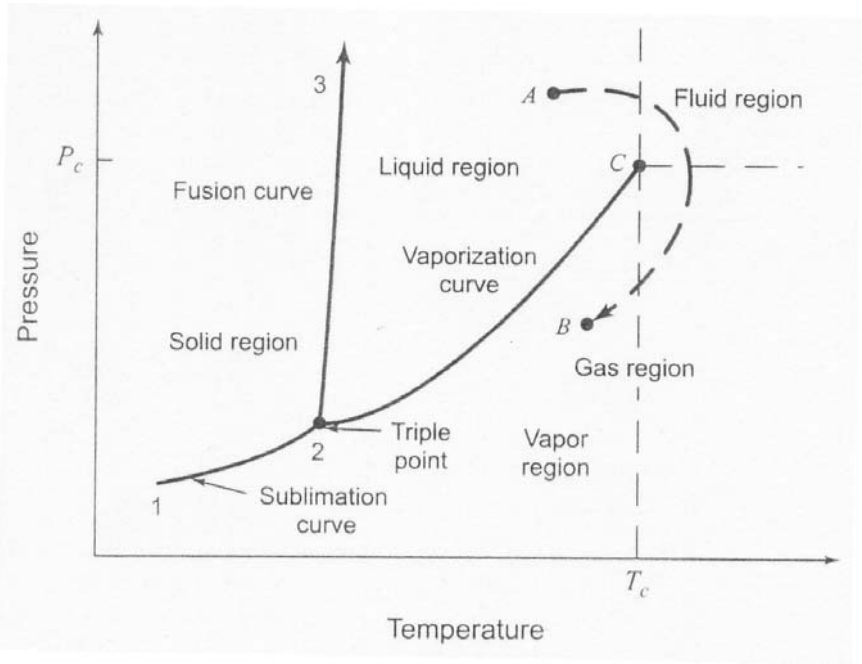
ch. 6 상태 방정식
(교재 212쪽)

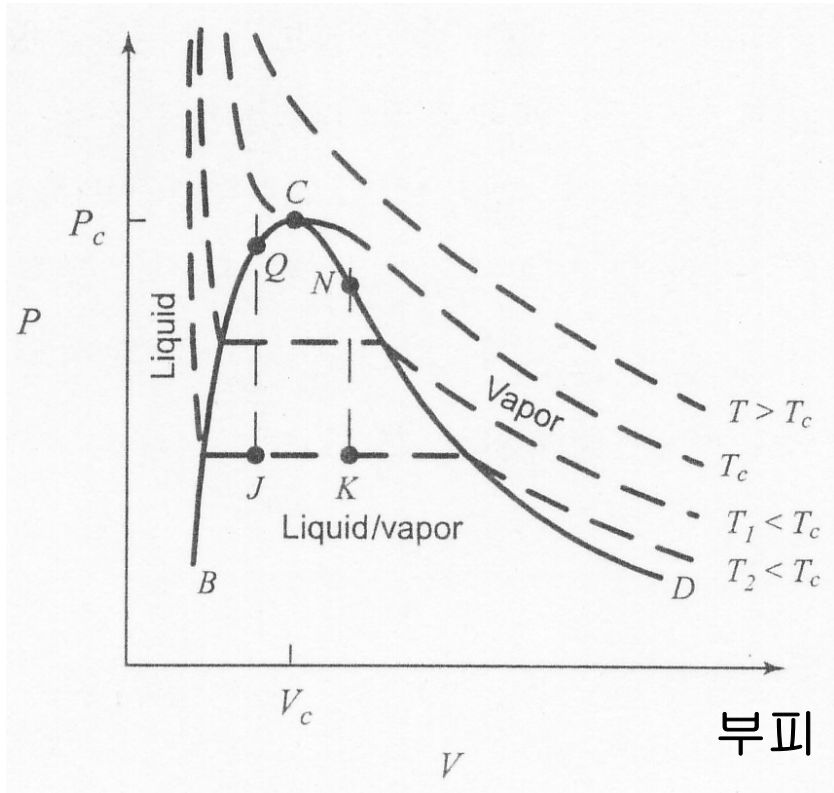
순수물질의 PVT 거동

압력



온도

압력



부피

기체 상태방정식 1: Virial equation

- Compressibility, z

  z=PV/RT

- Virial equation

$$z \equiv \frac{PV}{RT} = 1 + \frac{B}{V} + \frac{C}{V^2}$$

$$= 1 + B'P + C'P^2$$

- 이상기체

  z=1

기체 상태방정식 2: Pitzer equation

- Acentric factor, ω (교재 214쪽)

$$\omega = -1 - \log_{10}\left(\frac{P^{sat}}{P_c}\right)\Bigg|_{T_r=0.7}$$

- 환산 온도와 압력

$P_r = P/P_c$

$T_r = T/T_c$

Pitzer equation

$Z = Z^0 + \omega Z^1$

$Z = PV/(RT)$

전산실습

- 부록 D: 순수물질의 물성치 (563쪽)
- Component plus (new search)

Equation of State (EOS) for gas: 기체 상태방정식

- Ideal gas equation: P=RT/V
- Van der Waals equation: $P=RT/(V-b)-a/V^2$
- SRK (Soave-Redlich-Kwong) equation (non-spherical and non-polar molecules, hydrocarbons)
- Peng-Robinson equation (water)

- Critical point:

$$\left.\frac{\partial P}{\partial V}\right|_{T=T_c} = 0 \qquad a = \frac{9}{8} R T_c V_c$$

$$\left.\frac{\partial^2 P}{\partial V^2}\right|_{T=T_c} = 0 \qquad b = \frac{V_c}{3}$$

기체 상태방정식 : 예제

SRK (1972) model:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)}$$

$$a = \frac{27R^2T_c^2}{64P_c}$$

$$b = \frac{RT_c}{8P_c}$$

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

$$s = 0.48 + 1.574\omega - 0.176\omega^2$$

100 °C, 1 MPa 암모니아에 대하여 몰부피를 계산하시오.

R=8.314, T_c=405.5K, P_c=11.28×10^6 Pa, s=0.86546
T_r=373.1/T_c

비이상기체의 Gibbs 자유에너지

- 일정온도에서 (dT=0) Gibbs 자유에너지 : dG=VdP
  - 이상기체: $dG^* = \frac{RT}{P} dP$
  - 비이상기체: $dG = \frac{zRT}{P} dP$
  - 편차값:

$$dG - dG^* = \frac{RT}{P}(z-1)dP$$

$$\frac{dG}{RT} - \frac{dG^*}{RT} = (z-1)\frac{dP}{P}$$

$$d\left(\frac{G}{RT} - \frac{G^*}{RT}\right) = (z-1)\frac{dP}{P}$$

$$\left(\frac{G}{RT} - \frac{G^*}{RT}\right) = \int (z-1)\frac{dP}{P}$$

과제:
비이상기체의 Gibbs 자유에너지

예제: Virial 식이 다음과 같이 기체압력에 대하여 표현될 때,

$$z = 1 + B'P + C'P^2$$

일정한 온도에서 Gibbs 자유에너지의 편차값을 구하시오.