



Enhancement of the Lee–Kesler–Plöcker Equation of State for Calculating Thermodynamic Properties of Long-Chain Alkanes

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Abstract

Two optimization approaches to correct the physical limitations of the Lee–Kesler–Plöcker equation of state for the application to long-chain hydrocarbons are presented. The quality of the approaches is evaluated by comparisons with experimental data and reference equations of state. The calculation of thermodynamic properties for alkanes up to squalane is possible with both approaches, for some of which no highly accurate fundamental equation of state is available in the literature. For the first approach, the original parameter set was refitted with constraints guaranteeing correct behavior of the equation in the liquid state. The densities of long-chain hydrocarbons are reproduced with small deviations, while the results for some short-chain alkanes are worsened. For the second approach, existing Helmholtz energy equations of state are utilized, while keeping the linear interpolation scheme via the acentric factor. Significant improvements are achieved for all fluids considered.

Keywords Equation of state · Lee–Kesler–Plöcker equation · Long-chain hydrocarbons · Thermodynamic properties

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1 Introduction

The accurate prediction of thermodynamic properties is crucial for the design and operation of various industry processes, including petrochemical, oil and gas, and chemical and power engineering. Fossil fuels, such as natural gas and crude oil, will still be used in all these processes for the indefinite future. The primary constituents of these fossil fuels are hydrocarbons with varying chain lengths. One approach to calculate the thermodynamic properties of these hydrocarbons is the Lee–Kesler–Plöcker equation of state (LKP) developed by Lee and Kesler [1] and extended by Plöcker et al. [2] in the 1970s. Although this equation of state (EOS) is significantly less accurate than fundamental equations of state formulated in terms of the dimensionless Helmholtz energy, it has the advantage that only a few parameters are required to calculate the thermodynamic properties of any fluid.

Recently, Jäger et al. [3] investigated the behavior of the residual entropy scaling model for various equations of state, including the LKP. The required molar residual entropy s^r and the number density ρ_N were calculated using the equations of state and the fluid-specific scaling factor ξ was fitted for a large number of fluids in order to obtain a general relationship for ξ . The LKP performed well when applied to short-chain hydrocarbons and showed good agreement with the Helmholtz energy equations of state. For fluids with an acentric factor $\omega > 0.398$ (applies for hydrocarbons with longer chain lengths than *n*-octane), the LKP is evaluated by extrapolation. This leads to inaccurate or in some cases unphysical results, so that an application to longer hydrocarbons (e.g., *n*-hexadecane and higher) was practically impossible. The aim of this work is, thus, to optimize the LKP for better applicability to long-chain hydrocarbons.

2 Lee–Kesler–Plöcker Equation of State

2.1 Fundamentals

The Lee–Kesler–Plöcker equation of state is based on the principle of corresponding states. This approach was first introduced by van der Waals [4] using the critical temperature T_c and pressure p_c , since many fluids exhibit similar thermodynamic behavior under the same reduced conditions. Later, Pitzer et al. [5–7] extended this approach by using the acentric factor ω as a further correlating variable. The compressibility factor Z is obtained according to

$$Z = Z^{(0)} + \omega Z^{(1)}, \quad (1)$$

where ω is the acentric factor of the investigated fluid. $Z^{(0)}$ is the compressibility factor of a simple fluid, while $Z^{(1)}$ describes the deviation of Z and $Z^{(0)}$. The values for $Z^{(0)}$ and $Z^{(1)}$ were given as tabulated data as a function of reduced temperature and pressure. Lee and Kesler [1] introduced a reference fluid (superscript ref) to give an analytical expression for the deviation term $Z^{(1)}$:

$$Z^{(1)} = \frac{1}{\omega^{(\text{ref})}} (Z^{(\text{ref})} - Z^{(0)}). \quad (2)$$

Consequently, in the basic form of the LKP, the compressibility factor Z is then given by

$$\begin{aligned} Z &= Z^{(0)} + \frac{\omega}{\omega^{(\text{ref})}} (Z^{(\text{ref})} - Z^{(0)}) \\ &= \left(1 - \frac{\omega}{\omega^{(\text{ref})}}\right) Z^{(0)} + \frac{\omega}{\omega^{(\text{ref})}} Z^{(\text{ref})}. \end{aligned} \quad (3)$$

The equation can be interpreted as a linear interpolation as a function of ω between the two compressibility factors of the base points (0) and (ref) evaluated at corresponding states, assuming that the acentric factor of the simple fluid $\omega^{(0)}$ is zero. Later, Plöcker et al. [2] extended this approach by adding binary parameters for the calculation of mixtures. To analytically represent the compressibility factors, a modification of the Benedict-Webb-Rubin-EOS [8] (BWR) is used in reduced form

$$Z^{(0 \text{ or ref})} = 1 + \frac{B}{\Psi} + \frac{C}{\Psi^2} + \frac{D}{\Psi^5} + \frac{c_4 \tau^3}{\Psi^2} \left(\beta + \frac{\gamma}{\Psi^2} \right) \exp\left(-\frac{\gamma}{\Psi^2}\right), \quad (4)$$

where the constants B to D are obtained from temperature-dependent polynomials

$$B = b_1 - b_2 \tau - b_3 \tau^2 - b_4 \tau^3, \quad (5)$$

$$C = c_1 - c_2 \tau + c_3 \tau^3, \quad (6)$$

$$\text{and } D = d_1 + d_2 \tau. \quad (7)$$

The reciprocal reduced temperature τ is calculated using the reducing temperature T_r :

$$\tau = \frac{T_r}{T}. \quad (8)$$

Ψ is the reduced volume given as

$$\Psi = \frac{p_r v}{RT_r} = \frac{p_r}{RT_r \rho}, \quad (9)$$

with the reducing pressure p_r and the specific volume $v = 1/\rho$. The link between Ψ and the reduced density δ is, therefore, made by the following formula:

$$\delta = \frac{\rho}{\rho_r} = \frac{p_r}{RT_r \rho_r \Psi} = \frac{Z_r}{\Psi}. \quad (10)$$

For pure substances, the respective critical parameters are used as the reducing quantities

$$p_r = p_c, \quad \rho_r = \rho_c, \quad \text{and} \quad T_r = T_c, \quad (11)$$

while for mixtures, the determination of reducing quantities is explained in Sect. 2.2. For calculations with the LKP, two parameter sets for Eqs. 4–7 are required for the reference and simple fluid, respectively. Each of these consists of the 12 fluid-specific parameters b_1 to b_4 , c_1 to c_4 , d_1 , d_2 , β , and γ . The parameters determined by Lee and Kesler [1] are summarized in Table 1. According to Lee and Kesler [1], the reference fluid parameters were fitted to density and enthalpy data of *n*-octane. For the simple fluid, data for argon, krypton, and methane were selected. Since the reduced temperatures of the triple points of these fluids are $T_{tr}/T_c > 0.5$, additional data on light hydrocarbons such as propane (data covering temperatures down to $T_{tr}/T_c = 0.32$) were used to represent the low temperature regions. Moreover, Lee and Kesler [1] report that data from other hydrocarbons were additionally used in the fit in order to obtain the best possible fit of all available data.

2.2 Mixtures

For mixtures, pseudo-critical parameters are used as the reduction quantities. To obtain the pseudo-critical parameters, combining rules must be applied, which was summarized by Herrig [9]. This requires the critical temperatures $T_{c,i}$, critical pressures $p_{c,i}$, and acentric factors ω_i , as well as the molar fraction x_i of all substances in the mixture consisting of N different components. The combining rules can be extended by adjustable binary parameters k_{ij} (see Plöcker et al. [2]) to increase the accuracy of the equation.

Table 1 Parameters for Eqs. 4–7

Parameters	Simple fluid	Reference fluid
b_1	0.1181193	0.2026579
b_2	0.2657280	0.3315110
b_3	0.1547900	0.0276550
b_4	0.0303230	0.2034880
c_1	0.0236744	0.0313385
c_2	0.0186984	0.0503618
c_4	0.0427240	0.0415770
c_3	0.0000000	0.0169010
$d_1 \cdot 10^4$	0.1554280	0.4873600
$d_2 \cdot 10^4$	0.6236890	0.0740336
β	0.6539200	1.2260000
γ	0.0601670	0.0375400

The pseudo-critical temperature and molar volume of the compound can be calculated as follows:

$$T_r = T_{c,mix} = \frac{1}{v_{c,mix}^\eta} \sum_{i=1}^N \sum_{j=1}^N x_i x_j v_{c,ij}^\eta T_{c,ij} \tag{12}$$

$$\text{and } \frac{1}{\rho_r} = v_{c,mix} = \sum_{i=1}^N \sum_{j=1}^N x_i x_j v_{c,ij}. \tag{13}$$

$T_{c,ij}$ and $v_{c,ij}$ denote pseudo-critical quantities of the binary systems:

$$T_{c,ij} = k_{ij} (T_{c,i} \cdot T_{c,j})^{0.5} \tag{14}$$

$$\text{and } v_{c,ij} = 0.125 \left(v_{c,i}^{1/3} + v_{c,j}^{1/3} \right)^3. \tag{15}$$

The exponent η , similar to the k_{ij} in Eq. 14, could be adjusted to different mixtures, but is set to $\eta = 0.25$ as a global parameter, since good results were obtained for all binary systems considered in their original work [2]. Often, the critical molar volumes (or densities) of the pure substances are not known. Therefore, the value is calculated with the approximation in Eq. 16 using T_c , p_c and ω of the investigated substance [1]

$$v_{c,i} = (0.2905 - 0.085\omega_i) \frac{RT_{c,i}}{p_{c,i}}. \tag{16}$$

The acentric factor of the mixture is defined as

$$\omega_{mix} = \sum_{i=1}^N x_i \omega_i. \tag{17}$$

Using the same approximation from Eq. 16, the pseudo-critical pressure is given by

$$p_r = p_{c,mix} = (0.2905 - 0.085\omega_{mix}) \frac{RT_{c,mix}}{v_{c,mix}}. \tag{18}$$

2.3 Transformation to Helmholtz Energy Equation

A fundamental equation of state has the advantage of determining all thermodynamic properties of the system by combining the derivatives of the equation. In the fluid state, a fundamental equation in the form of the Helmholtz energy $a = a(T, \rho)$ is commonly used for this purpose. The equation is typically divided into an ideal part (superscript o) that describes the ideal gas behavior, and a

residual part (superscript r) that describes the deviation of the real fluid from the ideal gas behavior. Furthermore, a description in reduced form is used:

$$\alpha(\tau, \delta) = \frac{a(\tau, \delta)}{RT} = \frac{a^o(\tau, \delta) + a^r(\tau, \delta)}{RT} = \alpha^o(\tau, \delta) + \alpha^r(\tau, \delta). \quad (19)$$

The partial derivatives of the reduced Helmholtz energy with respect to τ and δ are abbreviated with the respective subscripts. As the LKP is expressed in terms of the compressibility factor $Z(T, \rho)$, only the residual part of the fundamental equation can be derived from it. Therefore, an additional formulation for the isobaric heat capacity of the ideal gas c_p^o is required to calculate α^o .

Using the relation $c_v^o = c_p^o - R$ between isobaric and isochoric heat capacities of the ideal gas, the link between the isobaric heat capacity and the reduced Helmholtz energy of the ideal gas according to Span [10] is

$$\alpha^o = \int \left(\int \frac{R - c_p^o}{R\tau^2} d\tau \right) d\tau + \ln \left(\frac{\delta}{\delta_0} \right). \quad (20)$$

The equation for c_p^o used in this work is the PPDS–Equation published by Kleiber and Joh [11]

$$c_p^o = RB + R(C - B) \left(\frac{T_r}{A\tau + T_r} \right)^2 \cdot \left[1 - \frac{A}{A + T_r/\tau} \left(D + E \frac{T_r}{A\tau + T_r} + F \left(\frac{T_r}{A\tau + T_r} \right)^2 + G \left(\frac{T_r}{A\tau + T_r} \right)^3 \right) \right]. \quad (21)$$

The constants A to G are fluid-specific. A detailed list of constants for many different fluids can be found in the work of Kleiber and Joh [11]. In Table 2, the constants for a selection of fluids considered in the course of this work are listed. By inserting the PPDS–Equation into the integral in Eq. 20, a correlation for α^o can be derived:

$$\alpha^o = \int \left[\xi(\lambda + 2) \frac{\ln(A\tau + T_r)}{AT_r} + (AC - AB)(\lambda + 2) \frac{\ln(\tau)}{T_r} - \frac{\xi(\lambda - D + 1)}{A(A\tau + T_r)} + (C - 1)/\tau - \xi \left(\frac{\lambda T_r}{2A(A\tau + T_r)^2} + \frac{(\lambda - D)T_r^2}{3A(A\tau + T_r)^3} + \frac{(G + F)T_r^3}{4A(A\tau + T_r)^4} + \frac{GT_r^4}{5A(A\tau + T_r)^5} \right) + c^I \right] d\tau + \ln \left(\frac{\delta}{\delta_0} \right) \quad (22)$$

and

Table 2 Constants of the PPDS–Equation(see Eq. 21 for selected fluids [11]. Since no parameters are available for *n*-docosane, the constants for *n*-eicosane were used here

Substance	A	B	C	D	E	F	G
Krypton	0.0000	2.5000	2.5000	0.0000	0.0000	0.0000	0.0000
Argon	0.0000	2.5000	2.5000	0.0000	0.0000	0.0000	0.0000
Methane	1530.8043	4.2038	− 16.6150	− 3.5668	43.0563	− 86.5507	65.5986
Ethane	903.4113	4.4815	11.6905	8.4792	77.0215	122.9766	74.0600
Propane	1089.3798	4.7246	1.1767	3.7776	129.3687	281.4223	216.9425
Butane	668.6492	8.9081	14.2467	41.0466	258.1830	411.8238	258.6880
<i>n</i> -Pentane	789.3078	10.6168	0.9888	24.2821	191.4972	315.5929	203.9787
<i>n</i> -Hexane	752.9844	13.4279	1.5402	29.6772	208.3733	342.0902	217.4263
<i>n</i> -Heptane	785.9090	14.6277	1.8476	21.5324	168.6597	283.0262	181.4694
<i>n</i> -Octane	662.4091	20.7046	4.6878	40.7644	232.4401	359.1133	215.4126
<i>n</i> -Nonane	828.9112	18.2983	− 7.0327	− 19.5401	163.6825	− 294.9747	195.6096
<i>n</i> -Decane	807.8718	20.1071	− 3.9883	− 22.5527	184.3994	− 327.2729	214.1176
<i>n</i> -Dodecane	844.185	21.6766	2.1683	− 25.2676	244.7925	− 447.8236	295.3902
<i>n</i> -Hexadecane	668.1744	18.2523	2.5022	− 4.1518	177.7261	− 329.3481	256.6324
<i>n</i> -Docosane	566.8372	54.1062	12.4032	− 44.8725	237.4861	− 374.5789	232.4371

$$\begin{aligned}
 \alpha^o = & \xi(\lambda + 2) \frac{(A\tau + T_r) \ln(A\tau + T_r) - A\tau}{A^2 T_r} + (AC - AB)(\lambda + 2) \frac{\tau(\ln(\tau) - 1)}{T_r} \\
 & - \xi(\lambda + 1) \frac{\ln(A\tau + T_r)}{A^2} + (C - 1) \ln(\tau) + \ln\left(\frac{\delta}{\delta_0}\right) + c^I \tau + c^{II} \\
 & + \xi \left[\frac{\lambda T_r}{2A^2(A\tau + T_r)} + \frac{(\lambda - D)T_r^2}{6A^2(A\tau + T_r)^2} + \frac{(G + F)T_r^3}{12A^2(A\tau + T_r)^3} + \frac{GT_r^4}{20A^2(A\tau + T_r)^4} \right]
 \end{aligned} \tag{23}$$

with

$$\lambda = G + F + E + D \quad \text{and} \quad \xi = A^2 B - A^2 C. \tag{24}$$

c^I and c^{II} are integration constants and can be set for any arbitrary reference state.

Using the PPDS–Equation is not applicable to the calculation of α^o for squalane, as there are no constants A to G given by Kleiber and Joh [11]. Unlike in the case of *n*-docosane, the fluids available in their work vary significantly from squalane, so that it is not possible to use the parameters of another fluid to calculate good approximations for squalane. Therefore, the group contribution method developed by Joback [12] is employed to determine the ideal part of the Helmholtz energy of squalane. The isobaric heat capacity of the ideal gas c_p^o is given by

$$c_p^o = \zeta + \theta(T_r/\tau) + \phi(T_r/\tau)^2 + \psi(T_r/\tau)^3 \tag{25}$$

with

$$\zeta = -34.474, \theta = 2.46936, \phi = 8.454 \cdot 10^{-4}, \text{ and } \psi = 3.428 \cdot 10^{-7}. \tag{26}$$

Once again, c_p^0 is inserted into Eq. 20 and the integrals are solved:

$$\begin{aligned} \alpha^0 &= \int \int \frac{R - \left(\zeta + \theta(T_r/\tau) + \phi(T_r/\tau)^2 + \psi(T_r/\tau)^3\right)}{R\tau^2} d\tau d\tau + \ln\left(\frac{\delta}{\delta_0}\right) \\ &= \int -\frac{(12R - 12\zeta)\tau^3 - 6\theta T_r \tau^2 - 4\phi T_r^2 \tau - 3\psi T_r^3}{12R\tau^4} + c^I d\tau + \ln\left(\frac{\delta}{\delta_0}\right) \\ &= -\left((12R - 12\zeta) \ln(\tau) + \frac{6\theta T_r \tau^2 + 2\phi T_r^2 \tau + \psi T_r^3}{\tau^3}\right) / (12R) + c^I \tau + c^{II} + \ln\left(\frac{\delta}{\delta_0}\right). \end{aligned} \tag{27}$$

The partial derivatives of α^0 with respect to τ and δ up to the third order for both approaches are included in the Supplementary Material.

To calculate the residual part of the Helmholtz energy α^r , the LKP is used. For this purpose, the relation between the compressibility factor Z and α^r is used [10]:

$$\alpha^r = \int_0^\delta \frac{1}{\delta} (Z - 1) d\delta. \tag{28}$$

Substituting the LKP gives:

$$\begin{aligned} \alpha^r &= \int_0^\delta \frac{1}{\delta} \left[\left(1 - \frac{\omega}{\omega^{(ref)}}\right) Z^{(0)} + \frac{\omega}{\omega^{(ref)}} Z^{(ref)} - 1 \right] d\delta \\ &= \int_0^\delta \frac{1}{\delta} \left[\left(1 - \frac{\omega}{\omega^{(ref)}}\right) (Z^{(0)} - 1) + \frac{\omega}{\omega^{(ref)}} (Z^{(ref)} - 1) \right] d\delta \\ &= \left(1 - \frac{\omega}{\omega^{(ref)}}\right) \int_0^\delta \frac{Z^{(0)} - 1}{\delta} d\delta + \frac{\omega}{\omega^{(ref)}} \int_0^\delta \frac{Z^{(ref)} - 1}{\delta} d\delta. \end{aligned} \tag{29}$$

The integrals can be solved by inserting the BWR EOS from Eq. 4 and using the link between Ψ and δ introduced in Eq. 10:

$$\begin{aligned} \int_0^\delta \frac{Z - 1}{\delta} d\delta &= \int_0^\delta \frac{1}{\delta} \left[1 + \frac{B}{\Psi} + \frac{C}{\Psi^2} + \frac{D}{\Psi^5} + \frac{c_4 \tau^3}{\Psi^2} \left(\beta + \frac{\gamma}{\Psi^2}\right) \exp\left(-\frac{\gamma}{\Psi^2}\right) - 1 \right] d\delta \\ &= \int_0^\delta \frac{B}{Z_r} + \frac{C\delta}{Z_r^2} + \frac{D\delta^4}{Z_r^5} + \frac{c_4 \tau^3 \delta}{Z_r^2} \left(\beta + \frac{\gamma \delta^2}{Z_r^2}\right) \exp\left(-\frac{\gamma \delta^2}{Z_r^2}\right) d\delta \\ &= \frac{B\delta}{Z_r} + \frac{C\delta^2}{2Z_r^2} + \frac{D\delta^5}{5Z_r^5} - \frac{c_4 \tau^3}{2\gamma} \left(\beta + 1 + \gamma \frac{\delta^2}{Z_r^2}\right) \exp\left(-\gamma \frac{\delta^2}{Z_r^2}\right) + \frac{c_4 \tau^3}{2\gamma} (\beta + 1). \end{aligned} \tag{30}$$

This results in the residual part of the Helmholtz energy α^r as

$$\alpha^r = \left(1 - \frac{\omega}{\omega^{(ref)}}\right) \alpha^{(r,BWR,0)} + \frac{\omega}{\omega^{(ref)}} \alpha^{(r,BWR,ref)} \tag{31}$$

with $\alpha^{(r,BWR)}$

$$\alpha^{(\tau, \text{BWR})} = \frac{B\delta}{Z_r} + \frac{C\delta^2}{2Z_r^2} + \frac{D\delta^5}{5Z_r^5} - \frac{c_4\tau^3}{2\gamma} \left(\beta + 1 + \gamma \frac{\delta^2}{Z_r^2} \right) \exp \left(-\gamma \frac{\delta^2}{Z_r^2} \right) + \frac{c_4\tau^3}{2\gamma} (\beta + 1). \quad (32)$$

The partial derivatives of α^r with respect to τ and δ up to the third order are included in the Supplementary Material.

3 Optimization Approaches

3.1 Adjusting New Parameters for the LKP Equation

The first optimization approach involves refitting of the parameters of the LKP EOS without altering its mathematical structure. In this section, the refitting procedure is described and the resulting set of parameters is presented. The fitting process was performed using the MATLAB-based fitter MFEOs [13] and a least-squares algorithm, while the calculations of the fluid properties were carried out using TREND [14]. Similar to the original work of Lee and Kesler [1], the parameters were fitted in two separate steps. First, the parameters of the reference fluid were adjusted using *n*-octane data. Since $\omega^{n\text{-octane}} = \omega^{\text{ref}}$ applies, the simple fluid part vanishes from the LKP equation and, thus, the parameters of the simple fluid do not influence the results of the LKP equation for the reference fluid. In a second step, the simple fluid parameters were fitted to a dataset of methane. Since the reduced temperature at the triple point T_{tr}/T_c of methane is about 0.48, further data points of propane had to be included to cover the lower reduced temperature range. The data points were generated by using the reference equations of state of the respective fluids. In both fits, homogeneous densities ρ , vapor pressures p_v , speeds of sound w , and isobaric heat capacities c_p were used. Minimizing the deviations of the density is prioritized. Therefore, all density data points were assigned twice the weighting of the remaining points. Table 3 provides more information about the used datasets, such as the data source, the number of data points in the set, and the temperature and pressure ranges.

Jäger et al. [3] highlight the limitations of the LKP when dealing with long-chain hydrocarbons, as observed during the numerical evaluation of pressure at a temperature of 298.15 K. Specifically, calculations for *n*-hexadecane and longer hydrocarbons resulted in negative values for the pressure p , as well as for the slopes $\left(\frac{\partial p}{\partial \rho}\right)_T$ and curvatures $\left(\frac{\partial^2 p}{\partial \rho^2}\right)_T$ of the isotherms in the homogeneous liquid state. These find-

Table 3 Fluids with their respective reference equation of state and the used properties in the fit

Substance	EOS	N	$(T_{\text{min}} - T_{\text{max}})$ (K)	$(p_{\text{min}} - p_{\text{max}})$ (MPa)	Properties
Methane	[15]	59	95 – 600	0.01 – 400	ρ, c_p, w, p_v
Propane	[16]	25	115 – 300	0.01 – 200	ρ, c_p, w
<i>n</i> -Octane	[17]	136	215 – 650	0.05 – 300	ρ, c_p, w, p_v

ings were important, because flash calculations, as implemented in TREND [14] or similar software tools, will not work as expected if physically incorrect behavior occurs. In order to avoid unphysical behavior of the courses of the isotherms, two constraint functions were used in the fitting process of the parameters to ensure the qualitatively correct physical behavior of the isotherms of long-chain hydrocarbons. The first constraint assures that p remains positive for squalane ($C_{30}H_{62}$) at $T = 260\text{ K}$ and $\rho = 2.8\text{ mol/dm}^3$, while the second constraint guarantees positive slope $\left(\frac{\partial p}{\partial \rho}\right)_T$ of the isotherm under the same conditions. The behavior of the isotherms becomes unphysical when the leading term κ is negative [3]:

$$\kappa = \left(1 - \frac{\omega}{\omega^{\text{ref}}}\right) \frac{D^{(0)}\delta^4}{Z_c^{(0)^5}} + \frac{\omega}{\omega^{\text{ref}}} \frac{D^{(\text{ref})}\delta^4}{Z_c^{(\text{ref})^5}}. \quad (33)$$

As D is temperature-dependent and increases with rising temperature, 260 K was selected for the constraint. This ensures correct behavior of the isotherms even at very low temperatures. An estimate of the maximum density of squalane was used as the density input to the constraint. As a rule of thumb, $\rho_{\text{max}} = 4 \cdot \rho_c$ is used for this. Using the estimations of the critical parameters given by Ambrose et al. [18] and the approximation from Eq. 16, $\rho_c = 0.7\text{ mol/dm}^3$ was chosen to calculate the upper limit.

The resulting parameters of the fit are presented in Table 4. In the further course of this paper, the version of the LKP with these parameters is referenced as LKP-mod.

3.2 Enhancement of the LKP Equation

In this section, an approach to further investigate the simplistic LKP approach, i.e., the interpolation between a simple and reference fluid as a function of the

Table 4 New parameters for Eq. 4–7

Constants	Simple fluid	Reference fluid
b_1	0.1331199	0.0243243
b_2	0.3392959	0.0640205
b_3	0.0786113	0.0899694
b_4	0.0498273	0.2313499
c_1	0.0218093	0.0647721
c_2	0.0109580	0.0928313
c_3	0.0050041	0.0154748
c_4	0.0309082	0.0444100
$d_1 \cdot 10^5$	1.9876201	2.0525725
$d_2 \cdot 10^5$	3.4930069	3.5470136
β	0.5859460	1.4003447
γ	0.0677684	0.0286862

acentric factor ω , is presented. For this purpose, highly accurate Helmholtz energy equations of state are used for the calculation of the simple and the reference fluid parts. This approach will be abbreviated as LKP-SJT in the further course of this work. As already shown in Eq. 19, these equations of state are typically split into ideal and residual parts. Here, only the residual part of the Helmholtz energy equation is adopted, while the ideal part is still calculated using the PPDS–Equation. This enables a direct comparison of the BWR and Helmholtz energy equation as basic functions, without altering any additional influencing factors. For the simple fluid, the equation for methane of Setzmann and Wagner [15] and for the reference fluid, the equation for n -octane of Beckmüller et al. [17] were used. Further information on the calculation of the residual Helmholtz energy and its derivations can be found in the corresponding papers. In contrast to the original LKP equation, where different fluids were used for the calculation of the simple fluid part, only the reference equation for methane is used for the LKP-SJT. Thus, the acentric factor of the simple fluid is changed to $\omega^{(0)} = 0.01142$ in accordance with the value of methane by Setzmann and Wagner [15]. The residual part of the reduced Helmholtz energy is consequently calculated with

$$\begin{aligned}\alpha^r &= \alpha^{r,\text{methane}} + \frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}} \cdot (\alpha^{r,n\text{-octane}} - \alpha^{r,\text{methane}}) \\ &= \left(1 - \frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \alpha^{r,\text{methane}} + \left(\frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \alpha^{r,n\text{-octane}}.\end{aligned}\quad (34)$$

Apart from modifying $\omega^{(0)}$, this approach is equivalent to exchanging the compressibility factors $Z^{(0)}$ and $Z^{(\text{ref})}$ from Eq. 3 with the compressibility factors calculated from the Helmholtz energy equations of state Z^{methane} and $Z^{n\text{-octane}}$. This is shown with the following transformation. Using Eq. 28, Eq. 34 can be rewritten as:

$$\begin{aligned}\alpha^r &= \left(1 - \frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \left[\int_0^\delta \frac{1}{\delta} (Z - 1) d\delta\right]^{\text{methane}} + \left(\frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \left[\int_0^\delta \frac{1}{\delta} (Z - 1) d\delta\right]^{n\text{-octane}} \\ &= \int_0^\delta \left[\left(1 - \frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \frac{Z^{\text{methane}}}{\delta} + \left(\frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) \frac{Z^{n\text{-octane}}}{\delta} - \frac{1}{\delta}\right] d\delta.\end{aligned}\quad (35)$$

Taking the derivative with respect to δ and rearranging the equation yields:

$$1 + \delta \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau = Z = \left(1 - \frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) Z^{\text{methane}} + \left(\frac{\omega - \omega^{(0)}}{\omega^{(\text{ref})} - \omega^{(0)}}\right) Z^{n\text{-octane}}.\quad (36)$$

The determination of the reducing quantities p_r , ρ_r , and T_r as well as the acentric factor ω follows the procedures explained in Section (2.2). This is why the assumed reducing density ρ_r differs from the ones originally used in the Helmholtz energy equations of state, which in turn alters the calculated δ . Therefore, when calculating α^r for the two fluids used as base points, the same accuracies as in the reference equations are not achieved.

The LKP-SJT will be implemented in TREND 6.0.

4 Results

4.1 Data Selection

The datasets required to validate the calculations from the equations of state presented were generated from the respective reference equations of state of the fluids. For this purpose, the minimum and maximum pressure and 10 to 15 isotherms were specified for each fluid. Along these isotherms, 15 points between p_{\min} and p_{\max} were chosen at irregular intervals. At all these state points, the density ρ , the speed of sound w , and the isobaric heat capacity c_p of the fluids were calculated using the respective reference equations of state. In addition, the vapor pressure p_v was calculated for all subcritical isotherms. The exception to these generated datasets are the datasets for methane [28–136], *n*-octane [136–429], and squalane [425–474]. Experimental datasets were compiled for methane and *n*-octane, in order to prove that the approach of fitting the parameters of the LKP-mod is a reasonable strategy. For squalane, a highly accurate Helmholtz energy equation of state is not available. Therefore, direct comparisons to experimental data are made. Table 5 provides an overview of the fluids under consideration and their respective reference equations of state. In addition, the total number of data points in each set N , the minimum and maximum temperature of the isotherms, p_{\min} , and p_{\max} as well as the parameters of the fluids that are required as input for the calculation are specified.

To analyze the results of the equations of state, the relative deviation (ΔX) in percent was calculated between each data point x_{Data} in these datasets and the computed

Table 5 Fluids utilized for the validation of results, together with their input parameters for the equations of state

Substance	Reference	N	T [K]	p [MPa]	T_1 [K]	p_1 [MPa]	ω [-]
Argon	[19]	635	90 – 700	0.07 – 400	150.687	4.8630	– 0.00219
Krypton	[20]	632	120 – 750	0.07 – 180	209.48	5.5250	– 0.000894
Methane	[15]	9505	–	–	190.564	4.5992	0.0114
Ethane	[21]	451	100 – 450	0.01 – 200	305.322	4.8722	0.0995
Propane	[16]	545	115 – 620	0.01 – 200	369.89	4.2512	0.1521
<i>n</i> -Butane	[22]	545	150 – 575	0.01 – 200	425.125	3.796	0.201
<i>n</i> -pentane	[23]	547	150 – 650	0.01 – 400	469.7	3.3675	0.251
<i>n</i> -Hexane	[24]	541	190 – 600	0.01 – 100	507.82	3.0441	0.3
<i>n</i> -Heptane	[25]	537	190 – 600	0.01 – 100	540.2	2.7357	0.349
<i>n</i> -Octane	[17]	6407	–	–	568.74	2.4836	0.3978
<i>n</i> -Nonane	[20]	686	250 – 600	0.01 – 100	594.55	2.103	0.4884
<i>n</i> -Decane	[20]	581	260 – 640	0.01 – 100	617.7	2.281	0.4433
<i>n</i> -Dodecane	[26]	629	280 – 700	0.01 – 100	658.1	1.817	0.574
<i>n</i> -Hexadecane	[27]	585	300 – 760	0.01 – 50	722.1	1.4799	0.749
<i>n</i> -Docosane	[27]	641	350 – 1000	0.01 – 50	792.2	1.174	0.978
Squalane	[18]	996	–	–	810	0.728	1.075

properties using the respective equation of state x_{LKP} , $x_{\text{LKP-mod}}$, and $x_{\text{LKP-SJT}}$ as follows:

$$\Delta X = \frac{x_{\text{Data}} - x_{\text{EOS}}}{x_{\text{Data}}} \cdot 100. \quad (37)$$

In order to evaluate the accuracy of the equations of state using entire datasets, the average absolute relative deviation (AARD) is defined, where N is the total number of points present in the dataset.

$$\text{AARD} = \frac{1}{N} \sum_{i=1}^N |\Delta X_i|. \quad (38)$$

4.2 Comparison with Respect to the LKP-mod

The results of the LKP-mod are compared to the original LKP EOS. Methane and n -octane, linear hydrocarbons between these two base points, as well as argon and krypton are considered. Analyzed properties are density ρ , speed of sound w , vapor pressure p_v , and isobaric heat capacity c_p . Additional properties are taken into account for methane and n -octane. The results for methane are displayed in Fig. 1(a). The total AARD of methane decreased significantly from 2.2% to 1.1% with the introduction of the new parameters listed in Table 4. Each individual property is better reproduced as well. The biggest improvements were made with respect to speed of sound and isochoric heat capacity. Similar results can also be observed in Fig. 1(b) for n -octane, where the overall AARD decreased from 1.4% to 0.7%. The deviations of the densities calculated with the new parameters are less than half the value of the LKP EOS. Deviations with respect to w , c_p , p_v , and ρ' are also smaller with the new parameter set. In contrast, the AARDs for h_{vap} and ρ'' increased slightly, while those for w' and w'' are significantly worse. For both methane and n -octane, additional plots showing the relative deviations ΔX of the experimental data points are included in the Supplementary Information.

The AARDs for propane as well as argon and krypton, which were originally used for the fit of the simple fluid [1], are illustrated in Fig. 2. Figures 2(a) and (b) show the improvements with respect to argon and krypton. The total AARDs of the fluids decreased from approximately 4% to less than 1%, even though the new parameters were not fitted to data of krypton and argon. Noteworthy are the deviations in the speed of sound w , which became significantly smaller due to the new parameters. The improvements are particularly visible at subcritical temperatures. For example for krypton, the AARD decreased from 11.5% to 1%. Propane is in contrast to these results. The AARDs of the LKP and LKP-mod to the values calculated with the reference equation of state of Lemmon et al. [16] are depicted in Fig. 2(c). The density ρ is slightly improved, while the isobaric heat capacity c_p , the speed of sound w , and the vapor pressure p_v are reproduced significantly worse than

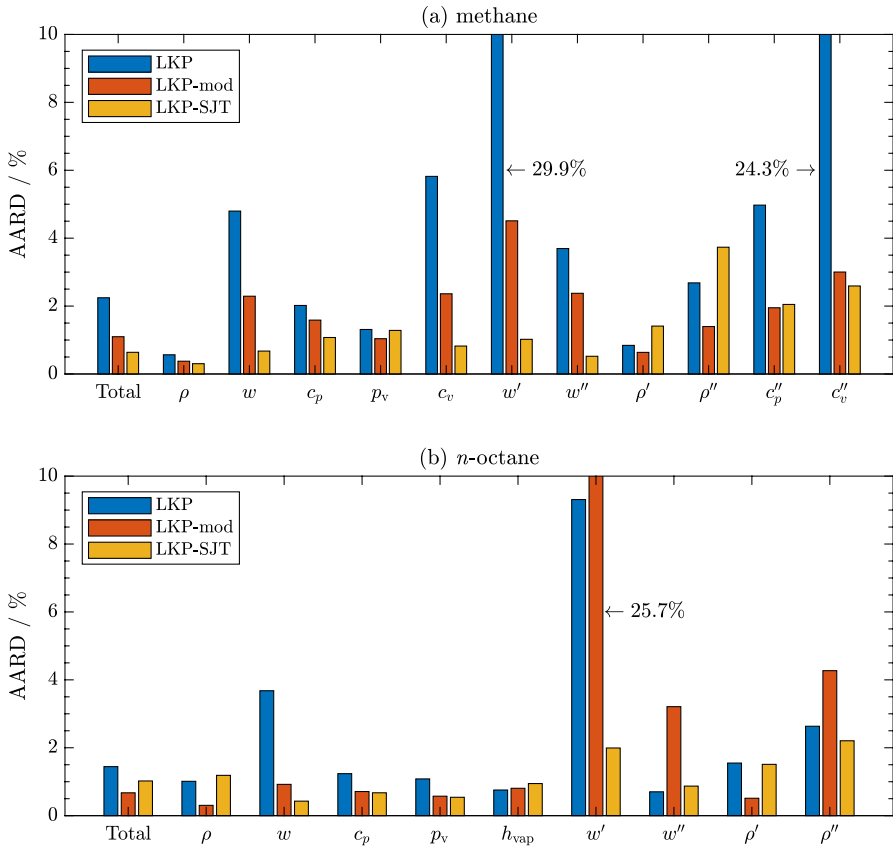


Fig. 1 AARD of methane (a) and *n*-octane (b) calculated with the LKP, LKP-mod, and LKP-SJT to selected experimental data from the literature [28–429]. The AARDs are displayed for each property and as an overall value

with the old parameter set. A better fit of these data worsens the representation of the properties for methane, argon, and krypton.

In Fig. 3, the AARDs of the LKP and LKP-mod to the datasets of the alkanes from methane to *n*-octane are illustrated. Although the representation of the base fluids methane and *n*-octane was significantly improved, the AARD has increased for the majority of the other alkanes. For propane, *n*-butane, and *n*-pentane, the total AARD increases by more than 1 percentage point. A smaller increase can be seen for ethane and *n*-hexane. The performance of *n*-heptane has improved slightly. In general, the densities have benefited from the change in the constants, but the speed of sound and isobaric heat capacities are less well reproduced, especially in the sub-critical temperature range.

Finally, the behavior of the isotherms for various long-chain hydrocarbons is examined. Figure 4 shows the numerical evaluations of the pressure for different long-chain hydrocarbons for the LKP, as similarly illustrated by Jäger et al. [3], and

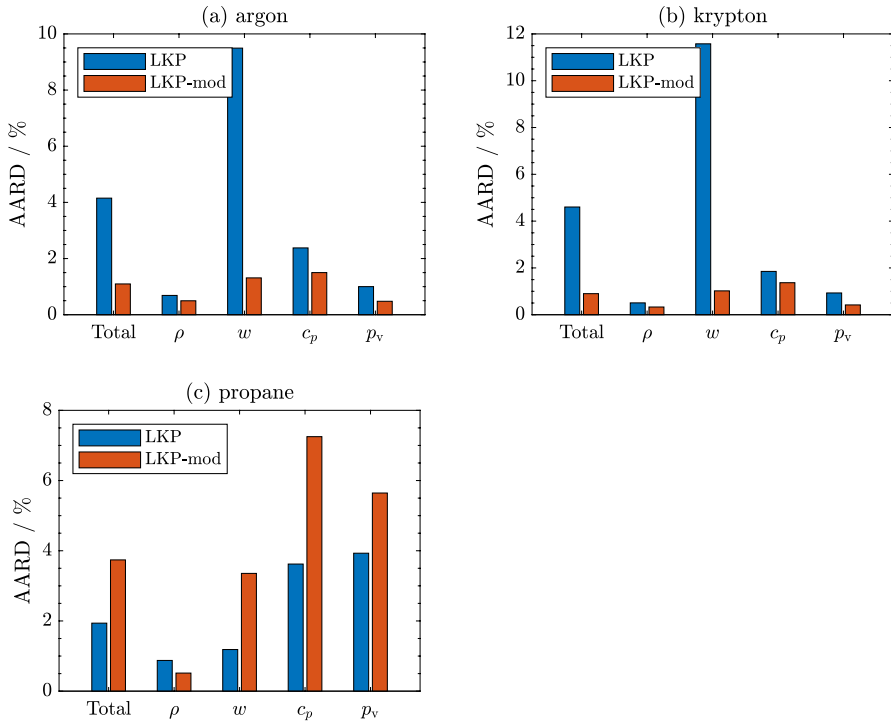


Fig. 2 AARD of argon (a), krypton (b), and propane (c) calculated with the LKP and LKP-mod to their respective reference equation of state. The AARDs are displayed for each property and as an overall value

the LKP-mod. The isotherms of *n*-hexadecane, *n*-docosane, and squalane calculated with the LKP exhibit negative values for the pressure p , as well as for the slopes $\left(\frac{\partial p}{\partial \rho}\right)_T$ and curvatures $\left(\frac{\partial^2 p}{\partial \rho^2}\right)_T$ in the homogeneous liquid state, see Fig. 4(a). By refitting the parameters of the LKP, the unphysical behavior was corrected. The new course of the isotherms in Fig. 4(b) is qualitatively correct, making them now suitable for flash calculations of long-chain hydrocarbons. This is a great advantage over the original LKP although the accuracy of calculated caloric properties of smaller hydrocarbons is worse. Since there are no Helmholtz energy EOS for many long-chain hydrocarbons, it is particularly important to have alternative EOS available.

4.3 Comparison with Respect to the LKP-SJT

In this section, the performance of the LKP-SJT is examined. First, the detailed AARDs of the two fluids are analyzed, which act as base points of the equation. Again, a comparison is made with the LKP. Figure 1(a) shows that the LKP-SJT agrees well with the dataset of methane, with a reduction in the total AARD from 2.2% to 0.6%. The vapor pressure data are reproduced with a comparable quality to the basic form of the LKP, while a clear deterioration can be seen in the saturated

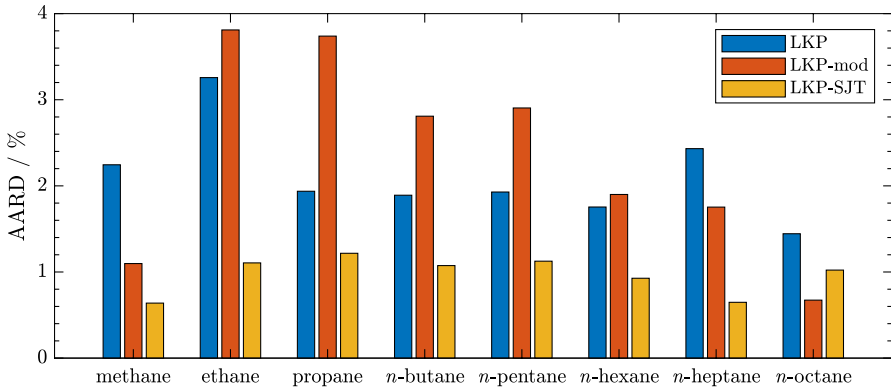


Fig. 3 AARD to the datasets of the alkanes between methane and *n*-octane calculated for the LKP, LKP-mod, and LKP-SJT. Experimental data are used for methane [28–136] and *n*-octane [136–429], while the datasets for the remaining fluids are generated from their respective reference equation of state

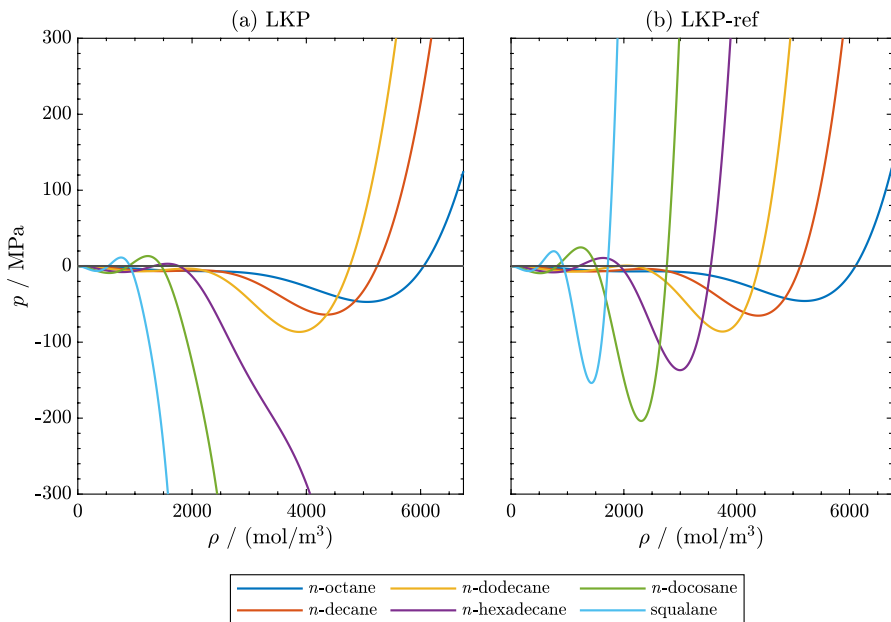


Fig. 4 Numerical evaluation of the pressure at $T = 298.15$ K for chosen long-chain hydrocarbons between *n*-octane and squalane using the LKP (a) and the LKP-mod (b)

densities. The AARDs of ρ' and ρ'' calculated with the LKP-SJT are 0.6 and 1.1 percentage points higher, respectively, than calculated with the LKP EOS. On the opposite, the remaining properties are reproduced much better. As an example, the AARD of w' is 1% (LKP-SJT) compared to 29.9% (LKP EOS). Similarly good results are illustrated in Fig. 1(b) for *n*-octane, where the total AARD is reduced from 1.4% to 1%. For ρ , w'' , and h_{vap} , the calculations are slightly inferior to the

calculations from the LKP EOS, but the LKP-SJT is more accurate with respect to the remaining properties, in some cases with considerable differences in the AARDs (see w and w').

With the results shown in Fig. 3, a comparison is made between the LKP and LKP-SJT for alkanes up to n -octane. The LKP-SJT shows a maximum AARD of 1.2% for propane, while the AARDs of the LKP are worse for all examined fluids. Thus, the equation significantly outperforms the basic form of the LKP for all alkanes over a wide range of acentric factors. In contrast to the LKP-mod approach, a reduction of the deviations from the respective datasets can be recognized throughout.

4.4 Comparison of the Approaches for Long Hydrocarbons

In this section, both optimization concepts discussed in the previous sections are compared in terms of their suitability for correctly calculating state points of long-chain hydrocarbons. Figure 5 shows the AARDs of n -nonane, n -decane, and n -dodecane. The LKP was also taken into account, as it still provides the results of the same order of magnitude as the LKP-mod for the fluids under consideration. For all three fluids, the LKP-SJT performs by far better. The differences are most noticeable for n -nonane and n -dodecane. Especially vapor pressures are predicted much more accurately. Overall, the LKP-mod achieves better results compared to the LKP EOS. The density reproduction is particularly good and even slightly better than the densities calculated with the LKP-SJT.

However, the most important advantage of the approaches becomes evident from Fig. 6, which shows the AARDs of both approaches to the reference equations of state of n -hexadecane and n -docosane. The LKP was not included in these bar charts, because an evaluation using the unmodified LKP is not possible for these fluids, as the flash calculations fail at lower temperatures due to the unphysical course of isotherms in the homogeneous liquid region. The LKP-mod, on the other hand, yields qualitatively correct results, but the deviations from the reference equations of state for w and p_v are fairly high. ρ and c_p are reproduced well for both fluids, including a lower AARD for ρ than the LKP-SJT. However, by comparison to the LKP-mod, the LKP-SJT provides consistently good results for both p_v and w . The overall AARDs for n -hexadecane and n -docosane are approximately 5% and 12.8% calculated with the LKP-SJT and 12.5% and 26% calculated with the LKP-mod, respectively.

Finally, the deviations of LKP-mod and LKP-SJT from the experimental data of squalane are presented. In Fig. 7, the deviations from the density data are illustrated. Both equations of state achieve higher accuracies for the density data of squalane than for n -docosane with AARDs of 9.2% for the LKP-mod and 1.6% for the LKP-SJT. In the range below 350 K, the LKP-SJT reproduces the data points with a maximum deviation of 2.7%. With higher temperature, the deviation increases with a maximum of 7%. The LKP-mod performs worse than the LKP-SJT, with deviations of 5 to 12%.

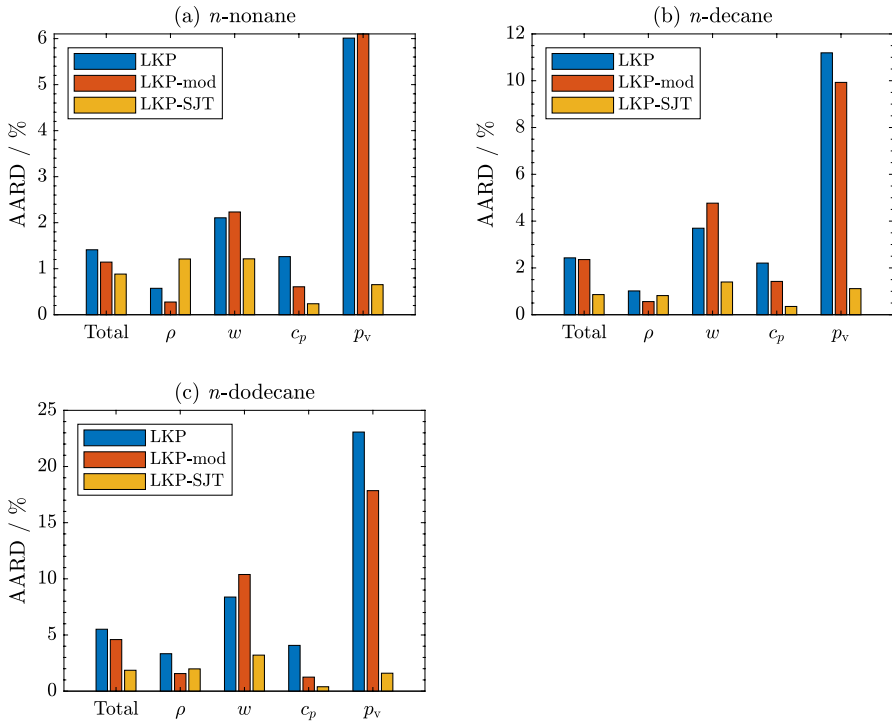


Fig. 5 AARD of *n*-nonane (a), *n*-decane (b) and *n*-dodecane (c) calculated by LKP, LKP-mod, and LKP-SJT to the datasets generated from the respective reference equation of state. The AARDs are displayed for each property and as an overall value

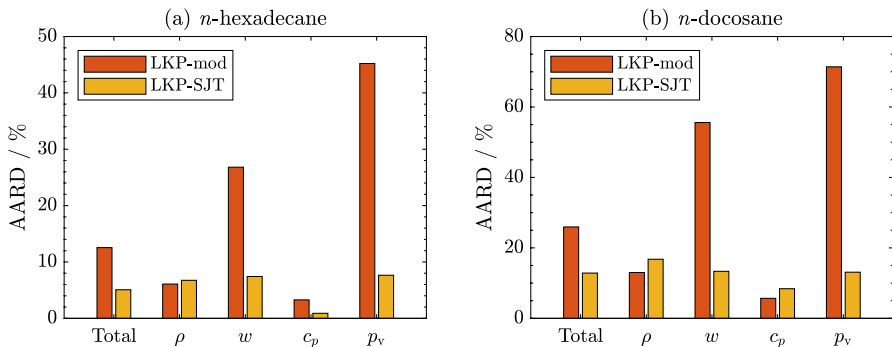


Fig. 6 AARDs of *n*-hexadecane (a) and *n*-docosane (b) calculated by LKP-mod and LKP-SJT to the datasets generated from the respective reference equation of state. The AARDs are displayed for each property and as an overall value

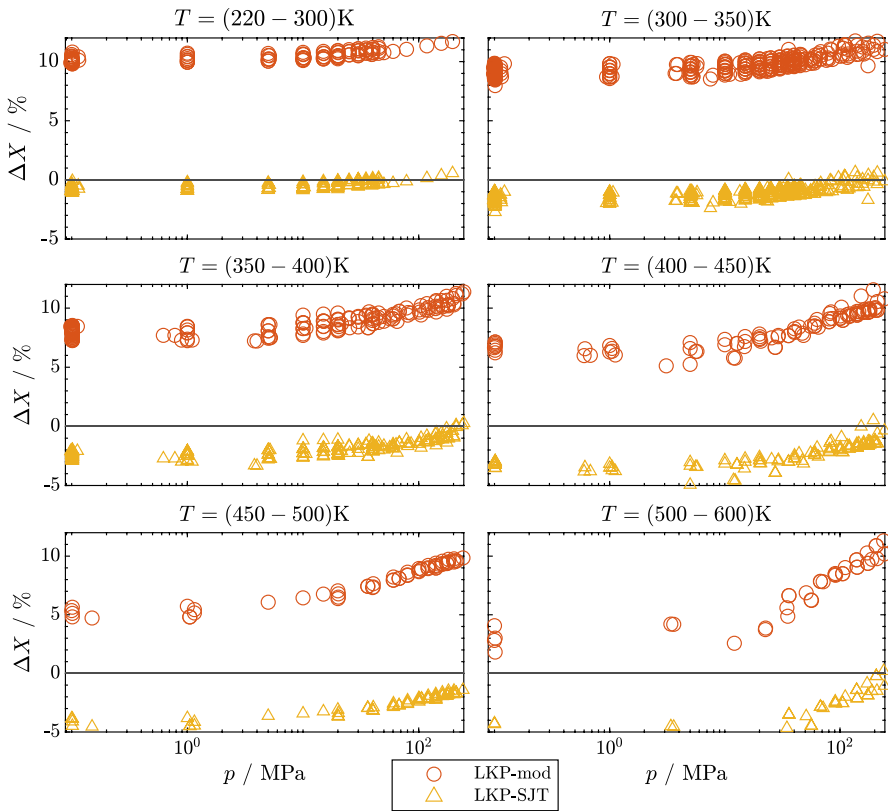


Fig. 7 Percentage deviation of experimental homogeneous density data ρ for squalane [425–474] from values calculated with the LKP-mod and LKP-SJT

Figure 8 shows the deviations from the remaining data as a function of temperature. In general, the LKP-SJT achieves better results compared to the LKP-mod. For w in Fig. 8(a), only data at ambient pressures are available. The deviations of speed of sound increase with rising temperature for both approaches. The LKP-SJT reproduces the data with deviations between 8% and 11%, while the deviations with the LKP-mod are between 26% and 37%. The deviations of the isobaric heat capacities calculated with the LKP-mod are between -18% and -10% , while the LKP-SJT reproduces the data with deviation between -14% and 5% , see Fig. 8(b). The deviations from the vapor pressure in Fig. 8(c) can be divided into two temperature ranges. For temperatures below 500 K, the average deviation for the LKP-SJT is about 30%, while the LKP-mod shows deviations of almost 100% when describing p_v . For higher temperatures, these mean deviations are reduced to 15% (LKP-SJT) and 55% (LKP-mod).

Based on the promising results, further investigations should be carried out in future, including the following aspects:

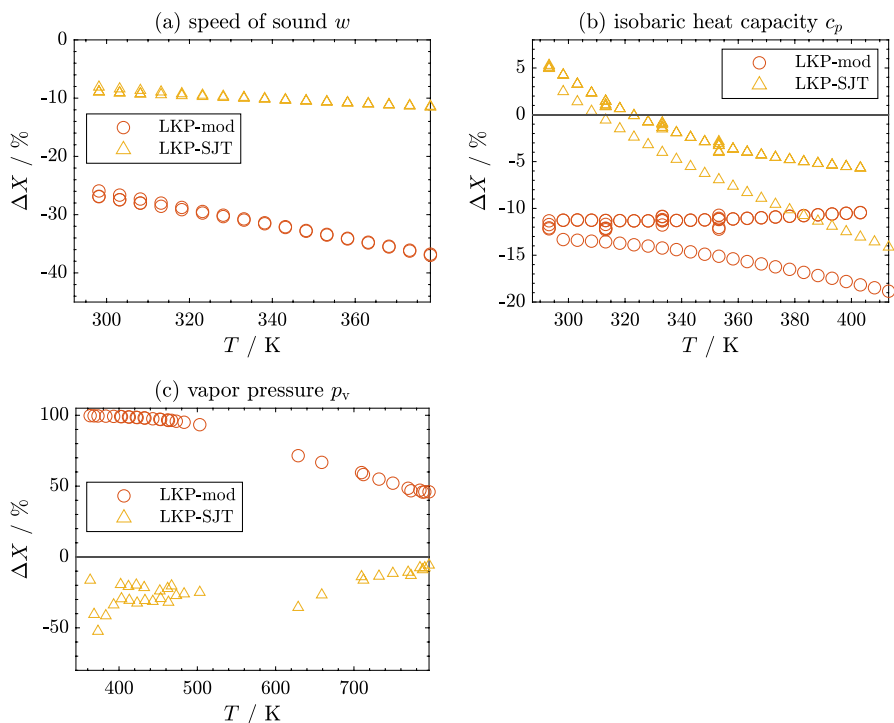


Fig. 8 Percentage deviation of experimental data [425–474] of speed of sound w (a), isobaric heat capacity c_p (b), and vapor pressure p_v (c) for squalane from values calculated with the LKP-mod and LKP-SJT

- Application to other fluid groups
- Application of different base functions other than methane and n -octane
- Introduction of a third base point (which would lead to a non-linear dependence on the acentric factor)
- Representation of mixture properties with the LKP-SJT EOS

5 Conclusions

In this paper, two different approaches were presented to optimize the LKP equation for the prediction of thermodynamic properties for long-chain hydrocarbons. Attention was also paid to the performance with respect to shorter hydrocarbons in order to make the equation applicable to a wide range of fluids.

The first approach is a refit of the original LKP parameters, called LKP-mod. Constraints were included to guarantee qualitatively correct behavior of the equation in the homogeneous liquid state. Thermodynamic properties of alkanes up to n -decane were reproduced with approximately the same accuracy on average. Unlike the LKP, calculations for hydrocarbons up to at least squalane are now feasible using

the LKP-mod. The densities of the long-chain alkanes in particular are described with good accuracy, while w and p_v only provide qualitatively correct results. The second approach is the LKP-SJT, which uses the existing reference state equations for methane [15] and n -octane [17] when calculating the two interpolation points (0) and (ref), while the linear interpolation via ω is preserved. This results in consistent improvements compared to the LKP. The equation also provides good results for the calculation of long-chain hydrocarbons. Based on these results, both approaches can be used to describe long-chain alkanes, for some of which no highly accurate fundamental equations of state are yet available. In general, the LKP-SJT yields much more accurate results, and therefore, when it comes to the requirement of accuracy, we recommend the use of this approach rather than LKP-mod or the original LKP.

The behavior of the equations for mixtures and fluid groups other than alkanes still needs to be investigated. It must be analyzed whether the binary parameters k_{ij} determined by Plöcker et al. [2] continue to yield satisfactory outcomes. In addition to the procedures presented, other approaches to optimize the LKP for long-chain hydrocarbons are also possible. For example, the base points of the equations could be changed to represent other fluids than methane or n -octane, or the equation could be extended by a third base point.

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Author Contributions FS: Conceptualization and methodology(supporting), investigation, software, visualization, and writing/original draft; AJ: Conceptualization and methodology, supervision, writing/review, and editing; MT: Conceptualization and methodology, supervision, writing/review, and editing

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Data Availability No datasets were generated or analyzed during the current study.

Declarations

Conflict of interest The authors declare no competing interests.

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