Journal of Chemical and Petroleum Engineering (JChPE)
Print ISSN: 2423-673X Online ISSN: 2423-6721

On the Solution of the Tao-Mason Equation of State by a Nonlinear Ordinary Differential Equation

Hooman Fatoorehchi *

School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran. E-mail: hfatoorehchi@ut.ac.ir

ARTICLE INFO

Article History:
Received: 29 July 2022
Revised: 25 August 2022
Accepted: 29 August 2022

Article type: Research

Keywords:
Asymptotic Solution,
Applied Thermodynamics,
Dormand-Prince Pair,
Nonlinear ODE,
Tao-Mason Equation of State

ABSTRACT

Based on the Tao-Mason equation of state, we have proposed a nonlinear ordinary differential equation that asymptotically converges to the compressibility factor of a pure substance or a mixture of chemical species. We have used the Dormand-Prince pair algorithm to solve the aforementioned differential equation in a purely numerical manner. Our method is devoid of the adverse convergence issues that are usually associated with Newton-type solvers. We have provided two case studies concerning two industrially common compounds namely ethane and carbon dioxide, for the sake of exposition. For 96 points of different temperatures and pressures, our method succeeded at calculating the compressibility factor of carbon dioxide with an average absolute error of 6.53×10^{-5} and a maximum absolute error of 4.79×10^{-4}. Unlike the previous root-finding algorithms, we only need to perform "*formal*" polynomial deflations in our method, which circumvents the computation-intensive synthetic divisions, to obtain all compressibility factors offered by the Tao-Mason EOS.

Introduction

An equation of state (EOS) is a valuable mathematical model that relates temperature, pressure, and the specific volume of a given pure fluid or a mixture. Other thermodynamic properties such as enthalpy, entropy, latent heat, vapor pressure as well as phase equilibrium data can be calculated from a suitable EOS. The aforementioned properties and data are essential for the design of many pieces of chemical engineering equipment, such as distillation columns [1-4].

Since the advent of the van der Waals EOS in 1873, dozens of equations of state have been proposed. They are either purely empirical, semi-empirical, or completely theoretical, each with its own strengths and weaknesses. A set of equations of states come in the form of polynomials of the specific volume or equivalently, the compressibility factor, with their coefficients being functions of temperature, pressure, and possibly some molecular indicators. Among them, cubic equations of states are well-known and popular due to their simplicity and their acceptable accuracy [5]. For instance, the Peng-Robinson EOS, as a two-parameter cubic equation, has gained a dependable reputation for predicting the properties of nonpolar hydrocarbons in the industrial community [6-9]. Several non-cubic equations of state have also been proposed in the literature having their strengths and limitations [10, 11].

* Corresponding Author: H. Fatoorehchi (E-mail address: hfatoorehchi@ut.ac.ir)

Journal of Chemical and Petroleum Engineering, 2022, 56(2): 233-243.
Publisher: University of Tehran, College of Engineering *DOI: 10.22059/JCHPE.2022.346496.1399*

The Tao-Mason EOS has been hailed by thermodynamists and physical chemists because of its accuracy and its sound theoretical basis. It is based on the statistical-mechanical perturbation theory for hard spheres and molecular fluids and provides accurate results for density as well as the phase boundaries (vapor pressures) [12]. The Tao-Mason EOS has been modified to predict the thermodynamic properties of ionic liquids with improved accuracy [13].

Nevertheless, the Tao-Mason EOS is actually a septic, i.e., of degree seven, polynomial in the specific volume or the compressibility factor, which makes it unfavorable from the computational viewpoint. This is deduced from the celebrated Abel-Ruffini theorem, which states that there can be no general algebraic solution to polynomial equations of degree five or higher. Inevitably, Newton-type solvers are recommended for solving the Tao-Mason EOS, yet they are inherently prone to convergence issues if not properly initialized [14-16].

The Dormand-Prince method is actually a variable-step numerical integrator and has been widely used in the simulation of dynamical systems in various branches of science and engineering. In fact, it is a hybridization of the fourth and the fifth Runge-Kutta algorithms. The Dormand-Prince method has been incorporated into the MATLAB software package as a default ODE solver under the name of "*ode45*".

In this paper, we modify the classical Tao-Mason EOS and convert it to a nonlinear ODE, which will be solved by the Dormand-Prince method numerically. Each converged solution of the aforementioned ODE is one zero of the original Tao-Mason EOS. Once combined with polynomial deflation or by changing the initial condition, we will obtain an algorithm for calculating all the zeros through a repetitive procedure.

The Proposed Method

The original Tao-Mason [17] can be written as a septic polynomial in the compressibility factor as follows:

$$\begin{aligned}
&z^7-(\lambda B+1)z^6+(B\lambda-C)z^5\\
&+\left(\lambda-A_1A_2+A_1e^{kT_c/T}\right)(C-A)Bz^4+\left(\frac{9B^4}{5}+B^2A_1\lambda(C-A)\left(A_2-e^{kT_c/T}\right)\right)z^3\\
&-\frac{9B^4}{5}(1+B\lambda)z^2+\frac{9B^4}{5}(B\lambda-C)z+\frac{9B^5\lambda}{5}(C-A)=0,
\end{aligned}\tag{1}$$

where $A=\frac{\alpha P}{kT}$, $B=\frac{bP}{kT}$, $C=\frac{B_2P}{kT}$, k is Boltzmann's constant, B_2 denotes the second virial coefficient, b is the effective Van der Waals co-volume, and α is a temperature-dependent parameter that quantifies the contribution of the repulsion forces to the second virial coefficient. Furthermore,

$$\begin{aligned}
&A_1=0.143\\
&A_2=1.64+2.65\left(e^{\kappa-1.093}-1\right)\\
&\kappa=1.093+0.26\left[\sqrt{\omega+0.002}+4.50(\omega+0.002)\right]
\end{aligned}\tag{2}$$

where ω is Pitzer's acentric factor. Also, λ is a characteristic parameter that has been correlated to the acentric factor as follows:

$$\lambda = 0.4324 - 0.3331\omega \tag{3}$$

Theoretically, it is possible to determine the three parameters B_2, b, and α accurately if the intermolecular potential is known. However, in the absence of experimental data, it has been found super convenient to use macroscopic corresponding states correlations that are based on critical temperature and pressure as well as the acentric factor for the calculation of B_2. Particularly, the following one that is due to Tsonopoulos is widely used [18]:

$$\frac{P_c B_2}{RT_c} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \tag{4}$$

where T_r is the reduced temperature, P_c and T_c denote the critical pressure and temperature respectively. The functions $f^{(0)}$ and $f^{(1)}$ are defined as:

$$f^{(0)}(T_r) = 0.1445 - \frac{0.330}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8} \tag{5}$$

$$f^{(1)}(T_r) = 0.0637 + \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8}. \tag{6}$$

Adopting the Lennard-Jones (Eqs. 6 and 12) intermolecular pair potential, it is possible can calculate the parameters α and b as functions of the Boyle temperature T_B and the Boyle volume V_B by

$$\frac{\alpha}{V_B} = -0.0648\exp\left(-2.6038\frac{T}{T_B}\right) + 1.8067\left[1 - \exp\left(-0.9726\left(\frac{T}{T_B}\right)^{-\frac{1}{4}}\right)\right] \tag{7}$$

and

$$\frac{b}{V_B} = -0.0648\left(1 - 2.6038\frac{T}{T_B}\right)\exp\left(-2.6038\frac{T}{T_B}\right) + 1.8067\left[1 - \left(1 + \frac{0.9726}{4\left(\frac{T}{T_B}\right)^{\frac{1}{4}}}\right)\exp\left(-0.9726\left(\frac{T}{T_B}\right)^{-\frac{1}{4}}\right)\right]. \tag{8}$$

Now, for brevity, we rewrite Eq. 1 as:

$$z^7 + k_1 z^6 + k_2 z^5 + k_3 z^4 + k_4 z^3 + k_5 z^2 + k_6 z + k_7 = 0, \tag{9}$$

where, obviously, k_1 to k_7 are known constants for a given substance at a prescribed temperature and pressure.

Next, we propose the following dynamical nonlinear ODE, which can converge to one zero of Eq. 9 as t tends to positive infinity. It is worthwhile to mention that the factor e^t is for convergence improvement and can possibly replaced by unity at the penalty of poor convergence.

$$\frac{dx}{dt} = e^t \left(x^7 + k_1 x^6 + k_2 x^5 + k_3 x^4 + k_4 x^3 + k_5 x^2 + k_6 x + k_7 \right), \tag{10}$$

Theorem 2.1

Consider the nonlinear ODE (Eq. 10) with an arbitrary finite initial condition. If dx/dt is asymptotically bounded, then the ODE converges to one zeros of the polynomial

$$P(x) = x^7 + k_1 x^6 + k_2 x^5 + k_3 x^4 + k_4 x^3 + k_5 x^2 + k_6 x + k_7 . \tag{11}$$

Proof: Since dx/dt is asymptotically bounded, we are assured that there exists a real number M such that

$$-M \leq \lim_{t \to +\infty} \frac{dx}{dt} \leq M . \tag{12}$$

Now, in view of Eq. 10, it follows that

$$-M \leq \lim_{t \to +\infty} e^t \left(x^7 + k_1 x^6 + k_2 x^5 + k_3 x^4 + k_4 x^3 + k_5 x^2 + k_6 x + k_7 \right) \leq M . \tag{13}$$

For the compound inequality (Eq. 13) to hold, we should have

$$\lim_{t \to +\infty} \left(x^7 + k_1 x^6 + k_2 x^5 + k_3 x^4 + k_4 x^3 + k_5 x^2 + k_6 x + k_7 \right) = 0 , \tag{14}$$

because e^t ultimately tends to infinity as t increases. Eq. 14 implies that the dynamic state function $x(t)$ asymptotically converges to one zero of polynomial $P(x)$ regardless of $x(0)$.

Remark 2.1

It is possible to translate the equilibrium point of Eq. 10 to the origin, i.e., $x = 0$, and then use the Lyapunov theorems for the stability of non-autonomous equations to develop theorems on the sufficient conditions for asymptotical stability of ODE (Eq. 10). However, it requires the knowledge of the zeroes of $P(x)$ or at least their signs. Therefore, it is safe to say that Theorem 2.1 is the best result that we can obtain regarding the convergence of Eq. 10.
In case the condition of Theorem 2.1 is not satisfied, the solution of Eq. 10 diverges to positive or negative infinity.

Once one zero of $P(x)$ is obtained, we can perform polynomial deflation and repeat the whole procedure to search for other zeroes.

Lemma 2.1

If the conditions of Theorem 2.1 hold, then the following nonlinear ODE also converges to one zero of $P(x)$:

$$\frac{dx}{dt} = -e^t \left(x^7 + k_1 x^6 + k_2 x^5 + k_3 x^4 + k_4 x^3 + k_5 x^2 + k_6 x + k_7 \right) . \tag{15}$$

Note 2.1

Since the Tao-Mason EOS is a septic polynomial with real coefficients, its complex zeros, if any, are conjugate. It is immediately followed by the complex conjugate root theorem [19]. This fact helps us to filter out the unwanted zeros faster, those without physical meaning, of the Tao-Mason EOS.

Illustrative Example

The First Case Study: Ethane

In this section, we will calculate the compressibility factors for ethane at 7 atm and 20 °C as provided by the Tao-Mason EOS for the sake of illustration. The required constants and thermophysical properties of ethane are listed in Table 1.

Table 1. Thermophysical properties of ethane [20]

V_B, Boyle volume	90.6×10^{-6} m^3/mol
T_B, Boyle temperature	770.8 K
T_C, Critical temperature	305.4 K
P_C, Critical pressure	48.8×10^5 Pa
ω , Acentric factor	0.098
MW, Molecular weight	30.0690 g/mol

Thus, the coefficients of the polynomial $P(X)$ are readily calculated and listed in Table 2.

Table 2. The numerical values of the coefficients of the polynomial (Eq. 11) for the first case study

k_1	-1.01181895514
k_2	0.0679401791848
k_3	-0.000593620506246
k_4	-0.00000408817520196
k_5	-0.00000138819887581
k_6	0.0000000932128024359
k_7	-0.00000000144827082441

Now, if we start with the arbitrary initial condition $x(0) = 1+i$, the Dormand-Prince method yields a solution that quickly converges to 0.058137 asymptotically. If we vary the initial condition $x(0)$, we will obtain other roots of the Tao-Mason equation of state as asymptotes. Table 3 lists these quantities.

Table 3. Different zeroes of the polynomial (Eq. 11) as a result of different initial conditions

$x(0)$	Converged Solution of ODE (Eq. 10)	Exact Zero of Polynomial (Eq. 11)
$1+i$	0.058137	0.058122
i	$0.021041+0.023124\,i$	$0.021041+0.023124\,i$

We can deflate the polynomial (Eq. 11) by factoring out the zero 0.058137 only formally, and focus on the following nonlinear ODE for obtaining the other zeroes of $P(x)$:

$$\frac{dx}{dt} = \frac{e^t\left(x^7 + k_1x^6 + k_2x^5 + k_3x^4 + k_4x^3 + k_5x^2 + k_6x + k_7\right)}{x - 0.058137} \tag{16}$$

Repeating the previous procedure, we can obtain the asymptotic solution of (Eq. 10) as 0.022290 by the arbitrary initial condition of $x(0) = 0.1$.

Also, once again, we will formally deflate polynomial (Eq. 11) and obtain a newer zero-generating ODE as

$$\frac{dx}{dt}=\frac{e^{t}\left(x^{7}+k_{1}x^{6}+k_{2}x^{5}+k_{3}x^{4}+k_{4}x^{3}+k_{5}x^{2}+k_{6}x+k_{7}\right)}{(x-0.058137)(x-0.022290)(x-0.021041-0.023124i)(x-0.021041+0.023124i)} \tag{17}$$

Similarly, Eq. 17 yields another zero of $P(x)$, using the initial condition $x(0)=0.5i$, which is −0.025453+0.023851*i*.

As pointed in Remark 2.1, the convergence of ODE (Eq. 10) is influenced by the sign of coefficients of $P(x)$. On the other hand, clearly, the zeroes of $P(x)=0$ are the same as those of $-P(x)=0$. Therefore, in view of Lemma 2.1, we modify Eq. 17 to have

$$\frac{dx}{dt}=\frac{-e^{t}\left(x^{7}+k_{1}x^{6}+k_{2}x^{5}+k_{3}x^{4}+k_{4}x^{3}+k_{5}x^{2}+k_{6}x+k_{7}\right)}{(x-0.058137)(x-0.022290)(x-0.021041\pm0.023124i)(x+0.025453\pm0.023851i.)} \tag{18}$$

whose solution with $x(0)=10$ tends to 0.940295 quickly.

As we have obtained all the seven zeroes of $P(x)$, we can list and assess their accuracy as given in Table 4.

Table 4. All zeroes of the polynomial (11) and their corresponding initial conditions

x(*0*)	Converged Solution of ODE (Eq. 10)	Exact Zero of Polynomial (Eq. 11)
1+*i*	0.058137	0.058122
i	0.021041+0.023124*i*	0.021041+0.023124*i*
0.1	0.022290	0.022282
0.5 i	-0.025713+0.023782*i*	-0.025453+0.023851*i*
10	0.940295	0.940238

The Second Case Study: Carbon Dioxide

For the further exposition, we have calculated the compressibility factor of carbon dioxide at different reduced temperatures and pressures by our method and the "*roots*" procedure of MATLAB. We consider the latter as the "exact" zero for the sake of comparison, henceforth. The built-in "*roots*" algorithm in MATLAB first finds the companion matrix associated to the given polynomial and then performs an eigenvalue computation using the Cholesky factorization or generalized Schur decomposition algorithms. The results for a total number of 96 points are given in Tables 5 to 12. As for our method, a nonlinear ODE of type (Eq. 15) was chosen and the initial condition $x(0)=10$ was used for all the simulations.

Furthermore, the absolute deviation of the calculated compressibility factors for the reduced temperature ranging from 0.5 to 1.2 and the reduced pressure ranging from 0.1 to 1.2 are depicted in the 3D plot of Fig. 1. The maximum value of the absolute error 4.79×10^{-4}, which corresponds to $(\mathrm{Tr},\mathrm{Pr})=(0.8,0.1)$ and the average absolute error is 6.53854×10^{-5}.

Table 5. The compressibility factors for CO_2 at T_r =0.5 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,0.5)	0.018047	0.018043
(0.2,0.5)	0.036085	0.036084
(0.3,0.5)	0.054131	0.054122
(0.4,0.5)	0.072170	0.072157
(0.5,0.5)	0.090192	0.090190
(0.6,0.5)	0.108265	0.108220
(0.7,0.5)	0.126334	0.126247
(0.8,0.5)	0.144275	0.144271
(0.9,0.5)	0.162314	0.162293
(1,0.5)	0.180323	0.180311
(1.1,0.5)	0.198362	0.198327
(1.2,0.5)	0.216376	0.216341

Table 6. The compressibility factors for CO_2 at T_r =0.6 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,0.6)	0.714281	0.714225
(0.2,0.6)	0.032107	0.032092
(0.3,0.6)	0.048135	0.048126
(0.4,0.6)	0.064161	0.064153
(0.5,0.6)	0.080191	0.080172
(0.6,0.6)	0.096208	0.096183
(0.7,0.6)	0.112197	0.112186
(0.8,0.6)	0.128192	0.128183
(0.9,0.6)	0.144207	0.144171
(1,0.6)	0.160158	0.160152
(1.1,0.6)	0.176130	0.176126
(1.2,0.6)	0.192102	0.192092

Table 7. The compressibility factors for CO2 at T_r =0.7 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,0.7)	0.867548	0.867484
(0.2,0.7)	0.629175	0.629134
(0.3,0.7)	0.044522	0.044517
(0.4,0.7)	0.059338	0.059323
(0.5,0.7)	0.074138	0.074114
(0.6,0.7)	0.088908	0.088888
(0.7,0.7)	0.103746	0.103647
(0.8,0.7)	0.118395	0.118390
(0.9,0.7)	0.133157	0.133118
(1,0.7)	0.147835	0.147830
(1.1,0.7)	0.162547	0.162528
(1.2,0.7)	0.177285	0.177210

Table 8. The compressibility factors for CO2 at T_r =0.8 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,0.8)	0.921568	0.921089
(0.2,0.8)	0.821692	0.821623
(0.3,0.8)	0.665943	0.665780
(0.4,0.8)	0.056803	0.056787
(0.5,0.8)	0.070907	0.070906
(0.6,0.8)	0.084996	0.084993
(0.7,0.8)	0.099078	0.099051
(0.8,0.8)	0.113096	0.113079
(0.9,0.8)	0.127083	0.127078
(1,0.8)	0.141056	0.141049
(1.1,0.8)	0.154997	0.154991
(1.2,0.8)	0.168914	0.168906

Table 9. The compressibility factors for CO_2 at T_r =0.9 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,0.9)	0.948292	0.948203
(0.2,0.9)	0.888927	0.888814
(0.3,0.9)	0.817498	0.817373
(0.4,0.9)	0.721855	0.721801
(0.5,0.9)	0.070467	0.070407
(0.6,0.9)	0.084332	0.084300
(0.7,0.9)	0.098137	0.098135
(0.8,0.9)	0.111959	0.111913
(0.9,0.9)	0.125672	0.125636
(1,0.9)	0.139382	0.139305
(1.1,0.9)	0.153018	0.152922
(1.2,0.9)	0.166510	0.166489

Table 10. The compressibility factors for CO_2 at T_r =1 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,1)	0.964128	0.964065
(0.2,1)	0.924797	0.924715
(0.3,1)	0.881017	0.880839
(0.4,1)	0.830740	0.830547
(0.5,1)	0.770462	0.770080
(0.6,1)	0.689485	0.689291
(0.7,1)	0.101897	0.101892
(0.8,1)	0.115920	0.115902
(0.9,1)	0.129811	0.129800
(1,1)	0.143728	0.143590
(1.1,1)	0.157286	0.157278

Table 11. The compressibility factors for CO_2 at T_r =1.1 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,1.1)	0.974269	0.974166
(0.2,1.1)	0.946889	0.946624
(0.3,1.1)	0.917081	0.917022
(0.4,1.1)	0.884941	0.884865
(0.5,1.1)	0.849607	0.849418
(0.6,1.1)	0.809578	0.809505
(0.7,1.1)	0.763184	0.763015
(0.8,1.1)	0.705380	0.705332
(0.9,1.1)	0.620609	0.620568
(1,1.1)	0.158564	0.158548
(1.1,1.1)	0.172520	0.172510

Table 12. The compressibility factors for CO_2 at T_r =1.2 and P_r ranging from 0.1 to 1.2

(Pr,Tr)	Converged Solution of ODE (Eq. 15)	Exact Zero of Polynomial (Eq. 11)
(0.1,1.2)	0.981188	0.980975
(0.2,1.2)	0.961105	0.961040
(0.3,1.2)	0.940215	0.940068
(0.4,1.2)	0.918022	0.917900
(0.5,1.2)	0.894433	0.894328
(0.6,1.2)	0.869155	0.869079
(0.7,1.2)	0.841886	0.841775
(0.8,1.2)	0.812033	0.811868
(0.9,1.2)	0.778653	0.778517
(1,1.2)	0.740453	0.740299
(1.1,1.2)	0.694468	0.694423

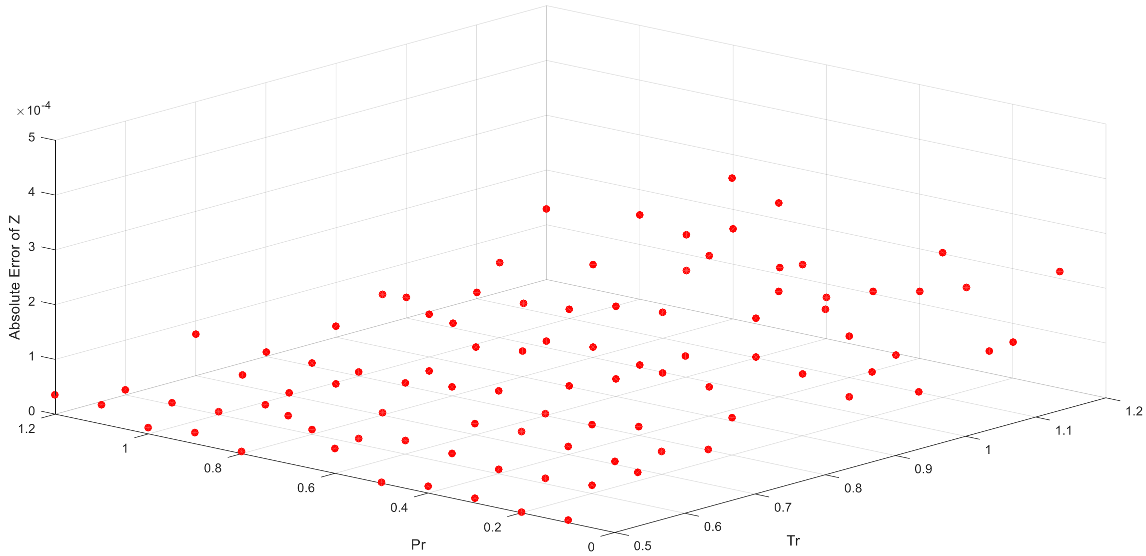

Fig. 1. Graphical representation of the absolute error values of the compressibility factor for CO_2 computed by our method at different reduced pressures and temperatures

Conclusion

As an unorthodox approach, we have proposed a nonlinear ODE based on the Tao-Mason EOS that can asymptotically converge to the compressibility factor of a given pure substance or mixture. The goal was to bypass the difficulties that are characteristic of the Newton-type polynomial root-finding algorithms. We employed the Dormand-Prince pair algorithm to numerically solve the aforementioned Z-factor generating ODE. Two case studies were carried out to demonstrate the accuracy and efficacy of our method. As it can be deduced from Sections 2 and 3, our method formally requires polynomial deflations in the search for other compressibility factors, or in other words, other zeroes of the polynomial (Eq. 11), and we actually are not forced to perform synthetic divisions. This is a remarkable advantage if we consider previous root-finding algorithms that entail polynomial deflations. It is also worthwhile to mention that the promising approximate analytical method, namely the Adomian decomposition could have been applied to solve the proposed nonlinear ODE in a parametric manner [21-24]. Doing so, a new analytical expression for the Tao-Mason EOS in the form of an infinite series would have been obtained. However, the approach would require the use of Padé approximants to extract the asymptotics of the solution out of the infinite series. We plan to follow this idea in our future research. Our approach can be extended to other equations of state, particularly those with more complicated mathematical formulations, such as the SAFT EOS.

Nomenclature

A	Parameter of the Tao-Mason EOS (-)
B	Parameter of the Tao-Mason EOS (-)
C	Parameter of the Tao-Mason EOS (-)
k	Boltzmann's constant ($J.K^{-1}$)
b	Effective van der Waals co-volume ($m^3.mol^{-1}$)
α	Temperature-dependent parameter of the Tao-Mason EOS
$A_1, A_2, \kappa, \lambda$	Parameters of the Tao-Mason EOS

T_c	Critical temperature (K)
P_c	Critical pressure (Pa)
T_B	Boyle temperature (K)
V_B	Boyle (specific) volume ($m^3.mol^{-1}$)
$k_1, k_2, k_3, k_4, k_5, k_6, k_7$	Auxiliary parameters
x, t	Indicator variables
z	Compressibility factor (-)

References

[1] Anderko A. Equation-of-state methods for the modelling of phase equilibria. Fluid Phase Equilibria. 1990; 61(1-2): 145-225.

[2] Fatoorehchi H, Rach R, Tavakoli O, Abolghasemi H. An efficient numerical scheme to solve a quintic equation of state for supercritical fluids. Chemical Engineering Communications. 2015; 202(3): 402-7.

[3] Fatoorehchi H, Abolghasemi H, Rach R, Assar M. An improved algorithm for calculation of the natural gas compressibility factor via the Hall-Yarborough equation of state. The Canadian Journal of Chemical Engineering. 2014; 92(12): 2211-17.

[4] Fatoorehchi H, Abolghasemi H, Rach R. An accurate explicit form of the Hankinson–Thomas–Phillips correlation for prediction of the natural gas compressibility factor. Journal of Petroleum Science and Engineering. 2014; 117: 46-53.

[5] Kontogeorgis GM, Liang X, Arya A, Tsivintzelis I. Equations of state in three centuries. Are we closer to arriving to a single model for all applications?. Chemical Engineering Science: X. 2020; 7:100060.

[6] Valderrama JO. The state of the cubic equations of state. Industrial & Engineering Chemistry Research. 2003; 42(8): 1603-18.

[7] Lopez-Echeverry JS, Reif-Acherman S, Araujo-Lopez E. Peng-Robinson equation of state: 40 years through cubics. Fluid Phase Equilibria. 2017; 447:39-71.

[8] Shojaeian A, Fatoorehchi H. Modeling solubility of refrigerants in ionic liquids using Peng Robinson-Two State equation of state. Fluid Phase Equilibria. 2019; 486: 80-90.

[9] Kedge CJ, Trebble MA. Improvements to a new equation of state for pure components. Fluid Phase Equilibria. 2004; 217(2): 257-62.

[10] Behar E, Simonet R, Rauzy E. A new non-cubic equation of state. Fluid Phase Equilibria. 1985; 21:237-55.

[11] Kedge CJ, Trebble MA. Development of a new empirical non-cubic equation of state. Fluid phase equilibria. 1999; 158:219-28.

[12] Fatoorehchi H, Mohammadi-Khanaposhtani M, Abolghasemi H. Erratum to “Performance assessment of Tao–Mason equation of state: Results for vapor–liquid equilibrium properties [J. Ind. Eng. Chem. 17 (4)(2011) 667–674]”. Journal of Industrial and Engineering Chemistry. 2020; 85: 308-9.

[13] Yousefi F, Karimi H. Modification of Tao–Mason equation of state to ionic liquids. Ionics. 2012; 18(1):135-42.

[14] Fatoorehchi H, Abolghasemi H. Finding all real roots of a polynomial by matrix algebra and the Adomian decomposition method. Journal of the Egyptian Mathematical Society. 2014; 22(3): 524-8.

[15] Fatoorehchi H, Abolghasemi H. On computation of real eigenvalues of matrices via the Adomian decomposition. Journal of the Egyptian Mathematical Society. 2014; 22(1): 6-10.

[16] Fatoorehchi H, Abolghasemi H, Zarghami R, Rach R, von Freeden S. A novel and computationally efficient algorithm for stability analysis of multi input-multi output process control systems. Korean Journal of Chemical Engineering. 2015; 32(9):1733-43.

[17] Tao FM, Mason EA. Statistical-mechanical equation of state for nonpolar fluids: prediction of phase boundaries. The Journal of chemical physics. 1994; 100(12): 9075-87.

[18] Tsonopoulos C. An empirical correlation of second virial coefficients. AIChE Journal. 1974; 20(2): 263-72.

[19] Jeffrey A. Analytic functions: Complex analysis and applications. CRC Press; 2005.

[20] National Institute of Standards and Technology (NIST) database, 2016, accessed on 25 July 2022.

[21] Fatoorehchi H, Rach R, Sakhaeinia H. Explicit Frost-Kalkwarf type equations for calculation of vapour pressure of liquids from triple to critical point by the Adomian decomposition method. The Canadian Journal of Chemical Engineering. 2017; 95(11): 2199-208.

[22] Fatoorehchi H, Rach R. Decomposition solution for nonlinear model describing diffusional growth of intermetallic layers. Acta Phys Pol A. 2021; 140(1): 91-6.

[23] Fatoorehchi H, Gutman I, Abolghasemi H. A combined technique for computation of energy-effect of cycles in conjugated molecules. Journal of Mathematical Chemistry. 2015; 53(4):1113-25.

[24] Fatoorehchi H, Rach R. An inversion-free method for computation of the square roots of real matrices. Romanian Journal of Physics. 2021; 66(7-8): 1-16.

How to cite: Fatoorehchi H. On the Solution of the Tao-Mason Equation of State by a Nonlinear Ordinary Differential Equation. Journal of Chemical and Petroleum Engineering. 2022; 56(2): 233-243.