FLASH PROBLEM: Multi component vapour liquid equilibrium calculations.

AUREL Systems Inc. Company Information:

CADSIM Plus, the chemical process simulation software is authored and marketed by Aurel Systems. Chemical process engineers to use our tools to;

- Visualize plant processes
- Perform heat and material balances of process flow sheets
- Design new plants, or modifications and expansions to, existing plants
- Help engineers to develop a better understanding of how their plants *really* operate
- Reduce costs and increase profits
- Predict operating efficiencies and anticipate problems
- Trouble-shoot process and control problems
- Assist operators to plan for production changes and disruptions
- Train operators

In addition to software sales, Aurel Systems provides many services, including training, modeling, custom simulation module development, and chemical engineering consulting expertise.

Problem Description:

Process simulation techniques involve mathematical calculations of process systems based on fundamental physical laws. Using first principles, the simulation tool calculates the state of the given system for the given conditions. For example, take the flow of a chemical mixture through a pipe. Typically the process engineer would know the composition of the mixture flowing through the pipe and also its temperature and pressure. Given these details, the simulation tool would calculate the state of the system, in other words the density, energy and entropy of the system. These calculations, when done assuming equilibrium, are known as the Flash calculations or the phase equilibrium calculations.

The flash calculations form the basis for most other calculations in the simulation system. These calculations give us the phase compositions (vapour and liquid) and also the amount of vaporization. The energy, entropy and density of the system are also simultaneously calculated along with the phase calculations. The equations used for these calculations are known as the Equations of State. Equations of State describe the relationship of pressure, volume and temperature for a given fluid and are based on parameters easily deduced from the physical property of the components.

Numerical Formulation of the Problem:

Given an Equation of State, we can define a set of equations that describe the different variables in the system. These equations are based on the basic laws of thermodynamics. Although the number of equations is relatively small, the numerical formulation is not very obvious. Variables are bounded and because of a large interdependency of the variables in the different equations, identifying the free variables correctly is a challenge.

Also, the partial derivative curves are not smooth, especially when vaporization of condensation occurs. For example, the energy can change abruptly with a small change in temperature creating a divergence of the solution. Accurate scaling of the different variables is also a challenge that will make convergence difficult.

Previous attempts, by numerous researchers and by our own engineers have not yielded satisfactory results with simultaneous calculation methods. Although some success with specific systems is recorded in literature, it is not reliable and the methods are easily broken with other mixtures. Our own research, at Aurel has not yielded a solution to the problem under certain conditions. And when the problem does solve, the low performance and lack of robustness prevent it from being useful in a simulator.

Currently, at Aurel, an iterative algorithm is used for solving the problem. Although this has proven to be faster than the simultaneous methods attempted so far, the performance is not nearly good enough. We believe that finding better solving methods is essential to make process simulation technology more useful to industry.