**First Attempt for Robust Bubble/Dew Problem Solution with Bender EoS**

Filippo Bisotti1, Flavio Manenti1\*

*1 Politecnico di Milano, DMIC Department “Giulio Natta”, Piazza Leonardo da Vinci, 32, 20133, Milan, Italy;*

*\*Corresponding author: flavio.manenti@polimi.it*

**Highlights**

* Thermodynamic package available only for Air Separation Unite
* Attractive to be used in simulation environment
* Presence of twenty fitting parameters makes Bender EoS very flexible and efficient
* Development of numerical tricks to avoid any trivial and unfeasible solutions

**1. Introduction**

The Bender Equation of State is a specific thermodynamic package available for Air Separation Unit. Bender EoS is essentially composed by twenty fitting parameters which let very flexible and efficient prediction of thermodynamic of air mixture. The model has been implemented to solve bubble/dew problems. The main difficulty is to avoid the convergence of the system toward trivial solution, which is actually unfeasible. In addition, strong nonlinearities in the formulation of the Equation of State and in the mixing rules make the solution quite stiff (Figure 1), where for very small change of the density value, pressure solution rapidly diverges. Therefore, some tricks have to be applied in order to drive the system toward the right solution



**Figure 1** – pressure prediction with Bender EoS for liquid (blue line) and vapor phase (red)

**2. Methods**

In order to solve a vapor-liquid equilibrium the following nonlinear system has to be solved

According to the thermodynamic model, pressure is function of temperature, density and composition of the phase (m): temperature and pressure dependence appear in mixing parameter

To prevent any possible divergence of the solution due to nonlinearities, a sensitivity analysis on the several mixing coefficients and, finally, on the global term appearing inside the square brackets has been done. This clearly depicts that exists for both phases a feasibility region owing to that absolute pressure cannot be negative. Obviously, this criterion is adopted to remove any potential unfeasible behavior of the model in any iteration during the nonlinear system solution. The system has been solved in VSC++ 2013 combined with the BzzMath Library numerical tools.

**3. Results**

Figure 2 compares the solutions of dew problem in pressure for dry air with the results of other EoS directly implemented in Aspen-Hysys: Peng-Robinson, BWR and Bender one. The experimental data are taken from NIST experimental campaigns’ results published in literature

**Figure 2** – relative error comparison of pressure and liquid density prediction with three different EoS

**4. Conclusion and future developments**

Bender model is an effective thermodynamic tool to predict the behavior if air components mixtures and its results are comparable to those obtained from commonly used Equation of State in ASU design. Indeed, it is also accurate near both the triple and the critical points of the mixture. In addition, more reliable results and convergence are ensured by forcing the solver to avoid the unfeasible region. Therefore, considering that Bender EoS’s parameters directly derive from a numerical fitting, the partial loss of physical meaning can be overcome by properly selecting and imposing physical constraints on the thermodynamic model itself. In the future, further numerical tricks may be applied not only to increase the predictive capacity and help the convergence but major efforts should be focus on decreasing the computational time without loss in accuracy and precision.

**References**

1. E. Bender, The Calculation of Phase Equilibria from a Thermal Equation of State Applied to the Pure Fluids Argon, Nitrogen, Oxygen and their Mixtures, C.F. Verlag Muller, Karlsruhe, 1973
2. E. Bender, An equation of state for predicting vapour-liquid equilibria for system N2-Ar-O2, *Cryogenics*, 13(1), 1973
3. G. Buzzi-Ferraris, F. Manenti, Nonlinear Systems and Optimization for Chemical Engineer – Solving numerical problems, Wiley-VCH, 2014
4. E.W. Lemmon, R.T. Jacobsen, S.G. Penoncello, D.G. Friend, Thermodynamic Properties of Air and Mixtures of Nitrogen, Argon and Oxygen From 60 to 2000K at Pressures to 2000MPa, *J. Phys. Chem. Ref. Data*, 29(3), 2000