RESEARCH ARTICLE

Chemical Engineering Numerical Analysis with R: Peng–Robinson Equation of State

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Abstract: Likely, many text on MATLAB, C++, FORTRAN, and Python programming languages exists in chemical engineering libraries, discussing their applications for chemical engineering numerical analysis. R programming language, which has been in existence for more than 40 years, is just evolving as a language of choice for data analytics in science and engineering. Here, it is shown that numerical analysis with equations of state (EOS), especially the Peng–Robinson EOS, typically taught in undergraduate chemical engineering introductory courses can be solved with a developed or existing R source codes. Out of several other mathematical methods, including fixed-point iteration, Regula-Falsi, bisection, and their modified/hybrid methods recently developed, only Secant and Newton’s method algorithm were followed to solve a sample problem by writing an R program. Although sufficient, in-depth study of the R language using some recommended manuals in this work can be a guide in implementing a solution with R for other numerical methods, for the same problem, as well as several other existing analytical and statistical chemical engineering problems out there.

Keywords: R programming, Secant method, Peng–Robinson, chemical engineering, equations of state

1. Introduction

Based on the S language collectively designed by Rick Becker, John Chambers, Doug Dunn, Jean McRae, and Judy Schilling in the 1970s, Ross Ihaka and Robert Gentleman developed the R programming language in 1991 (Femi & Samuel, 2022; Hackenberger, 2020; Vidoni, 2021b). R is applied in linear regression, statistical inference, processing and computation (e.g., machine and deep learning to parallel computing, Bayesian statistics, big data processing, data visualization, and meta-analysis), bioinformatics, machine learning algorithms, elaboration of analysis (e.g., correlation, clustering and data reduction), time series, data manipulation (e.g., data analysis, calculation, and management), and graphical display (Hackenberger, 2020; Pfeiffer & Pia, 2013; Pothigai & Sundararajan, 2021). In 2017, R ranked 6th in terms of popularity among all data science languages, rapidly becoming one of the most extensively employed tools (around 2 million users globally) in statistical analysis (Diaz-Bejarano et al., 2019; Jalal et al., 2017; Staples, 2022). R developers (or software engineers) are continuously contributing new functions and packages to the programming software making them different from R users applying them to do any of the listed uses (Pothigai & Sundararajan, 2021; Vidoni, 2021a). Example of such is an R package (Overview R) created by R developing team from the University of Mannheim, in which, according to Ndaba (2022), it gives an overview of data and identifies gaps inherent in them with a particular emphasis on a time series cross-sectional consideration (Meyer & Hammerschmidt, 2022). Another R package called STEM (spatio-temporal models) was developed by Professor Michela Cameletti from the Department of Economics at the University of Bergamo, Italy. The package uses estimation of the parameters of a spatio-temporal model using the expectation–maximization (EM) algorithm and estimation of the parameter of standard errors using a spatio-temporal parametric bootstrap and spatial mapping (Ndaba, 2022). R users can attest to its functional flavor due to the absence of pointers, many libraries for specific tasks, exponentially growing add-ons, beautiful plots, resistance to hacking and little syntactic

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overhead, ease, less verbosity, free open-source multi-paradigm language, effective data storage and handling flair, immeasurable data processing capabilities, support installation on UNIX, MacOS, and Windows platforms, and a provision for internet distribution and automatic installation (Hackenberger, 2020; Pfeiffer & Pia, 2013; Pothigai & Sundararajan, 2021; Schneider & Lauber, 2020).

Scope of a case sensitive R in accounting, health sciences, medicine, chemistry, civil engineering, mathematics and statistics, biology, physics, and chemical engineering has been described in the literature (Beckerman et al., 2017; Calderon et al., 2022; Dehmer et al., 2016; Gentry & Hiatt, 2022; Lowe, 2013; Pothigai & Sundararajan, 2021). Lowe (2013) is the first to use R for particle physics analysis and opens door for its application in nuclear physics, bio-medical physics, and astrophysics research, earlier foretold by Pfeiffer & Pia (2013). Currently, R is evolving in health sciences departments of universities as a teaching tool for decision making (Jalal et al., 2017). Chemical engineering is not void of statistical data analysis problems prompting utilization of computing systems (Kantor & Edgar, 2020; Krijnen & Wit, 2022). However, programming is not listed as a problem in the chemical engineering domain, introducing it to students interested in statistics and data science would be a good idea (Diaz-Bejarano et al., 2019; Garnier, 2014). Because, in order to build mathematical models to comprehend, find, run, regulate, or optimize the processes, chemical engineers collect and use data on a variety of scales, from laboratories to pilot plants to large-scale industrial settings (Lazic, 2004; Samavedham & Lakshminarayan, 2021).

Thankfully, Coelho et al. (2019) begin a practical application of R in chemical engineering by developing an R package for data analysis of aqueous two-phase systems. Also, R root finding algorithm using Newton–Raphson and Secant methods, provided by Woollett (2015), would be helpful in solving the Peng–Robinson (PR) equation of state (EOS), including its over 220 modifications and other developed or existing models that are nonlinear or unsolvable without numerical analysis (Lopez-Echeverry et al., 2017). In this domain and other fields of application, R users would complain of its sluggishness and the fact that user’s data have to fit into RAM (Lowe, 2013). Objectives of the study are to extensively review and show R language application in all fields of study, highlight the most basic requirement for R teaching and learning, explain briefly the importance of the PR EOS, and employ the Newton–Raphson and Secant method in solving the PR EOS using R.

2. Materials and Methods

2.1. Materials

Secondary information sourced from popular databases such as Google Scholar and ResearchGate is Webinar and Conference paper, Journal articles, Books, Book Chapters, and Lecture Slide Presentations.

R software version 4.2.2 (2022-10-31 ucrt) and Excel 2013 were used to implement the solution of selected variables in PR EOS, as well as show plots were necessary.

2.2. Research methodology

Extent of R application in various fields of study was investigated. Requirements for use in desktop and personal computers were clearly presented. Manuscripts highlighting how to perform basic programming in R were suggested for beginners who wish to take on from where the authors stop, regarding its application in chemical engineering.

Specifically, the PR EOS used to predict natural gas behaviors in oil-based drilling fluid was identified as type of equation that can be solved by mathematical methods. In a nutshell, the basic functions, model development, and its previous application to solve fundamental gas problems were first highlighted.

Newton–Raphson and Secant method syntax in R programming language presented by Woollett (2020) was carefully studied in order to implement it to solve volume, molar volume, and number of moles tied to the PR EOS (see Base Question).

2.3. Base problem

Working with a problem that states that: Methane has a critical temperature of 191.15 K, a critical pressure of 4.641 MPa, and an acentric factor of 0.0115. Estimate the molar volume (Vm) for this compound in the vapor phase at T = 180K and P = 4.5 MPa using the PR equation by taking R = 8.314413 J/mol K.

Solution begins by calculating, electronically, all unknown parameters in Excel Spreadsheet that would help in finding Vm. After the root is determined using Newton’s method, R codes were tested several times to implement a solution to the problem by specifying all the known parameters and setting tolerance error, maximum iterations, and initial Vm guess.

R source code in terms of the Secant method was written for the same problem. An R plot of the function over a range of the independent variable (i.e., Vm) was generated. Volume and number of moles were further determined using Newton and Secant method by modifying the old R source code. Equations used for the implementation, R source code written, and plots generated were presented in the Appendix.

3. Results and Discussion

3.1. R applications

In terms of deployment, R was ranked 15th in 2019 and 13th a year after (2020) by TIOBE INDEX (Sabri, 2020). It is therefore important to showcase various aspects, and the R language can be deployed in the field (Table 1).

All indications point to growing research utilization of the R programming language between 2015 and 2022, as several

<table>
<thead>
<tr>
<th>Field</th>
<th>Uses</th>
<th>Source</th>
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<td>Geography</td>
<td>• Analysis of Spatial Data</td>
<td>(Akinwumiju, 2021; Battul et al., 2020;)</td>
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<td></td>
<td>• Earthquake Data Analysis</td>
<td>Kaya et al., 2019; Kobal et al., 2013;</td>
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<td>• Geoinformatics</td>
<td>Lemenkova, 2018; Murugadoss et al., 2022;</td>
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<td>• Geomorphology</td>
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<td></td>
<td>• Spatial-Temporal Trends</td>
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<td>• The Precipitation Concentration Index (PCI)</td>
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<td>• Mann–Kendall Trend Test</td>
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<td>• Autocorrelation Function (ACF)</td>
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<td>• Relative Percentage Change (RPC)</td>
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<td>• Change Point Detection</td>
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<td>Architecture</td>
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<td>(Basha et al., 2020; Hussain et al., 2015)</td>
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<td>• Over-fitting Research Data</td>
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<td>(Briz-Redon &amp; Serrano-Aroca, 2018)</td>
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<td>• Calculus and Matrix Operation</td>
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<td>• Set Operation and Recursion</td>
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<td>(Kaheh &amp; Shahanzadeh, 2018)</td>
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<td>• Metallurgy</td>
<td>(Bora et al., 2020; Dakubo, 2022; Kwaame et al., 2020)</td>
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<td>Engineering</td>
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<td>Health and</td>
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<td>(Aliyu et al., 2022; Barua, 2021; Hymond and Master, 2020;</td>
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<td>Medicine</td>
<td>• Improving Case Notification Procedures</td>
<td>Jahandideh &amp; Krishnamurthy, 2013; Kothei &amp; Patil, 2022; Mente &amp; Kuhn, 2012; Nakh, 2019;</td>
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<td>• Extracting COVID-19 Data</td>
<td>Robinson &amp; Wayman, 2020; Ruas et al., 2022; Ummaheswari et al., 2021; Weeks et al., 2020;</td>
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<td>• Medicinal Chemistry</td>
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<td>• Eyam Plague Mathematical Modeling</td>
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<td>Chemistry</td>
<td>• Infectious Disease Prediction</td>
<td>(Altintas, 2022; Guha, 2007)</td>
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<td>Ecology</td>
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<td></td>
<td>• Balancing Chemical Equations</td>
<td>(Charalamopoulos, 2020; Forrester et al., 2022; Lai et al., 2019; Plant, 2019;</td>
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<td>• Ecology</td>
<td>Popov &amp; Secerov, 2019; Rajesh &amp; Ravishankar, 2021</td>
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<td>Civil Engineering</td>
<td>• Fetching and Transforming Survey Data</td>
<td>(Barbosa et al., 2021; Hasan &amp; Jamaluddin, 2019; Maurer, 2021)</td>
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<td>• Geotechnical Engineering</td>
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<td>• Structural Analysis</td>
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<td>Safety and Risk</td>
<td>• Fault Tree Analysis</td>
<td>(Antonov, et al., 2018; Antonov, et al., 2018; Vacciana &amp; Ascoli, 2015)</td>
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<td>Management</td>
<td>• Rothermel Fire Spread Model</td>
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<tr>
<td>Food Science</td>
<td>• Prediction of Wine Quality</td>
<td>(Akanbi et al., 2022; Alkarkhi &amp; Alqaraghuli, 2019; Lakhani &amp; Manjre, 2021)</td>
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<td>Sociology</td>
<td>• Sensitivity Analysis of Diet Problem</td>
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<td>• Policing Olympic games</td>
<td>(Brostrom, 2021; Congelio, 2022; Nasri, 2022; Roy et al., 2018)</td>
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<td>• Event decision</td>
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<td>• Event History Analysis</td>
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researchers have found R applications in many fields of study. Yet in engineering, works employing the services of the program are limited. Breakthrough in solving technical problems in chemical engineering with R, if identified, will facilitate probable adoption or recommendation of the programming language to academicians, process engineers, and students. Its potential utilization or adoption could be to fashion a design of experiments; solve chemical plant cost optimization using simplex linear programming approach; solve differential equations from material and energy balances, kinetic data analysis (Chau, 2021), thermodynamic problems (Dick, 2022; Saenz et al., 2018) and in biochemical engineering; perform linear regression parameter estimations (Hoffmann, 2021); and in chemometrics (Kucheryavskiy, 2020).

### 3.2. Installation know-how

R Consortium, Inc. is responsible for maintaining R (Gentry & Hiatt, 2022). Executing R follows the Read-Eval-Print-Loop (REPL) condition (Ayyappa et al., 2018; Gillespie & Lovelace, 2017). An interface (RStudio) that makes R easy to use can be downloaded alongside R via: [https://mirrors.nics.utk.edu/cran/](https://mirrors.nics.utk.edu/cran/) and [https://www.rstudio.com](https://www.rstudio.com) (Doyle et al., 2022; Turner, 2020). Users can then follow the step-wise installation guide lectured byJayasankar et al. (2017).

### 3.3. R programming scholarship

R (Berry et al., 2021) as a statistical tool for scientific and engineering analysis is hitherto gaining serious recognition. Though versatile like Python, the best among the two had been a subject of debate among users (Lee & Lee, 2023; Odhiambo et al., 2020; Ozgur et al., 2020; Ozgur et al., 2018a, 2018b). According to Odhiambo et al. (2020), almost 65% of developers use Python compared to 25% that use the R language – who agree to the fact that R is difficult to learn (even though easy to code) while syntax for coding certain problems is not very obvious. It suffices to say that if statistical/programming languages were cars, then the analogy in Figure 1 holds.

### Figure 1

Durability comparison of statistical/programming languages

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<td><strong>Field</strong></td>
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<td>Business and Finance</td>
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<td>Agriculture and Forestry and Environmental Protection</td>
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<td>Conservation</td>
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<td>Communications</td>
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Proposal to adopt R as a meaningful statistical software in various fora and institutions is not new (Ababaei, 2020; Amine et al., 2021; Redón & Aroca, 2018; Staples & Wagge, 2020). Table 2 points to tutorial lessons prepared by experts in R programming that would serve the requirements for non-majors in R programming.

Already, course certificates are ongoing, both virtual and full course (non-online). “The Carpentries,” a global non-profit organization that teaches practical data science skills to researchers through active learning workshops, has R as part of their programming languages. It also provides workshops for badged instructors to hold workshops which are sponsored by the organization. R certificates obtained by Salahi (2020), Kesavan (2021), and (Singh, 2020) are good to have in one’s curriculum vitae.

### 3.4. Peng–Robinson equation of state

EOS such as the PR EOS is majorly applied in the petroleum and chemical industries to model compositional and volumetric phase behaviors of pure compounds and mixtures (Mansour, 2020; Shi, 2017). Example is its application to forecast natural gas phase behaviors of pure compounds and mixtures (Mansour, 2021). The PR EOS as presented in equation (1) given by Al-Kindi & Babadagli (2021):

\[
P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m^2 + 2bV_m - b^2}
\]  

(1)

where \(P\), \(T\) = pressure and temperature, \(a, b\) = PR constants (unique for every substance), \(R\) = universal gas constant, and \(V_m\) = molar volume. Alpha or \(\alpha\) is a temperature-dependent function connected to the critical temperature \(\left( T_c = \frac{T}{T_c} \right)\) and acentric factor \(\omega\), given by equation (2) and equation (3) in Shi (2017):

\[
\alpha = \left[ 1 + k\left(1 - \frac{T}{T_c}\right)^{\frac{1}{2}} \right]^2
\]  

(2)

\[
k = \left\{ \begin{array}{ll}
0.374646 + 1.54226a - 0.26992a^2, & a < 0.49 \\
0.379642 + 1.48503a - 0.164423a^2 + 0.016666a^3, & a > 0.49 
\end{array} \right.
\]  

(3)

where \(T_c\) = critical temperature and \(k\) = a dimensionless function of \(\omega\). Now, four sets of new alpha functions have been proposed by Sun et al. (2022), which extends the list of modifications done to the PR EOS earlier presented by Lopez-Echeverry et al. (2017).

### 3.5. Software solutions to PR EOS

Remarkably, Nasri & Binous (2009) illustrate, convincingly, the application of the PR EOS using MATLAB. Relative to this work, Abubakar & Mustapha (2021) used C++ to solve the PR EOS for \(V_m\), while Li et al. (2015) predict the same parameter for pure compounds. To replicate this using the R programming software, functions of \(V_m\) and its derivative, as given in equations (4) and (5), had to be considered.

\[
f(V_m) = V_m^3 + \left( b - \frac{RT}{P} \right) V_m^2 - \left( 3b^2 + 2\frac{RTb}{P} - \frac{a\alpha}{P} \right) V_m
\]  

\[
f'(V_m) = 3V_m^2 + 2\left( b - \frac{RT}{P} \right) V_m - \left( 3b^2 + 2\frac{RTb}{P} - \frac{a\alpha}{P} \right)
\]  

(4)

(5)

Equations (4) and (5) are considered since they form parts of functional parameters in both Newton’s and Secant methods. The Newton equation and the Secant equation (which had been in existence before the invention of the Newton–Raphson method) are, respectively, given in equations (6) and (7).

\[
v_{i+1} = v_i - \frac{f(v_i)}{f'(v_i)}
\]  

(6)

\[
v_{i+1} = v_i - \frac{f(v_i)(v_i - v_{i-1})}{f(v_i) - f(v_{i-1})}
\]  

(7)
In Excel (Figure 2), coefficients of the independent variable ($V$) of the cubic equations defined as $C_1$, $C_2$, and $C_3$ help eliminate unknowns from the functions in order to easily implement equation (6) as shown in cell address E85 ($v_{i+1}$). Where $v_i$ is in cell E84, $f(v_i)$ in F84 and $f'(v_i)$ in G84.

Both in Excel and the R source code shown in Figure 3, "c" was used to represent the $\alpha$ symbol.

Based on Equation (7) or the Secant method, an R source as shown in Figure 4 confirms $V$ ("m" or "MV") obtained from Excel and the R-Newton’s solution, as 54.27034 m$^3$; for tolerance error $= 10^{-10}$ and maximum iteration $= 100$.

Unlike Newton’s method where because a single guess (hinted as value calculated from ideal gas law) will converge to the root, Secant method requires two initial guesses.
(m₀ & m₁ or vᵢ & vᵢ₋₁) to begin, which is not likely close to \( V_m \) from ideal gas equation. This keeps problem solvers without prior knowledge of the root, blinded, as to what and what value it might bracket. Again, the function can be plotted by writing short R code, as shown in Figure 5.

The span of the x-axis values can be specified in R while R selects the interval independently. In addition, color type, width, or thickness of the line and the line type can be selected by defining them under “col,” “lwd,” and “lty” as shown in Figure 6.

Figure 6 is a plot of molar volume function against molar volume (taken as “x”). The points on the y-axis are kept in standard form, where “e” stands for “\( 10 \)” and the figure with “+” sign next to it implies the “\( 10 \) raised to the power of the integer.” To check for different width sizes (lwd) and line types (lty), simply vary the numbers used in Figure 5. For instance, a green color was selected for moles function plot in the Appendix with a long-dash broken line type.

---

**Figure 4**
Secant method molar volume calculation algorithm with R

```r
secant <- function(f, m0, m1, tol=1e-10, maxiter=100) 
+ { 
+   # f = Function of Molar Volume (m) from Peng-Robinson EOS 
+   # df = Derivative of f 
+   # m0 = Initial guess for the root (from ideal gas law) 
+   # tol = Tolerance for the error 
+   # maxiter = Maximum number of iterations 
+   for (i in 1:maxiter) 
+     { 
+       m2 <- m1 - f(m1) / ((f(m1) - f(m0)) / (m1 - m0)) # Update m using Newton's Method 
+     if (abs(m1 - m0) < tol) return(m1) # Check for Convergence 
+       m0 <- m1 
+       m1 <- m2 
+     } 
+   return(m1) # Return the result if convergence was not achieved 
+ } 
> f <- function(m) m^3+(b-0.6*T/P)*m^2-(3*b^2+2*0.6*T*b/P-a*c/P)*m+(b^3+(0.6*T*b^2)/P-a*b*c/P)/P 
> m0 <- 40 
> m1 <- 60 
> 
> # Declaring Given Variables 
> T <- 180 # Temperature 
> P <- 4.5 # Pressure 
> R <- 8.314413 # Molar Gas Constant 
> To <- 191.159 # Critical Temperature 
> Pc <- 4.64 # Critical Pressure 
> c <- 1.023364405 # Peng-Robinson Parameter 
> a <- (0.45724/Pc)*(R*To)^2 # a & b = Peng-Robinson EOS Constants 
> b <- (0.07780*R*To)/Pc 
> 
> # Molar Volume after Convergence 
> result <- secant(f, m0, m1) 
> print(result) 
[1] 54.27034
```

**Figure 5**
Molar volume function plot implementation using R

```r
mvfunc <- function(m) 
+ { 
+   m^3-305.9340844*m^2+36742.18176*m-1252793.101 
+ } 
> curve(mvfunc, xlim=c(0,350), col='red', lwd=2.5, lty=4) 
> abline(h=0) 
> abline(v=0) 
```

---

**Figure 6**
Plot created with R source code
R programming source code has the advantage of simplicity as regards solving for molar volume in PR EOS, but there is however no basis for comparing it to other programming languages. PYTHON, Java, C++, FORTRAN, and MATLAB can also be used to perform the same task, as would be seen in the next write-up by the corresponding author. This would allow users to gauge R’s portability, speed, reliability, and flexibility to solve PR EOS or other EOS (e.g., Van der Waals, Redlich–Kwong, and Soave–Redlich–Kwong EOS) compared to other programming tools for this type of chemical engineering problem.

4. Conclusion

R source codes for implementing volume, molar volume, and number of moles calculations from PR EOS were painstakingly formulated for Secant and Newton–Raphson algorithm to validate Excel solution. To use on different problems encountered, the declared variables and initial guess(es) may be replaced. The work demonstrates, practically, the significance of the R programming language in computing complex numerical problems in chemical engineering using a sample problem. With this, future recognition of R as a tool for teaching and learning in tertiary institutions, especially in chemical engineering, is anticipated.

Conflicts of Interest

The authors declare that they have no conflicts of interest to this work.

References


Normal University (Natural Science), 1, 124–135, 143. https://doi.org/10.3969/j.issn.1000-5641.2019.01.014


Singh, G. (2020). One week online faculty development programme on R programming: Certificate of participation. Deemed to Be University.


Thupeng, W. M., & Thekiso, T. B. (2019). Change point analysis: A practical tool for detecting abrupt changes in rainfall and


APPENDIX

A. Attention

In Abubakar & Mustapha (2021), reader’s attention is drawn to a mistake in Equation (7) which is a function of molar volume, \( f(V_m) \). The author solved for \( V_m \) in C++ using the wrong equation and so made a mistake in line 220 of his coding. The correct root is 4.5811 ft\(^3\) and the correct line of code is:

```
220     |
```

Request the C++ coding via abdulhalim@mau.edu.ng

B. Volume Calculation

B.1. Excel result

Since “\( n \)” was not given, 1 mole basis for the CH4 gas was taken. After 9 iterations with Newton’s method, \( V = 54.27034 \) m\(^3\).
B.2. R program solution

```r
> prbnewton <- function(f, df, v0, tol=1e-10, maxiter=100)
+ { # f = Function of Volume (v) from Peng-Robinson EOS
+ # df = Derivative of f
+ # v0 = Initial guess for the root (from ideal gas law)
+ # tol = Tolerance for the error
+ # maxiter = Maximum number of iterations
+ #
+ # for (i in 1:maxiter)
+ #
+ # v1 <- v0 - f(v0)/df(v0) # Update v using Newton's Method
+ # if (abs(v1 - v0) < tol) return(v1) # Check for Convergence
+ # v0 <- v1 # Update v0 for the next iteration
+ #
+ # Return the result if convergence was not achieved
+ }
> f <- function(v) v^3+n*(b-R*T/P)*v^2+n^2*(a*c/F-3*b^2-2*R*T*b/F)*v+(b^3+(R*T*b^2)/P-a*b*c/F)*n^3
> df <- function(v) 3*v^2+2*n*(b-R*T/P)*v+n^2*(a*c/F-3*b^2-2*R*T*b/F)
> v0 <- 332.57652
> # Declaring Given Variables
> T <- 180 # Temperature
> n <- 1 # Number of Molecules (Basis)
> P <- 4.5 # Pressure
> R <- 8.314419 # Molar Gas Constant
> Tc <- 191.15 # Critical Temperature
> Pc <- 4.641 # Critical Pressure
> c <- 1.023364405 # Peng-Robinson Parameter
> a <- (0.45724/Pc)*(R*Tc)^2 # a & b = Peng-Robinson EOS Constants
> b <- (0.07780*R*Tc)/Pc
> # Volume after Convergence
> result <- prbnewton(f, df, v0)
> print(result)
[1] 54.27034
```

*Newton–Raphson method*
**Secant Method**

The unit moles taken resulted in equal $V_m$ and $V$. In problems where “$n$” is provided, unique value of $V_m$ and $V$ will be obtained.

Note: The signs “+” and “<” at the beginning of every line in the R source codes are not part of the code text. Also, functions plot of both $V_m$ and $V$ are same.
It took 23 iterations to arrive at $n = 1$ moles for CH4, assuming V is known, as it is not provided in the base problem.
C.2. R program solution

```r
# C.2. R program solution

f <- function(n) c1*n^3+c2*n^2+c3*n+c4
df <- function(n) 3*c1*n^2+2*c2*n+c3
n0 <- 0.163181

# Declaring Given Variables
T <- 180# Temperature
P <- 4.5# Pressure
V <- 54.27034# Volume
R <- 8.314413# Molar Gas Constant
Tc <- 191.15# Critical Temperature
Pc <- 4.641# Critical Pressure

# Peng-Robinson Parameter
a <- (0.45724/Pc)*(R*Tc)^2
b <- (0.07780*R*Tc)/Pc

c1 <- b*3*(R*T+b^2)/(P-a*b*c/P)
c2 <- V*(a*c/P-(3*b^2)-(2*b*R*T/P))
c3 <- (V^2)*(b*R*T/P)
c4 <- V^3*c1, c2, c3, c4 are Coefficients of n

# Number of Moles after Convergence
result <- prbnnewton(f, df, n0)
print(result)

[1] 1
```

* Newton–Raphson method
Secant Method

For easy execution, coefficients of “n” were shortened as c1, c2, c3, and c4 both in Excel and R. After running the program, n = 1 mole was obtained (in R-Newton and R-Secant source codes) as the value of V used was calculated taking a unit mole as basis. In Secant, the root was found over an interval of (0, 1.5).

C.3. Number of moles function plot

An interval that brackets the root (0, 2) was taken. Corresponding value on x-axis, where the horizontal line at zero touches the curve, indicates the root as shown below.
D. Critical Conditions for Gases and Liquids

<table>
<thead>
<tr>
<th>Compound</th>
<th>Formula</th>
<th>Molecular weight</th>
<th>Critical pressure (psi)</th>
<th>Critical temperature (°F)</th>
<th>Critical volume (ft³/lb)</th>
<th>Liquid specific gravity (water = 1)</th>
<th>Gas specific (air = 1)</th>
<th>Acentric factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>16.042</td>
<td>667</td>
<td>-116.66</td>
<td>0.0985</td>
<td>0.3</td>
<td>0.554</td>
<td>0.0115</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td>30.069</td>
<td>706.6</td>
<td>89.92</td>
<td>0.0775</td>
<td>0.35643</td>
<td>1.0383</td>
<td>0.0994</td>
</tr>
<tr>
<td>Propane</td>
<td>C₃H₈</td>
<td>44.096</td>
<td>615.5</td>
<td>205.92</td>
<td>0.0728</td>
<td>0.59738</td>
<td>1.5277</td>
<td>0.1529</td>
</tr>
<tr>
<td>Isobutane</td>
<td>C₄H₁₀</td>
<td>58.122</td>
<td>527.9</td>
<td>274.41</td>
<td>0.0715</td>
<td>0.56295</td>
<td>2.0071</td>
<td>0.1865</td>
</tr>
<tr>
<td>n-butane</td>
<td>C₅H₁₂</td>
<td>58.122</td>
<td>550.9</td>
<td>305.55</td>
<td>0.0703</td>
<td>0.58408</td>
<td>2.0071</td>
<td>0.2003</td>
</tr>
<tr>
<td>iso-pentane</td>
<td>C₅H₁₂</td>
<td>72.149</td>
<td>490.4</td>
<td>369</td>
<td>0.0685</td>
<td>0.6246</td>
<td>2.4914</td>
<td>0.2284</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>C₅H₁₂</td>
<td>72.149</td>
<td>488.8</td>
<td>385.8</td>
<td>0.0676</td>
<td>0.63113</td>
<td>2.4914</td>
<td>0.2515</td>
</tr>
<tr>
<td>n-hexane</td>
<td>C₆H₁₄</td>
<td>86.175</td>
<td>436.9</td>
<td>453.3</td>
<td>0.0688</td>
<td>0.66404</td>
<td>2.9758</td>
<td>0.2993</td>
</tr>
<tr>
<td>n-heptane</td>
<td>C₇H₁₆</td>
<td>100.202</td>
<td>396.8</td>
<td>512.9</td>
<td>0.0682</td>
<td>0.68819</td>
<td>3.4602</td>
<td>0.3483</td>
</tr>
<tr>
<td>n-Octane</td>
<td>C₈H₁₈</td>
<td>114.229</td>
<td>360.7</td>
<td>564.2</td>
<td>0.0673</td>
<td>0.70698</td>
<td>3.9445</td>
<td>0.3977</td>
</tr>
<tr>
<td>n-nonane</td>
<td>C₉H₂₀</td>
<td>128.255</td>
<td>330.7</td>
<td>610.8</td>
<td>0.0693</td>
<td>0.72186</td>
<td>4.4289</td>
<td>0.4421</td>
</tr>
<tr>
<td>n-Decane</td>
<td>C₁₀H₂₂</td>
<td>142.282</td>
<td>304.6</td>
<td>652.2</td>
<td>0.0703</td>
<td>0.73406</td>
<td>4.9133</td>
<td>0.4875</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>28.01</td>
<td>506.7</td>
<td>-220.63</td>
<td>0.0527</td>
<td>0.79265</td>
<td>0.9672</td>
<td>0.051</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO₂</td>
<td>44.01</td>
<td>1070</td>
<td>87.76</td>
<td>0.0343</td>
<td>0.82203</td>
<td>1.5197</td>
<td>0.2239</td>
</tr>
<tr>
<td>Hydrogen sulfide</td>
<td>H₂S</td>
<td>34.082</td>
<td>1306.5</td>
<td>212.81</td>
<td>0.0462</td>
<td>0.80269</td>
<td>1.1769</td>
<td>0.101</td>
</tr>
<tr>
<td>Air</td>
<td></td>
<td>28.9586</td>
<td>551.9</td>
<td>-220.97</td>
<td>0.0458</td>
<td>0.87603</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>2.0159</td>
<td>190.7</td>
<td>-399.9</td>
<td>0.5319</td>
<td>0.87087</td>
<td>0.06961</td>
<td>-0.214</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>31.9988</td>
<td>731.4</td>
<td>-181.43</td>
<td>0.0367</td>
<td>1.1423</td>
<td>1.105</td>
<td>0.0222</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>28.0135</td>
<td>492.5</td>
<td>-232.53</td>
<td>0.0511</td>
<td>0.80687</td>
<td>0.9674</td>
<td>0.0372</td>
</tr>
<tr>
<td>Water</td>
<td>H₂O</td>
<td>18.0153</td>
<td>3200.1</td>
<td>705.1</td>
<td>0.04975</td>
<td>1.06221</td>
<td>0.3443</td>
<td></td>
</tr>
</tbody>
</table>

Molecular weight, Tc, Pc, Vc, and ω, can be look up for a particular compound from the table.

To convert to: (1) “MPa”, multiply by 0.00689476, (2) Kelvin, insert value into K = \frac{9}{5} (°F–32) + 273 and (3) “m³/kg”, multiply by 0.062428.