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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 verboseness, 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 & Lakshminarayanan, 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 (V_m) 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 V_m. After the root is determined using Newton's method, R codes were tested severally to implement a solution to the problem by specifying all the known parameters and setting tolerance error, maximum iterations, and initial V_m 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., V_m) 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 1
R Language utilization in various fields

Field	Uses	Source
Geography	• Analysis of Spatial Data • Earthquake Data Analysis • Geoinformatics • Geomorphology • Characterizing Hypsometric Curve	(Akinwumiju, 2021; Battul et al., 2020; Kaya et al., 2019; Kobal et al., 2013; Lemenkova, 2018; Murugadoss et al., 2022; Na-U-Dom, 2019; Pérez-Molina et al., 2020)

(*Continued*)

Table 1
(*Continued* **)**

Field	Uses	Source
Climatology	• Rescaled range (R/S analysis) • Spatial-Temporal Trends • The Precipitation Concentration Index (PCI) • Mann–Kendall Trend Test • Theil–Sen's Slope Estimator (β) • Autocorrelation Function (ACF) • Relative Percentage Change (RPC) • Change Point Detection	(Gökçekuş et al., 2021; Thupeng & Thekiso, 2019; Zhou et al., 2005)
Architecture	• Real Estate Analytics • Anthropometrics	(Basha et al., 2020; Hussain et al., 2015)
Statistics	• Data Visualization • Big Data Analysis • Correlation Coefficient • Bivariate Probability • Statistical Analysis • TOBIT Regression • Over-fitting Research Data	(Ayanwale et al., 2022; Brennan, 2021; Elshahhat, 2022; Mary et al., 2022; Ndaba, 2022; Nitnaware, 2021; Pavlenko et al., 2020; Rajan, 2020; Rimal, 2019, 2020; Sapanji et al., 2021; Sevil & Yildiz, 2022;
Mathematics	• Plane Geometry • Algebra and Numerical Methods • Calculus and Matrix Operation • Set Operation and Recursion	(Briz-Redon & Serrano-Aroca, 2018; Matloff, 2011; Rajan, 2020; Redón & Aroca, 2018)
Biology	• Bioinformatics • Biological Data Analysis • Graphics in Biological Research	(Dean, 2019; Doyle et al., 2022; Eglen, 2009; Gentleman, 2009; Giorgi et al., 2022; Lewis, 2010; Seefeld & Linder, 2007; Lan et al., 2019)
Electrical Engineering	Electric Load Forecasting	(Kaheh & Shabanzadeh, 2018)
Education	• Educational Measurement and Psychometrics • Educational Data Mining • Multi-choice Test • Social Science Research	(Ayanwale & Ndlovu, 2021; Bulut & Sunbul, 2017; Hussain, 2015; Wong et al., 2019)
General	Simulation Studies	(Hallgren, 2013; Nikitina & Chernukha, 2021; Prihhapso et al., 2022)
Mechanical Engineering	• Metallurgy • Friction stir welded joint mathematical model	(Bora et al., 2020; Dakubo, 2022; Kwame et al., 2020)
Health and Medicine	• Diagnosis System for Lung Cancer • Improving Case Notification Procedures • Extracting COVID-19 Data • Medicinal Chemistry • Clinical Laboratories • Eyam Plague Mathematical Modeling • Healthcare Management • Infectious Disease Prediction	(Aliyu et al., 2022; Barua, 2021; Haymond & Master, 2020; Jahandideh & Krishnamurthy, 2013; Kothari & Patil, 2022; Mente & Kuhn, 2012; Nath, 2019; Robinson & Wayman, 2020; Ruas et al., 2022; Umamaheswari et al., 2021; Weeks et al., 2020)
Chemistry	• Chemical Informatics • Balancing Chemical Equations	(Altintas, 2022; Guha, 2007)
Ecology	• Ecology • Climate Change Analysis • Biometeorological Research • Spatial Data Analysis in Ecology • Drought Monitoring	(Charalampopoulos, 2020; Forrester et al., 2022; Lai et al., 2019; Plant, 2019; Popov & Secerov, 2019; Rajesh & Ravishankar, 2021)
Civil Engineering	• Fetching and Transforming Survey Data • Geotechnical Engineering • Structural Analysis	(Barbosa et al., 2021; Hasan & Jamaluddin, 2019; Maurer, 2021)
Safety and Risk Management	• Fault Tree Analysis • Rothermal Fire Spread Model	(Antonov, et al., 2018; Antonov, et al., 2018; Vacchiano & Ascoli, 2015)
Food Science	• Prediction of Wine Quality • Sensitivity Analysis of Diet Problem	(Akanbi et al., 2022; Alkarkhi & Alqaraghuli, 2019; Lakhani & Manjre, 2021)
Sociology	• Policing Olympic games • Event decision • Event History Analysis	(Brostrom, 2021; Congelio, 2022; Nasri, 2022; Roy et al., 2018)

(*Continued*)

Table 1
(*Continued*)

Field	Uses	Source
Business and Finance	• Sentiment Analysis in Sales • Stock Prices and Business Forecasting • Determination of Consumer Behavior • Process Mining (business intelligence) • Analyzing Customer Shopping Data • Predict Bank Failure and Financial Stability • Banking Research • Econometrics	(Apichatibutarapong, 2015; Booth et al., 2018; Cao, 2021; Celik, 2020; Gürsoy, 2019; Hanck et al., 2020; Kabir & Karim, 2020; Akhil Kumar et al., 2018; Sussolaikah, 2021)
Agriculture and Forestry and Environmental Protection	• Forestry • Biomedical Waste Management • Construction Waste Reduction • Spatial Data Analysis in Agriculture • Agricultural Monitoring Exercises • Plant Breeding and Crop Yield Prediction	(Chandol et al., 2021; Duveiller, 2015; Edmondson, 2019; Emerald et al., 2012; Jeelani et al., 2014; Plant, 2019; Thenmozhi & Divakar, 2020; Values, 2020)
Conservation	• Hierarchical Cluster Analysis • Dendrogram Graphing • Decision Tree Analysis • Aerial Strip Surveys • Line Transects • Fisher Test	(Kaufman & Rousseeuw, 1990; Keeping et al., 2018; Nichols & Alexander, 2019)
Communications	• Controlling the Phonetics software • Social media (e.g., Facebook) big data analysis • Fuzzy Logic	(Albin, 2014; Chen et al., 2021; Shukla & Thaker, 2018; Wagner et al., 2011)

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/ and https://www.rstudio.com) (Doyle et al., 2022; Turner, 2020). Users can then follow the step-wise installation guide lectured by Jayasankar 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

Table 2
R programming language learning texts

Learning material	Reference
Introduction to R Programming Handout	(Srinivasavaradhan, 2019)
R Programming Tutorials	(Joshua, 2020)
R Basics	(Kostadinov, 2016)
Qualitative Research using R: A Systemic Approach	(Chandra & Shang, 2019)
R Programming for Beginners-Mathematical Perspectives	(Rajan, 2020)
Deep R Learning	(Gagolewski, 2022)
Ten Simple Rules for Teaching Yourself R	(Lawlor et al., 2022)
Exploratory Data Analysis with R Programming Language	(Sharma, 2019)
An Introduction to R	(Venables & Smith, 2022)
R Programming in Statistics	(Thiagarajan, 2020)
R for Data Science	(Wickham & Grolemund, 2016)

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, certificate courses 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 characteristics in oil-based drilling fluid (Adeyanju & Olafuyi, 2008; Ashour et al., 2011). This is in addition to using PR EOS to evaluate gas injection candidate reservoirs, provision of quick and accurate engineering estimates of phase behavior, mapping phase envelopes and separator gas compositions prediction, and the calculation of reservoir fluid properties (e.g., densities of complex mixtures, like liquefied natural gas) (Ashour et al., 2011 Majidi et al., 2021; Shanshool et al., 2007). The PR EOS is as presented in equation (1) given by Al-Kindi & Babadagli (2021):

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m^2 + 2bV_m - b^2} \tag{1}$$

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 α is a temperature-dependent function connected to the critical temperature $\left(T_r = \frac{T}{T_c}\right)$ and acentric factor (ω), given by equation (2) and equation (3) in Shi (2017):

$$\alpha = \left[1 + k\left(1 - T_r^{\frac{1}{2}}\right)\right]^2 \tag{2}$$

$$k = \begin{cases} 0.37464 + 1.54226\omega - 0.26992\omega^2, & \omega < 0.49 \\ 0.379642 + 1.48503\omega - 0.164423\omega^2 + 0.016666\omega^3, & \omega > 0.49 \end{cases} \tag{3}$$

where T_C = critical temperature and k = a dimensionless function of ω. 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.

$$f(V_m) = V_m^3 + \left(b - \frac{RT}{P}\right)V_m^2 - \left(3b^2 + \frac{2RTb}{P} - \frac{a\alpha}{P}\right)V_m + \left(b^3 + \frac{RTb^2 - ab\alpha}{P}\right) \tag{4}$$

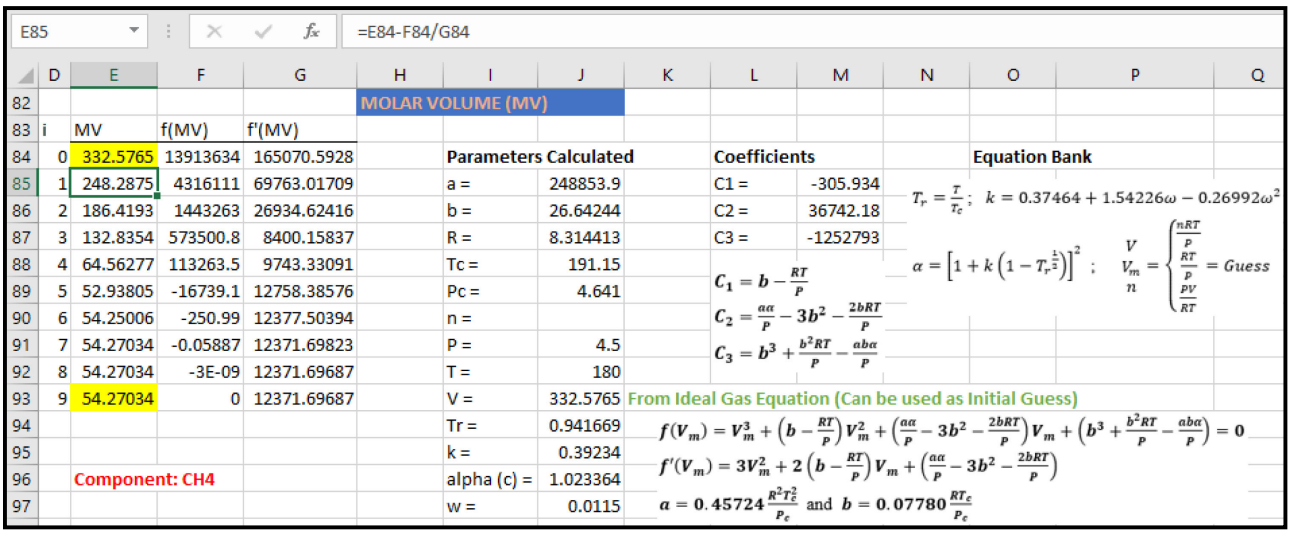
$$f'(V_m) = 3V_m^2 + 2\left(b - \frac{RT}{P}\right)V_m - \left(3b^2 + \frac{2RTb}{P} - \frac{a\alpha}{P}\right) \tag{5}$$

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).

$$v_{i+1} = v_i - \frac{f(v_i)}{f'(v_i)} \tag{6}$$

$$v_{i+1} = v_i - \frac{f(v_i)(v_i - v_{i-1})}{f(v_i) - f(v_{i-1})} \tag{7}$$

Figure 2
Excel Newton–Raphson method molar volume root finding from PR EOS



In Excel (Figure 2), coefficients of the independent variable (V) of the cubic equations defined as C1, C2, and C3 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 α 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

Figure 3
Newton–Raphson molar volume calculation algorithm with R

```
> prbnewton <- function(f, df, m0, 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)
+   {
+     m1 <- m0 - f(m0)/df(m0)              # Update m using Newton's Method
+     if (abs(m1 - m0) < tol) return(m1)   # Check for Convergence
+     m0 <- m1                             # Update m0 for the next iteration
+   }
+   return(m1)                             # Return the result if convergence was not achieved
+ }
> f <- function(m) m^3+(b-R*T/P)*m^2-(3*b^2+2*R*T*b/P-a*c/P)*m+(b^3+(R*T*b^2)/P-a*b*c/P)
> df <- function(m) 3*m^2+2*(b-R*T/P)*m-(3*b^2+2*R*T*b/P-a*c/P)
> m0 <- 332.57652
>
> # Declaring Given Variables
> T <- 180# Temperature
> P <- 4.5# Pressure
> R <- 8.314413# 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
>
> # Molar Volume after Convergence
> result <- prbnewton(f, df, m0)
> print(result)
[1] 54.27034
```

Figure 4
Secant method molar volume calculation algorithm with R

```
> prbsecant <- 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                                          # Update m0 for the next iteration
+     m1 <- m2
+   }
+   return(m1)                    # Return the result if convergence was not achieved
+ }
> f <- function(m) m^3+(b-R*T/P)*m^2-(3*b^2+2*R*T*b/P-a*c/P)*m+(b^3+(R*T*b^2)/P-a*b*c/P)
> m0 <- 40
> m1 <- 60
>
> # Declaring Given Variables
> T <- 180# Temperature
> P <- 4.5# Pressure
> R <- 8.314413# 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
>
> # Molar Volume after Convergence
> result <- prbsecant(f, m0, m1)
> print(result)
[1] 54.27034
```

Figure 5
Molar volume function plot implementation using R

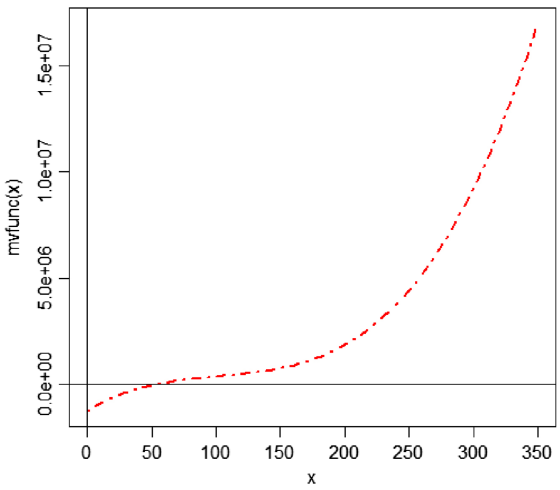
```
> mvfunc <- function(m)
+   {
+    m^3-305.9340844*m^2+36742.18176*m-1252793.101
+   }
> curve(mvfunc, xlim=c(0,350), col='red', lwd=2.5, lty=4)
> abline(h=0)
> abline(v=0)
```

(m0 & m1 or v_i & v_{i-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 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.

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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 ft3 and the correct line of code is:

```
220        SE14=pow(bPENG,3)+(R*T*pow(bPENG,2)-aPENG*bPENG*alphaPENG)/P;
```

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

B. Volume Calculation

B.1. Excel result

M63: =(J64-(J65*J70/J69))*J68

	i	V	f(V)	f'(V)		Parameters	Calculated		Coefficients	
60					VOLUME (V)					
61	i	V	f(V)	f'(V)						
62	0	332.5765	13913634	165070.5928		a =	248853.9		C1 =	-305.934
63	1	248.2875	4316111	69763.01709		b =	26.64244		C2 =	36742.18
64	2	186.4193	1443263	26934.62416		R =	8.314413		C3 =	-1252793
65	3	132.8354	573500.8	8400.15837		Tc =	191.15			
66	4	64.56277	113263.5	9743.33091		Pc =	4.641			
67	5	52.93805	-16739.1	12758.38576		n =	1	Basis		
68	6	54.25006	-250.99	12377.50394		P =	4.5			
69	7	54.27034	-0.05887	12371.69823		T =	180			
70	8	54.27034	-3E-09	12371.69687						
71	9	54.27034	0	12371.69687		V =	332.5765	From Ideal Gas Equation (Can be used as Initial Guess)		
72						Tr =	0.941669			
73						k =	0.39234			
74		Component: CH4				alpha (c) =	1.023364			
75						w =	0.0115			

Equation Bank

$$T_r = \frac{T}{T_c};\quad k = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$\alpha = \left[1 + k\left(1 - T_r^{\frac{1}{2}}\right)\right]^2;\quad V_m = \begin{cases} \frac{nRT}{P} \\ \frac{RT}{P} \\ \frac{PV}{RT} \end{cases} = Guess$$

$$C_1 = n\left(b - \frac{RT}{P}\right)$$

$$C_2 = n^2\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)$$

$$C_3 = n^3\left(b^3 + \frac{b^2RT}{P} - \frac{ab\alpha}{P}\right)$$

$$f(V) = V^3 + n\left(b - \frac{RT}{P}\right)V^2 + n^2\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)V + n^3\left(b^3 + \frac{b^2RT}{P} - \frac{ab\alpha}{P}\right) = 0$$

$$f'(V) = 3V^2 + 2n\left(b - \frac{RT}{P}\right)V + n^2\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)$$

$$a = 0.45724\frac{R^2T_c^2}{P_c} \text{ and } b = 0.07780\frac{RT_c}{P_c}$$

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

```
> 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(v1)                             # Return the result if convergence was not achieved
+ }
> f <- function(v) v^3+n*(b-R*T/P)*v^2+n^2*(a*c/P-3*b^2-2*R*T*b/P)*v+(b^3+(R*T*b^2)/P-a*b*c/P)*n^3
> df <- function(v) 3*v^2+2*n*(b-R*T/P)*v+n^2*(a*c/P-3*b^2-2*R*T*b/P)
> v0 <- 332.57652
>
> # Declaring Given Variables
> T <- 180# Temperature
> n <- 1# Number of Moles (Basis)
> P <- 4.5# Pressure
> R <- 8.314413# 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

```
> prbsecant <- function(f, v0, v1, 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)
+   {
+     v2 <- v1 - f(v1) / ((f(v1) - f(v0)) / (v1 - 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
+     v1 <- v2
+   }
+   return(v1)                    # Return the result if convergence was not achieved
+ }
> f <- function(v) v^3+n*(b-R*T/P)*v^2+n^2*(a*c/P-3*b^2-2*R*T*b/P)*v+(b^3+(R*T*b^2)/P-a*b*c/P)*n^3
> v0 <- 40
> v1 <- 60
>
> # Declaring Given Variables
> T <- 180# Temperature
> P <- 4.5# Pressure
> n <- 1# Number of Moles (Basis)
> R <- 8.314413# 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 <- prbsecant(f, v0, v1)
> print(result)
[1] 54.27034
```

**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.

C. Number of Moles Calculation

C.1. Excel result

F43: =(M44*E43^3)+(M45*E43^2)+(M46*E43)+M47

NUMBER OF MOLES (n)

i	n	f(n)	f'(n)
0	0.16	61586.5	-359188.65
1	0.33146	34627.51	7894.475068
2	-4.05484	1.2E+08	-78865949.8
3	-2.53174	35552225	-35087899.6
4	-1.51851	10512700	-15623267.8
5	-0.84562	3105221	-6960962.19
6	-0.39953	918038	-3094340.16
7	-0.10285	274970.2	-1350982.05
8	0.100683	88053.84	-537628.946
9	0.264465	37833.73	-109232.881
10	0.610824	67915.67	132646.7912
11	0.09882	89061.43	-543663.973
12	0.262637	38036.8	-112902.497
13	0.599536	66381.82	138978.6523
14	0.121896	77364.38	-470778.041
15	0.286229	35917.18	-67483.4404
16	0.818466	71235.26	-154687.291
17	1.278977	-351830	-1948364.67
18	1.0984	-84345.6	-1055037.78
19	1.018455	-13000.1	-737819.88
20	1.000835	-562.433	-674367.278
21	1.000001	-1.22872	-671421.631
22	0.999999	-5.9E-06	-671415.174
23	999999	0	-671415.174

Parameters Calculated

a =	248853.9
b =	26.64244
R =	8.314413
Tc =	191.15
Pc =	4.641
n =	0.163181
P =	4.5
T =	180
V =	54.2703
Tr =	0.941669
k =	0.39234
alpha (c) =	1.023364
w =	0.0115

Coefficients

C1 =	-1252793.1
C2 =	1994009.227
C3 =	-901057.093
C4 =	159840.4402

From Ideal Gas Equation (Can be used as Initial Guess)

$$C_1 = b^3 + \frac{b^2RT}{P} - \frac{ab\alpha}{P}$$

$$C_2 = V\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)$$

$$C_3 = V^2\left(b - \frac{RT}{P}\right)$$

$$C_4 = V^3$$

Equation Bank

$$T_r = \frac{T}{T_c};\quad k = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$\alpha = \left[1 + k\left(1 - T_r^{\frac{1}{2}}\right)\right]^2;\quad \frac{V}{n} V_m = \begin{cases} \frac{nRT}{P} \\ \frac{RT}{P} \\ \frac{PV}{RT} \end{cases} = Guess$$

$$f(n) = \left(b^3 + \frac{b^2RT}{P} - \frac{ab\alpha}{P}\right)n^3 + V\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)n^2 + V^2\left(b - \frac{RT}{P}\right)n + V^3 = 0$$

$$f'(n) = 3\left(b^3 + \frac{b^2RT}{P} - \frac{ab\alpha}{P}\right)n^2 + 2V\left(\frac{a\alpha}{P} - 3b^2 - \frac{2bRT}{P}\right)n + \left(b - \frac{RT}{P}\right)V^2$$

$$a = 0.45724\frac{R^2T_c^2}{P_c} \text{ and } b = 0.07780\frac{RT_c}{P_c}$$

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

```
> prbnewton <- function(f, df, n0, tol=1e-10, maxiter=100)
+ {
+   # f = Function of Number of Moles (n) from Peng-Robinson EOS
+   # df = Derivative of f
+   # n0 = Initial guess for the root (from ideal gas law)
+   # tol = Tolerance for the error
+   # maxiter = Maximum number of iterations
+   for (i in 1:maxiter)
+   {
+     n1 <- n0 - f(n0)/df(n0)              # Update n using Newton's Method
+     if (abs(n1 - n0) < tol) return(n1)   # Check for Convergence
+     n0 <- n1                             # Update n0 for the next iteration
+   }
+   return(n1)                             # Return the result if convergence was not achieved
+ }
> 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
> 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
> 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 <- prbnewton(f, df, n0)
> print(result)
[1] 1
```

* Newton–Raphson method

```
> prbsecant <- function(f, n0, n1, tol=1e-10, maxiter=100)
+ {
+   # f = Function of Number of Moles (n) from Peng-Robinson EOS
+   # df = Derivative of f
+   # n0 = Initial guess for the root (from ideal gas law)
+   # tol = Tolerance for the error & 'maxiter' = Maximum number of iterations
+   for (i in 1:maxiter)
+   {
+     n2 <- n1 - f(n1) / ((f(n1) - f(n0)) / (n1 - n0))  # Update n using Newton's Method
+     if (abs(n1 - n0) < tol) return(n1)                # Check for Convergence
+     n0 <- n1                                          # Update n0 for the next iteration
+     n1 <- n2
+   }
+   return(n1)                    # Return the result if convergence was not achieved
+ }
> f <- function(n) c1*n^3+c2*n^2+c3*n+c4
> n0 <- 0
> n1 <- 1.5
> # 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
> 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
> 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 <- prbsecant(f, n0, n1)
> print(result)
[1] 1
```

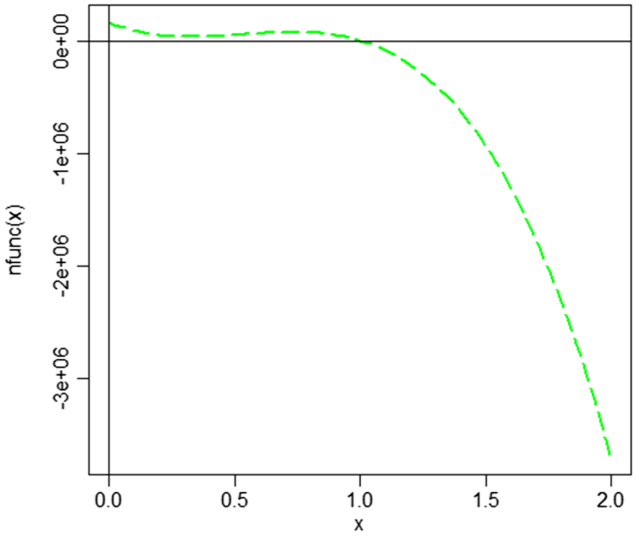
**Secant Method

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

```
> nfunc <- function(n)
+   {
+    -1252793.101*n^3+1994009.227*n^2-901057.0925*n+159840.4402
+   }
> curve(nfunc, xlim=c(0,2), col='green', lwd=2.5, lty=5)
> abline(h=0)
> abline(v=0)
```

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

Compound	Formula	Molecular weight	Critical pressure (psia)	Critical temperature (°F)	Critical volume (ft^3/lb)	Liquid specific gravity (water = 1)	Gas specific (air = 1)	Acentric factor
Methane	CH_4	16.042	667	-116.66	0.0985	0.3	0.554	0.0115
Ethane	C_2H_6	30.069	706.6	89.92	0.0775	0.35643	1.0383	0.0994
Propane	C_3H_8	44.096	615.5	205.92	0.0728	0.50738	1.5227	0.1529
Isobutane	C_4H_{10}	58.122	527.9	274.41	0.0715	0.56295	2.0071	0.1865
n-butane	C_4H_{10}	58.122	550.9	305.55	0.0703	0.58408	2.0071	0.2003
Isopentane	C_5H_{12}	72.149	490.4	369	0.0685	0.6246	2.4914	0.2284
n-Pentane	C_5H_{12}	72.149	488.8	385.8	0.0676	0.63113	2.4914	0.2515
n-Hexane	C_6H_{14}	86.175	436.9	453.3	0.0688	0.66404	2.9758	0.2993
n-Heptane	C_7H_{16}	100.202	396.8	512.9	0.0682	0.68819	3.4602	0.3483
n-Octane	C_8H_{18}	114.229	360.7	564.2	0.0673	0.70698	3.9445	0.3977
n-Nonane	C_9H_{20}	128.255	330.7	610.8	0.0693	0.72186	4.4289	0.4421
n-Decane	$C_{10}H_{22}$	142.282	304.6	652.2	0.0703	0.73406	4.9133	0.4875
Carbon monoxide	CO	28.01	506.7	-220.63	0.0527	0.79265	0.9672	0.051
Carbon dioxide	CO_2	44.01	1070	87.76	0.0343	0.82203	1.5197	0.2239
Hydrogen sulfide	H_2S	34.082	1306.5	212.81	0.0462	0.80269	1.1769	0.101
Air	–	28.9586	551.9	-220.97	0.0458	0.87603	1	–
Hydrogen	H_2	2.0159	190.7	-399.9	0.5319	0.07087	0.06961	-0.214
Oxygen	O_2	31.9988	731.4	-181.43	0.0367	1.1423	1.105	0.0222
Nitrogen	N_2	28.0135	492.5	-232.53	0.0511	0.80687	0.9674	0.0372
Water	H_2O	18.0153	3200.1	705.1	0.04975	1	0.6221	0.3443

Molecular weight, T_c, P_c, V_c, 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 $K = \frac{5}{9}(°\text{F}–32) + 273$ and (3) "m^3/kg", multiply by 0.062428.