Generalized equation predicts vapor pressure of hydrocarbons

M. Edalat, R. B. Bozor-Jomehri Sharif University of Technology Teheran
G. A. Mansoori University of Illinois at Chicago

One of the most important physical properties of hydrocarbons needed by practicing engineers in the oil and gas industries is vapor pressure.\(^1,2\) But until now, no reliable equation could predict hydrocarbon vapor pressures accurately, with only one set of generalized parameters.

A new equation addresses this critical industry need. The accuracy of this generalized equation for predicting 1,106 vapor pressure data points for 94 different fluids has been successfully tested.

This testing has demonstrated that the simple equation performs better than the other vapor pressure equations for all data points tested.

The equation also requires only critical pressure, critical temperature, and acentric factor.

It should be noted that several equations for vapor pressures exist in the literature.\(^3,4\)

The Antoine equation (Equation 1) is the oldest and simplest of such equations (see Equations and Nomenclature).\(^9\)

Equation 1 contains the constants A, B, and C, which must be obtained by fitting the equation to the experimental vapor pressure data of every hydrocarbon separately. As a result, the use of this equation for all hydrocarbons requires a large data bank for the equation coefficients.

On the other hand, an equation developed by Wagner is a bit more generalized (Equation 2).\(^11\) In Wagner's equation, a, b, c, and d are characteristic constants for the fluid under study, and \(P^\theta\) is the vapor (saturation) pressure. If parameters a, b, c, and d are available for a pure hydrocarbon, the equation predicts vapor pressures within the acceptable accuracy down to a reduced temperature (see Nomenclature) of 0.5.

The simple generalized equation presented here accurately estimates vapor pressure of hydrocarbons, nonhydrocarbons, and polar fluids, using only the critical properties \((P_c\) and \(T_c\)) and acentric factor \((\omega)\).

The equation has been successfully tested for a variety of fluids and can be readily used in the oil and gas industry.

### Equations

\[
\begin{align*}
\text{ln} P^\theta &= A - B(T + C) \\
\text{ln} P^\theta &= (a + b - c + d\omega)(1 - \tau)^{-1} \\
\text{ln} P^\theta &= [a(\omega) + b(\omega)] - c(\omega) + d(\omega) - 1 \\
\omega &= \text{Log(P^\theta)}^{1.97} - 1 \\
a(\omega) &= -6.1559 - 4.0856\omega \\
b(\omega) &= 1.5737 - 1.0540\omega - 4.4365 \times 10^{-3} d(\omega) \\
c(\omega) &= -0.8747 - 7.8874\omega \\
d(\omega) &= (0.4893 - 0.9912\omega + 3.1551\omega^2)^{-1}
\end{align*}
\]

### Nomenclature

- \(a, b, c, d\) = Parameters in the Wagner equation
- \(A, B, C\) = Parameters in the Antoine equation
- \(\text{ln}\) = Natural logarithm
- \(P\) = Pressure
- \(P_c\) = Critical pressure
- \(P_r\) = Reduced pressure \((- P/P_c\))
- \(P^\theta\) = Reduced vapor temperature \((- P/P_c\))
- \(T\) = Absolute temperature
- \(T_c\) = Critical temperature
- \(T_r\) = Reduced temperature \((- T/T_c\))
- \(\tau\) = \(1 - T/T_c\)
- \(\omega\) = Acentric factor
Generalized equation

To develop a generalized vapor pressure equation with a simple form, applicable to wide ranges of temperature and a variety of fluids, the authors propose the use of Equation 2, but with its parameters defined as functions of $\omega$.

The result of this is Equation 3.

Based on coefficient data of Equation 2—available for 73 compounds—and applying a regression method by considering Pitzer’s definition of acentric factor (Equation 4), the parameters of Equation 3 can be defined by Equations 5-8.

Equation 3, together with Equations 5-8, constitute the new generalized, accurate correlation for vapor pressure.

The applicability of this equation has been tested for a variety of fluids.

Equation comparability

The results of calculations indicate that Equations 3, 5, 6, 7, and 8 can predict vapor pressures of hydrocarbons, nonhydrocarbons, and polar fluids more accurately than the vapor pressure equations available in the literature without the need for information about any additional parameters.

Table 1 compares vapor pressures of pure liquids, as predicted by the Ambrose and Patel (AP) equation, the Lee-Kessler (LK) equation, and Equation 3.

The new equation predicts vapor pressure more accurately than the AP interpolation method. The prediction of the new equation is also superior to the LK equation for all hydrocarbons and other substances, excluding alcohols.

Also reported in Table 1 are the overall average percentage errors of the present and other equations for all 94 substances, tested with a total of 1,106 vapor pressure data points. This comparison shows that, overall, the new equation predicts vapor pressure more accurately than the other equations.

It should be pointed out that the application of the other vapor pressure equations requires knowledge of the coefficients of those equations for every individual substance. The new equation, however, does not require such knowledge, and is accurate and suitable for engineering design calculations.

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References


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The Authors

Edalat

M. Edalat is a professor of chemical engineering at Sharif University of Technology, Tehran. He received his PhD and MS degrees in chemical engineering from the University of Illinois, and his BS degree in chemical engineering from the University of Teheran.

Mansoori

G. A. Mansoori is a professor of chemical engineering at the University of Illinois, Chicago. He was a postdoctoral fellow at Rice University, Houston, from 1960-70. He has been a consultant to the United Nations, Argonne National Laboratory, U.S. Department of Commerce, and numerous chemical, petroleum, and natural gas companies. He has a PhD from the University of Oklahoma, an MS from the University of Minnesota, and a BS from the University of Teheran, all in chemical engineering.

R. R. rozar-jomeheh is an instructor of chemical engineering at Sharif University of Technology. He received BS and MS degrees in chemical engineering from the same institution.

BOOK

Saudi Arabia and the Gulf War, by Nasser Ibrahim Rashid and Esber Ibrahim Shaleen. Published by International Institute of Technology Inc., 830 Wall St., Joplin, Mo., 64801. 564 pp., $35.95.

Here is the story of the recent Gulf War from the viewpoint of Saudi Arabia. It includes events leading up to the conflict and the role played by Saudi Arabia in the war. The book provides a fresh look at the war as seen from the perspective of a Gulf ally which had both its civilians and military directly involved.