AN IMPROVED SCHEME TO HANDLE NONLINEAR EQUATIONS OF SCFS

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ABSTRACT- In this study, an improved iterative mathematical scheme is employed to handle nonlinear equations arising in estimation of thermodynamic properties at supercritical conditions. The method takes the classical Newton-Raphshon method as a starting point. It is demonstrated that the proposed method enjoys higher degrees of accuracy and requires less iteration numbers to reach to a specific solution compared to that of by the Newton-Raphson technique. To illustrate the efficiency of the mentioned solution technique, some numerical examples are also given. The proposed method has easily been implemented into computer codes to provide parametric, not numeric, solutions to the target equations. Consequently, one can derive other thermodynamic properties which have not been treated parametrically yet, based on this approach.

KEYWORDS: Quintic EOS, Iterative scheme, Supercritical region

INTRODUCTION

Precise thermodynamic data at supercritical conditions are vital for design, modeling and simulation of supercritical systems. Equations of states (EOSs), while chosen appropriately, can provide reliable huge sets of data in a most condensed manner and serve as strong tools for many thermodynamic calculations. Many EOSs have been proposed for simulate the behavior of pure components/mixture in supercritical regions (see for example [1-4]). Almost recently and on the basis of Nakamura-Bredveld-Prausnitz (NBP) equation of state [5], Koziol has come up with a quintic equation of state applicable to substances both in sub- and supercritical conditions [6]. The equation is:

$$p(T,v)=\frac{RT\left[(v-d)^2+e^2\right]}{(v-b)^3}-\frac{a(T)}{v^2+c(v-b)} \tag{1}$$

where a, b, c, d, e are five temperature-dependent parameters to be discussed later. Obviously, the preceding equation is quintic with respect to v (molar volume). As the classical Abel's impossibility theorem suggests that no general formula for achieving zeroes of most polynomials with degree greater than 4 exists [7], robust computation of the roots of eq.(1) entails complexity.

It is the objective of this paper to present a Newton-Raphson type improved iterative scheme to treat eq.(1) elegantly. The initial idea stems from [8]. The approach is based on incorporating a powerful analytical solution technique namely, Adomian Decomposition Method (ADM) into the traditional Newton-Raphson routine. ADM has established a good reputation in various braches of science and engineering, particularly for treating nonlinear functional equations. The interested reader is recommended to consult [9] for background knowledge on ADM and [10-12] for its applications. For better reference, hereinafter, we abbreviate the eq.(1) by EOS5 and the proposed method by EOS5-ADM-NR.

FOUNDATIONS OF ADM

In this section we provide a quick review of basics of ADM for the convenience of the reader. Consider a general functional equation as follows:

$$Lu + Nu + Ru = g \tag{2}$$

where L is an easily invertible linear operator, N is a nonlinear operator which maps a Hilbert space H to H, and R denotes the remaining part (and obviously u is a unknown function). By defining the inverse operator of L as L^{-1}, it is directly concluded that:

$$L^{-1}Lu + L^{-1}Nu + L^{-1}Ru = L^{-1}g \tag{3}$$

Choosing L as an n-th order derivative operator into account, L^{-1} becomes an n-fold integration operator. Thus, it is followed that $L^{-1}Lu=u+a$, where a is appeared from the integrations. ADM suggests the final solution in form of $u = \sum_{n=0}^{\infty} u_n$. Letting $u_0 = L^{-1}g - a$, eq. (2) yields:

$$u = u_0 - L^{-1}Nu - L^{-1}Ru \tag{4}$$

Furthermore, ADM forces the representation of Nu be in form of a special infinite series called Adominan polynomials as follows:

$$Nu = \sum_{n=0}^{\infty} A_n \tag{5}$$

where A_n is classically suggested to be computed from [9]:

$$A_n\left(u_0, u_1, \ldots, u_n\right) = \frac{1}{n!}\left[\frac{d^n}{d\lambda^n} N\left(\sum_{i=0}^{\infty} \lambda^i u_i\right)\right]_{\lambda=0} \tag{6}$$

Hence, a recurrence can be constructed to calculate the remnant solution terms as:

$$u_{i+1} = -L^{-1}A_i - L^{-1}Ru_i \quad ; \quad i \geq 0 \tag{7}$$

DESCRIPTION OF THE METHOD (EOS5-ADM-NR)

The five temperature-dependent parameters of eq.(1) are determined by the following formula:

$$a(T) = \Omega_a \frac{(RT_{cr})^2}{P_{cr}} \alpha(T) \tag{8}$$

$$b = \Omega_b \frac{RT_{cr}}{P_{cr}} \tag{9}$$

$$c = \gamma b \tag{10}$$

$$d = \delta b \tag{11}$$

$$e = \varepsilon b \tag{12}$$

where;

$$\alpha(T) = (T_r)^{-m} \tag{13}$$

$$m = m_0 + m_1\Theta + m_2\Theta^3 \tag{14}$$

$$\Theta = \frac{T - T_0}{T_{cr}} \tag{15}$$

The aforementioned T_0 represents the temperature of an arbitrary saturation point and is used in determination of parameters m_0, m_1 and m_2. The formula for derivation of these quantities is beyond the scope of this paper and is available elsewhere [6].

One can easily rearrange eq.(1) as follows:

$$\begin{aligned} & v^5 + \left(c - 3b - \frac{RT}{p}\right)v^4 + \left(3b^2 - 4cb + \frac{a - RTc + 2RTd}{p}\right)v^3 \\ & + \left(6cb^2 - b^3 + \frac{2RTdc + RTcb - 3ab - RTd^2 - RTe^2}{p}\right)v^2 \\ & + \left(\frac{3ab^2 - 2RTdcb - RTd^2c - RTe^2c}{p} - 4cb^3\right)v \\ & + cb^4 + \frac{RTd^2cb + RTe^2cb - ab^3}{p} = 0 \end{aligned} \tag{16}$$

For the sake of brevity, the prior equation is written as:

$$v^5 + k_4v^4 + k_3v^3 + k_2v^2 + k_1v + k_0 = 0 \tag{17}$$

where,

$$k_0 = cb^4 + \frac{RTd^2cb + RTe^2cb - ab^3}{p} \tag{18}$$

$$k_1 = \frac{3ab^2 - 2RTdcb - RTd^2c - RTe^2c}{p} - 4cb^3 \tag{19}$$

$$k_2 = 6cb^2 - b^3 + \frac{2RTdc + RTcb - 3ab - RTd^2 - RTe^2}{p} \tag{20}$$

$$k_3 = 3b^2 - 4cb + \frac{a - RTc + 2RTd}{p} \tag{21}$$

$$k_4 = c - 3b - \frac{RT}{p} \tag{22}$$

Now, let us construct the mathematical basis of EOS5-ADM-NR.
Assume that we are after the solution of the following nonlinear equation:

$$f(x) = 0 \tag{23}$$

By Taylor's expansion we can write:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{iv}(x) + \frac{h^5}{120}f^{v}(x) + O\left(h^6\right) \tag{24}$$

Consider a small value for h, such that:

$$f(x-h) = 0 \approx f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{iv}(x) - \frac{h^5}{120}f^{v}(x) \tag{25}$$

Therefore,

$$h = \frac{f(x)}{f'(x)} + \frac{h^2}{2}\frac{f''(x)}{f'(x)} - \frac{h^3}{6}\frac{f'''(x)}{f'(x)} + \frac{h^4}{24}\frac{f^{iv}(x)}{f'(x)} - \frac{h^5}{120}\frac{f^{v}(x)}{f'(x)} \tag{26}$$

According to ADM, we have:

$$\begin{aligned} h &= \sum_{i=0}^{\infty} h_i \\ &= \frac{f(x)}{f'(x)} + \frac{1}{2}\frac{f''(x)}{f'(x)}\sum_{i=0}^{\infty} A_i - \frac{1}{6}\frac{f'''(x)}{f'(x)}\sum_{i=0}^{\infty} B_i + \frac{1}{24}\frac{f^{iv}(x)}{f'(x)}\sum_{i=0}^{\infty} C_i - \frac{1}{120}\frac{f^{v}(x)}{f'(x)}\sum_{i=0}^{\infty} D_i \end{aligned} \tag{27}$$

where A_i, B_i, C_i, D_i denote i-th component of Adomian polynomials correspond to h^2, h^3, h^4, h^5, respectively.
In keeping with principles of ADM, it is deduced that:

$$\begin{cases} h_0 = \dfrac{f(x)}{f'(x)} \\ h_{i+1} = \dfrac{1}{2}\dfrac{f''(x)}{f'(x)}A_i - \dfrac{1}{6}\dfrac{f'''(x)}{f'(x)}B_i + \dfrac{1}{24}\dfrac{f^{iv}(x)}{f'(x)}C_i - \dfrac{1}{120}\dfrac{f^{v}(x)}{f'(x)}D_i; \quad i \geq 0 \end{cases} \tag{28}$$

So,

$$x - h = x - \frac{f(x)}{f'(x)} - \frac{1}{2}\frac{f''(x)}{f'(x)}\sum_{i=0}^{\infty}A_i + \frac{1}{6}\frac{f'''(x)}{f'(x)}\sum_{i=0}^{\infty}B_i - \frac{1}{24}\frac{f^{iv}(x)}{f'(x)}\sum_{i=0}^{\infty}C_i + \frac{1}{120}\frac{f^{v}(x)}{f'(x)}\sum_{i=0}^{\infty}D_i \tag{29}$$

which gives us the sought-after iterative solution formula as,

$$x_{n+1} = x_n - \frac{f(x)}{f'(x)} - \frac{1}{2}\frac{f''(x)}{f'(x)}\sum_{i=0}^{\infty}A_i + \frac{1}{6}\frac{f'''(x)}{f'(x)}\sum_{i=0}^{\infty}B_i - \frac{1}{24}\frac{f^{iv}(x)}{f'(x)}\sum_{i=0}^{\infty}C_i + \frac{1}{120}\frac{f^{v}(x)}{f'(x)}\sum_{i=0}^{\infty}D_i \tag{30}$$

As convergence speed of Adomian polynomials are very high, there is no need to expand the summations in eq.(30) up to more than their first 4 terms. Also, note that the resulted formula is general and can be applied to any other nonlinear equation arising in supercritical engineering discipline. Now all is needed is to apply the implement the eq.(30) to eq.(17).

ILLUSTRATIVE EXAMPLES

To demonstrate the reliability and efficiency of EOS5-ADM-NR, we have computed the molar density of five substances in their supercritical state and compared the estimates with Newton-Raphson algorithm. Table 1 lists the parameters required for the selected substances. As shown in table 2, EOS5-ADM-NR yields an identical solution after less number of iterations required by the classical Newton-Raphson. Moreover, as depicted in Fig.1, EOS5-ADM-NR has provided estimations which are in excellent agreement with experimental data for supercritical Argon.

Table 1. Parameters of EOS5 for some famous substances [6]

Substance	T_{cr} $[K]$	P_{cr} $[MPa]$	Ω_a	Ω_b	m_0	m_1	m_2	γ	δ	ε	T_0 $[K]$
CO_2	304.128	7.3773	0.543196	0.0981227	0.36484	-0.30053	0.266	2.70831	1.03674	0.048102	216.60
H_2O	647.096	22.064	0.629121	0.0420773	0.83638	0.333144	1.01617	15.1849	1.4506	1.12124	400.00
CH_4	190.564	4.5992	0.511565	0.0813664	0.307615	0.011752	0.06538	3.10726	1.03165	0.293246	108.0
C_2H_6	305.33	4.8718	0.528567	0.0896589	0.314602	-0.09748	0.126795	2.83565	1.01956	0.098953	184.31
Ar	150.687	4.863	0.513023	0.0895572	0.247433	-0.07123	0.07171	2.57258	1.01665	0.151369	87.178

Table 2. Comparison of Results by EOS5-ADM-NR and Newton-Raphson Methods*

Substance	$T_{cr}+150$ $[K]$	$2\times P_{cr}$ $[MPa]$	Number of Iterations (Newton-Raphson)	Number of Iterations (EOS5-ADM-NR)	Iteration Tolerance	Calculated molar density $\rho\left[kmol\cdot m^{-3}\right]$
CO_2	454.128	14.7546	21	17	1E-10	5.06320284150
H_2O	747.096	44.128	24	21	1E-10	7.10757099045
CH_4	340.564	9.1984	21	16	1E-10	5.73176549787
C_2H_6	455.33	9.726	17	14	1E-10	3.29338717954

*Ideal gas assumption is taken as the initial guess for both methods.

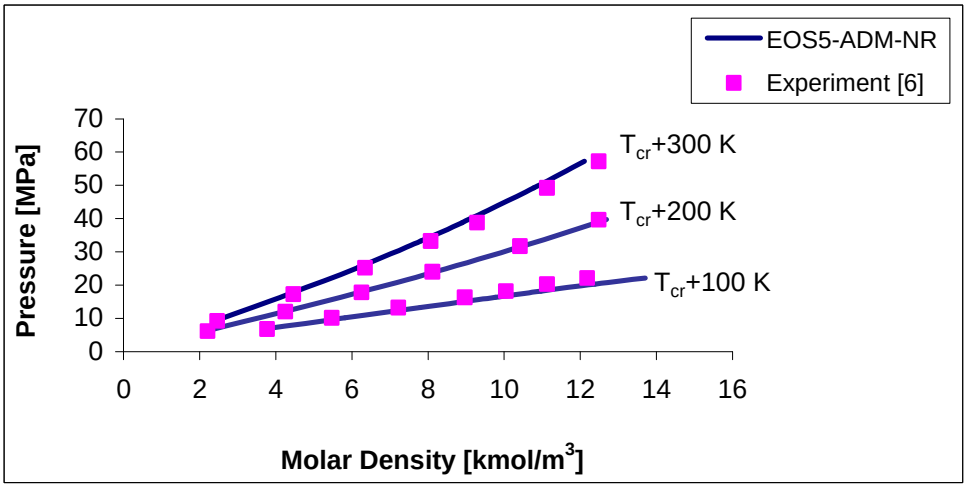

Figure 1. Pressure-Density Relation of Supercritical Argon

CONCLUSION

An improved iterative scheme was proposed for treatment of a quintic equation of state which is dedicated to supercritical regions. Based on the results, the proposed method was shown to be efficient and accurate and superior to the traditional Newton-Raphson in terms of the necessary numbers of iterations for convergence. This fact can be of interest for relevant massive computer simulations. As demonstrated for Argon as a case study, the chosen equation of state combined with the proposed solution technique admirably simulates the experimental data.

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