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Fundamental equation of state for ethylene oxide based on a hybrid dataset



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HIGHLIGHTS

- An empirical fundamental equation of state (FEOS) is presented for ethylene oxide.
- The FEOS can be used to calculate all thermodynamic properties.
- The underlying dataset consists of experimental and molecular simulation data.

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ABSTRACT

An empirical fundamental equation of state correlation is presented for ethylene oxide. The correlation is explicit in terms of the Helmholtz energy and it can be used to calculate all thermodynamic properties. The underlying dataset consists of experimental and molecular simulation data. The experimental data cover almost exclusively the gaseous phase and are available for temperatures from the triple point up to the critical point. Molecular simulation data are used to extend the validity to the liquid state and up to a maximum temperature of 1000 K and a maximum pressure of 700 MPa.

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1. Introduction

A sufficient amount of reliable thermodynamic data is essential for the design and optimization of almost any process in the chemical industry. Currently, databases alone cannot meet the increasing requirements of process engineering. Mapping the entire thermodynamic property spectrum of a given fluid is often impossible using laboratory experiments due to the associated financial cost, time investment, and potentially extreme measuring conditions. Empirical equations of state (EOS) correlations are one solution for this problem, because they rationalize and summarize experimental data, offering a built-in interpolation and extrapolation scheme for general engineering purposes. Empirical correlations that represent the fundamental equation of state (FEOS) are particularly beneficial (Span, 2000). A FEOS can be expressed in terms of various thermodynamic potentials. However, independent on which representation is chosen, it contains

the complete property information about the system: once a thermodynamic potential is explicitly given as a function of its natural variables, every other thermodynamic property is simply a combination of its derivatives with respect to its natural variables.

The construction of a FEOS that covers the entire fluid region of industrial relevance typically faces the problem of scarce experimental input data. Molecular modeling and simulation have evolved to a point of acceptance in the applied sciences and are a potential solution to satisfy the need for thermodynamic data. Molecular simulation yields macroscopic properties exclusively from microscopic information. Accordingly, its predictive capabilities are, in principle, only limited by the quality of the molecular interaction model that represents the investigated substance. While molecular simulation techniques (Monte Carlo and molecular dynamics) have a huge advantage over experimental measurements when it comes to speed and cost efficiency, the number of molecular interaction models that can really offer an alternative to laboratory measurements, not just on the qualitative, but also on the quantitative level, increased significantly only over the last decade (Industrial fluid properties simulation collective). Extreme temperatures or pressures are not limiting factors for molecular

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Table 1
Parameters for the residual part of the reduced Helmholtz energy $\alpha^r(\tau, \delta)$ according to Eq. (4).

k	n_k	t_k	d_k	l_k	η_k	λ_k	γ_k	ϵ_k
1	0.3805675D-01	1.000	4					
2	0.1359482D+01	0.312	1					
3	-0.1833370D+01	0.860	1					
4	-0.5754450D+00	1.114	2					
5	0.1536490D+00	0.500	3					
6	-0.1598130D+01	2.100	1	2				
7	-0.6826090D+00	1.700	3	2				
8	0.6436960D+00	0.754	2	1				
9	-0.5353070D+00	2.500	2	2				
10	-0.1872220D-01	0.900	7	1				
11	0.1238840D+01	2.180	1		1.010	1.12	0.874	0.7202
12	-0.4315460D+00	3.500	1		1.650	2.16	0.617	0.9110
13	-0.2295870D+00	2.340	3		0.896	0.91	0.476	0.6880
14	-0.1931280D+02	4.330	3		22.000	196.00	1.24	0.9100
15	-0.5283590D-01	3.900	2		1.730	0.13	0.562	1.2100

Table 2
Experimental data for ethylene oxide from the literature. The original units were converted into SI units and the temperature is given in terms of the international temperature scale of 1990 standard (ITS-90). Data points calculated from an ancillary equation are marked with an asterisk.

Source	Year	Data points	Temperature range (K)	Pressure range (MPa)
Homogeneous density				
Lide (2005) ^a	2005	1	273.15	0.101325
Walters and Smith (1952) ^a	1952	81	294–428	0.006–3.448
Overall ^b		82	273–428	0.006–3.448
Vapor pressure				
Calado et al. (1996)	1996	1	182.33	0.0001
Chao et al. (1986)	1986	1	283.71	0.101325
Coles and Popper (1950)	1950	17	273–305	0.067–0.221
Giauque and Gordon (1949)	1949	14	223–286	0.004–0.108
Giles and Wilson (2006)	2006	2	298–349	0.174–0.767
Gillespie et al. (1985)	1985	2	283–299	0.101–0.174
Hess and Tilton (1950)	1950	1	293.14	0.1462
Kistiakowsky and Rice (1940)	1940	1	283.84	0.101325
Lide (2005)	2005	3	283–284	0.101–0.100
Maass and Boomer (1922)	1922	21	216–286	0.002–0.110
McDonald et al. (1959)	1959	11	284–239	0.103–0.012
Mock and Smith (1950)	1950	10	322–423	0.379–3.827
Olson (1977)	1977	3	273–324	0.065–0.394
Frenkel et al. (2013)*	2013	17	160–469	0.000–7.207
Walters and Smith (1952)	1952	12	294–469	0.151–7.192
Overall ^b		99	182–423	0.000–3.827
Saturated liquid density				
Auwers (1918)	1918	2	279.20	–
Comelli and Francesconi (1991)	1991	11	288–304	–
Comelli and Francesconi (1995)	1995	1	298.15	–
Comelli and Francesconi (1996)	1996	2	298–314	–
Francesconi and Comelli (1994)	1994	1	298.15	–
Francesconi and Comelli (1995)	1995	1	298.15	–
Maass and Boomer (1922)	1922	16	222–294	–
Olson (1977)	1977	3	273–324	–
Perkin (1893)	1893	1	280.15	–
Frenkel et al. (2013)*	2013	17	160–469	–
Walters and Smith (1952)	1952	12	294–469	–
Wurtz (1859)	1859	1	273.15	–
Overall ^b		51	222–469	–
Saturated vapor density				
Olson (1977)	1977	3	273–324	–
Frenkel et al. (2013)	2013	20	377–469	–
Walters and Smith (1952)	1952	12	294–469	–
Overall ^b		15	273–469	–
Speed of sound				
Hurly (2002)	2002	334	285–440	0.049–1.020
Overall ^b		334	285–440	0.049–1.020
Isobaric heat capacity				
Giauque and Gordon (1949)	1949	22	166–284	Vapor pressure
Overall ^b		22	166–284	Vapor pressure

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