

## **Project Vision**

This document provides details concerning the projected new features, which will be pursued for MSE within the framework of Phase IV. Your participation in the next phase of the Consortium will assure that the new technology can be applied to your most pressing applications at the earliest possible date.

In Phase IV of the MSE consortium, we propose to select for implementation among the following development topics, based upon how many companies support this proposal and the priorities expressed by these supporters:

### **1. Development of a model and associated parameters for mutual diffusivity**

Mutual diffusivity is required for implementation of a first-principles model for mass transfer calculations.

### **2. Development of a model and associated parameters for interfacial tension**

Interfacial tension would enable a number of important calculations in the future including, but not limited to emulsions.

### **3. Calibration of the thermodynamic model for chemical systems of common interest to consortium members.**

We recognize that databank coverage is at the core of the usefulness of the software. In this section, we summarize the chemical systems that we are proposing to include as part of MSE IV. These systems have already been suggested to us by MSE III consortium members and other software users. In particular, most of these systems were indicated as priority items at the MSE Technical Partner Meeting held on October 21, 2008. This list should not be regarded as exhaustive. We are asking for further input regarding the systems that should be added and the priority ranking of those that are already on the list. Strong support was provided, at this meeting, for:

- a. Metal silicates**
- b. Transition metal cyanides**
- c. Scaling and corrosion inhibitors**
- d. Supercritical CO<sub>2</sub> in the presence of various minerals and brines**
- e. Remaining inorganic and organic chemistry that is needed to model oil- and gas-related systems; this will include Sr, Fe<sup>II</sup>, sulfide, formate, acetate, and ammonia chemistry in aqueous systems and in the presence of methanol and glycols**

### **4. Comprehensive treatment of ionic liquids**

Recently, we started a preliminary project to examine the applicability of MSE to ionic liquids. It is already evident that MSE makes it possible to reproduce both phase equilibria and transport properties of ionic fluid mixtures. However, more work is needed to establish a comprehensive treatment of common ionic liquids.

## **5. Correlations to enable prediction of gas solubility in MSE chemical environments**

This would extend prior work in the area of predicting hydrocarbon gas solubility to cover the solubility of other industrially important gases in environments that may contain dissolved electrolytes and nonaqueous solvents. Such a capability is available to a degree for aqueous environments via the Setschenow framework but is not available in the current MSE.

## **6. Restructuring redox calculations to enable selection of individual oxidation states**

This would give the user more flexibility to eliminate oxidation states that are not produced in reality even though they are thermodynamically stable. Such phenomena are quite common in practice, for example with nitrogen and halogen species.

## **7. Implementation of a first-principles model for prediction of mass transfer**

Utilizing the new, mutual diffusivity model noted above as part of MSE IV, we would be able to implement a first-principles model based on the Stefan-Boltzmann formalism resulting in a highly predictive heat and mass transfer limited tower program including the ability to simulate packed columns.