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Joule–Thomson inversion curve prediction by using equation of state

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Abstract

In this paper five equations of state are tested for checking their ability to predict the Joule–Thomson inversion curve. These five equations of state are: Mohsennia–Modarres–Mansoori (MMM), Ji-Lemp (JL), modified Soave–Redlich–Kwang (SRK) equation of state by Graboski (MSRK1), modified SRK equation of state by Peneloux and Rauzy (MSRK2), and modified Peng–Robinson (PR) equation of state by Rauzy (PRmr). The investigated equations of state give good prediction of the low-temperature branch of the inversion curve, except for MMM equation of state. The high-temperature branch and the peak of the inversion curve have been observed, in general, to be sensitive to the applied equation of state. The values of the maximum inversion temperature and maximum inversion pressure are calculated for each component used in this work.

Keywords: Equation of state; Joule–Thomson coefficient; Inversion curve

Equation of state (EoS) is commonly used to correlate thermodynamic properties for computer-aided design of chemical processes [1–3]. On the other hand, it has been recognized for a long time that the prediction of the Joule–Thomson (JT) inversion curve is an extremely severe test of an equation of state [4]. The prediction of adiabatic Joule–Thomson coefficient for the inert gases on the basis of numerous intermolecular potentials have been calculated by Nain and Aziz [5]. To date, inversion curves have been calculated both numerically and via simulation methods [6–11].

Meanwhile, it is the objective of this article to compare the predictive capabilities of five equations of state for Joule–Thomson inversion curve. These equations of state are as follows: Mohsennia–Modarres–Mansoori (MMM) [12,13], Ji-Lemp (JL) [14,15], modified Soave–Redlich–Kwang (SRK) equation of state by Graboski (MSRK1) [16], modified SRK equation of state by Peneloux and Rauzy (MSRK2) [17,18], and modified Peng–Robinson (PR) equation of state by Rauzy (PRmr) [19,20]. We will present the results of our numerical study.

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1. Theory and calculation

The locus of points at which the Joule–Thomson coefficient μ is zero is called the inversion curve. The inversion condition, $\mu = 0$ is given by the equation

$$T_r\left(\frac{\partial P_r}{\partial T}\right)_{V_r} + V_r\left(\frac{\partial P_r}{\partial V_r}\right)_{T_r} = 0 \quad (1)$$

By solving the above-mentioned equation simultaneously with a given equation of state, one can calculate the locus of points for which the Joule–Thomson coefficient is zero. In this work, we employ five different equations of state to predict the inversion curve of some fluids. The equations of state used in the present work are given in the appendix.

2. Results and discussion

The calculated Joule–Thomson inversion curves from various equation of state are shown in Figs. 1–5 for Ar, CO_2, CH_4, C_2H_6, and C_3H_8, respectively. It has been found from Figs. 1–5 that the low-temperature region of the inversion curve is well matched by all equations of state, except for MMM EoS. The inversion locus predicted by the MMM equation of state does not agree with experimental data [21] in any region. The calculated maximum inversion pressure by MMM equation of state is considerably less than their reference values. Therefore, the weakness of this equation in predicting of Joule–Thomson inversion curve can not be set within reliable limits of operating conditions. There is poor agreement between JL equation of state with experimental of Joule–Thomson inversion data in sub-critical region. The predicted maximum inversion pressure is less than their reference value except for Ar. The predicted inversion curve of methane by JL equation of state shows desirable agreement at low temperatures and the calculated maximum inversion pressure is comparable to that obtained from the reference values. The inversion curve predicted by MSRK1 equation of state shows good predictions at low temperatures. The low-temperature region of the inversion curve is well matched by MSRK1 equation of state for hydrocarbons. The predicted maximum inversion pressure is less than the reference value except for Ar. The inversion curve locus predicted using the MSRK2 equation of state is same as that predicted by MSRK1 equation of state at low temperatures.

The inversion curve predicted by PRmr equation of state shows good predictions at low temperatures. The low-temperature region of the inversion curve is well matched by PRmr equation of state for hydrocarbons. Therefore, the PRmr equation can safely be considered as a reference for the evaluation of the low-temperature inversion curve predicted by other equations of state. Reasonable agreement between PPmr equation of state with experimental data is observed for heavier hydrocarbons at high temperature portion and at the peak of curves.

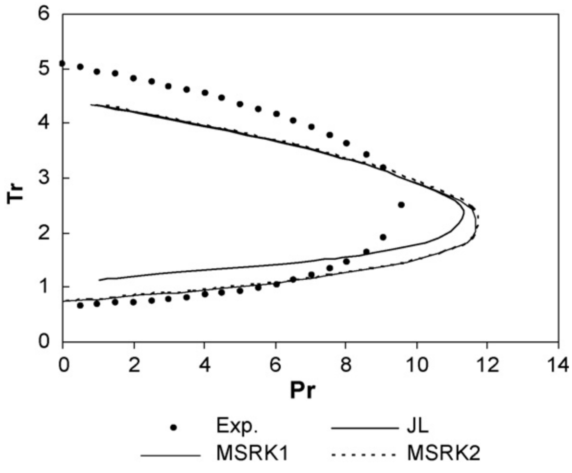

Fig. 1. Joule–Thomson inversion curves for Argon.

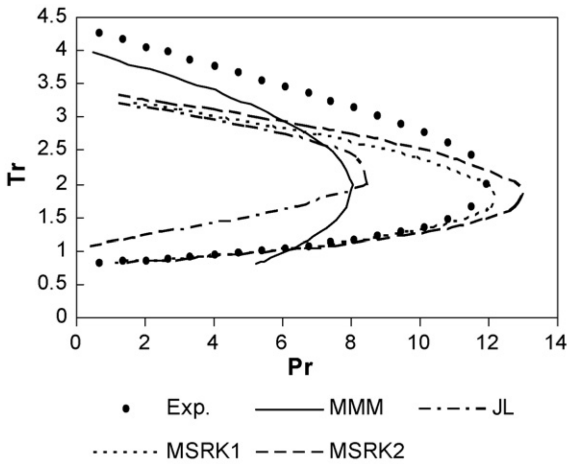

Fig. 2. Joule–Thomson inversion curves for CO_2.

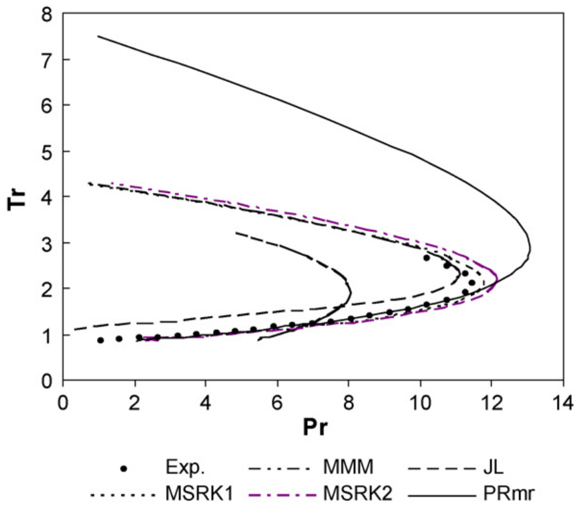

Fig. 3. Joule–Thomson inversion curves for CH_4.

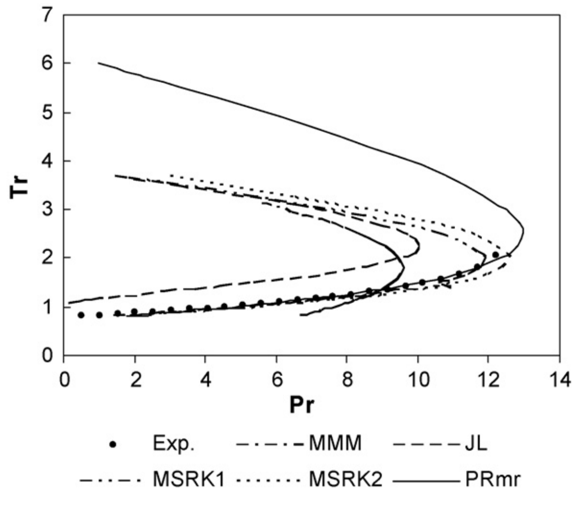

Fig. 4. Joule–Thomson inversion curves for C_2H_6.

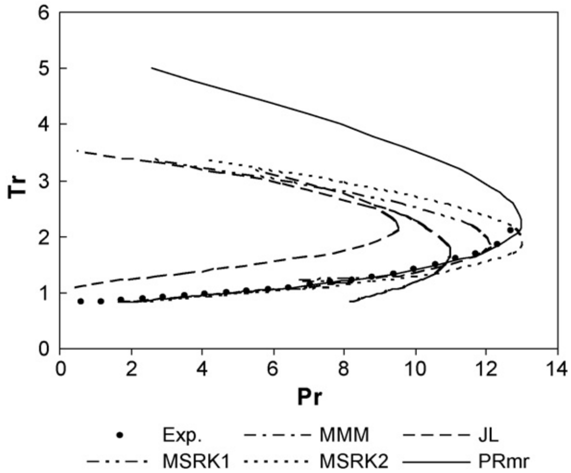

Fig. 5. Joule–Thomson inversion curves for C_3H_8.

3. Conclusion

In the present study, we have provided a comparison among Mohsennia–Modarres–Mansoori, Ji-Lemp, modified Soave–Redlich–Kwang equation of state by Graboski, modified SRK equation of state by Peneloux and Rauzy, and modified Peng–Robinson equation of state by Rauzy. A conclusion central to our study seems to be that the investigated equations of state give good prediction of the low-temperature branch of the inversion curve, except for MMM equation of state. The high-temperature branch and the peak of the inversion curve have been observed, in general, to be sensitive to the applied equation of state. The maximum inversion pressure, $P_{r,max}$, and the corresponding temperature, $T_{r,i}$, for the five equations are calculated and given in Table 1. The maximum inversion temperatures, $T_{r,max}$ obtained in the ideal gas limit ($P_r \to 0$), is also calculated and are given in Table 1.

Table 1
The calculated maximum inversion pressures $P_{r,max}$, the corresponding temperature $T_{r,i}$, and maximum inversion temperature $T_{r,max}$

Equation of state	Component	$P_{r,max}$	$T_{r,i}$ [a]	$T_{r,max}$
MMM	Methane	8.0643	1.91	3.9957
MMM	Ethane	9.6108	1.79	3.9550
MMM	Propane	11.0056	1.7	3.9016
MMM	Carbon dioxide	8.0696	1.998	3.9955
JL	Argon	11.2050	2.49	4.4215
JL	Methane	11.1554	2.29	4.3410
JL	Ethane	10.0603	2.3	3.8141
JL	Propane	9.5414	2.15	3.5650
JL	Carbon dioxide	8.4745	1.998	4.6825
MSRK1	Argon	11.5474	1.91	4.4052
MSRK1	Methane	11.7944	2.1	4.3292
MSRK1	Ethane	11.9481	2.05	3.8316
MSRK1	Propane	12.1019	1.85	3.6020
MSRK1	Carbon dioxide	12.0944	1.63	3.3246
MSRK2	Argon	11.6164	1.91	4.4400
MSRK2	Methane	12.1401	2.1	4.4187
MSRK2	Ethane	12.6459	2.05	3.9376
MSRK2	Propane	13.0329	1.85	3.7237
MSRK2	Carbon dioxide	12.9055	1.998	3.4008
PRmr	Methane	13.0691	2.9	7.5875
PRmr	Ethane	12.9555	2.5	6.0884
PRmr	Propane	12.9735	2.2	5.3633

[a] The number of significant figures are exactly adopted from their reference values [21].

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