

## THE PITZER-LEE-KESLER-TEJA (PLKT) STRATEGY AND ITS IMPLEMENTATION BY META-COMPUTING SOFTWARE

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### Abstract

An extension of the corresponding states approach of Pitzer and of Lee and Kesler (Pitzer-Lee-Kesler (PLK) strategy) based on the work of Teja et al. (PLKT strategy) provides a clear pedagogical setting for describing the underlying basis of the PLK strategy itself and also its extension to families of non-normal fluids. Application of the strategy to two families of non-normal fluids is illustrated. Furthermore, the PLKT implementation using meta-computing software provides a convenient tool to perform quantitatively accurate calculations while simultaneously emphasizing the thermodynamic problem structure. Procedures and an example are given for illustration.

Keywords:

extended Lee-Kesler strategy, meta-computing software,  $PvT$  behavior, generalized corresponding states

One way of utilizing an equation of state (EOS) for pure fluids is to determine the EOS parameters by fitting them to experimental data for each individual fluid. Instead of a particular parameter set for each fluid, in a variant of this approach, an EOS is extended to broad classes of fluids by expressing at least one of the parameters in terms of critical properties,  $P_c$  and  $T_c$ , and at least one additional parameter such as the acentric factor,  $\omega$ . The resulting generalized form of EOS, while less accurate for each individual fluid, is intended to provide a compact and reasonably accurate representation of the volumetric (and thermodynamic) properties of the entire class of fluids. An important aspect of chemical engineering education is the study of this strategy of EOS construction and generalization, and its extension to fluid mixtures. A recent example of this strategy for pure polar and nonpolar fluids and their mixtures is described by Platzner and Maurer<sup>(1,2)</sup>.

A different and less common way of utilizing an EOS for classes of fluids is to follow an approach originally proposed by Pitzer. This utilizes parameter sets corresponding to accurate representations of the behavior of selected reference fluids, and then approximates the properties of a class of fluids by incorporating an additional parameter such as  $\omega$  in the form of corrections to the principle of corresponding states, in terms of an expression for  $z(P_r, T_r)$  (where  $T_r = T/T_c$  is the reduced temperature and  $P_r = P/P_c$  is the reduced pressure). In this note, we explore the general basis for and the utility of this latter approach, which we believe has been insufficiently exploited in the pedagogical literature.

The correlation of Lee and Kesler<sup>(3)</sup> for volumetric and thermodynamic properties of normal fluids, based on the acentric factor ( $\omega$ ) of Pitzer et al.<sup>(4-7)</sup> (PLK strategy), is the most favored three-parameter corresponding states correlation (Smith et al.<sup>(8)</sup>, p. 88). In spite of this accolade, introductory books on thermodynamics almost all either ignore it, or deal only

with its implementation in graphical or tabular form. Such pedagogical treatments of the correlation for the most part ignore the underlying basis, thus obscuring its possible extension to other classes of fluids, and by default its dependence on a particular representation of  $PvT$  behavior. Such treatments also disregard the emphasis placed by Lee and Kesler on an analytical implementation in a form convenient for computer use. The graphical form is useful for a qualitative representation of the behavior of pure fluids, but both tables and charts are inadequate for the best quantitative results. The extension of the PLK strategy by Teja et al.<sup>(9–13)</sup> (PLKT strategy), applicable to broader families of fluids, is not discussed at all in introductory texts.

The somewhat complex computer implementation necessary at the time of its original development has probably led to the emphasis on the use of graphs and tables in the teaching of the PLK approach. However, current computer implementation technology has advanced considerably beyond that available twenty-five years ago. Implementations are now available in the form referred to by Edgar<sup>(14)</sup> as “meta-computing” software, involving the use of packages such as Maple<sup>(15)</sup>, Mathematica<sup>(16)</sup>, Mathcad<sup>(17)</sup>, and MATLAB<sup>(18)</sup>. We agree with Sandler<sup>(19,20)</sup> that this type of software is especially useful in a pedagogical setting, since in addition to allowing the treatment of problems previously considered too complex at the undergraduate level, it “can let the student concentrate on the subject matter at hand, ..., rather than being distracted by computational methods, algorithms, and programming languages”<sup>(20)</sup>. This type of software is becoming increasingly accessible to engineering undergraduates, and lends itself to an efficient implementation of the PLK and the PLKT approaches.

Our purpose in this note is two-fold:

1. to describe and emphasize the pedagogical importance of the PLKT strategy, both as a setting for understanding the essential basis of the PLK strategy for normal fluids, and for extending it to other classes of fluids; and
2. to describe an efficient analytical implementation of the PLKT strategy using meta-computing software

We first describe the Pitzer-Lee-Kesler-Teja (PLKT) strategy, and give an example of its application to two families of non-normal fluids. This description points up the generic nature of the original PLK strategy so as to remove any dependence on a particular equation of state and choice of reference fluids. We then describe, with an example, its implementation using meta-computing software. Throughout, we focus on representation of the compressibility factor,  $z = PV/nRT$ , for pure fluids, but the determination of thermodynamic properties follows from this, as outlined, for example, by Lee and Kesler.<sup>(3)</sup>

## THE PLKT STRATEGY

In 1955, Pitzer et al.<sup>(4,5)</sup> added a third parameter,  $\omega$ , to the two-parameter  $(P_c, T_c)$  principle of corresponding states for determining the thermodynamic properties of “normal fluids”. This was based on the concepts of (1) “simple” fluids with spherically symmetric intermolecular potentials/shapes, and (2) “normal” fluids with moderate departures from simple-fluid behavior, and expressed as a linear relation for  $z$  in terms of  $\omega$ :

$$z(P_r, T_r; \omega) = z^{(0)}(P_r, T_r) + \omega z^{(1)}(P_r, T_r) \quad (1)$$

where  $P_r (= P/P_c)$  and  $T_r (= T/T_c)$  are the reduced pressure and temperature, respectively, and  $\omega$  is defined by

$$\omega = -\log_{10} p_r^*(T_r = 0.7) - 1.000 \quad (2)$$

where  $p_r^*$  is the reduced vapor pressure ( $= p^*/P_c$ ) of the substance at  $T_r = 0.7$ . Since the analytical representation of  $z^{(0)}(P_r, T_r)$  and  $z^{(1)}(P_r, T_r)$  is not feasible, Pitzer et al. provided tables of their values based on analysis of experimental data. Curl and Pitzer<sup>(21)</sup> provided a criterion for normal fluids based on surface tension.

In 1975, Lee and Kesler<sup>(3)</sup>, seeking to improve the Pitzer results for fluids involved in hydrocarbon processing, developed an analytical implementation for  $z(v, T_r)$  using a modified Benedict-Webb-Rubin (BWR) equation of state (EOS)<sup>(22)</sup> to represent the behavior of two reference fluids which served to determine  $z^{(0)}$  and  $z^{(1)}$  in equation (1). Lee and Kesler<sup>(3)</sup> described a procedure to implement this strategy to obtain  $z$  for a hydrocarbon fluid of interest at a given  $(P, T)$ , and they provided tables and charts of values of  $z^{(0)}$  and  $z^{(1)}$  as functions of  $(P_r, T_r)$ . We call this the Pitzer-Lee-Kesler (PLK) strategy.

In the 1980s, Teja and co-workers<sup>(9-13)</sup> generalized the PLK approach in three ways. First, they considered it as a special case of interpolation/extrapolation involving  $z(P_r, T_r)$  using two arbitrary, but conveniently chosen, reference fluids, and thus extended its use to “families” of fluids other than normal fluids. Second, they allowed the reference fluids to be represented by any convenient EOS. Third, they extended their approach to mixtures and to other properties, including viscosity<sup>(23-26)</sup>, surface tension<sup>(27)</sup>, and thermal conductivity<sup>(28)</sup>. We call this the Pitzer-Lee-Kesler-Teja (PLKT) strategy. No extensive published calculations show the utility of this approach for pure non-normal fluids, perhaps because the primary focus of their work was on mixtures<sup>(29)</sup>.

The basis of the PLKT strategy is to recognize that the essential assumption underlying the Pitzer approach is that  $z(P_r, T_r)$  is represented as a linear function of the acentric factor

(equation (1)). To determine this linear relationship with  $\omega$ , we may select, from a family of fluids, two appropriate reference fluids,  $r_1$  and  $r_2$  (according to some specified criterion), with corresponding acentric factors  $\omega^{(r_1)}$  and  $\omega^{(r_2)}$ . The equation for the linear  $z(\omega)$  relation for any member of the family may be determined from the two points  $(\omega^{(r_1)}, z^{(r_1)})$  and  $(\omega^{(r_2)}, z^{(r_2)})$  as:

$$z(P_r, T_r, \omega) = z^{(r_1)}(P_r, T_r) + \frac{z^{(r_2)}(P_r, T_r) - z^{(r_1)}(P_r, T_r)}{\omega^{(r_2)} - \omega^{(r_1)}}(\omega - \omega^{(r_1)}) \quad (3)$$

Lee and Kesler used equation (3) for the family of normal fluids, with the reference fluids  $r_1$  and  $r_2$  chosen as a simple fluid ( $\omega^{(r_1)} = 0$ ) and (essentially) *n*-octane ( $\omega^{(r_2)} = 0.3978$ ), respectively. However, equation (3) allows the use of *any* two reference fluids within a family. The original PLK strategy was developed for normal fluids; the following example illustrates the appropriateness of equation (3) for two families of non-normal fluids.

**Example 1:** Consider (a) the family of halogenated hydrocarbon refrigerants, and (b) the family of normal alkanols. Investigate whether the PLKT strategy of equation (3) can be applied to these fluid families.

**Solution:**

(a) Figure 1 (similar to Figure 2 of Pitzer et al.<sup>(5)</sup>) shows values of  $z(P_r, T_r)$  for nine halogenated hydrocarbon refrigerants (ranging from C<sub>1</sub> to C<sub>4</sub>) as a function of  $\omega$  at 4 values of  $(P_r, T_r)$ , together with the corresponding results for normal fluids. The  $z$  points for the refrigerants were calculated using the NIST *REFPROP* software package<sup>(32)</sup>; the full lines are least-squares fits through these points and are for comparison only. The dotted lines for normal fluids were calculated using a quantitative numerical implementation of the PLK strategy, as described in the next section. Figure 1 indicates that the linear relationship of equation (3) holds for the family of refrigerants, and that it is somewhat different from that

for normal fluids (the agreement of the results at  $T_r = 1.30$  is coincidental).

(b) Figure 1 also shows values of  $z(P_r, T_r)$  for the normal alkanols from methanol ( $\text{CH}_4\text{O}$ ) to  $n$ -eicosanol ( $\text{C}_{20}\text{H}_{42}\text{O}$ ). Experimental data<sup>(33)</sup> were used for  $z_c$  (at  $P_r = T_r = 1$ ), and at the other state points  $z$  was calculated for the first five  $n$ -alkanols using the Patel-Teja EOS,<sup>(35,36)</sup> the full line at  $P_r = T_r = 1$  is a least-squares fit through the points and is shown for comparison only. Away from  $T_r = 1$ , there is perhaps an insufficient number of family members to draw a conclusion (and the first member, methanol, is anomalous according to the particular EOS used). However, the data at  $T_r = 1$  indicate that the linear relationship of equation (3) likely holds for the family of  $n$ -alkanols, and that it is also somewhat different from that for normal fluids.

Finally, we remark that another way to extend the PLKT approach to non-normal fluids is to incorporate parameters in addition to  $\omega$ . For example, if parameters  $(\omega, \xi)$  are used,  $z(P_r, T_r)$  may be fitted to the plane through 3 points corresponding to 3 reference systems,  $\{(z^{(r_1)}, \omega^{(r_1)}, \xi^{(r_1)}), (z^{(r_2)}, \omega^{(r_2)}, \xi^{(r_2)}), (z^{(r_3)}, \omega^{(r_3)}, \xi^{(r_3)})\}$ , and the analogue of equation (3) is

$$z = z_1 + a(\omega - \omega^{(r_1)}) + b(\xi - \xi^{(r_1)}) \quad (4)$$

where  $a$  and  $b$  are determined from the 3 reference systems. Essentially this approach has been considered by Wu and Stiel<sup>(30)</sup>, by Platzer and Maurer<sup>(1)</sup>, and by Rowley and co-workers<sup>(31)</sup>, who selected as reference systems two specific nonpolar fluids and either water or methanol as the third reference system. Platzer and Maurer<sup>(1)</sup> compared their implementation of this approach with the alternative approach of expressing the EOS parameters in terms of  $\omega$  and  $\xi$ . This extension of the PLKT approach is beyond the scope of this note.

# IMPLEMENTATION OF PLKT STRATEGY USING META-COMPUTING SOFTWARE

In the typical case when the reference fluid EOS is expressed in terms of  $v$  and  $T$ , implementation of the PLKT strategy for calculating  $z$  or  $P$  given  $(v, T)$  is an explicit calculation. In contrast, calculating  $z$  or  $v$  given  $(P, T)$  involves an implicit calculation entailing the solution of certain nonlinear equations. The underlying structure of this calculation is made transparent by the use of meta-computing software. We describe the approach in both cases, and provide an example calculation for the latter situation.

When the EOS for the reference fluids is given explicitly in terms of  $v$  and  $T$ , we write

$$z = f(v, T; \mathbf{p}) \quad (5)$$

where  $\mathbf{p}$  denotes a set of parameters that take on particular values for individual fluids. The particular EOS that Lee and Kesler used in the implementation of their approach<sup>(3)</sup> is written in the form

$$z = f(v'_r, T_r, \mathbf{p}) \quad (6)$$

where  $v'_r$  is the ideal-gas reduced volume defined by

$$v'_r = \frac{P_c v}{RT_c} \equiv z_c v \quad (7)$$

and  $v$  is the actual reduced volume,  $v/v_c$ . Now,

$$z = \frac{Pv}{RT} = \frac{P_r}{T_r} \frac{P_c v}{RT_c} \equiv \frac{P_r}{T_r} v'_r \equiv \frac{P_r}{T_r} z_c v_r \quad (8)$$

Equation (8) shows that, in the use of an EOS to calculate  $z$  at a given  $(P_r, T_r)$ , the set of reduced variables  $\{P_r, T_r, v'_r\}$  is more appropriate than the set  $\{P_r, T_r, v_r\}$ , since the former



requires neither an assumption about the constancy of  $z_c$ , nor a knowledge of  $v_c$ . Since the usual form of an arbitrarily chosen EOS, equation (5), involves  $v$ ,  $v$  must first be converted to  $v'_r$  to use the PLKT strategy in conjunction with it. This is a subtle point that is not apparent in the pedagogical literature, and affects the calculation of  $z$  both from a given  $(v, T)$  and from a given  $(P, T)$ .

### Calculation of $z(v, T)$ via equation (5)

To calculate  $z(v, T)$  for a substance with critical constants  $(P_c, T_c)$  and acentric factor  $\omega$ , the following (explicit) equations are used when the EOS is expressed in terms of  $(v, T)$  (*i.e.*, via equation (5)):

$$z^{(r_1)} = f \left( \frac{RT_c^{(r_1)}}{P_c^{(r_1)}} v'_r, T_r T_c^{(r_1)}; \mathbf{p}^{(r_1)} \right) \quad (9)$$

$$z^{(r_2)} = f \left( \frac{RT_c^{(r_2)}}{P_c^{(r_2)}} v'_r, T_r T_c^{(r_2)}; \mathbf{p}^{(r_2)} \right) \quad (10)$$

where  $v'_r$  and  $T_r$  are calculated using the properties of the fluid of interest. The value of  $z$  is then obtained from equation (3).

### Calculation of $z(P, T)$ via equation (5)

To calculate  $z(P, T)$  when the EOS is expressed in terms of  $(v, T)$ , equation (5), an implicit calculation must be performed involving the solution of nonlinear equations for the reference fluids as follows:

1. calculate  $T_r$  and  $P_r$  using the properties of the fluid of interest
2. calculate  $z^{(r_1)}$  as the solution of of the nonlinear equation:

$$z = f \left( R \frac{T_c^{(r_1)}}{P_c^{(r_1)}} \frac{T_r}{P_r} z, T; \mathbf{p}^{(r_1)} \right) \quad (11a)$$

4. calculate  $z^{(r_2)}$  as the solution of the nonlinear equation:

$$z = f \left( R \frac{T_c^{(r_2)}}{P_c^{(r_2)}} \frac{T_r}{P_r} z, T; \mathbf{p}^{(r_2)} \right) \quad (11b)$$

5. calculate  $z$  from equation (1)

### Calculation of $z(v, T)$ and $z(P, T)$ via equation (6)

When the EOS is expressed in terms of  $(v'_r, T_r)$  (as is the case for the Lee-Kesler EOS<sup>(3)</sup>), equations (9,10), and (11a, 11b) are, respectively:

$$z^{(r_1)} = f(v'_r, T_r; \mathbf{p}^{(r_1)}) \quad (12)$$

$$z^{(r_2)} = f(v'_r, T_r; \mathbf{p}^{(r_2)}) \quad (13)$$

for  $z(v, T)$ , and

$$z = f \left( \frac{zT_r}{P_r}, T_r; \mathbf{p}^{(r_1)} \right) \quad (14)$$

$$z = f \left( \frac{zT_r}{P_r}, T_r; \mathbf{p}^{(r_2)} \right) \quad (15)$$

for  $z(P, T)$ .

The calculation procedure is illustrated in Figure 2, which shows a Maple<sup>(15)</sup> script for calculating  $z(P, T)$  using the PLKT strategy in conjunction with an EOS expressed in terms of  $(v, T)$ . To make the approach itself transparent, a simple technique is incorporated in the script to calculate only the largest value of  $z$ ; this suffices for the supercritical case, but for the subcritical case only the “vapor-like” root is found. It is left as a student exercise to modify the script to calculate the appropriate result in any given circumstances, which requires either a (somewhat complicated) calculation of the vapor pressure using equation (3), or use of the vapor pressure correlation of Lee and Kesler<sup>(3)</sup>.

Corresponding scripts for Mathematica<sup>(16)</sup>, Mathcad<sup>(17)</sup>, and MATLAB<sup>(18)</sup> may be obtained from the web site at <http://www.chemical-stoichiometry.net/PLKT/>. Scripts for the calculation of  $z$  given an EOS expressed in terms of  $(v'_r, T_r)$  are also available at this location. Use of the Maple<sup>(15)</sup> script is illustrated by the following example:

**Example 2:** *n*-propanol ( $C_3H_8O$ ) is to be stored in a 200-liter cylinder at 230°C. What is the maximum amount (kg) that can occupy the cylinder as vapor? For *n*-propanol,  $P_c = 5170$  kPa,  $T_c = 536.71$  K,  $\omega = 0.628$ ,  $M = 60.10$ , and  $p^*(230^\circ\text{C}) = 2996$  kPa. (Data are from Yaws<sup>(33)</sup>, except for the vapor pressure, which is from the DIPPR Student Chemical Database web site<sup>(34)</sup>.) Use the PLKT strategy with ethanol ( $\omega^{(r_1)} = 0.637$ ) and *n*-pentanol ( $\omega^{(r_2)} = 0.594$ ) as reference fluids  $r_1$  and  $r_2$ , respectively, and the Patel-Teja EOS<sup>(35,36)</sup> in conjunction with equation (3). Values of the parameters  $\mathbf{p}^{(r_1)}$  and  $\mathbf{p}^{(r_2)}$  are given by Patel and Teja.

**Solution:** For the amount of vapor to be a maximum, the highest pressure is  $P = p^*(230^\circ\text{C}) = 2996$  kPa. The amount is

$$m = nM = \frac{p^*VM}{zRT} \quad (16)$$

All quantities in equation (16) are known except  $z(p^*, T)$ . Using the PLKT procedure described above and the Maple script shown in Figure 2, we obtain the values

$$z = 0.6279, \quad m = 13.71 \text{ kg}$$

(For comparison, direct use of the Patel-Teja EOS<sup>(35,36)</sup> gives  $z = 0.6283$ ,  $m = 13.70$  kg.)

## CONCLUSIONS

1. We believe that it is important in teaching the  $PvT$  behavior of fluids to emphasize the general basis for the Pitzer-Lee-Kesler-Teja (PLKT) strategy as an implementation of the 3-parameter principle of corresponding states. This makes clear the underlying basis for the Pitzer corresponding-states approach, and makes extensions more self-evident; we have provided an example of possible extensions to the family of halogenated hydrocarbon refrigerants and to the family of  $n$ -alkanols.
2. We believe that it is important pedagogically to emphasize the quantitative (analytical) implementation of the PLKT strategy, rather than the use of tables and charts, although the latter are useful qualitatively. This quantitative implementation is easily carried out using meta-computing software.
3. We have shown an implementation for a three-parameter corresponding states prediction of the compressibility factor to calculate  $z(P, T)$  when the EOS is given in the form  $z(v, T)$  using meta-computing software. We have illustrated this with an example using MAPLE<sup>(15)</sup>; files for Mathematica<sup>(16)</sup>, Mathcad<sup>(17)</sup>, and MATLAB<sup>(18)</sup> may be obtained from the web site at <http://www.chemical-stoichiometry.net/PLKT/>. Also contained on this web site are four corresponding files for calculating  $z(P, T)$  when the EOS is given in the form  $z(v'_r, T_r)$ .

## ACKNOWLEDGMENT

Financial assistance has been received from the Natural Sciences and Engineering Research Council of Canada. We are grateful for discussions with A. S. Teja.

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## FIGURE CAPTIONS

### Figure 1.

Compressibility factor,  $z(P_r, T_r)$ , as a function of acentric factor,  $\omega$ , for a family of refrigerants (filled circles), some members of the family of  $n$ -alkanols (open circles and triangles), and the family of normal fluids (dotted lines). Where present, the full lines are linear fits to the data points, and are shown for comparison only. For the refrigerants,  $z$  was calculated using the NIST *REFPROP* software package<sup>(32)</sup>; for the  $n$ -alkanols, at  $T_r = 1.00$ , experimental critical data were used<sup>(33)</sup> for C1 to C20; at other temperatures,  $z$  was calculated only for C1 to C5 using the Patel-Teja EOS<sup>(35,36)</sup> and values of parameters provided; for the normal fluids, the dotted line is the original PLK strategy<sup>(3)</sup>. The refrigerants on the graph (in order of their  $\omega$  values) are R13, R21, R22, R23, R125, R218, R134a, RC318, R236ea; the corresponding order for the  $n$ -alkanols is C1, C6, C7, C11, (C5, C8, C9, C4, shown as one point), C10, C13, C3, C2, C12, C14, C16, C17, C18, C20, C19, C15 at  $T_r = 1$ , and C1, C5, C4, C3, C2 at other temperatures.

**Figure 2.** MAPLE<sup>(15)</sup> script for Example 2. This and scripts in Mathematica<sup>(16)</sup>, Mathcad<sup>(17)</sup>, and MATLAB<sup>(18)</sup> may be obtained from the web site at

<http://www.chemical-stoichiometry.net/PLKT/>



Figure 1

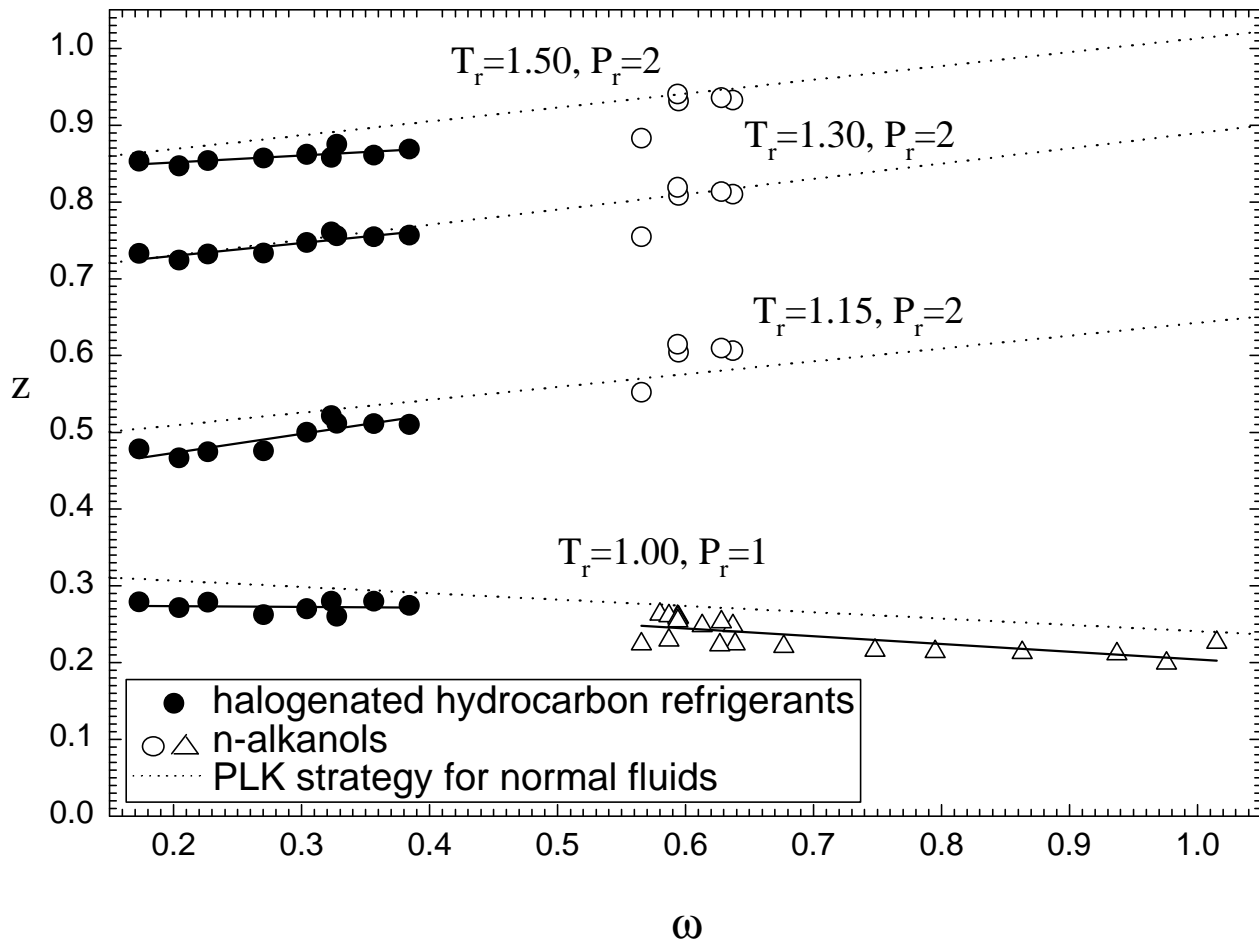


Figure 2

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# PLKT strategy for z(Pr,Tr) using Patel-Teja EOS for n-alkanols
# Reference fluids are ethanol, n-pentanol
restart;R:=8.3145;
omega1:=0.637;Tc1:=516.25;Pc1:=6384000.;zeta1:=0.300;F1:=1.230395;
omega2:=0.594;Tc2:=586.15;Pc2:=3880000.;zeta2:=0.311;F2:=1.242855;
omega_b1:=fsolve(x^3+(2-3*zeta1)*x^2+3*zeta1^2*x-zeta1^3,x,0..10.);
omega_b2:=fsolve(x^3+(2-3*zeta2)*x^2+3*zeta2^2*x-zeta2^3,x,0..10.);
omega_a1:=3*zeta1^2+3*(1-2*zeta1)*omega_b1+omega_b1^2+1-3*zeta1;
omega_a2:=3*zeta2^2+3*(1-2*zeta2)*omega_b2+omega_b2^2+1-3*zeta2;
omega_c1:=1-3*zeta1;omega_c2:=1-3*zeta2;
alpha:=(F,Tr)->(1+F*(1-Tr^(0.5)))^2;
a1:=omega_a1*R^2*Tc1^2/Pc1;a2:=omega_a2*R^2*Tc2^2/Pc2;
b1:=omega_b1*R*Tc1/Pc1;b2:=omega_b2*R*Tc2/Pc2;
c1:=omega_c1*R*Tc1/Pc1;c2:=omega_c2*R*Tc2/Pc2;
zPT:=(v,T,a,b,c)->(R*T/(v-b)-a/(v*(v+b)+c*(v-b)))*v/R/T;
# Example 2 re n-propanol
omega:=0.628;Pc:=5170000.;Tc:=536.71;
T:=230.+273.15;P:=2996000.;Tr:=T/Tc;Pr:=P/Pc;
T1:=Tc1*Tr;P1:=Pc1*Pr;T2:=Tc2*Tr;P2:=Pc2*Pr;
if Tr>1 then
  z1:=fsolve(xx=zPT(xx*R*T1/P1,T1,a1*alpha(F1,Tr),b1,c1),xx,0..10);
  z2:=fsolve(xx=zPT(xx*R*T2/P2,T2,a2*alpha(F2,Tr),b2,c2),xx,0..10);
else
  x:=5.;
  while x-zPT(x*R*T1/P1,T1,a1*alpha(F1,Tr),b1,c1)> 0 do x:=x-0.01 end do;
  z1:=fsolve(zz=zPT(zz*R*T1/P1,T1,a1*alpha(F1,Tr),b1,c1),zz,x..x+.01);
  x:=5.;
  while x-zPT(x*R*T2/P2,T2,a2*alpha(F2,Tr),b2,c2)> 0 do x:=x-0.01 end do;
  z2:=fsolve(zz=zPT(zz*R*T2/P2,T2,a2*alpha(F2,Tr),b2,c2),zz,x..x+.01);
end if;
z:=z1+(omega-omega1)/(omega2-omega1)*(z2-z1);
m:=P*0.2*60.1/(z*R*T);

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