AQUAnews

The Newsletter for *AQUAlibrium* Users

Volume 1 Number 2 **Winter 1996**

Welcome to the second issue of ***AQUAnews***. As with the previous issue, feel free to make additional copies for your colleagues -- provided they are distributed *free of charge*. We are always seeking ideas for articles. The address is provided on the last page. Information about purchasing a copy of ***AQUAlibrium*** can also be obtained by writing to the address given on the last page.

New Release of *AQUAlibrium*

A new release of ***AQUAlibrium***, Version 2.0e, is now available. A new release, as opposed to a new version, indicates that relatively minor changes were made to the program and releases are noted by the letter following the version number. Users of earlier releases of Version 2.0 will automatically receive updates in the mail.

Version 2.0e is a result of some fine-tuning of the parameters in the model to better fit the available experimental data. In particular, the values for the system propane-water have been adjusted resulting in an improvement of the prediction for that system.

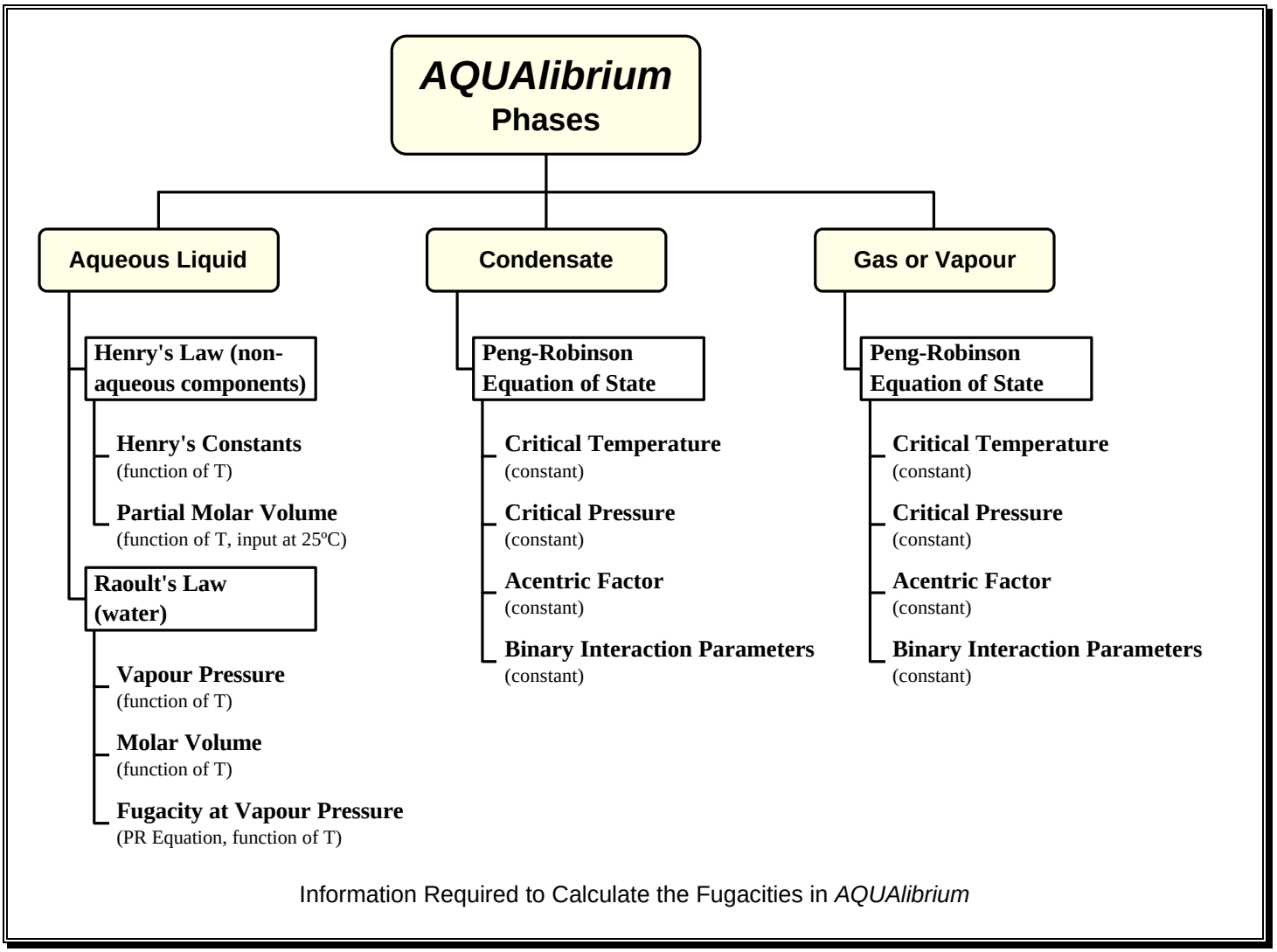
In the last edition of this newsletter, results were present based on Version 2.0d. If you re-run these examples you will see that the calculations based on version 2.0e are slightly different. The output shown above is for one of those calculations.

```
                        |======================|
                        |     AQUAlibrium      |
                        | Version 2.0e (c)1993 |
                        |======================|

THREE-PHASE NORMAL DEW POINT CALCULATION IN A NATURAL GAS-WATER SYSTEM
    Temperature  50.00 deg C     Pressure     3003.4 kPa

Component   ----------------- Mole Fraction ----------------     Fugacity
              Feed       Condensate    Aqueous       Vapor        (kPa)
Water       .3333E+00    .1182E-02    .9996E+00    .3728E-02    .1260E+02
Ethane      .3333E+00    .3331E+00    .2268E-03    .4981E+00    .1244E+04
Propane     .3333E+00    .6657E+00    .1405E-03    .4982E+00    .9481E+03

Component    ------------- K-factors -------------
               gas/aq       gas/con        con/aq
Water        .3729E-02     .3155E+01     .1182E-02
Ethane       .2197E+04     .1495E+01     .1469E+04
Propane      .3545E+04     .7483E+00     .4737E+04

                                Vapor      Condensate      Aqueous
   Mole Per Cent                66.90          .00          33.10
   Mole Per Cent (Non-aqu.)    100.00          .00            -
   Weight Per Cent              80.59          .00          19.41
   Weight Per Cent (Non-aqu.)  100.00          .00            -
   Volume Per Cent              98.42          .00           1.58
   Volume Per Cent (Non-aqu.)  100.00          .00            -
   Molecular Weight (g/mol)     37.01        39.39          18.02
   z-factor (z=Pv/RT)           .6279        .1127          .0204
   Density (kg/m**3)              65.90      390.8          988.6

Water content of gas       = 2.996E-03 kg/m**3 (STP) = 2.835E-03 kg/m**3 (std)
                           = 3.728E+03 ppm
Water content of condensate= 9.497E-04 kg/m**3 (STP) = 8.984E-04 kg/m**3 (std)
                           = 1.182E+03 ppm
```

How Does *AQUAlibrium* Work?

AQUAlibrium performs all of its equilibrium calculations based on the principle of equal fugacities. The fugacities are calculated on a phase basis. A different model is used for each phase and they require different input data. The chart below summarizes the information required for each phase in order to calculate the fugacities.

In order to use an equation of state, the critical temperature, critical pressure and acentric factor are required for the pure component. For each pair of components, a binary interaction parameter is required. The same data are used for both the gas and condensate phases.



Information Required to Calculate the Fugacities in *AQUAlibrium*

Henry's law requires a Henry's constant as a function of temperature. The partial molar volumes at infinite dilution are required for the Poynting correction, the effect of pressure on the reference fugacity. Finally, the properties of water are also required: the vapor pressure and the molar volume. The molar volume is used in the Poynting correction for the solvent.

Those readers interested in more information about Henry's law are referred to the following papers:

Carroll, J.J., "What is Henry's Law?", *Chemical Engineering Progress*, **87**, (9), 48-52, (1991).

Carroll, J.J., "Use Henry's Law for Multicomponent Mixtures." *Chemical Engineering Progress*, **88**, (8), 53-58, (1992).

Registered owners of ***AQUAlibrium*** can receive copies of these at no charge by writing to the address given to the right.

AQUAnews is published by

John Carroll, Ph.D., P.Eng.
P.O. Box 52163
Garneau Postal Outlet
8210 - 109 Street
Edmonton, Alberta
CANADA TG6 2A4

Information about purchasing copies of ***AQUAlibrium*** can be obtained from the above address.