



Group Contribution Method for the Residual Entropy Scaling Model for Viscosities of Branched Alkanes

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Abstract

In this work it is shown how the entropy scaling paradigm introduced by Rosenfeld (Phys Rev A 15:2545–2549, 1977, <https://doi.org/10.1103/PhysRevA.15.2545>) can be extended to calculate the viscosities of branched alkanes by group contribution methods (GCM), making the technique more predictive. Two equations of state (EoS) requiring only a few adjustable parameters (Lee–Kesler–Plöcker and PC-SAFT) were used to calculate the thermodynamic properties of linear and branched alkanes. These EOS models were combined with first-order and second-order group contribution methods to obtain the fluid-specific scaling factor allowing the scaled viscosity values to be mapped onto the generalized correlation developed by Yang *et al.* (J Chem Eng Data 66:1385–1398, 2021, <https://doi.org/10.1021/acs.jced.0c01009>) The second-order scheme offers a more accurate estimation of the fluid-specific scaling factor, and overall the method yields an AARD of 10% versus 8.8% when the fluid-specific scaling factor is fit directly to the experimental data. More accurate results are obtained when using the PC-SAFT EoS, and the GCM generally outperforms other estimation schemes proposed in the literature for the fluid-specific scaling factor.

Keywords Group contribution method · Lee–Kesler–Plöcker equation of state · Machine learning · PC-SAFT equation of state · Residual entropy scaling · Viscosity

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1 Introduction

Rosenfeld [1] suggested a link between the residual entropy and transport properties of dense fluids. Since its development, the model was applied, modified, and improved by several authors, see, *e.g.*, [2–6]. Yang *et al.* [7] proposed a predictive entropy scaling model for mixtures focusing on refrigerants. Basically, only one parameter of this model, *i.e.*, the fluid-specific scaling factor ξ , needs to be fitted to experimental viscosity data for each fluid of interest. In order to make the model entirely predictive, Yang *et al.* [8] suggested to estimate the fluid-specific scaling factor based on the residual entropy of the fluid at the critical point according to $\xi = 0.7 \cdot s_{\text{crit}}^+$ with $s^+ = -s_{\text{res}}/R$ with s_{res} being the residual entropy and R the universal gas constant. In order to evaluate the predictive method suggested by Yang *et al.* [8], Jäger *et al.* [9] studied linear and branched alkanes, for which multiparameter equations of state (EoS) are available, many of which have been established by the group of Prof. Roland Span, and developed an improved estimation scheme for the fluid-specific scaling factor depending on the longest carbon chain in the molecule. It has been demonstrated that their proposed estimation method yields better results than the method originally proposed by Yang *et al.* [8]. The linear relationship between the fluid-specific scaling factor and the investigated linear and branched alkanes also holds when equations of state other than multiparameter equations of state are used to calculate the required properties (*i.e.*, the p - T - ρ relationship as well as the residual entropy s_{res}).

In this work, the method proposed by Jäger *et al.* [9] is extended to branched alkanes for which no multiparameter equations of state are available. Overall, 60 linear and branched alkanes have been investigated. In order to make the method fully predictive, the Lee–Kesler–Plöcker [10, 11] (LKP) equation of state (EoS) and the perturbed chain statistical associating fluid theory EoS of Gross and Sadowski [12] (PC-SAFT) were used and all required model parameters were estimated. For applying the LKP EoS [10, 11], critical temperatures, critical pressures, and acentric factors for the alkanes are required, which have been estimated by the group contribution method (GCM) of Constantinou and Gani [13]. The required parameters m , σ , and ϵ for the PC-SAFT [12] EoS have been estimated using the second-order GCM of Tihic *et al.* [14]. Besides the linear relationship between the longest carbon chain and the fluid-specific scaling factor, group contribution methods have been tested in order to predict the fluid-specific scaling factor for the investigated hydrocarbons.

All of the developed models have been implemented in the property software TREND [15], which is developed under the lead of Prof. Roland Span.

2 Residual Entropy Scaling for Viscosities Theory

Residual entropy scaling (RES) is a semi-empirical “universal” model for fluids that relates transport properties to thermodynamic properties. The viscosity can be formulated as the sum of the dilute-gas viscosity $\eta_{\rho \rightarrow 0}(T)$ and the residual part of the viscosity $\eta_{\text{res}}(s_{\text{res}})$:

$$\eta = \eta_{\rho \rightarrow 0}(T) + \eta_{\text{res}}(s_{\text{res}}) \quad (1)$$

The dilute-gas viscosity is a function of the temperature T and was formulated according to the Chapman–Enskog theory [16]

$$\eta_{\rho \rightarrow 0}(T) = \frac{5}{16} \sqrt{\frac{mk_{\text{B}}T}{\pi}} \frac{1}{\sigma^2 \Omega^{(2,2)*}}. \quad (2)$$

In this equation, m is the mass of one molecule in kg, $k_{\text{B}} = 1.380649 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$, σ is the collision diameter of a 6–12 Lennard–Jones particle in m, and $\Omega^{(2,2)*}$ is the reduced collision integral. A simplified correlation for the collision integral of Neufeld *et al.* [17] has been used in the residual entropy scaling model by Yang *et al.* [7] in the following form:

$$\Omega^{(2,2)*} = 1.16145 \cdot (T^*)^{-0.14874} + 0.52487 \cdot \exp(-0.77320 \cdot T^*) + 2.16178 \cdot \exp(-2.43787 \cdot T^*) \quad (3)$$

with $T^* = k_{\text{B}}T/\varepsilon$ being the dimensionless temperature and ε the Lennard–Jones pair potential energy. As in our previous work [9], the Lennard–Jones parameters, σ and ε , have been predicted using the method of Chung *et al.* [18] according to

$$\frac{\varepsilon}{k_{\text{B}}} = T_{\text{c}}/1.2593 \quad (4)$$

and

$$\sigma = 0.809 \cdot \rho_{\text{c}}^{-1/3}. \quad (5)$$

T_{c} is the critical temperature in K and ρ_{c} the critical density in $\text{mol}\cdot\text{cm}^{-3}$. The unit of σ in Eq. 5 is in Å and needs to be converted to m when used in Eq. 2.

The residual part of the viscosity has been introduced by Bell [6] and reads:

$$\eta_{\text{res}}(s_{\text{res}}) = \frac{\eta_{\text{res}}^+ \rho_{\text{N}}^{2/3} \sqrt{mk_{\text{B}}T}}{(s^+)^{2/3}} \quad (6)$$

η_{res}^+ denotes the dimensionless plus-scaled residual viscosity; ρ_{N} is the number density in m^{-3} ; the dimensionless quantity s^+ is defined according to

$$s^+ = -s_{\text{res}}/R \quad (7)$$

with the universal gas constant $R = 8.31446261815324 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ [19]; s_{res} is the residual molar entropy as the difference of the entropy s and the entropy of the ideal gas s^0 at the same temperature and density

$$s_{\text{res}} = s(T, \rho) - s^0(T, \rho) \quad (8)$$

The empirical formulation of Yang *et al.* [7] was used to calculate the plus-scaled dimensionless residual viscosity η_{res}^+ according to

$$\ln(\eta_{\text{res}}^+ + 1) = n_{g1} \cdot (s^+/\xi) + n_{g2} \cdot (s^+/\xi)^{1.5} + n_{g3} \cdot (s^+/\xi)^2 + n_{g4} \cdot (s^+/\xi)^{2.5}. \quad (9)$$

In this equation, the global parameters n_{gk} as proposed by Yang *et al.* [7] were used, *cf.* Table 1. ξ is the fluid-specific scaling parameter which has been adjusted to experimental viscosity data for 39 refrigerants by Yang *et al.* [7] and later has been extended to 124 fluids by Yang *et al.* [20].

3 Estimated Parameters for LKP EoS and PC-SAFT EoS

When it comes to process modeling and screening of new working fluids for different applications, it is favorable to utilize the best model available, *i.e.*, for pure fluids reference equations of state formulated in the dimensionless Helmholtz energy α [21] and preferably for mixtures the multi-fluid mixture model [22]. However, if no adjusted mixture models and/or multiparameter equations of state for pure components are available, simpler equations of state need to be used, such as cubic equations of state, *e.g.*, [23, 24], the Lee–Kesler–Plöcker equation of state (LKP) [10, 11], or the PCP-SAFT equation of state [12, 25, 26]. In our previous works, we found that especially the LKP [10, 11] and PCP-SAFT [12, 25, 26] are promising substitutes if there is no multiparameter EoS for a specific substance available [27, 28]. Jäger *et al.* [9] developed a predictive scheme for estimating the fluid-specific scaling parameter ξ . In [9], the estimation method was restricted to all linear and branched alkanes for which multiparameter equations of state exist, *i.e.*, methane [29], ethane [30], propane [31], *n*-butane [32], *n*-pentane [33, 34], *n*-hexane [34, 35], *n*-heptane [36], *n*-octane [37], *n*-nonane [38], *n*-decane [38], *n*-undecane [39], *n*-dodecane [40], *n*-hexadecane [41], *n*-docosane [41], isobutane [32], isopentane [38], isohexane [38], and isooctane [34, 42]. Additionally, results have been compared when using the LKP [10, 11] and Peng–Robinson equation of state [23] for calculating the required thermodynamic properties for applying entropy scaling. It was found that the LKP [10, 11] should rather be used than the Peng–Robinson [23] for entropy scaling as generally better results for the studied hydrocarbons are obtained with the LKP [10, 11] (note that there are some restrictions of the LKP [10, 11] in its present form for hydrocarbons of large chain-lengths, see Jäger *et al.* [9]).

In this work, the predictive scheme is extended to branched alkanes up to decane for which experimental viscosity data exist. The focus is set on good predictive capabilities of the model; therefore, the LKP [10, 11] and the PC-SAFT [12] equations of state are used with appropriate estimation schemes available in the literature in order to estimate the required model parameters.

Table 1 Global parameters n_{gk} according to Yang *et al.* [7]

k	n_{gk}
1	−0.448 046
2	1.012 681
3	−0.381 869
4	0.054 674

3.1 Estimation of LKP Parameters

For the estimation of the critical temperature, critical pressure, and normal-boiling-point temperature, the second-order group contribution method of Constantinou and Gani [13] was used (Table 2). The model can be formulated with the following equation:

$$f(X) = \sum_i N_i C_i + \sum_j M_j D_j, \quad (10)$$

where C_i is the first-order contribution of group type i for the specific property occurring N_i times and D_j is the contribution of the second-order groups occurring M_j times in the molecule. $f(X)$ is a function of the property X as defined in Table 3.

For linear and branched alkanes, the first-order groups CH_3- , $-\text{CH}_2-$, $-\text{CH}<$ and $>\text{C}<$ are needed and the second-order groups $(\text{CH}_3)_2-\text{CH}-$, $(\text{CH}_3)_3-\text{C}-$, $-\text{CH}(\text{CH}_3)-\text{CH}(\text{CH}_3)-$, and $-\text{CH}(\text{CH}_3)-\text{C}(\text{CH}_3)_2-$ were selected. An additional second-order group for ethane (CH_3-CH_3) was used according to Constantinou and Gani [13]. The first- and second-order group parameters of the GCM of Constantinou and Gani [13] for the selected functional groups are listed in Tables 4 and 5. The resulting normal-boiling-point temperatures, critical temperatures, and critical pressures for all investigated fluids are summarized in Table 2.

Another parameter needed for the description of the LKP EoS [10, 11] is the acentric factor ω introduced by Pitzer [43] and can be calculated by the following equation:

$$\omega = -\log\left(\frac{p_s}{p_c}\right)_T - 1 \quad (11)$$

with p_c being the critical pressure and p_s the saturation pressure at the temperature $T = 0.7 \cdot T_c$ with T_c being the critical temperature. The Antoine equation (Eq. 12) was used to calculate the pressure p_s by adjusting the parameters A and B to the critical temperature, critical pressure, and normal-boiling-point temperature estimated by the second-order GCM method of Constantinou and Gani [13].

$$p_s = 10^{A-B/T} \quad (12)$$

The resulting acentric factors ω are listed in Table 2.

3.2 Estimation of PC-SAFT Parameters Using a Second-Order Group Contribution Method

There are several publications on estimation schemes for PC-SAFT [12] parameters. Among others, there are first and second-order group contribution methods, where the latter is used for a better distinction of structural isomers. Vijande *et al.* [44] incorporated proximity effects in the GCM for linear alkanes, alkanes with one branch, linear mono-ethers, and esters. No multiple branches and mixed tertiary

Table 2 Names, formula, CAS number, molar weight and critical temperature T_c , critical pressure p_c , normal-boiling-point temperature T_b and acentric factor ω estimated by Constantinou and Gani [13] and the Antoine equation (Eq. 12) as well as PC-SAFT [12] parameters estimated by Tihic *et al.* [14] of all investigated alkanes sorted by the number of carbon atoms N_C and number of branches N_B

N_C	N_B	Name	Formula	CAS number	Molar weight (g·mol ⁻¹)	Critical temperature T_c (K)	Critical pressure p_c (MPa)	Normal boiling point T_b (K)	Acentric factor ω (-)	m (-)	σ (Å)	ϵ/k_B (K)
2	0	Ethane	C ₂ H ₆	74-84-0	30.07	305.42	4.880	184.55	0.101	1.2887	3.7570	200.80
3	0	Propane	C ₃ H ₈	74-98-6	44.10	348.49	4.547	203.08	-0.011	1.6731	3.8120	215.83
4	0	<i>n</i> -Butane	C ₄ H ₁₀	106-97-8	58.12	423.12	3.988	263.12	0.124	2.0574	3.8457	225.25
5	0	<i>n</i> -Pentane	C ₅ H ₁₂	109-66-0	72.15	475.82	3.529	309.46	0.229	2.4417	3.8685	231.70
6	0	<i>n</i> -Hexane	C ₆ H ₁₄	110-54-3	86.18	516.60	3.147	347.22	0.311	2.8260	3.8849	236.40
7	0	<i>n</i> -Heptane	C ₇ H ₁₆	142-82-5	100.20	549.86	2.827	379.07	0.375	3.2104	3.8973	239.97
8	0	<i>n</i> -Octane	C ₈ H ₁₈	111-65-9	114.23	577.95	2.555	406.63	0.426	3.5947	3.9070	242.78
9	0	<i>n</i> -Nonane	C ₉ H ₂₀	111-84-2	128.25	602.26	2.322	430.90	0.466	3.9790	3.9147	245.04
10	0	<i>n</i> -Decane	C ₁₀ H ₂₂	124-18-5	142.285	623.69	2.121	452.60	0.498	4.3634	3.9211	246.91
11	0	<i>n</i> -Undecane	C ₁₁ H ₂₄	1120-21-4	156.312	642.85	1.947	472.21	0.522	4.7477	3.9265	248.48
12	0	<i>n</i> -Dodecane	C ₁₂ H ₂₆	112-40-3	170.338	660.18	1.795	490.10	0.542	5.1320	3.9310	249.81
16	0	<i>n</i> -Hexadecane	C ₁₆ H ₃₄	544-76-3	226.446	716.53	1.344	549.20	0.579	6.6693	3.9438	253.59
22	0	<i>n</i> -Docosane	C ₂₂ H ₄₆	629-97-0	310.6	777.61	0.948	614.53	0.568	8.9753	3.9547	256.84
4	1	2-Methylpropane	C ₄ H ₁₀	75-28-5	58.122	399.33	3.983	242.22	0.054	1.9769	3.8910	230.85
5	1	2-Methylbutane	C ₅ H ₁₂	78-78-4	72.149	450.48	3.506	287.26	0.161	2.3775	3.9005	230.85
6	2	2,2-Dimethylpropane	C ₅ H ₁₂	463-82-1	72.149	435.65	3.563	272.63	0.108	2.1268	4.0423	234.94
6	1	2-Methylpentane	C ₆ H ₁₄	107-83-5	86.177	496.65	3.128	328.94	0.252	2.7618	3.9126	235.78
1	3	Methylpentane	C ₆ H ₁₄	96-14-0	86.177	502.77	3.144	333.61	0.261	2.7456	3.9181	240.76
2	2	2,2-Dimethylbutane	C ₆ H ₁₄	75-83-2	86.177	485.27	3.176	317.08	0.209	2.5111	4.0338	239.73
2	2	2,3-Dimethylbutane	C ₆ H ₁₄	79-29-8	86.177	500.47	3.202	326.60	0.207	2.6188	3.9559	247.12
7	1	2-Methylhexane	C ₇ H ₁₆	591-76-4	100.204	533.41	2.810	363.53	0.323	3.1462	3.9217	239.50

Table 2 (continued)

N_C	N_B	Name	Formula	CAS number	Molar weight (g·mol ⁻¹)	Critical temperature T_c (K)	Critical pressure p_c (MPa)	Normal boiling point T_b (K)	Acentric factor ω (-)	m (-)	σ (Å)	ϵ/k_B (K)
1		3-Methylhexane	C ₇ H ₁₆	589-34-4	100.204	538.43	2.824	367.49	0.331	3.1299	3.9266	243.89
1		3-Ethylpentane	C ₇ H ₁₆	617-78-7	100.204	538.43	2.824	367.49	0.331	3.1299	3.9266	243.89
2		2,2-Dimethylpentane	C ₇ H ₁₆	590-35-2	100.204	524.17	2.851	353.57	0.287	2.8955	4.0275	243.25
2		2,3-Dimethylpentane	C ₇ H ₁₆	565-59-3	100.204	536.54	2.873	361.56	0.286	3.0031	3.9598	249.57
2		2,4-Dimethylpentane	C ₇ H ₁₆	562-49-2	100.204	515.33	2.794	346.71	0.269	3.0820	3.9469	239.01
2		3,3-Dimethylpentane	C ₇ H ₁₆	108-08-7	100.204	529.26	2.891	355.34	0.274	2.8540	4.0364	249.20
3		2,2,3-Trimethylbutane	C ₇ H ₁₆	464-06-2	100.204	536.11	3.045	354.13	0.233	2.6721	4.1078	261.77
8	1	2-Methylheptane	C ₈ H ₁₈	592-27-8	114.231	563.96	2.541	393.11	0.380	3.5305	3.9288	242.41
1		3-Methylheptane	C ₈ H ₁₈	589-81-1	114.231	568.20	2.552	396.54	0.387	3.5142	3.9331	246.33
1		4-Methylheptane	C ₈ H ₁₈	589-53-7	114.231	568.20	2.552	396.54	0.387	3.5142	3.9331	246.33
1		3-Ethylhexane	C ₈ H ₁₈	619-99-8	114.231	568.20	2.552	396.54	0.387	3.5142	3.9331	246.33
2		2,2-Dimethylhexane	C ₈ H ₁₈	590-73-8	114.231	556.18	2.575	384.52	0.349	3.2798	4.0227	245.94
2		2,3-Dimethylhexane	C ₈ H ₁₈	584-94-1	114.231	566.60	2.594	391.41	0.348	3.3874	3.9628	251.46
2		2,4-Dimethylhexane	C ₈ H ₁₈	589-43-5	114.231	553.41	2.538	382.32	0.340	3.4500	3.9557	246.02
2		2,5-Dimethylhexane	C ₈ H ₁₈	592-13-2	114.231	548.80	2.527	378.64	0.332	3.4663	3.9512	242.03
2		3,3-Dimethylhexane	C ₈ H ₁₈	563-16-6	114.231	560.46	2.610	386.04	0.338	3.2384	4.0304	251.22
2		3,4-Dimethylhexane	C ₈ H ₁₈	583-48-2	114.231	566.60	2.594	391.41	0.348	3.3874	3.9628	251.46
2		2-Methyl-3-ethylpentane	C ₈ H ₁₈	609-26-7	114.231	553.41	2.538	382.32	0.340	3.4500	3.9557	246.02
2		3-Methyl-3-ethylpentane	C ₈ H ₁₈	1067-08-9	114.231	560.46	2.610	386.04	0.338	3.2384	4.0304	251.22
3		2,2,3-Trimethylpentane	C ₈ H ₁₈	564-02-3	114.231	566.24	2.740	385.00	0.304	3.0564	4.0929	262.33
3		2,2,4-Trimethylpentane	C ₈ H ₁₈	540-84-1	114.231	540.33	2.561	369.41	0.299	3.2156	4.0475	245.60
3		2,3,3-Trimethylpentane	C ₈ H ₁₈	560-21-4	114.231	566.24	2.740	385.00	0.304	3.0564	4.0929	262.33
3		2,3,4-Trimethylpentane	C ₈ H ₁₈	565-75-3	114.231	560.66	2.625	382.54	0.301	3.2769	3.9894	252.71

Table 2 (continued)

N_C	N_B	Name	Formula	CAS number	Molar weight (g·mol ⁻¹)	Critical temperature T_c (K)	Critical pressure P_c (MPa)	Normal boiling point T_b (K)	Acentric factor ω (-)	m (-)	σ (Å)	ϵ/k_B (K)
9	1	2-Methyloctane	C ₉ H ₂₀	3221-61-2	128.258	590.09	2.310	418.95	0.425	3.9148	3.9345	244.75
	1	4-Methyloctane	C ₉ H ₂₀	2216-34-4	128.258	593.77	2.320	421.97	0.431	3.8986	3.9384	248.29
	2	2,3-Dimethylheptane	C ₉ H ₂₀	3074-71-3	128.258	592.38	2.356	417.45	0.398	3.7718	3.9652	252.96
	2	3,5-Dimethylheptane	C ₉ H ₂₀	926-82-9	128.258	584.86	2.318	412.63	0.396	3.8181	3.9628	251.68
	3	2,2,4-Trimethylhexane	C ₉ H ₂₀	16747-26-5	128.258	573.93	2.338	401.55	0.361	3.5837	4.0455	251.67
	2	3-Methyl-4-ethylhexane	C ₉ H ₂₀	3074-77-9	128.258	593.77	2.320	421.97	0.431	3.8986	3.9384	248.29
	1	3-Ethylheptane	C ₉ H ₂₀	15869-80-4	128.258	584.86	2.318	412.63	0.396	3.8181	3.9628	251.68
10	1	2-Methylnonane	C ₁₀ H ₂₂	871-83-0	142.282	612.92	2.111	441.88	0.460	4.2992	3.9392	246.67
	1	3-Methylnonane	C ₁₀ H ₂₂	5911-04-6	142.282	616.17	2.119	444.58	0.466	4.2829	3.9427	249.90
	1	4-Methylnonane	C ₁₀ H ₂₂	17301-94-9	142.282	616.17	2.119	444.58	0.466	4.2829	3.9427	249.90
	1	5-Methylnonane	C ₁₀ H ₂₂	15869-85-9	142.282	616.17	2.119	444.58	0.466	4.2829	3.9427	249.90
	1	4-Propylheptane	C ₁₀ H ₂₂	3178-29-8	142.282	616.17	2.119	444.58	0.466	4.2829	3.9427	249.90
	2	2,7-Dimethyloctane	C ₁₀ H ₂₂	1072-16-8	142.282	601.47	2.101	430.57	0.422	4.2350	3.9576	246.42
	2	3,6-Dimethyloctane	C ₁₀ H ₂₂	15869-94-0	142.282	608.32	2.118	436.24	0.434	4.2024	3.9649	253.01
	2	2-Methyl-5-ethylheptane	C ₁₀ H ₂₂	13475-78-0	142.282	604.93	2.109	433.42	0.428	4.2187	3.9613	249.70
	2	2,2,4,4-Tetramethylhexane	C ₁₀ H ₂₂	51750-65-3	142.282	592.23	2.178	417.36	0.363	3.6921	4.1286	257.88

Table 3 Function $f(X)$ for the property X and additional parameters according to Constantinou and Gani [13]

Property X	$f(X)$	Additional parameter	Value
Normal boiling point T_b (K)	$\exp(T_b/t_{b0})$	t_{b0}	204.359 K
Critical temperature T_c (K)	$\exp(T_c/t_{c0})$	t_{c0}	181.128 K
Critical pressure p_c (bar)	$(p_c - p_{c1})^{-0.5} - p_{c2}$	p_{c1} p_{c2}	1.3705 bar 0.100 220 bar ^{-0.5}

Table 4 First-order group contributions for the normal-boiling-point temperature T_b , the critical temperature T_c , and the critical pressure p_c of selected groups for linear and branched alkanes according to Constantinou and Gani [13]

First-order groups	$T_{1b,i}$ (K)	$T_{1c,i}$ (K)	$p_{1c,i}$ (K)
-CH ₃	0.8894	1.6781	0.019 904
-CH ₂ -	0.9225	3.492	0.010 558
-CH<	0.6033	4.033	0.001 315
>C<	0.2878	4.8823	-0.010 404

Table 5 Second-order group contributions for the normal-boiling-point temperature T_b , the critical temperature T_c , and the critical pressure p_c of selected groups for linear and branched alkanes according to Constantinou and Gani [13]

Second-order groups	$T_{2b,i}$ (K)	$T_{2c,i}$ (K)	$p_{2c,i}$ (K)
(CH ₃) ₂ -CH-	-0.1157	-0.5334	0.000 488
(CH ₃) ₃ -C-	-0.0489	-0.5143	0.00 141
-CH(CH ₃)-CH(CH ₃)-	0.1798	1.0699	-0.001 849
-CH(CH ₃)-C(CH ₃) ₂ -	0.3189	1.9886	-0.005 198
CH ₃ -CH ₃	0.6884	2.0427	0.005 175

aliphatic carbon groups with quaternary aliphatic carbon groups have been investigated. Habicht *et al.* [45] used machine learning and extended-connectivity fingerprints as input to estimate PC-SAFT [12] parameters. Sauer *et al.* [46] compared homo- and heterosegmented, also known as first- and second-order groups, GCM for estimating PC-SAFT [12] parameters and came to the conclusion that the heterosegmented GC approach agrees significantly better with the experimental data. The second-order contributions are not adjusted individually to experimental data, but binary group connections are calculated using Lorentz–Berthelot combining rules with the appropriate group contributions of that binary group connection. Tihic *et al.* [14] applied the second-order GCM to PC-SAFT [12] parameters of polymers, but also used linear and branched alkanes as experimental reference for the model adjustment. Structural isomers for branched alkanes can be distinguished up to methylhexane. Starting with methylheptane, the second-order GCM cannot distinguish all isomers. Despite this shortcoming, this model has been chosen in this work for the estimation of PC-SAFT [12] parameters as it is applicable to the branched

Table 6 First-order group contributions for m , $m\sigma^3$, and $m\epsilon$ of selected groups for branched alkanes of Tihic *et al.* [14]

First-order groups	m	$m\sigma^3$ (Å)	$m\epsilon/k_B$ (K)
-CH ₃	0.644 362	34.16 955	129.3866
-CH ₂	0.384 329	24.33 981	102.3238
-CH<	0.043 834	13.95 391	68.2084
>C<	-0.49 208	2.325 415	-10.983

Table 7 Second-order group contributions for m , $m\sigma^3$, and $m\epsilon$ of selected groups for branched alkanes of Tihic *et al.* [14]

Second-order groups	m	$m\sigma^3$ (Å)	$m\epsilon/k_B$ (K)
(CH ₃) ₂ -CH-	0.016263	0.280872	-9.83615
(CH ₃) ₃ -C-	0.041437	1.472296	-6.89516
-CH(CH ₃)-CH(CH ₃)-	-0.04634	-2.464521	-6.81456
-CH(CH ₃)-C(CH ₃) ₂ -	-0.10148	-1.913722	-4.68034

alkanes investigated here and it is based on the second-order GCM method by Constantinou and Gani [13] with identical first- and second-order groups. Selected first- and second-order group contributions for groups specific to branched alkanes are listed in Tables 6 and 7. The resulting PC-SAFT [12] parameters for the individual molecules investigated in this work are summarized in Table 2. The number of occurrences of each group for the investigated alkanes is indicated in Table S1 in the Supplementary Information.

4 Adjusting the Fluid-Specific Scaling Factor ξ to Experimental Data

The fluid-specific scaling factors ξ have been adjusted against experimental data. In order to perform this step, the viscosity Eq. 1 has been fitted against experimental dynamic and kinematic viscosity data taken from NIST TDE 103.b [47]. The selected fitting methodology relies on a machine-learning algorithm based on the covariance matrix evolutionary strategy (CMA-ES) as offered in the DEAP computation framework [48, 49]. The algorithm is a modification of the formulation introduced by Grau Turuelo *et al.* [50] with no weight factors, which is based on the method developed by Hansen and Ostermeier [51]. Such machine-learning methods do not need any derivatives, providing stable solutions for non-linear functions, as well as poorly conditioned ones. The same algorithm was already used by Jäger *et al.* [9] in order to fit the fluid-specific scaling factors ξ for the linear and branched alkanes to experimental viscosity data.

The first step of this method is to define the objective function that must be globally minimized. In the present case study, the objective function consists of the sum of the normalized squared residuals (SNR) of the measured and calculated values through the least-squares formulation:

$$\text{SNR} = \sum_{i=0}^n \left(\frac{\eta_{i,\text{calc}} - \eta_{i,\text{exp}}}{\eta_{i,\text{exp}}} \right)^2 \quad (13)$$

Due to the large amount of processed data, a pre-filtering step was applied as suggested by Yang *et al.* [7]. In general, the first filter consists of discarding experimental data lying outside of the temperature/pressure/density range of validity of the employed multiparameter EoS. For this certain instance, the first filter has no effective consequence, as there are no set ranges of validity for the LKP [10, 11] and PC-SAFT [12] EoS. The second filter excludes data points that do not agree with the reported phase. The third filter, following the formulation of Jäger *et al.* [9], discards experimental data points, which deviate by more than 30% to the calculated viscosity when using the following fluid-specific scaling factor ξ as a first estimate:

$$\xi = 0.0571n_{\text{chain}} + 0.8019 \quad (14)$$

where n_{chain} is the number of carbon atoms of the longest carbon chain.

To obtain the residuals and the fitted values of ξ with the suggested genetic evolution method, each iteration consists of the following steps:

- (1) Definition of the number of individuals of the population. The individuals are the number of ξ values that are tested at the same time. During the first iteration, their values are randomly chosen within a predefined selection range. These are taken as the first possible solutions. In this work, a value of 10 individuals is selected.
- (2) The selected values of ξ are then used as an input in an extended (to be released) version of TREND 5.0 for the calculation of the viscosity with the combination of the selected EoS, entering the pressure and temperature of every existing experimental point.
- (3) The output solution of TREND 5.0 is the searched value $\eta_{i,\text{calc}}$, with which the residuals (see Eq. 11) are obtained.
- (4) The residuals are then calculated for each individual and a ranking (the so-called “hall of fame”) of the best individuals is stored.
- (5) Just before the next iteration, the obtained information is stored and used in the covariance matrix, which is reinitialized after a recombination (new average distribution value) and mutation (averaged zero value random vector addition) step.
- (6) New individuals are chosen, following the direction of the best-ranked individuals of the previous step, due to the operations performed in the covariance matrix, and the process starts again, beginning a new iteration.

After a predefined number of iterations, the highest ranked individual is chosen as the solution. The goodness of the solution is checked through the residuals plot. If during the two or three last iterations, the residuals converge to a minimum value, the solution is stored. For this specific problem, 20 iterations are generally sufficient to achieve a converged solution.

Another advantage of the employed algorithm is the definition of constraints to accelerate the convergence. For instance, it is known that ξ cannot be negative. Therefore, a penalty factor, *i.e.*, a high-valued residual, is forced when an individual is negative, forcing the individual to be at the end of the ranking and preventing the algorithm to spend time into searching further negative ξ values. A scheme of the algorithm can be seen in Fig. 1.

In some cases, where the scaling parameter estimated with Eq. 14 significantly deviates from the adjusted value, the fitting process may be repeated with the adjusted fluid-specific scaling factors ξ as starting value. This causes changes in the data selection due to the modification of the third filter. Consequently, the amount of experimental data in the range of the 30 % of the new reference scaling parameter ξ is higher. The final adjusted scaling parameters ξ_{exp} are listed in Table 8.

5 GCM Methods for Predicting the Fluid-Specific Scaling Factor ξ

Different methods for describing the fluid-specific scaling factor ξ have been studied when there are no experimental viscosity data available to adjust that parameter. Yang *et al.* [8] related this parameter to the residual critical entropy with varying results. Jäger *et al.* [9] proposed a linear equation depending on the longest carbon chain for alkanes. This method displayed good results for the investigated linear alkanes, but for branched alkanes this method should be less accurate as it cannot account for the structure of more complicated molecules. In this work, the applicability to predict ξ is extended for branched alkanes utilizing a group contribution method.

Second-order GCMs, such as the method used by Tihic *et al.* [14], expand the first-order groups with second-order groups, allowing the description of some

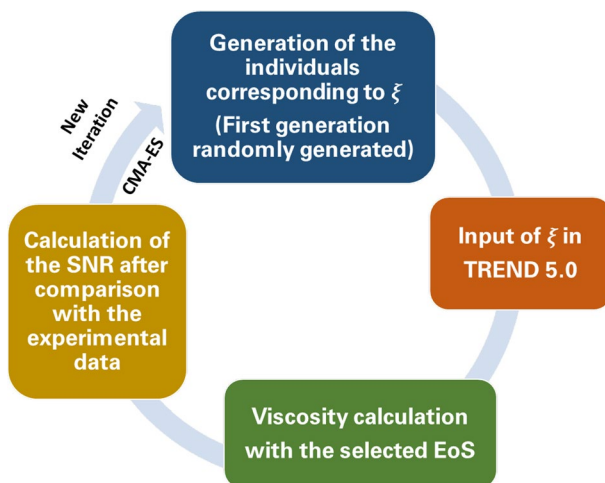


Fig. 1 Scheme of one iteration of the employed machine-learning algorithm in combination with TREND 5.0

Table 8 Fluid-specific scaling factor ξ_{exp} adjusted to experimental data, ξ_{GCM} values using the proposed GCM, and AARD values applying the LKP [10, 11] and PC-SAFT [12] EoS

Name	ξ_{exp}		ξ_{GCM}		AARD _{exp} (%)		AARD _{GCM} (%)	
	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT
Ethane	0.96242	0.77958	0.92289	0.82600	7.43	7.15	8.83	14.94
Propane	0.79391	0.86146	0.98751	0.88219	15.56	5.20	22.97	10.17
<i>n</i> -Butane	0.92805	0.93672	1.05213	0.93838	7.01	5.46	22.05	8.09
<i>n</i> -Pentane	1.04927	1.00205	1.11676	0.99457	8.57	7.09	16.42	11.81
<i>n</i> -Hexane	1.15994	1.06863	1.18138	1.05075	8.82	5.52	11.18	9.10
<i>n</i> -Heptane	1.25225	1.12791	1.24600	1.10694	9.44	5.18	9.55	10.84
<i>n</i> -Octane	1.33675	1.18420	1.31063	1.16313	8.06	5.37	11.87	8.52
<i>n</i> -Nonane	1.39268	1.22610	1.37525	1.21932	5.34	4.51	8.61	5.25
<i>n</i> -Decane	1.45795	1.28456	1.43987	1.27551	7.80	5.72	9.28	6.83
<i>n</i> -Undecane	1.48599	1.33042	1.50449	1.33169	8.90	7.61	9.98	7.60
<i>n</i> -Dodecane	1.61127	1.40341	1.56912	1.38788	23.50	10.32	18.27	8.18
<i>n</i> -Hexadecane	1.71634	1.61117	1.82761	1.61263	42.58	13.20	58.69	10.12
<i>n</i> -Docosane	1.38053	1.92254	2.21534	1.94976	15.05	3.63	93.61	12.01
2-Methylpropane	0.76022	0.89531	0.97858	0.96367	11.24	8.08	51.67	22.63
2-Methylbutane	0.93073	0.97701	1.01781	0.99645	11.75	4.70	23.24	7.80
2,2-Dimethylpropane	0.71874	0.77406	0.90397	0.89481	5.43	9.61	67.51	54.43
2-Methylpentane	1.02972	1.05706	1.08243	1.05264	3.52	2.95	16.06	2.98
3-Methylpentane	1.04774	1.06580	1.10782	1.07605	2.93	2.60	17.72	3.54
2,2-Dimethylbutane	0.89131	0.90675	0.96859	0.95100	2.13	9.93	25.52	15.41
2,3-Dimethylbutane	0.92421	1.00266	1.02810	1.05031	7.12	5.89	31.62	16.01
2-Methylhexane	1.13685	1.12131	1.14706	1.10883	4.66	3.04	5.05	4.50
3-Methylhexane	1.17915	1.15092	1.17245	1.13223	1.35	0.81	1.66	2.77
3-Ethylpentane	1.17232	1.14403	1.17245	1.13223	0.97	1.58	0.97	2.18
2,2-Dimethylpentane	1.05802	1.05128	1.03321	1.00719	4.85	4.21	7.65	11.20
2,3-Dimethylpentane	1.07609	1.10732	1.09272	1.10649	2.81	1.73	5.80	1.77
2,4-Dimethylpentane	1.03577	1.12029	1.04811	1.11071	14.60	1.70	15.42	14.52
3,3-Dimethylpentane	1.01332	1.02797	1.05422	1.05160	2.0E-3*	2.6E-4*	14.72	8.85
2,2,3-Trimethylbutane	0.91322	0.95686	0.96498	0.99194	3.87	3.84	10.08	7.76

Table 8 (continued)

Name	ξ_{exp}		ξ_{GCM}		AARD _{exp} (%)		AARD _{GCM} (%)	
	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT
2-Methylheptane	1.23 247	1.18 096	1.21 168	1.16 502	7.52	5.29	10.21	8.59
3-Methylheptane	1.25 542	1.19 467	1.23 707	1.18 842	5.41	4.60	7.63	5.05
4-Methylheptane	1.27 782	1.21 619	1.23 707	1.18 842	4.01	3.21	10.93	7.80
3-Ethylhexane	1.28 881	1.22 676	1.23 707	1.18 842	3.62	2.86	13.43	10.12
2,2-Dimethylhexane	1.14 308	1.10 373	1.09 784	1.06 337	5.62	4.70	15.75	13.79
2,3-Dimethylhexane	1.18 419	1.18 164	1.15 735	1.16 268	4.72	3.74	8.73	6.61
2,4-Dimethylhexane	1.15 328	1.18 861	1.13 812	1.19 031	5.50	4.05	6.97	4.08
2,5-Dimethylhexane	1.14 377	1.16 536	1.11 273	1.16 690	5.02	3.99	11.03	3.98
3,3-Dimethylhexane	1.15 556	1.13 565	1.11 884	1.10 779	2.79	1.28	15.32	11.62
3,4-Dimethylhexane	1.19 280	1.18 928	1.15 735	1.16 268	5.95	4.88	10.43	8.39
2-Methyl-3-ethylpentane	1.15 416	1.18 815	1.13 812	1.19 031	2.27	1.36	6.18	1.59
3-Methyl-3-ethylpentane	1.12 303	1.10 357	1.11 884	1.10 779	2.54	0.96	2.80	1.83
2,2,3-Trimethylpentane	1.06 904	1.07 880	1.02 960	1.04 812	2.13	2.94	9.58	8.95
2,2,4-Trimethylpentane	1.06 531	1.10 079	0.99 889	1.06 526	9.71	5.04	32.87	15.32
2,3,3-Trimethylpentane	1.04 191	1.05 252	1.02 960	1.04 812	2.43	0.37	5.57	1.99
2,3,4-Trimethylpentane	1.07 978	1.11 887	1.05 223	1.11 354	5.57	7.52	10.44	7.75
2-Methylotane	1.28 683	1.21 908	1.27 630	1.22 120	4.35	3.59	5.04	3.63
4-Methylotane	1.32 927	1.25 267	1.30 169	1.24 461	4.07	3.35	8.77	3.68
2,3-Dimethylheptane	1.22 510	1.20 947	1.22 197	1.21 887	12.93	10.79	13.21	10.07
3,5-Dimethylheptane	1.21 312	1.22 296	1.22 814	1.26 990	4.45	2.86	5.98	15.29
2,2,4-Trimethylhexane	1.15 074	1.17 275	1.08 890	1.14 485	4.1E-4*	1.3E-3*	32.09	12.63
3-Methyl-4-ethylhexane	1.33 217	1.25 633	1.30 169	1.24 461	3.36	1.43	9.25	3.59

Table 8 (continued)

Name	ξ_{exp}		ξ_{GCM}		AARD _{exp} (%)		AARD _{GCM} (%)	
	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT	LKP	PC-SAFT
3-Ethylheptane	1.26277	1.27020	1.22814	1.26990	4.57	2.84	7.74	2.88
2-Methylnonane	1.36429	1.29795	1.34092	1.27739	11.11	13.77	9.16	11.29
3-Methylnonane	1.35900	1.29306	1.36632	1.30080	3.08	1.89	3.05	3.48
4-Methylnonane	1.36722	1.30097	1.36632	1.30080	3.04	1.87	3.16	1.85
5-Methylnonane	1.37582	1.30906	1.36632	1.30080	3.41	1.42	4.60	3.33
4-Propylheptane	1.42696	1.34939	1.36632	1.30080	2.92	2.36	22.47	14.22
2,7-Dimethyloctane	1.24222	1.25796	1.24198	1.27928	4.56	4.24	4.56	8.22
3,6-Dimethyloctane	1.28423	–	1.29276	1.32609	2.87	–	3.83	13.33
2-Methyl-5-ethylheptane	1.29362	1.30126	1.26737	1.30268	3.19	2.61	9.35	2.42
2,2,4,4-Tetramethylhexane	1.09952	1.13754	1.03530	1.12041	1.3E–3*	8.7E–4*	41.48	8.88
Total					10.33 %	8.76 %	16.11 %	10.51 %

*The fluid-specific scaling parameter has been adjusted to 1 data point available for this fluid

special structures formed by first-order groups. The same method has been adopted here for describing the fluid-specific scaling factor ξ . This results in the subsequent equation

$$\xi = \sum_i N_i \xi_{1,i} + \sum_j M_j \xi_{2,j} \quad (15)$$

with $\xi_{1,i}$ being the first-order contribution of group type i occurring N_i times and $\xi_{2,j}$ being the contribution of the second-order groups occurring M_j times in the molecule.

The groups were adjusted in a stepwise fashion individually for both LKP [10, 11] and PC-SAFT [12] EoS. First, only molecules were selected that contain CH_3 and CH_2 groups (linear alkanes) and the group contributions of the groups CH_3 and CH_2 were adjusted to the available experimental data of the selected fluids. These groups represent the basis for all other groups. Second, only molecules were selected that contain CH groups additionally to the CH_3 and CH_2 groups and the CH group was adjusted to the experimental data using the already adjusted parameters for CH_3 and CH_2 . Third, molecules were selected that also contain C groups in addition to the previous groups and the process was repeated. The procedure was also used

for the second-order contribution in the following order: $(\text{CH}_3)_2\text{-CH-}$, $(\text{CH}_3)_3\text{-C-}$, $-\text{CH}(\text{CH}_3)\text{-CH}(\text{CH}_3)\text{-}$, and $-\text{CH}(\text{CH}_3)\text{-C}(\text{CH}_3)_2\text{-}$.

6 Results and Discussion

6.1 Fluid-Specific Scaling Factor ξ

The fluid-specific scaling factors ξ of the residual entropy scaling model for viscosities, described in Sect. 2 were adjusted to the available experimental data of linear and branched alkanes, which are listed in Table 2, for both the LKP [10, 11] and PC-SAFT [12] EoS. In total, 13 373 experimental data points [52–484] were available in the NIST ThermoData Engine (TDE), database version 10 [47], for the investigated pure fluids. The number of literature sources and data points for each fluid can be found in Table S2 in the Supplementary Information. The parameters of both equation types have been calculated using the predictive estimation schemes outlined in Sect. 3. The experimental data has been filtered using the scheme proposed by Yang *et al.* [7] as described in Sect. 4. The number of available and used data points for each fluid and EoS are listed in Table S2.

The resulting values for the adjusted parameter to the experimental data ξ_{exp} as well as the values obtained with the GCM ξ_{GCM} can be found in Table 8. When applying the LKP [10, 11] and PC-SAFT [12] EoS in the fitting procedure, the fluid-specific scaling factor ξ_{exp} of all investigated fluids could be fitted, for which 89% and 87% of the experimental data could be used, respectively. In the case of the PC-SAFT EoS [12], 3,6-dimethyloctane could not be used because all experimental data were excluded during the preselection process.

On a side note, it has to be mentioned that the number of data points for some of the investigated fluids is rather small, with as few as only one data point. A validation of the values was accomplished by means of the absolute average relative deviation (AARD) according to

$$\text{AARD} = \frac{1}{N} \sum_{i=1}^N \frac{|\eta_{\text{exp},i} - \eta_{\text{RES},i}|}{\eta_{\text{exp},i}} \quad (16)$$

with N representing the total number of data points, $\eta_{\text{exp},i}$ being the experimental viscosity of data point i and $\eta_{\text{RES},i}$ the viscosity calculated using the residual entropy scaling model of data point i . The AARD_{exp} for each of the investigated fluids is listed in Table 8. The AARD over all data points is 10% and 8.8% for LKP and PC-SAFT, respectively.

Yang *et al.* [7] collapsed all experimental pure fluid viscosity data onto one single curve in a $\ln(\eta_{\text{res}}^+ + 1)$ over s^+/ξ plot in their work using the entropy scaling for viscosity approach. The same general behavior should be observed for the PC-SAFT EoS and LKP EoS used in this work and are shown in Figs. 2 and 3. Even though the experimental data for all investigated alkanes collapse onto one

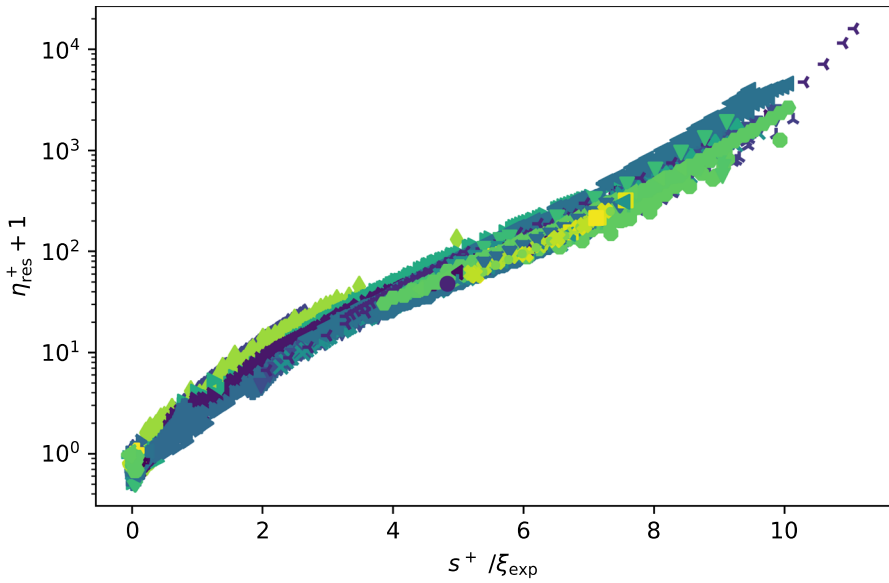


Fig. 2 Plus-scaled residual viscosity $\eta_{res}^+ + 1$ as a function of the plus-scaled dimensionless entropy s^+ divided by the fluid-specific scaling factor ξ for the LKP EoS [10, 11] for all investigated alkanes

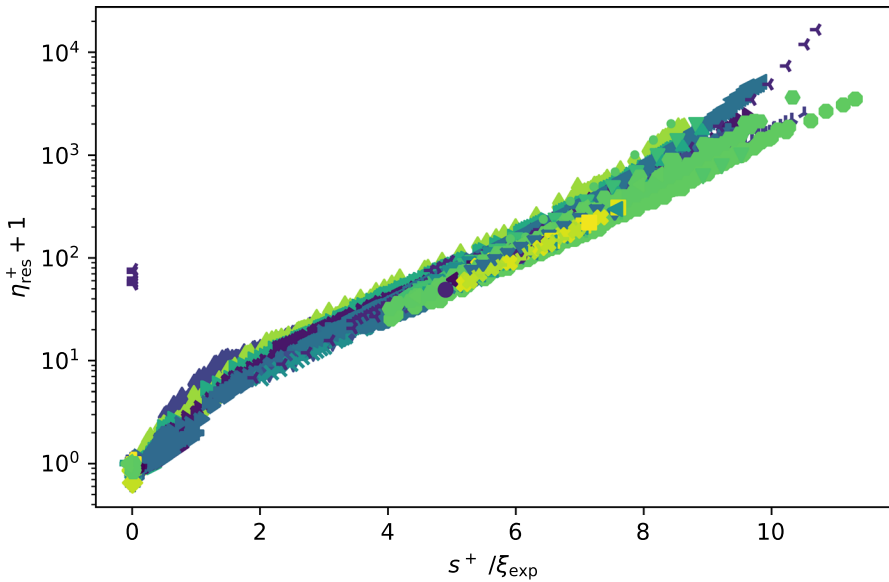


Fig. 3 Plus-scaled residual viscosity $\eta_{res}^+ + 1$ as a function of the plus-scaled dimensionless entropy s^+ divided by the fluid-specific scaling factor ξ for the PC-SAFT EoS [12] for all investigated alkanes

single curve as well, there is a slight wavy course for the LKP EoS and a sharp bend at the ratio s^+/ξ of roughly 2 for the PC-SAFT EoS, which highlights the limitation of the purely predictive parameters for both LKP EoS and PC-SAFT EoS. One possible reason for this behavior might be the deviations of the EoS parameters due to the estimation methods employed in this work to the literature values which have been adjusted for the respective fluids. For the linear alkanes, a comparison of the critical temperature, critical pressure, normal-boiling-point temperature, and the acentric factor has been done and the relative deviations to the literature data [30–33, 35–41] have been illustrated in Fig. 4. The critical temperature T_c agrees with the literature values the most with relative deviations of less than 6% for all the investigated linear alkanes. Similar deviations were found for the critical pressure p_c . Larger deviations in the normal-boiling-point temperature T_b and the acentric factor ω can be observed for the short chain alkanes, propane, and n -butane, with the exception being ethane due to an additional second-order group solely for ethane. These two alkanes, propane and n -butane, show large deviations of 107% and 38% in the acentric factor, respectively. Additionally, the long chain alkanes n -hexadecane and n -dodecane show larger deviations in the prediction of the acentric factor with a relative deviation of 21% and 42%, respectively.

Other estimation methods for describing the acentric factor for the LKP EoS might yield more accurate overall results when used for the calculation of the viscosity in the residual entropy scaling model.

The PC-SAFT parameters also exhibit deviations when compared to the literature data. In Fig. 5, the relative deviations of the parameters ϵ , σ , and m to the literature data as reported by Gross and Sadowski [12] are shown. The relative deviations of PC-SAFT parameters decrease with an increasing number of carbon atoms for the linear alkanes and are within 5% and 7% for the parameters ϵ and

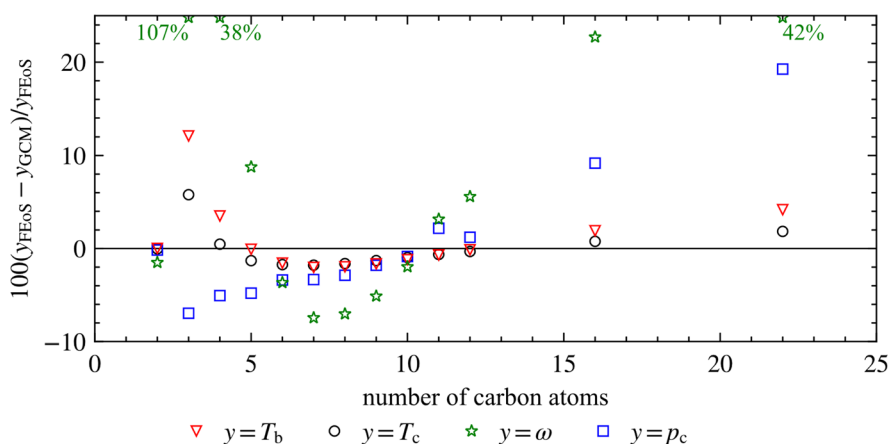


Fig. 4 Relative deviations of the GCM-based critical temperature T_c , critical pressure p_c , normal boiling point temperature T_b , and the acentric factor ω of Table 2 against literature values (FEOS) [30–33, 35–41] for the investigated n -alkanes denoted by their number of carbon atoms

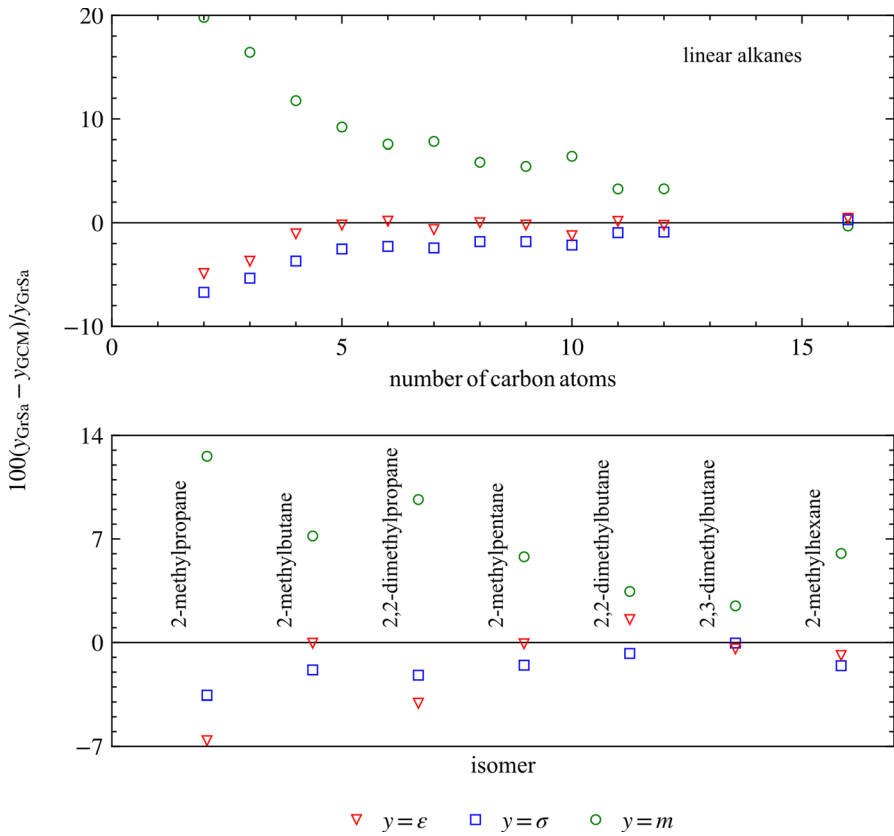


Fig. 5 Relative deviations of the GCM-based PC-SAFT parameters m , σ , and ϵ of Table 2 against values reported by Gross and Sadowski [12] (GrSa) for the investigated n -alkanes (denoted by their carbon atoms) and branched alkanes for which literature values were available

σ , respectively. The relative deviations of the parameter m have a maximum of 20% for ethane. The branched alkanes show similar relative deviations with ϵ and σ being within 5% and m within 13%.

None of the GCM have been adjusted using experimental data for transport properties such as the viscosity, obviously. As an outlook, the accuracy for the calculation of the viscosity (or any other transport property) by use of GCM for EoS parameters may be improved when used in residual entropy scaling models by incorporating experimental viscosity data while imposing the restriction to collapse $\ln(\eta_{\text{res}}^+ + 1)$ over s^+/ξ into a single curve in the fitting procedure.

Table 9 First- and second-order group contributions $\xi_{1,i}$ and $\xi_{2,i}$ (in short ξ_i) of Eq. 15 for the scaling parameter ξ of the proposed GCM for both LKP [10, 11] and PC-SAFT [12] EoS

Group i		$\xi_{i,\text{LKP}}$	$\xi_{i,\text{PCSAFT}}$
First-order	$-\text{CH}_3$	0.461 445	0.413 001
	$-\text{CH}_2-$	0.064 623	0.056 188
	$-\text{CH}<$	-0.405 755	-0.275 332
	$>\text{C}<$	-0.920 802	-0.712 776
Second-order	$(\text{CH}_3)_2-\text{CH}-$	-0.025 391	-0.023 406
	$(\text{CH}_3)_3-\text{C}-$	-0.021 007	-0.044 416
	$-\text{CH}(\text{CH}_3)-\text{CH}(\text{CH}_3)-$	-0.006 167	-0.051 032
	$-\text{CH}(\text{CH}_3)-\text{C}(\text{CH}_3)_2-$	-0.015 691	-0.084 959

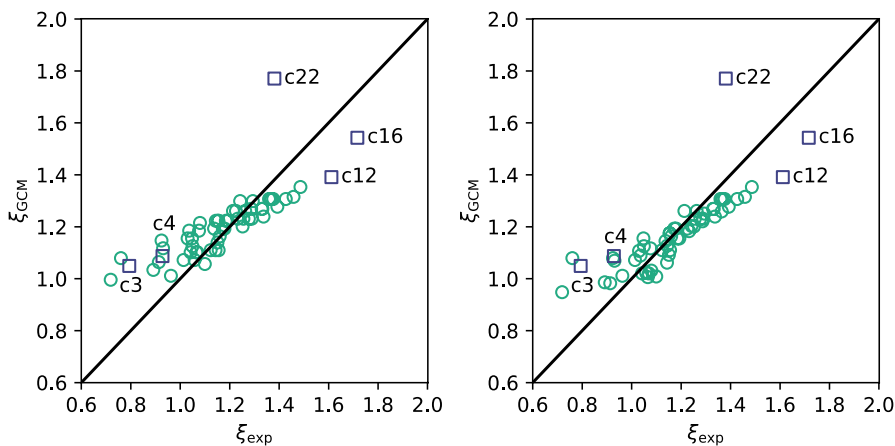


Fig. 6 Parity plots of the ξ_{GCM} parameter obtained by the first-order GCM (left) and second-order GCM (right) for the LKP [10, 11] EoS vs. ξ_{exp} adjusted to experimental data including propane (c3), *n*-butane (c4), *n*-decane (c12), *n*-hexadecane (c16), and *n*-docosane (c22) which are marked in the plot as purple squares with the corresponding carbon atom number (Color figure online)

6.2 Correlation of the Group Contribution Method

The resulting first- and second-order group contributions have been adjusted using the groups according to Constantinou and Gani [13] method and can be found in Table 9 for both LKP and PC-SAFT EoS. Parity plots for the first-order and second-order GCMs when using the LKP [10, 11] and PC-SAFT [12] EoS are illustrated in Figs. 6 and 7, respectively. Overall, the second-order GCM returns a better match of the fluid-specific scaling factor adjusted to the experimental data ξ_{exp} for both EoS.

For the LKP EoS, the fluid-specific scaling factor ξ_{GCM} obtained with the GCM vary from the experimentally adjusted fluid-specific scaling factor ξ_{exp} as displayed in Fig. 6. When using the LKP EoS [10, 11] for *n*-docosane, the resulting scaling parameter is $\xi = 1.38053$. This does not match other *n*-alkanes, which are showing an increasing value for the scaling parameter with the longest carbon chain. The adjustment of the CH_3- and $-\text{CH}_2-$ groups of the *n*-alkanes are the

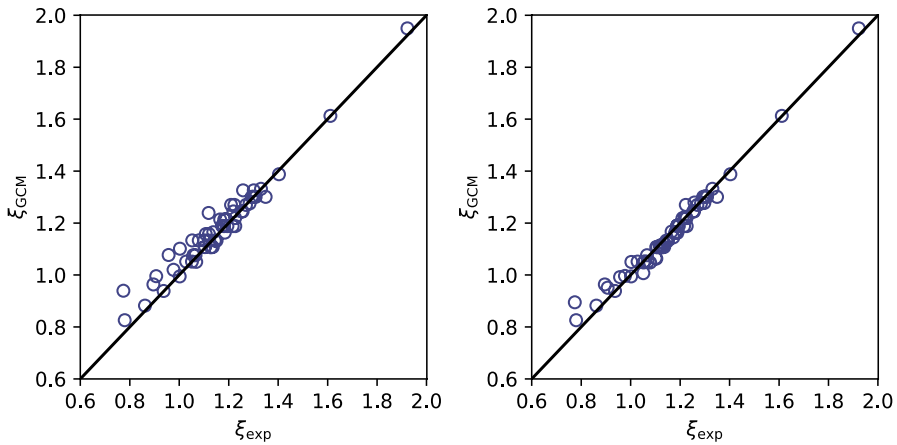


Fig. 7 Parity plots of the ξ_{GCM} parameter obtained by the first-order GCM (left) and second-order GCM (right) for the PC-SAFT EoS [12] vs. ξ_{exp} adjusted to experimental data

basis of the GCM, so having one outlier in a very limited amount of ξ parameters can have a significant effect on the correlation. The LKP parameters, critical temperature, critical pressure, and acentric factor, have been calculated using the estimation scheme by Constantinou and Gani [13] and the Antoine equation. In Fig. 4, the resulting parameters for the n -alkanes have been plotted over the literature values to check how much these values deviate. Propane, n -butane, n -hexadecane, and n -docosane, plotted as purple squares in Fig. 6, exhibit rather large deviations from the literature values, which might explain why the resulting scaling parameters seem to be off. That is why these fluids have been excluded

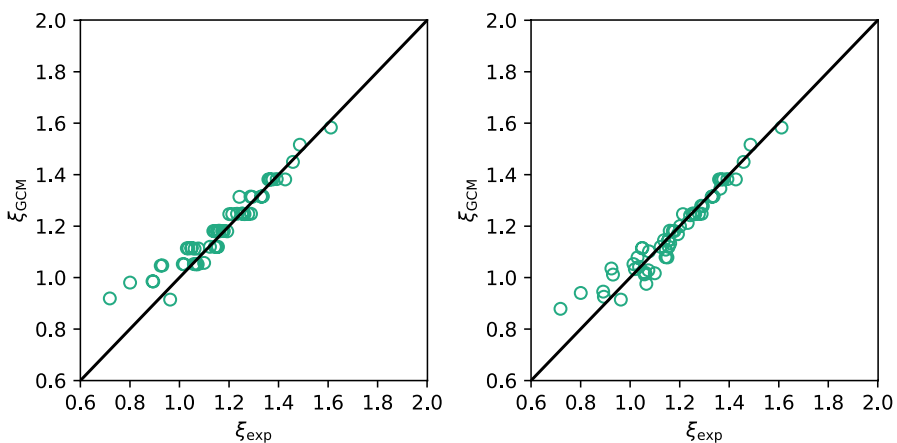


Fig. 8 Parity plots of the ξ_{GCM} parameter obtained by the first-order GCM (left) and second-order GCM (right) for the LKP [10, 11] EoS vs. ξ_{exp} adjusted to experimental data excluding propane, n -butane, n -hexadecane, and n -docosane

from the dataset and the GCM model has been readjusted for the remaining fluids, see Fig. 8. The results excluding the aforementioned fluids show an improved regression of the scaling parameters $\xi_{\text{GCM}}^{\text{E}}$ for the LKP EoS [10, 11] obtained with the GCM fitted to the experimentally adjusted fluid-specific scaling factors $\xi_{\text{exp}}^{\text{E}}$ (AARD=16%). Applying the PC-SAFT [12] EoS did not yield any outliers. Therefore, no fluid had to be excluded from the fitting procedure of the GCM. The AARD over all fluids to the experimental viscosity data for the GCM-based fluid-specific scaling factor $\xi_{\text{GCM}}^{\text{E}}$ adjusted using the PC-SAFT EoS is 11%.

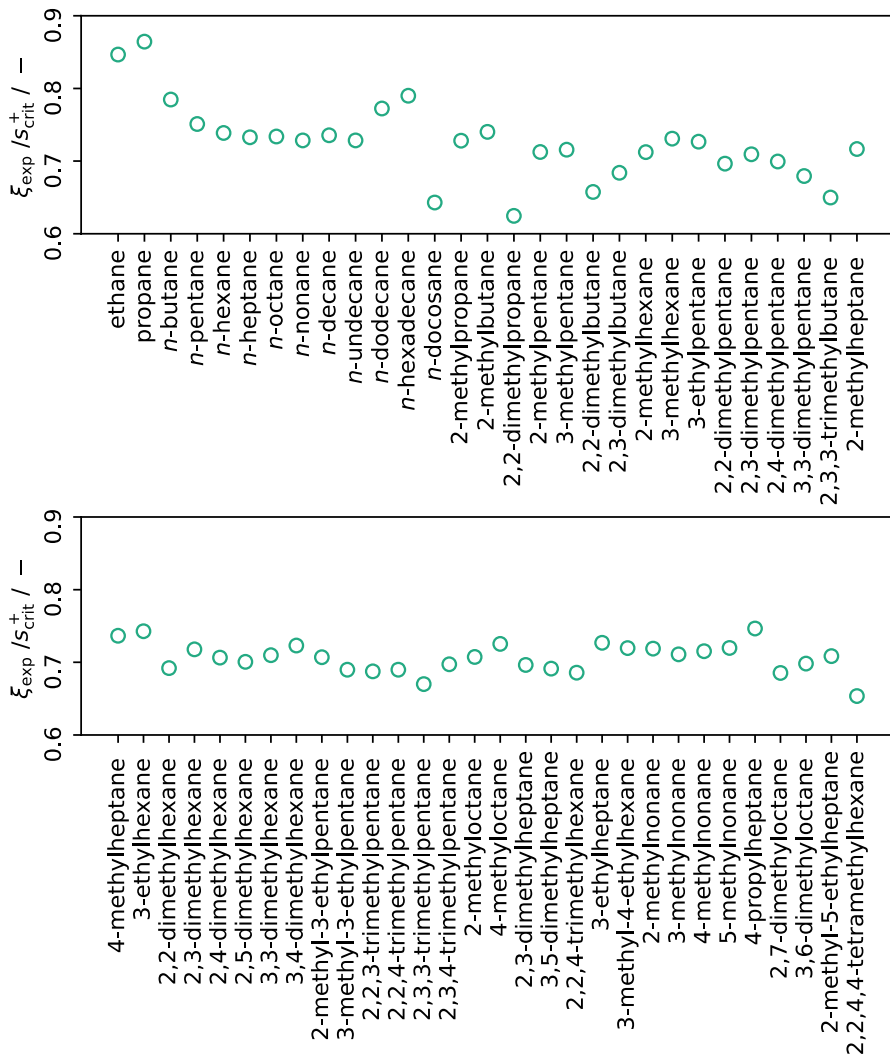


Fig. 9 Fluid-specific scaling factor $\xi_{\text{fit}}^{\text{E}}$ for the viscosity obtained in this work over the dimensionless plus-scaled entropy at critical point s_{crit}^+ for the LKP EoS

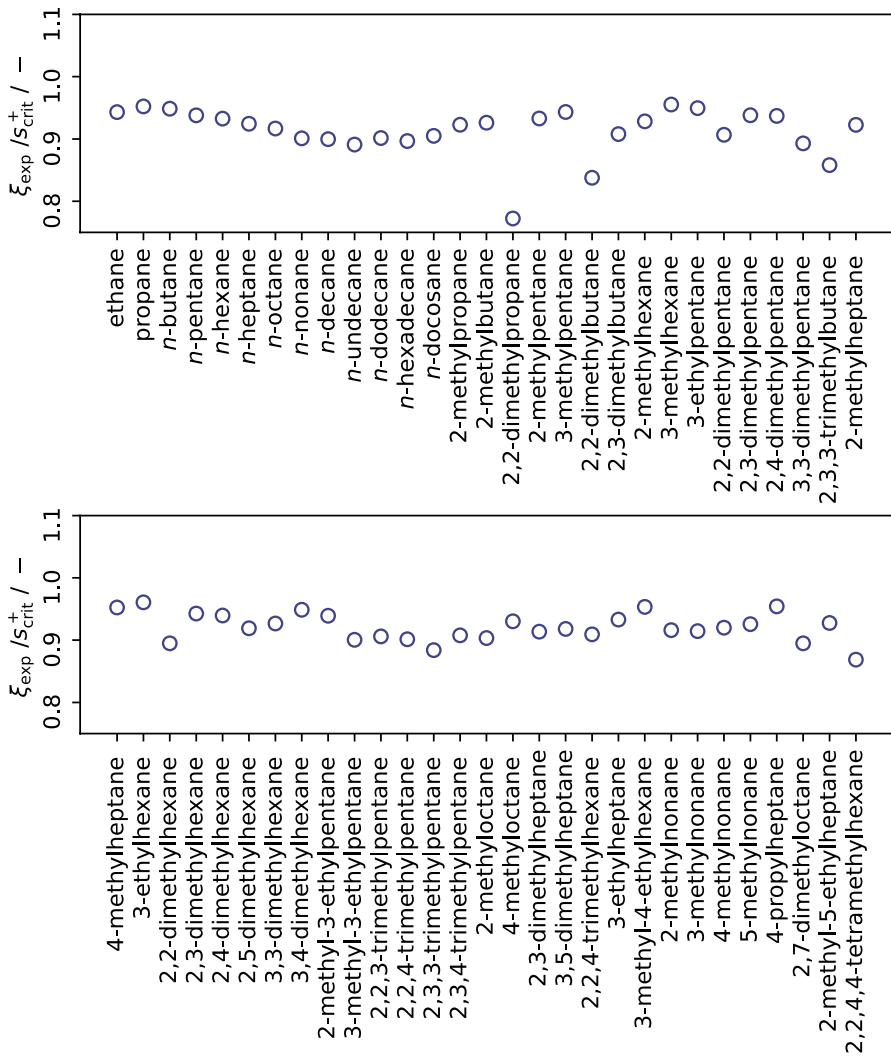


Fig. 10 Fluid-specific scaling factor ξ_{fit} for the viscosity obtained in this work over the dimensionless plus-scaled entropy at critical point s_{crit}^+ for the PC-SAFT EoS

Other estimation schemes for the scaling parameters are compared to the method proposed in this work. These estimation schemes include the $\xi/s_{\text{crit}}^+ = 0.7$ estimation method of Yang *et al.* [8] and longest carbon chain model of Jäger *et al.* [9]. As a check whether the $\xi/s_{\text{crit}}^+ = 0.7$ estimation method agrees with the LKP [10, 11] and PC-SAFT [12] EoS with the GCM-based parameters used in this work, $\xi_{\text{fit}}/s_{\text{crit}}^+$ has been plotted for all the investigated alkanes in this work and can be seen in Figs. 9 and 10 for the LKP [10, 11] and PC-SAFT [12] EoS, respectively. The ratio $\xi_{\text{fit}}/s_{\text{crit}}^+ = 0.7$ seems to agree with the LKP [10, 11] EoS and the parameters used in this work. PC-SAFT [12] EoS underestimates the

plus scaled entropy at the critical point by roughly 30%. That is why instead of $\xi/s_{\text{crit}}^+ = 0.7$, as proposed by Yang *et al.* [8], here $\xi/s_{\text{crit}}^+ = 0.9$ has been chosen to account for the differences in the plus scaled critical entropy calculation. The longest carbon chain model of Jäger *et al.* [9] has been adjusted using other parameters for the LKP EoS [10, 11]. To have a fair comparison, the linear equation according to Eq. 12 has been adjusted for the LKP [10, 11] and PC-SAFT [12] EoS using the fitted fluid-specific scaling factor ξ of the *n*-alkanes (as was done by Jäger *et al.* [9]), resulting in:

$$\xi_{\text{LKP}} = 0.06635n_{\text{chain}} + 0.77753 \quad (17)$$

$$\xi_{\text{PCSAFT}} = 0.05895n_{\text{chain}} + 0.69149 \quad (18)$$

The resulting AARDs for all models and all data can be found in Table S2 in the Supplementary Information. Only data points were selected that were calculable with all the models within a deviation range which has been set to the arbitrarily chosen value of 200%. This resulted in the evaluation of 11 956 out of the total 13 373 data points for the investigated EoSs and estimation schemes. The fluid-specific AARD values for the experimentally adjusted scaling factors and GCM-based scaling factors for LKP EoS and PC-SAFT EoS are illustrated in Fig. 11.

In general, the results in the viscosity calculation are more accurate for the PC-SAFT EoS [12] combined with any of the estimation schemes for the fluid-specific scaling factor ξ compared to the LKP EoS [10, 11]. The AARDs for the calculated viscosities when using the experimentally adjusted fluid-specific scaling factor ξ_{exp} range from 5.3% for *n*-nonane to 44% for *n*-hexadecane for the linear alkanes for the LKP EoS and from 3.6% for *n*-docosane to 13% for *n*-hexadecane for the PC-SAFT EoS [12]. The AARDs for the branched alkanes are up to 15% for 3,3-dimethylpentane for the LKP EoS and 14% for 2-methylnonane for the PC-SAFT EoS [12]. For some of the branched alkanes, rather low AARDs are calculated. This is because the underlying database contains only 25 or less data points with often as much as one data source. Exceptions are 2-methylpropane (isobutane), 2-methylbutane (isopentane), 2,2,4-trimethylpentane (isooctane), which were investigated experimentally in much more detail. Therefore, the adjusted fluid-specific scaling factor for the branched alkanes are subject to higher uncertainty as they are adjusted to only very few data points.

The parameters for the LKP EoS [10, 11] have been determined in a predictive way as has been discussed in Sect. 3.1. Calculated viscosities are less accurate for alkanes with only 3 and 4 carbon atoms as longest chain, *e.g.* propane, *n*-butane, 2-methylpropane, 2-methylbutane, and also less accurate for alkanes with 12 and more carbon atoms as longest chain, *e.g.* *n*-dodecane, *n*-hexadecane, and *n*-docosane. The former is due to larger inaccuracies when predicting the critical parameters of short hydrocarbons, because such molecules were not the focus of the GCM of Constantinou and Gani [13]. Only for ethane an additional second-order group has been introduced to improve the accuracy. The latter is caused by an inherent issue concerning the LKP EoS [10, 11] and long chain hydrocarbons as has been discussed by Jäger *et al.* [9]. Even though it is possible to adjust the scaling parameter

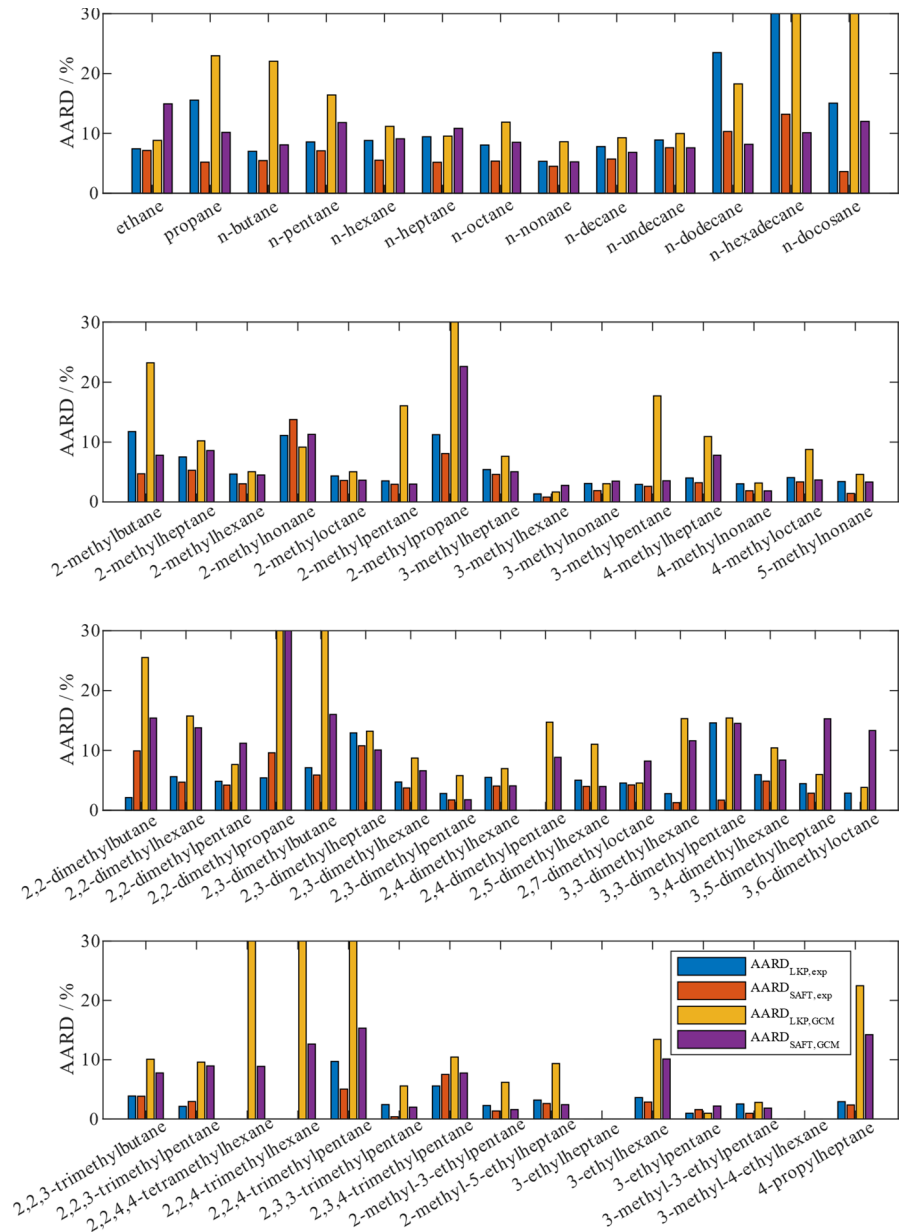


Fig. 11 AARD values in % for each alkane using the experimentally adjusted scaling parameter ξ_{exp} as blue columns for LKP EoS and orange columns for PC-SAFT EoS and the scaling parameter obtained by the GCM ξ_{GCM} as yellow columns for LKP EoS [10, 11] and purple columns for PC-SAFT EoS [12] (Color figure online)

with the LKP EoS [10, 11] to obtain good agreement of the calculated viscosities with experimental data, less accurate results will be obtained when using the scaling

parameters calculated with the GCM proposed in this work. An example for this is *n*-butane, which shows an AARD of 7% and 22% for the adjusted ξ_{exp} and ξ_{GCM} , respectively. This is due to weaknesses of the correlated GCM as these fluids do not fit the scheme very well.

Other estimation methods yield similar or worse results compared to the proposed model. The AARDs for all investigated fluids can be found in Table S3 in the Supplementary Information. The longest carbon chain method of Jäger *et al.* [9] yields good agreement with the experimental data for the linear alkanes, but exhibits weaknesses for the more complex branched alkanes. The $\xi/s_{\text{crit}}^+ = 0.7$ estimation scheme of Yang *et al.* [8] shows an overall good agreement to the experimental data for most branched alkanes. However, especially for the LKP EoS [10, 11], this method results in large AARDs of more than 20% for 11 out of the 13 linear hydrocarbons. More accurate results are achieved when modifying the estimation method, corrected to $\xi/s_{\text{crit}}^+ = 0.9$, for PC-SAFT [12]. As a result, the linear hydrocarbons show improved AARDs ranging from 5.1% to 15%. The AARDs increase for the more complex branched alkanes when the fluid-specific scaling factor is estimated using the plus-scaled dimensionless entropy at the critical point s_{crit}^+ .

Note, that the total AARD over all investigated alkanes in Table S3 might be misleading, because if a model happens to describe a fluid with many data points accurately, it can happen that the overall AARD is comparatively low, while other fluids with less data are not well described, and vice versa. Therefore, it is advisable to compare the individual AARDs for the fluids additionally to the overall AARDs.

All estimation schemes seem to overestimate the scaling parameter for 2,2-dimethylpropane (neopentane) with AARDs for the calculated viscosities ranging from 48% to 76%.

7 Conclusion

In this work, a GCM approach was developed to estimate the fluid-specific scaling factor ξ of the residual entropy scaling model for the viscosity of Yang *et al.* [7] using two equations of state. The parameters for the LKP [10, 11] and PC-SAFT [12] equations of state have been estimated using predictive methods. Two approaches were tested. The first method is the adjustment of the fluid-specific scaling factors to available filtered experimental data. For the second method, the fluid-specific scaling factors were fitted by means of the group contribution method. Both approaches were tested with both equations of state. According to the results, it is possible to calculate the viscosities within reasonable deviations with AARDs over the filtered dataset of 10.33% and 8.76% when the fluid-specific scaling factors are adjusted to the experimental data. The GCM-based fluid-specific scaling parameter proposed in this work yields AARDs of 16.11% and 10.51% for the LKP and PC-SAFT EoS, respectively. The results were compared to other estimation methods, showing an improved accuracy compared to the longest carbon chain linear regression from Jäger *et al.* [9]. For the filtered data points of all investigated hydrocarbons, the GCM method proposed in this work also performs better than the estimation scheme by Yang *et al.* [8].

The presented GCM can be extended to other functional groups according to the method proposed in this work and has, therefore, a great potential to be used for a significant number of substances. A potential and interesting application would be the use in polymers. The fluid-specific scaling factor ξ can be calculated for the repeating group of the polymer chain and then be normalized by the molar mass of that certain group. This has been already proposed for the PC-SAFT [12] parameters in the work of Tihic *et al.* [14], where the fluid-specific scaling factor ξ seems to have some relation to the size of the molecule. Furthermore, more functional groups can be added to include other fluids to increase the applicability of this model.

Identifying structural isomers has its limits when using the GCM by Constantinou and Gani [13]. For instance, 2-methylhexane, which shows one $(\text{CH}_3)_2\text{-CH-}$ group, can be distinguished from other isomers. However, that is not the case for 3-methylhexane and 3-ethylpentane as both show identical groups (3 $-\text{CH}_3$, 3 $-\text{CH}_2-$, 1 $-\text{CH}<$ group). This leads to increased uncertainties for such substances when predicting the viscosity by means of the GCM. Therefore, to increase the accuracy of the introduced estimation scheme, the underlying method for describing the molecule should be revised. Other more sophisticated options may include natural language learning algorithms for accurate molecular description not only of branched alkanes, but also more complex molecules. In addition, new insights into the physics of residual entropy [485–487] could pave the way for something closer to first principles predictive approaches of transport properties.

A shortcoming of the general entropy scaling approach presented here is that even when fitting fluid-specific scaling factors ξ , it is still not possible to fit the experimental data within its experimental uncertainty. As the fluids studied here can be expected to follow entropy scaling, it could also be possible to use the transport property measurements to develop simultaneously thermodynamic and transport property models. Thermal conductivity could be a more fruitful path than viscosity for this process because it can be measured with a lower uncertainty in the liquid phase.

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Data Availability There are no new data available. The applied data are taken from literature and marked with the corresponding references.

Declarations

Competing Interests The authors have no competing interests to declare.

Ethical Approval Not applicable.

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