Estimation of Physical Properties for Hydrogen Isotopes Using Aspen Plus Simulator

Jungho Cho [a*], Seungyon Cho [b], Sei-Hun Yun [a], Min Ho Chang [b], Hyun-Goo Kang [b], Ki Jung Jung [b], Dong Min Kim [c]
[a]*Dept. of Chemical Eng., Kongju National Univ., 275 Budae-dong, Cheonan, Chungnam, 330-717, Korea*
[b]*National Fusion Research Institute, Daejeon, 305-806, Korea*
[c]*Dept. of Materials Scienc and Eng., Hongik Univ.,Jochiwon, Yongi, Chungnam, 339-701, Korea*
[*]*Corresponding author: jhcho@kongju.ac.kr*

1. Introduction

Hydrogen isotopes are H_2, HD, D_2, H_2, HD, D_2, HT, DT and T_2. Among the hydrogen isotopes, the physical properties of H_2, HD and D_2 are included in the Aspen Plus, however HT, DT and T_2 are not included. In this study, various thermodynamic properties were estimated for six components of isotopes by use of the fixed properties and temperature-dependent properties. To estimate thermodynamic properties, Soave modified Redlich-Kwong equation of state and Aspenplus simulator was used. The results were verified and compared with by PRO/II with PROVISION of Invensys.

2. Physical Properties Estimation

Data in Table I are needed to estimate the physical properties of pure components. Among the molecular weight and critical properties, critical pressure and critical temperature are urgently necessary to use the equation of state. Critical volume and compressibility factor can be calculated by selected equation of state. Since saturation pressure at boiling point is the same with atmospheric pressure, boiling point of the pure components can be estimated by vapor pressure change with temperature. Gibbs free energy of formation and heat of formation are related with the estimation of the equilibrium constant of chemical reaction and the heat reaction. Since the reactions between hydrogen isotopes are not considered in this study, these properties were not entered to Aspen Plus simulator.

Table I: Pure Component Properties

Parameter	Description	Unit
MW	Molecular weight	g/gmol
NBP	Normal boiling point	K
Tc	Critical temperature	K
Pc	Critical pressure	Pa
Vc	Critical volume	m^3/gmol
Zc	Critical compressibility facor	
P_i^{vap}	Vapor pressure	Pa
$\Delta G_{f,i}^0$	Gibbs free energy of formation	J/gmol
$\Delta H_{f,i}^0$	Heat of formation	J/gmol

Table II show the physical properties of pure components for each isotopes.

Table II

Parameter	H_2	HD	D_2	HT	DT	T_2
MW		3.0238		4.0236	5.0319	6.0320
Tc (K)		35.91		37.13	39.42	40.22
Pc (kPa)		1,484		1,570	1,770	1,850

Physical properties of hydrogen isotopes can be calculated by the equation of state and the data in table II. Additionally, vapor pressure change with temperature is necessary for the estimation. The vapor pressures of H_2, HD, D_2 are shown in Fig. 1 as a function of temperature by Aspen Plus. However, experimental data are used for HT, DT and T_2 components as shown in table III because it is not included in the Aspen Plus simulator.

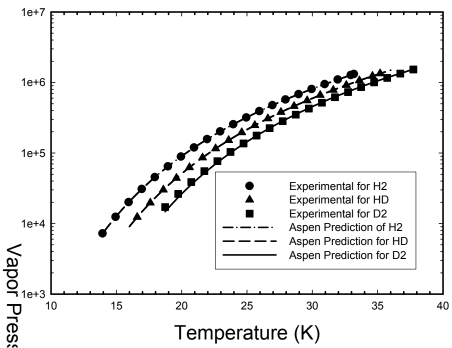

Fig. 1. Experimental vapor pressure for H_2, HD and D_2 and its prediction with Aspen Plus modeling.

Table III: Vapor Pressures of HT, DT and T_2

Temperature, K	HT, Pa	DT, Pa	T_2, Pa
4.2	$5x10^{-4}$	$4x10^{-10}$	$2x10^{-11}$
6	$1x10^{-3}$	$4x10^{-5}$	$6x10^{-6}$
8	$3.9x10^{-1}$	$4x10^{-3}$	$1x10^{-2}$
10	15	2.6	1.0
12	$2.0x10^{2}$	47	22
14	$1.27x10^{3}$	$4.2x10^{2}$	$2.2x10^{2}$
16	$5.37x10^{3}$	$2.06x10^{3}$	$1.26x10^{3}$
18	$1.68x10^{4}$	$7.63x10^{3}$	$5.06x10^{3}$
20	$3.84x10^{4}$	$2.20x10^{4}$	$1.58x10^{4}$
22	$7.68x10^{4}$	$4.74x10^{4}$	$3.74x10^{3}$
24	$1.38x10^{5}$	$9.08x10^{4}$	$7.41x10^{4}$
26	$2.29x10^{5}$	$1.58x10^{5}$	$1.33x10^{5}$
28	$3.55x10^{5}$	$2.56x10^{5}$	$2.20x10^{5}$
30	$5.24x10^{5}$	$3.92x10^{5}$	$3.41x10^{5}$
32	$7.43x10^{5}$	$5.76x10^{5}$	$5.06x10^{5}$
34	$1.02x10^{6}$	$8.13x10^{5}$	$7.21x10^{5}$
35	$1.18x10^{6}$	$9.54x10^{5}$	$8.50x10^{5}$
36	-	$1.10x10^{6}$	$9.94x10^{5}$
37	-	$1.28x10^{6}$	$1.16x10^{6}$
38	-	-	$1.33x10^{6}$

Experimental vapor pressures of HT, DT and T_2 in Table III are plotted and compared by Aspen Plus in Fig. 2 to Fig. 4.

They show that the estimated data by Aspen plus are matched well with the experimental data.

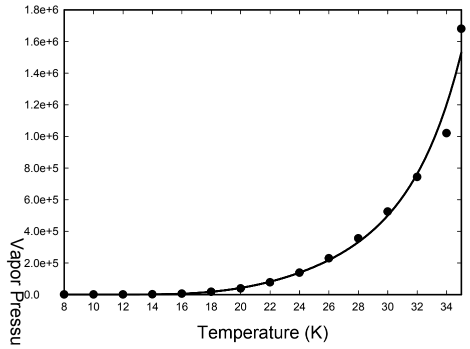

Fig. 2. Experimental vapor pressure for HT and its prediction with Aspen Plus modeling.

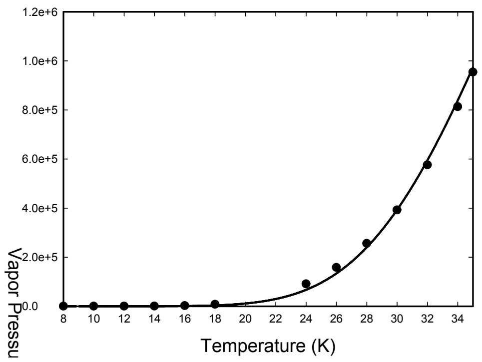

Fig. 3. Experimental vapor pressure for DT and its prediction with Aspen Plus modeling.

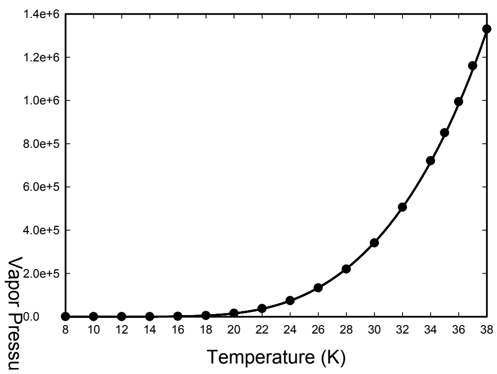

Fig. 4. Experimental vapor pressure for T_2 and its prediction with Aspen Plus modeling.

3. Conclusions

Thermodynamic properties of hydrogen isotopes were estimated by using Aspen Plus simulator and SRK equation of state. For the estimation of the thermodynamic properties for the component which are not built-in Aspen Plus data such as HT, DT and H_2, molecular weight, critical temperature, critical pressure and pure component vapor pressure experimental data versus temperature were used for the prediction of pure component properties. Experimental vapor pressures are well matched with Aspen plus estimation.

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