

is, eq 20, not the maximum of H of eq 12, becomes the necessary condition.

Specifically, Lovland claims that the optimal policy should be $v = 0.1$ for $\tau_0 \in [c, d]$ to maximize H , since $(x(\tau_0, 1) - x^d) < 0$. This claim is incorrect. Since over the time interval the flow rate is constant, i.e., $v(\theta) = v_*$, H becomes

$$H = \int_c^d x(\theta, 1)^2 [x(\theta, 1) - x^d] d\theta \quad (21)$$

How can eq 21 be used to select $v = 0.1$? The same question applies to the interval of $\tau \in [0, a]$, while choosing $v = 1$. The only apparent reason for choosing v as Lovland did can be $x(\tau, 1) > x^d$ for $\tau \in [c, d]$ and $x(\tau, 1) < x^d$ for $\tau \in [b, c]$. However, this is his starting assumption. Further, without

justification he assumed that $H = 0$ for $\tau_0 \in [b, d]$ and the control is singular.

In summary, the relationship between H and Lovland's choice of the control policy is not clear. What is lacking is the generality and constructiveness in his necessary condition. The above analytical method seems to be preferred to solving the two-point boundary value problem for this problem.

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Comments on: "A New Two-Constant Equation of State"

Sir: In their publication, Peng and Robinson (1976) presented an equation of state obtained by modifying the "cohesive pressure" term of the van der Waals equation of state (1873). In the modification of this term, they included a temperature-dependent function that had already been proposed by Soave (1972). This function is of the form

$$f(T) = (1 + m(1 - (T/T_c)^{1/2}))^2 \quad (1)$$

The Peng–Robinson and the Soave equations of state can be expressed in a polynomial form as

$$Z^3 - (1 - \bar{B})Z^2 + (A - 3\bar{B}^2 - 2\bar{B})Z - (\bar{A}\bar{B} - \bar{B}^2 - \bar{B}^3) = 0 \quad (2)$$

where $\bar{A} = 0.45724P_R f(T)/T_R^2$, and $\bar{B} = 0.0778P_R/T_R$, and

$$Z^3 - Z^2 + (A - B^2 - B)Z - AB = 0 \quad (3)$$

where $A = 0.42748P_R f(T)/T_R^2$, and $B = 0.08664P_R/T_R$, respectively.

Both eq 2 and eq 3 were claimed to yield one real root in the one-phase region and three real roots in the two-phase region. In this connection, when considering the case of argon, using the methods suggested by Peng–Robinson and Soave, the parameters to be used in eq 1 can be calculated to be: $\bar{m} = 0.3617$ for the Peng–Robinson equation and $m = 0.4769$ for the Soave equation. Equations 2 and 3 were solved using the method given by Abramowitz and Stegun (1965) for supercritical reduced temperatures ranging from 2.0 to 6.0 and reduced pressures ranging from 0.001 to 5.0. For these conditions of temperature and pressure, the equations of state should predict the one-phase region. But the two polynomial equations, eq 2 and 3, yielded in some instances three real unequal roots.

From the three real roots, the largest root is the value of the compressibility factor with physical meaning. The

other two roots are of extraneous nature and can be positive or negative.

The Peng–Robinson equation yielded extraneous roots for all temperatures larger than $T_R = 2.9$ for all pressures considered. The Soave equation yielded spurious roots for all reduced temperatures larger than 4.9 for all the values of pressure considered. This indicates that these equations of state should be used with caution when applied to large temperature values. In the event of multiplicity of real roots, the largest root must be used for the further evaluation of thermodynamic properties.

Nomenclature

A, B, m = parameters of the Soave equation, eq 3
 $\bar{A}, \bar{B}, \bar{m}$ = parameters of the Peng–Robinson equation, eq 2
 P = pressure, N/m²
 P_C = critical pressure, N/m²
 P_R = reduced pressure, P/P_C
 R = gas constant
 T = temperature, K
 T_C = critical temperature, K
 T_R = reduced temperature, T/T_C
 v = molar volume, L/mol
 z = compressibility factor, Pv/RT

Literature Cited

Abramowitz, M., Stegun, I. A., "Handbook of Mathematical Functions", p. 17, Fourth Printing, U.S. Government Printing Office, Washington, D.C., 1965.
Peng, D., Robinson, D. B., *Ind. Eng. Chem. Fundam.*, **15**, 59 (1976).
Soave, G., *Chem. Eng. Sci.*, **27**, 1197 (1972).
van der Waals, J. D., Doctoral Dissertation, Leiden, 1873.

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Sir: Professor Gómez-Nieto has correctly pointed out that two-constant cubic equations can yield three real roots for volume in some supercritical regions. Of these only the largest root has a real physical meaning. We have always assumed users of these equations took this for granted. We

do not believe the point deserves further comment.

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