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CALCULATION OF DOUBLE RETROGRADE VAPORIZATION: NEWTON'S METHODS AND HYPERHEURISTIC APPROACH

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Abstract. Double retrograde vaporization is a thermodynamic phenomenon that, instead of an ordinary dew point curve, its loci can exhibit two domes, at temperatures slightly above the critical temperature of the more volatile component (under specified pressure). Besides, this curve has an S-shape, at temperatures slightly below referred critical temperature. These facts imply, respectively, in the existence of four or three roots for the phase coexistence problem. We investigate the numerical aspects of dew point calculations of a system that depicts double retrograde vaporization – the mixture ethane+limonene. In order to evaluate regions of convergence/non-convergence, we construct basins of attraction for the dew point calculations. These diagrams indicate a fractal behavior arising from application of Newton's type methods and still some roots have small convergence radii. Moreover, a new technique – called hyperheuristic, which uses five recurrent metaheuristics to overcome the peculiarities of this physical problem – was applied to dew point calculations in this system. These complex characteristics make this problem a "challenging" nonlinear system, useful to evaluate/validate methodologies for solving nonlinear equations (including optimization algorithms), even when globalization techniques are applied.

Keywords. Phase equilibria, Newton's method, Double retrograde vaporization, Hyperheuristic, Optimization.

1 Introduction

Nonlinear systems of equations are present in many engineering situations, and solving techniques are continuously being developed for this kind of problem (see, for example, [1, 2, 3, 4]). Therefore, new solving techniques are usually applied to some "benchmark" problems, as initial tests. For example, we can cite chemical equilibrium systems [5, 6, 7] and robot kinematics [8]. As indicated by Hirsch et al. [2, 9], some of these problems are challenging ones, mainly if they exhibit multiple solutions (roots) and some roots have *domains of attraction* in relation to others (as indicated by Allgower and George [10]). In this context, Shacham et al. [11] developed a web-based library for testing methodologies applied to nonlinear systems.

In this paper, we analyze some convergence aspects related to the calculation of a thermodynamic phenomenon called double retrograde vaporization, which occurs at high pressures and can be used as a hard test problem for validating new methodologies for nonlinear systems. This kind of nonlinear phenomenon arises from real world situations and has applications in petroleum science and supercritical extraction processes.

Double retrograde vaporization (DRV) was firstly reported by [12] for methane+n-butane system. This thermodynamic phenomenon is characterized by the existence of three dew-point pressures for a specified composition of vapor phase, at temperatures closely below the critical temperature of methane. These facts produce a dew-point locus with a S-shaped structure when the mixture is enriched in methane. The same authors [13] present dew-point loci for methane + n-pentane system at temperatures above the critical temperature of methane. In this case, the dew-point locus shows a double-dome aspect. [14] presents simulations of DRV phenomena using the Peng-Robinson equation of state. Recently, [15] indicates, by numerical calculations, that many hydrocarbon systems can show double retrograde vaporization, including the system n-butane + hexadecane and mixtures with aromatic compounds (like naphtalene). In the present work, we show calculations of dew-point pressures for the system ethane + limonene. This problem is represented by a system of nonlinear algebraic equations, which is solved by some variations of Newton's method (essentially, damping strategies) with numerical derivatives (using forward finite differences). For each initial estimate, the root-finding method can converge to a particular solution of the problem. Thus, we construct basins of attraction that indicate the attraction domain for each root of the nonlinear system and the region where there is no convergence. One can point that dew point curves can be produced by bubble point calculations or even flash calculations. However, there are some situations where dew point problem must be solved: (i) when experimental data are measured for vapor phase at high pressures (for instance, in parameter estimation), which is particularly interesting for prediction of DRV (as pointed by [14]) and

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