ISS (Isotope Separation System)

초저온증류 공정시뮬레이션

공주대학교 화학공학부

조 정 호

목 차

4. Pure Component Properties

4. Pure Component Properties

- **The following pure component data are required for the simulation.**

Parameter	Description
MW	Molecular weight
TC	Critical temperature
PC	Critical pressure
VC	Critical volume
ZC	Critical compressibility factor
PL	Vapor pressure coefficients
CPIG	Ideal gas heat capacity coefficients
DHFORM	Heat of formation
DGFORM	Gibbs free energy of formation
DHVLWT	Watson heat of vaporization coefficients

4. Pure Component Properties

- **Temperature-dependent properties**

✓ Vapor pressure vs. temperature
✓ Enthalpy vs. temperature
✓ Specific heat vs. temperature
✓ Heat of vaporization vs. temperature
✓ Liquid density vs. temperature
✓ Liquid and vapor viscosities vs. temperature
✓ Liquid and vapor thermal conductivities vs. temperature
✓ Surface tension vs. temperature

4. Pure Component Properties

Description	H_2	HD	D_2	HT	DT	T_2
Ideal gas heat capacity coefficients	○	○	○	X	X	X
Heat of vaporization coefficients	○	○	○	X	X	X
Liquid density coefficients	○	○	○	X	X	X
Solid density coefficients	X	○	○	X	X	X
Liquid thermal conductivity coefficients	○	○	○	X	X	X
Vapor thermal conductivity coefficients	○	○	○	X	X	X
Liquid viscosity coefficients	○	○	○	X	X	X
Vapor viscosity coefficients	○	○	○	X	X	X
Surface tension coefficients	○	○	○	X	X	X

4. Pure Component Properties

- Fixed Properties Built-in Aspen Plus Database & Newly Added

Properties	H_2	HD	D_2	HT	DT	T_2
MW	2.01588	3.02194	4.028	4.0236	5.0319	6.032
NBP (K)	20.39	22.14	22.92	23.66	24.38	25.04
Tc (K)	33.19	35.19	38.35	37.13	39.42	40.22
Pc (kPa)	1,313.0	1,484.0	1,667.1	1,570	1,770	1,850
w (OMEGA)	-0.22	-0.18	-0.15	-0.12	-0.13	-0.14
DGFORM (kJ/kmol)	0	-1,464.65	0	-1,169.89	-1,661.12	0

DGFORM: Standard Gibbs free energy of formation

4. Pure Component Properties

➢ Coefficients in Vapor Pressure Correlation

$$\ln P_i^{vap} = C_{1i} \times \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i} \ln T + C_{6i} T^{C_{7i}}$$

Components	H_2	HD	D_2	HT	DT	T_2
Temperature units	**K**	**K**	**K**	**K**	**K**	**K**
Property units	**kPa**	**kPa**	**kPa**	**kPa**	**kPa**	**kPa**
C_{1i}	5.782245	14.77644	12.03924	600.9424	-44.2099	118.44
C_{2i}	-94.896	-154.269	-154.47	-4394.55	0.999352	-922.336
C_{3i}	0	0.512593	0	6.921281	-8.35385	4.581168
C_{4i}	0	0.060997	0	2.330207	-0.37298	0.39025
C_{5i}	1.1125	-1.51724	-0.57226	-160.417	18.03123	-28.7063
C_{6i}	3.29E-04	0	0.038899	0	0	0
C_{7i}	2	0	1	0	0	0

4. Pure Component Properties

➢ *SRK Equation of State Model*

✓ In 1972, Soave (Italian) introduced an acentric factor (nonsphericity) to explain the size and shape differences and the intermolecular forces between molecules but used same functional form with RK equation of state.

$$P = \frac{RT}{v-b} - \frac{a\,\alpha}{v\left(v+b\right)}$$

4. Pure Component Properties

- ✓ In SRK equation of state, energy and size parameters, a and b are functions of critical temperature and pressure.

$$a = 0.42747 \frac{R^2 T_c^2}{P_c} \qquad b = 0.08664 \frac{R T_c}{P_c}$$

- ✓ Alpha function is also introduced to predict pure component vapor pressures more accurately.

$$\alpha(T) = \left[1 + m\left(1 - \sqrt{T_r}\right)\right]^2$$

$$m = 0.48508 + 1.55171\omega - 0.15613\omega^2$$

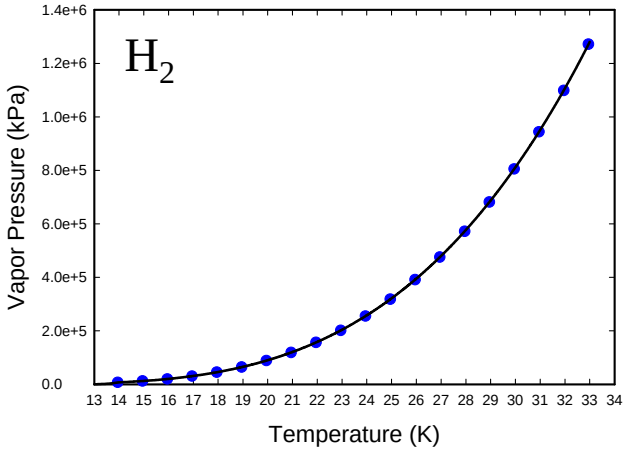
4. Pure Component Properties

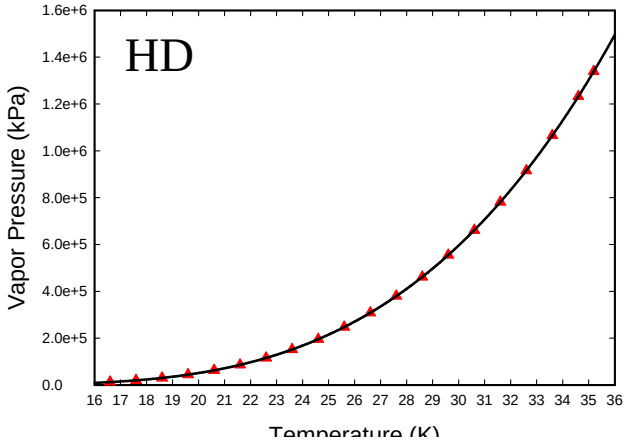
Exterminate Data vs. Calculation Data

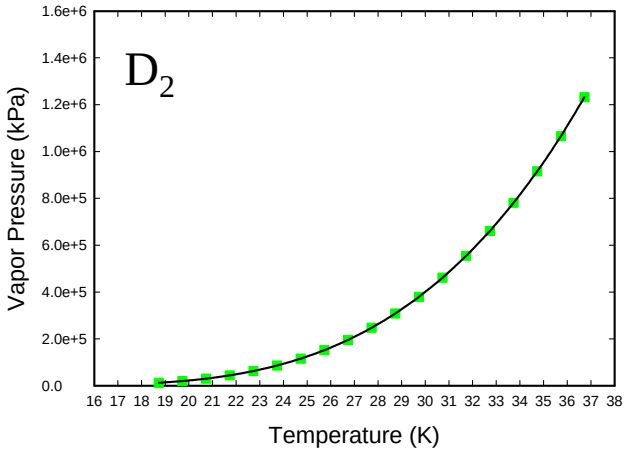
		H_2	HD	D_2	HT	DT	T_2
vapor pressure at 25K (mmHg)	Exp.	2,483.19	1,620.17	1,117.77	1,346.05	915.77	759.05
	Calc.	**2,411.75**	**1,612.90**	**1,103.09**	**1,316.65**	**721.25**	**757.05**
boiling point (K)	Exp.	20.39	22.14	22.92	23.66	24.38	25.04
	Calc.	**20.39**	**22.34**	**22.81**	**23.50**	**24.44**	**25.00**

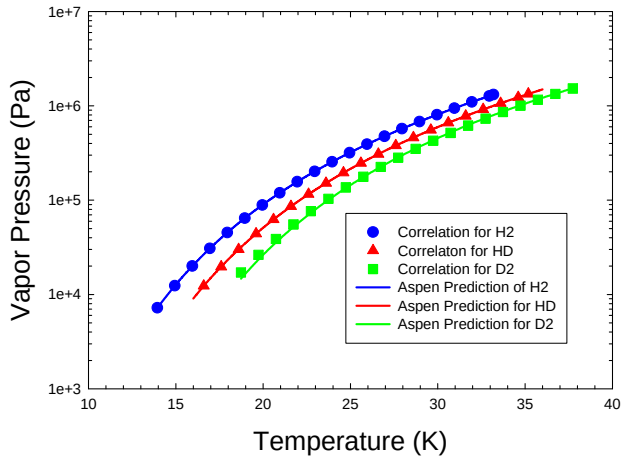
4. Pure Component Properties

Vapor Pressure Estimation for H_2, HD, D_2, HT, DT & T_2 Using Aspen Plus



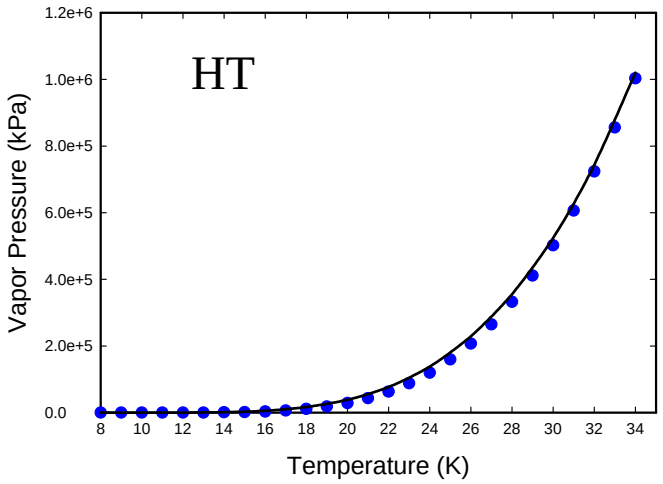


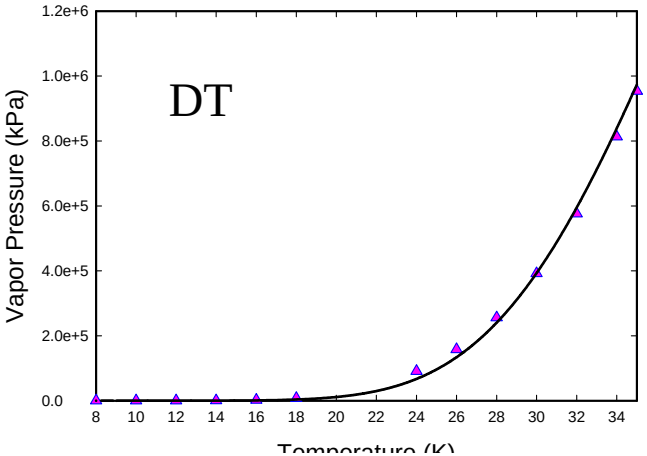


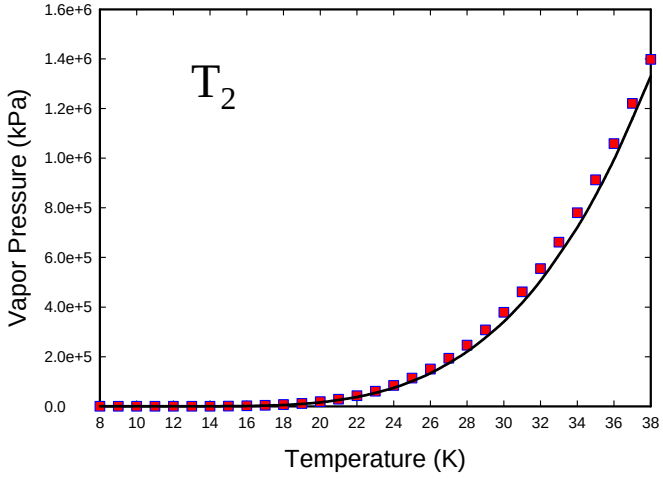


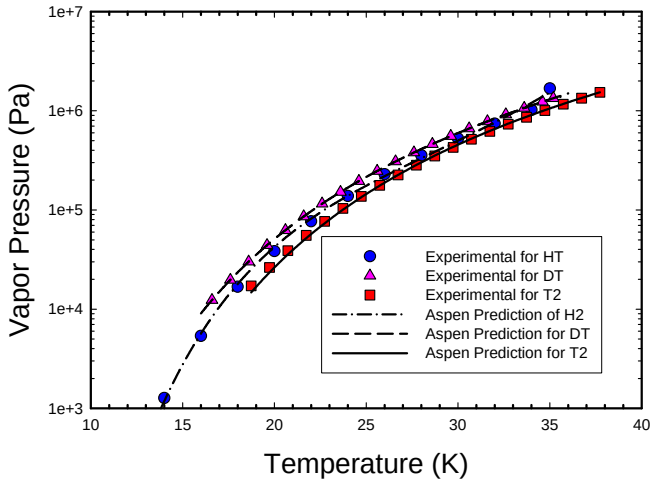
4. Pure Component Properties

Vapor Pressure Estimation for H_2, HD, D_2, HT, DT & T_2 Using Aspen Plus



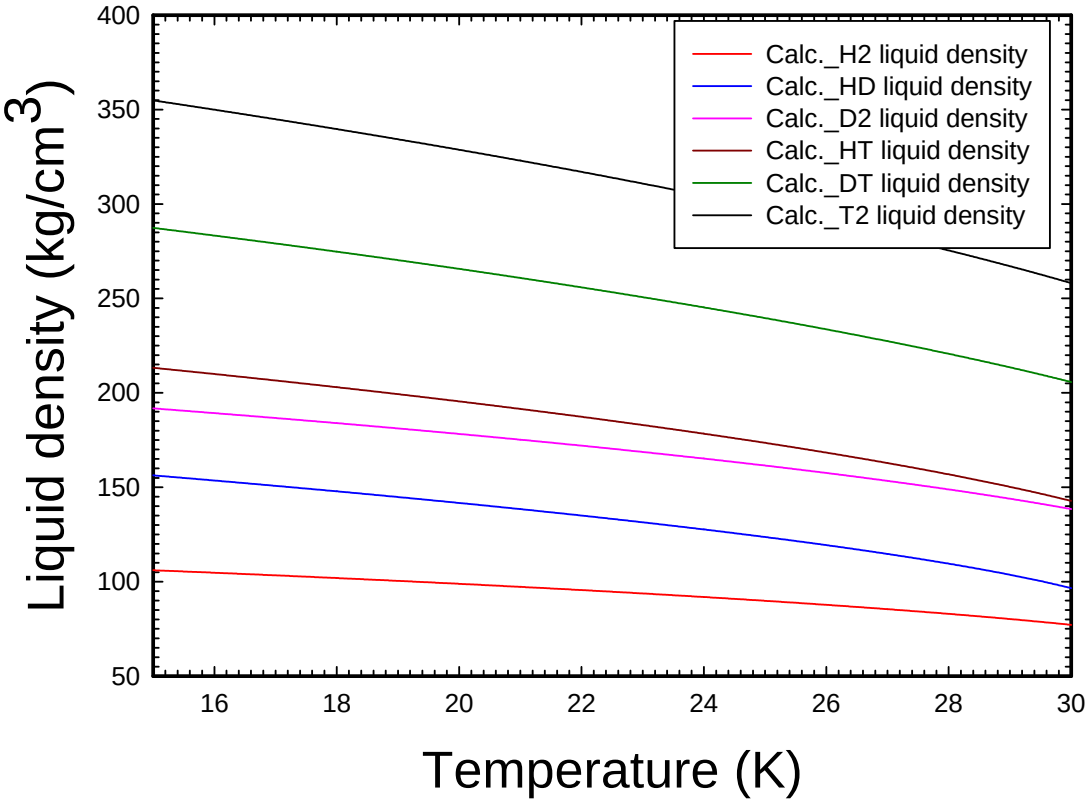






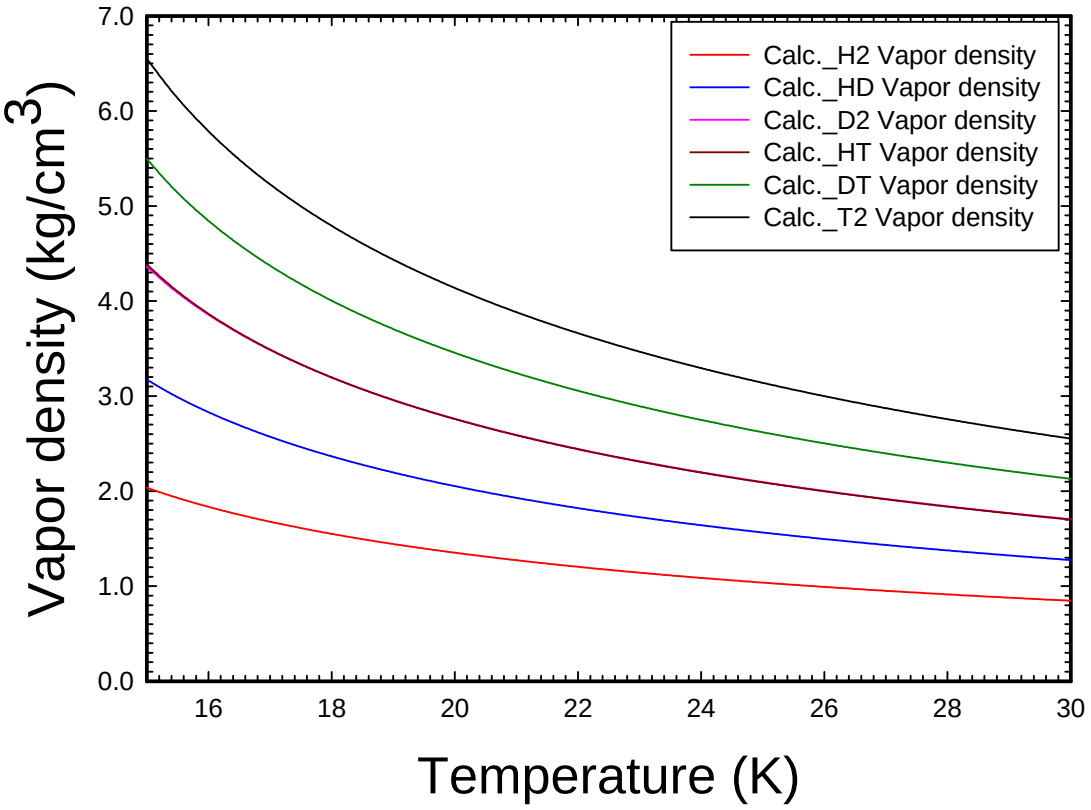
4. Pure Component Properties

Liquid Density



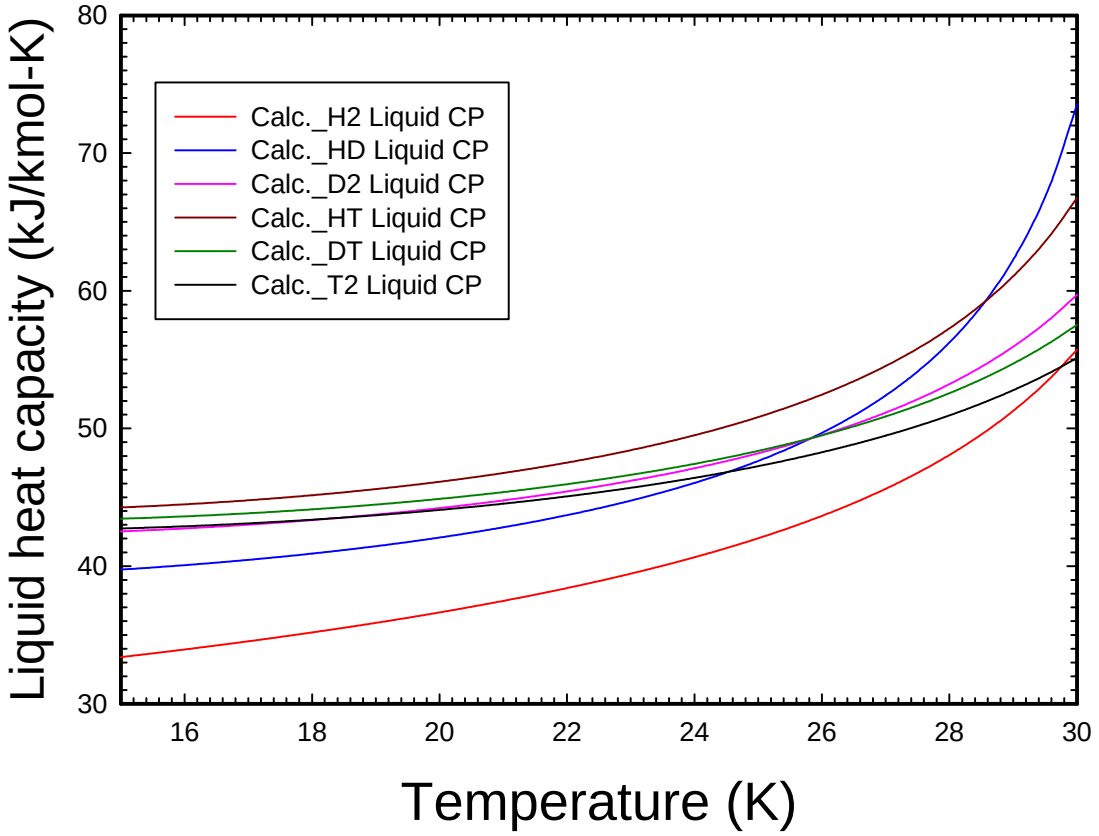
4. Pure Component Properties

Vapor Density



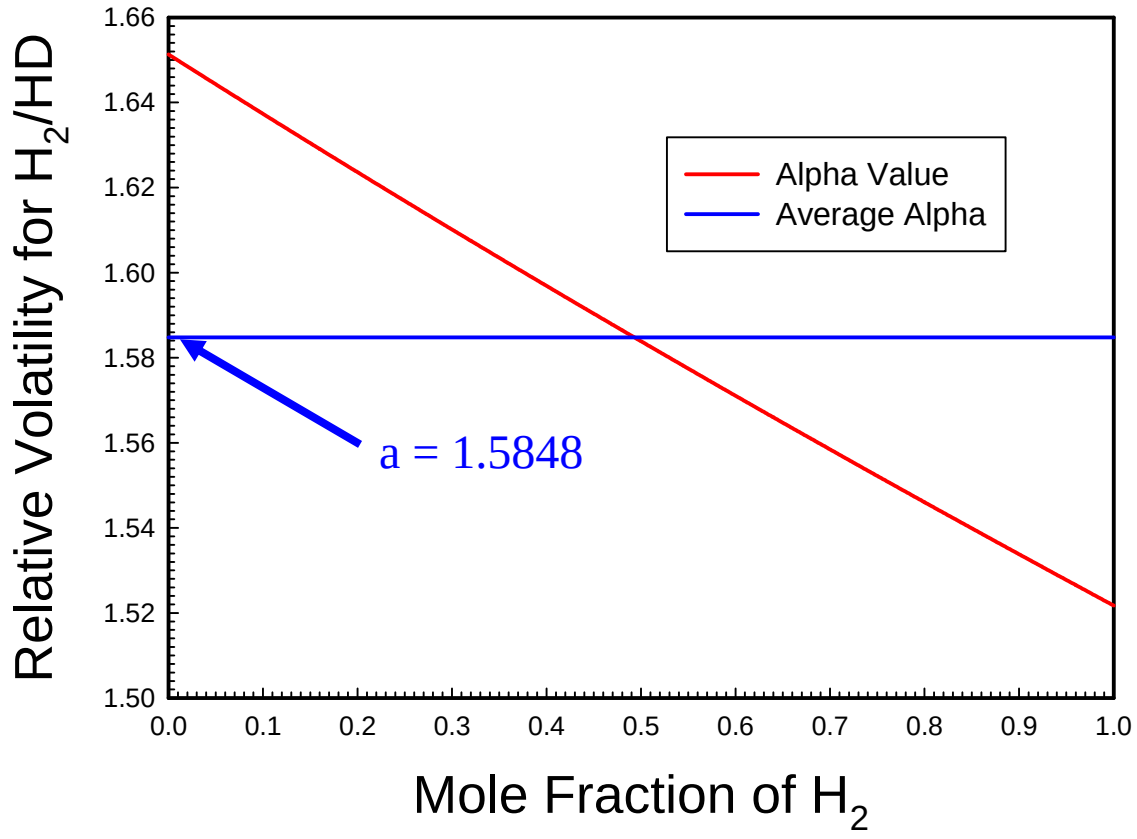
4. Pure Component Properties

Liquid heat capacity



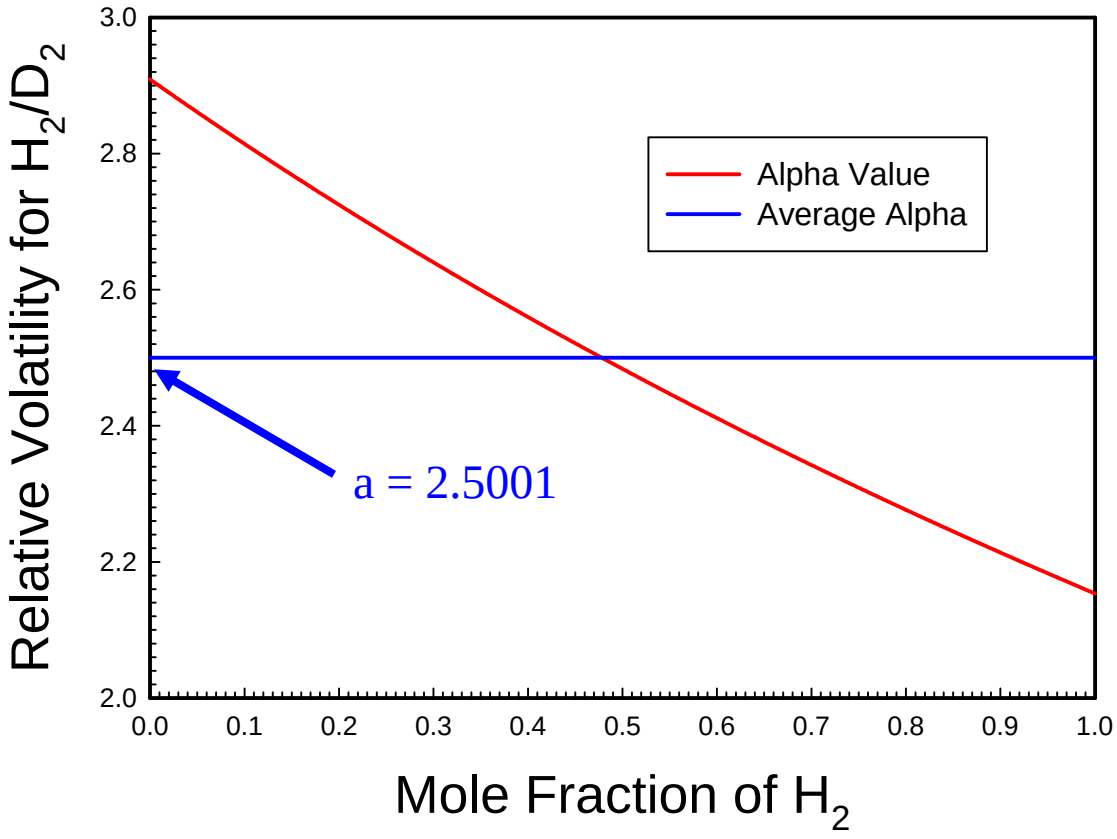
4. Pure Component Properties

- **Average Relative Volatility at 22K for H_2/HD = 1.6 (문헌치)**



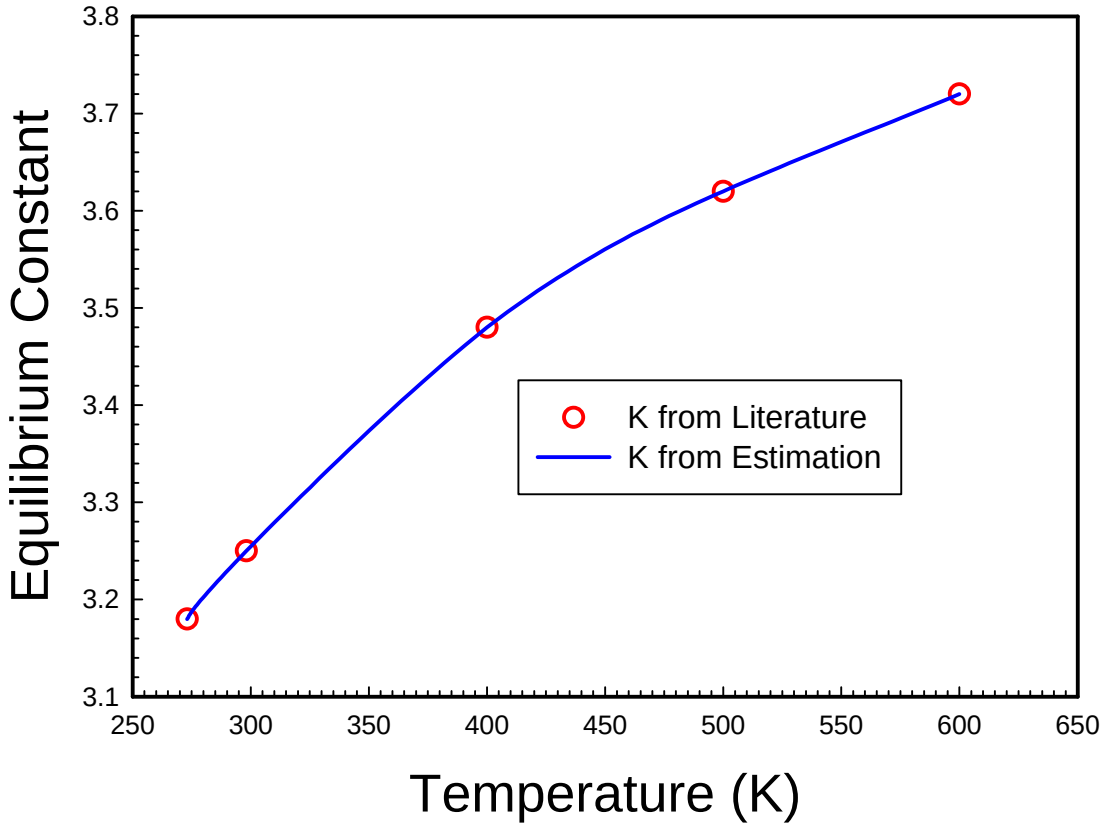
4. Pure Component Properties

- **Average Relative Volatility at 22K for H_2/D_2 = 2.6 (문헌치)**



4. Pure Component Properties

- **Equilibrator: H_2+D_2 = HD**



감사합니다