Chapter 4. Reaction network and thermodynamic properties

All reactor models will, as a minimum, require the following information for each species:

- chemical formulas
- standard heat of formation
- Gibbs free energy of formation
- heat capacity

The above information can be obtained from several sources. In this book, the information has been obtained from Reid et al (1977). Another source could be a process simulation program because they usually include a large database of physical properties. Also, the standalone program, Prode Physical Properties (PPP), can be used in conjunction with either Mathcad or SMath. An example of its use with SMath is provided for Example 1.

The reaction network must also be known. For very complex systems, such as biochemical reactions, this information may not be readily available. However, all of the models developed in this course require a reaction network that conserves mass.

The list above is sufficient to determine the effluent composition of an equilibrium controlled reactor, but not the amount of catalyst needed. For that and for a reactor not at or near equilibrium, a kinetic model of the rates of each reaction is needed. In addition, other properties of the fluid and catalyst will be needed.

Example 1: Methane Reforming

With the above information, heats of reaction and free energies as functions of temperature can be easily defined for use in the model. To demonstrate this step in building a reactor model, steam reforming of methane will be used as the reaction system. This system is a commonly used example in textbooks, so the model developer can check a model against published results, e.g. Rase (1990) pf 232.

Please read Example 1 in the file "Example 1.pdf" or execute either the Mathcad file, "**Example 1.xmcd**", or the SMath file, "**Example 1.sm**". The SMath/PPP version is also provided in PDF.