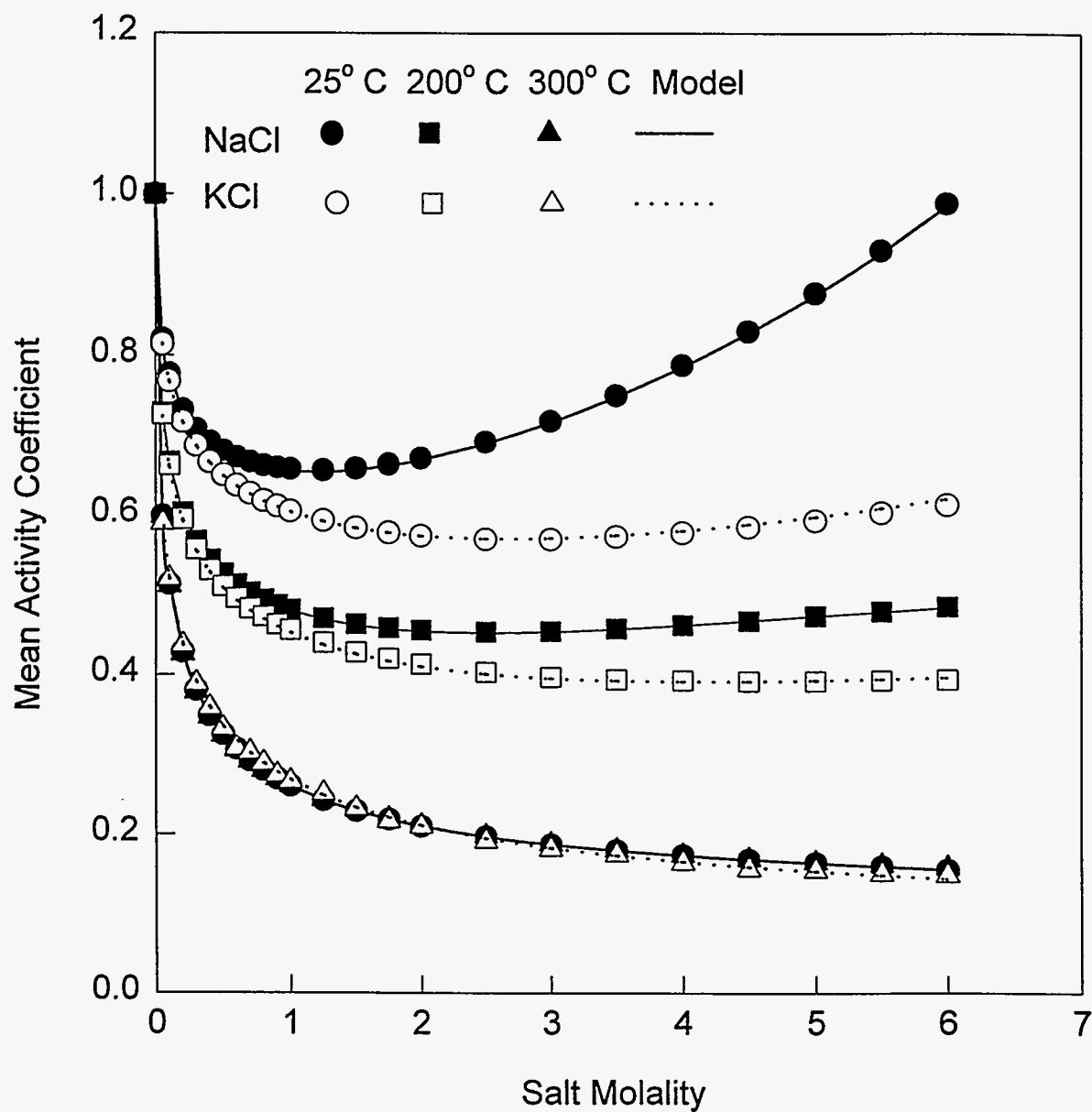
Properties of Water as a Function of Temperature and Pressure



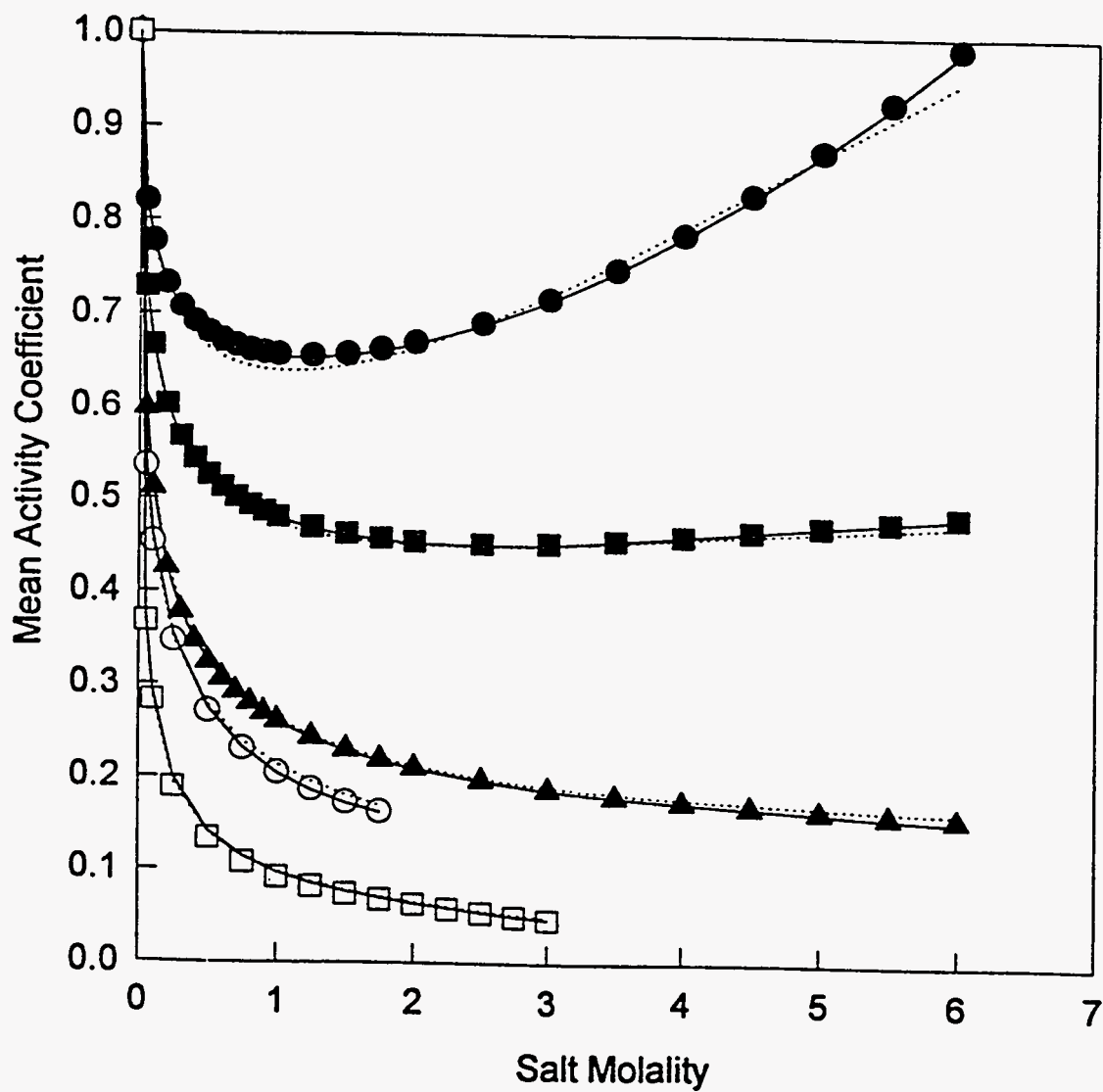
ASPEN PLUS Chen NRTL Model Activity Coefficient Predictions for NaCl and KCl



ASPEN PLUS Pitzer Model Activity Coefficient Predictions for NaCl and KCl

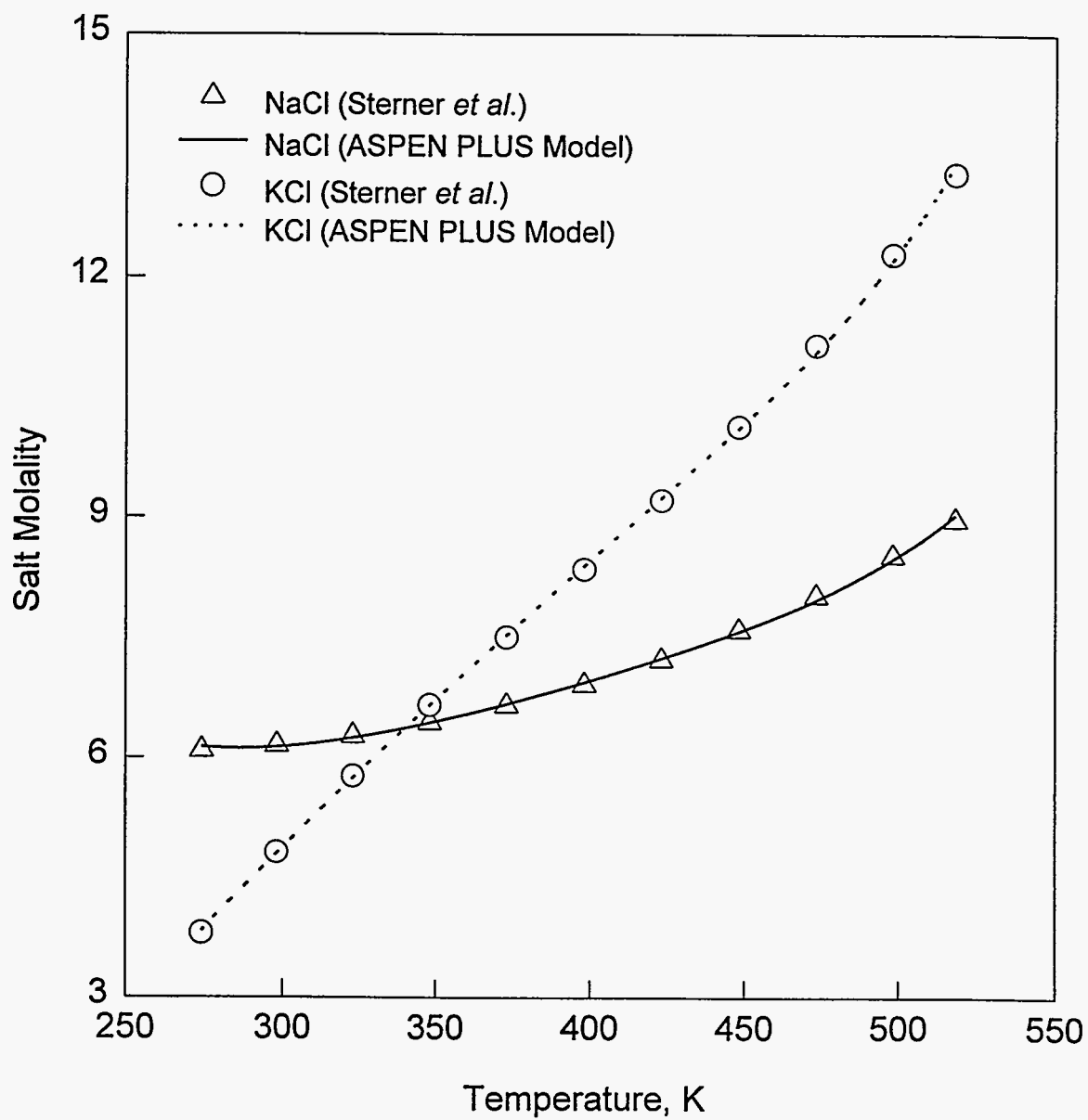


Demonstration of Mean Activity Coefficient Models in ASPEN PLUS

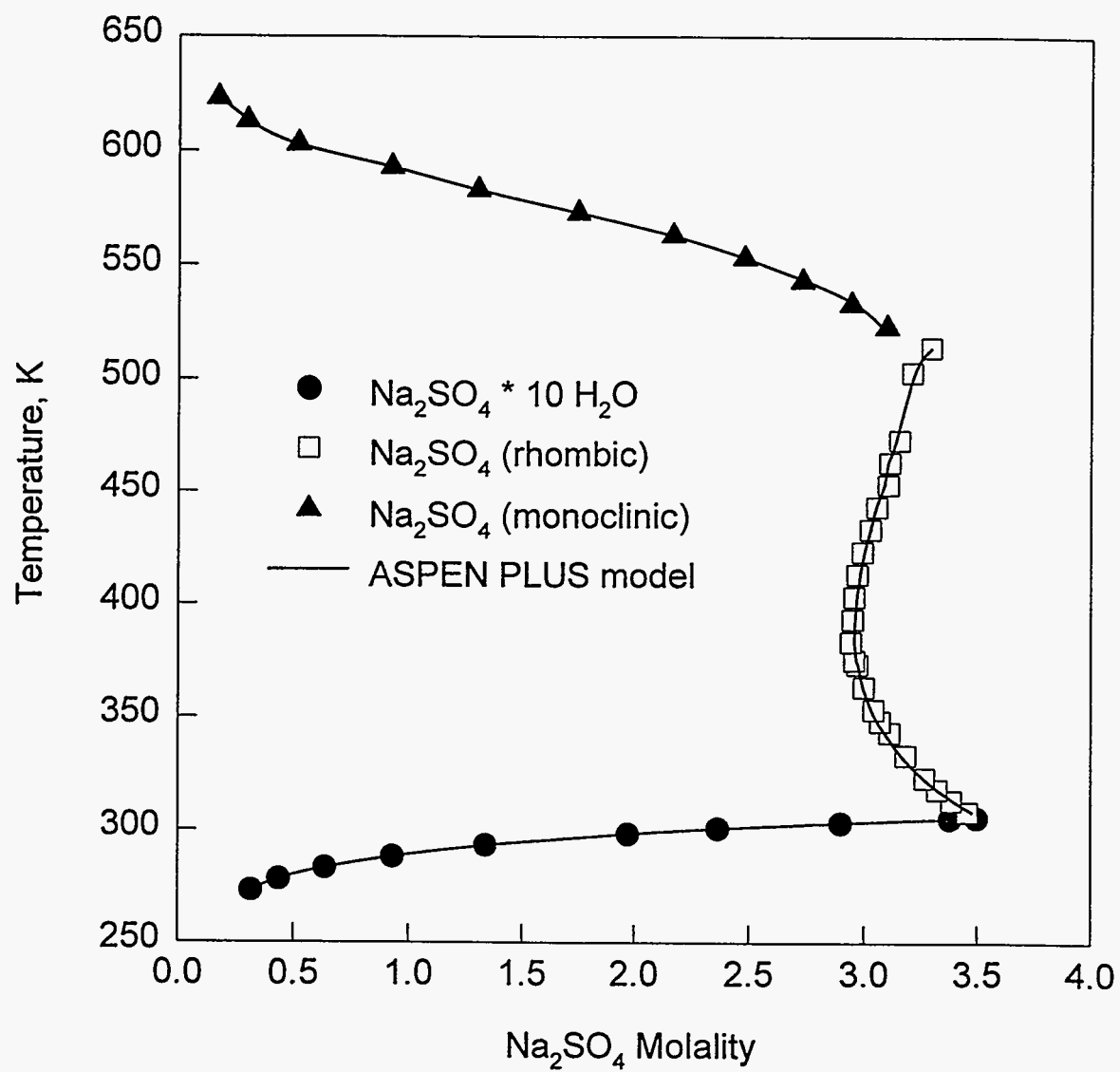


Data	25 C	200 C	300 C	Model	Pitzer	Chen
NaCl	●	■	▲	NaCl	—
Na ₂ SO ₄	○	□		Na ₂ SO ₄	—

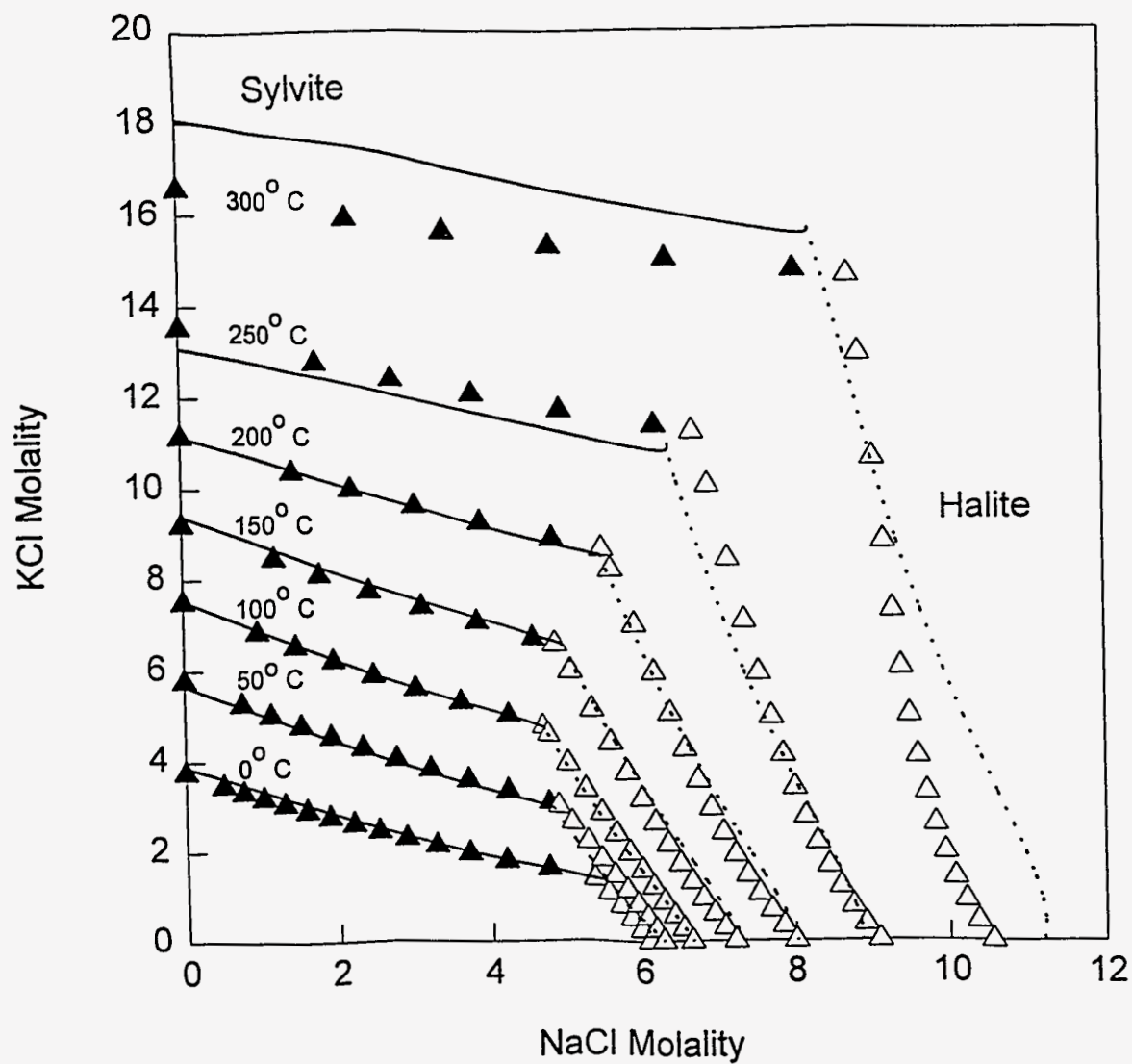
Solubility of NaCl and KCl from 0 to 250 °C



Solubility of Na_2SO_4 and its Hydrates

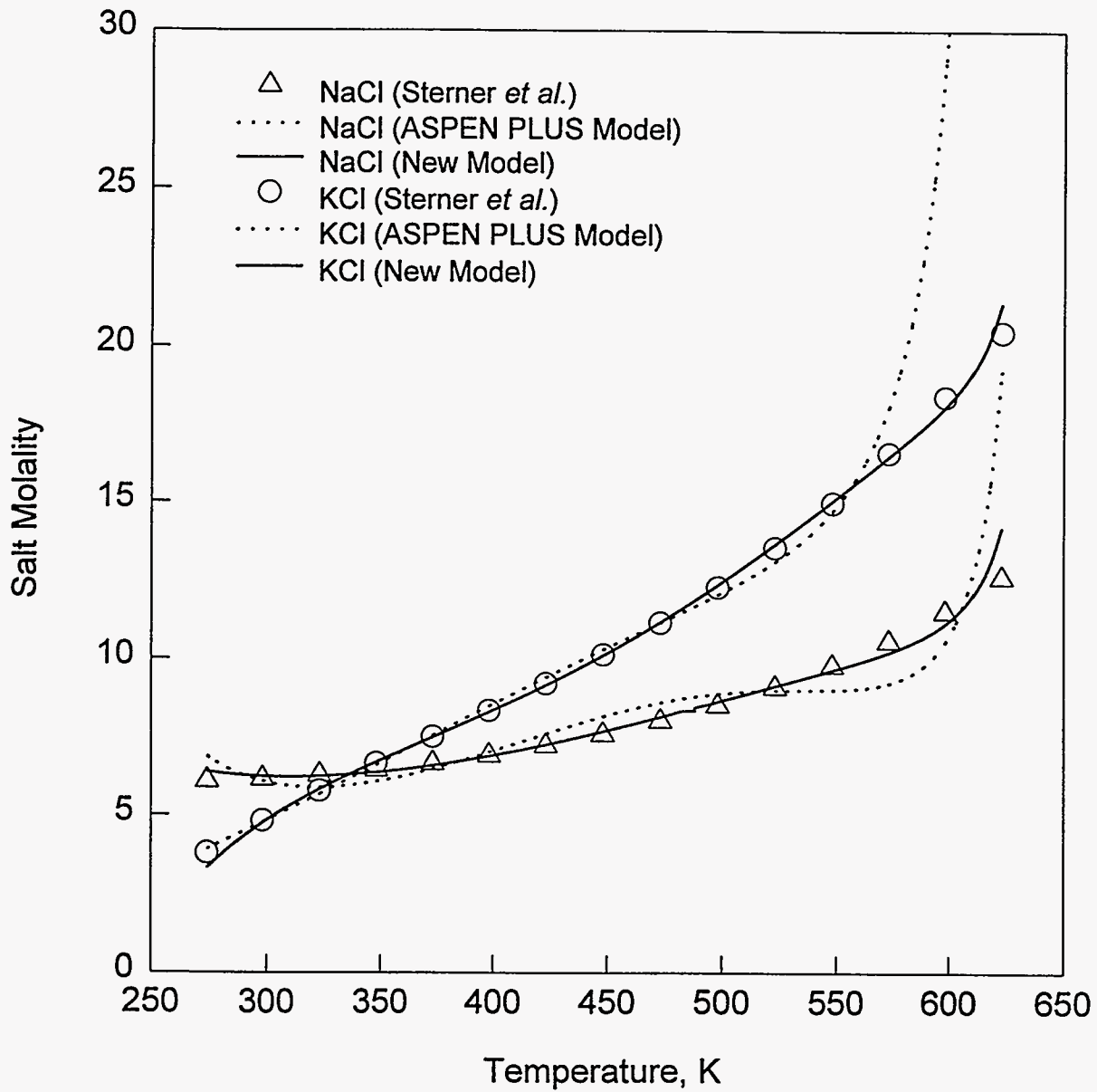


Solubility of NaCl and KCl in the NaCl-KCl-H₂O System



Solubility of NaCl and KCl

from 0 to 350 °C



Summary and Conclusions

- **The increasing reliance of the chemical processing industry on computer simulation of their processes provides a clear incentive toward insuring accuracy in the modeling of physical properties.**
- **Accurately simulating the behavior of aqueous electrolyte systems represents both a great challenge and a great need to the chemical industry.**
- **ASPEN PLUS, a chemical process simulator provides a useful framework for modeling electrolyte solutions in industrial applications.**
- **Many of the difficulties inherent in modeling electrolyte systems at elevated temperatures and pressures may be minimized through data regression and the use of new user models.**

Future Work

- **It is our goal to produce an integrated package allowing the modeling of electrolyte systems to be extended beyond the present range of the simulator.**
- **The work discussed today is being applied to other chemical systems and to elevated temperature and pressure.**
- **As temperatures and pressures increase, less data is available for regression and the systems themselves increase in complexity. We are working to improve our ability to predict electrolyte behavior in increasingly extreme conditions.**