2. Thermodynamics of fuel cell systems (Mench, ch. 3)

1. Physical nature of thermodynamic variables
2. Heat of formation, sensible enthalpy, latent heat
3. Change in enthalpy for nonreacting species & mixtures
4. Change in enthalpy for reacting species & mixtures
5. Thermodynamics of moist air mixtures
6. Thermodynamic efficiency of fuel cell
7. Maximum expected open circuit voltage: Nernst voltage

1. Physical nature of thermodynamic variables

-thermodynamics: the study of equilibrium at a macroscopic level

(1) Physical meaning of parameters

-Temperature (T)
-Pressure (P)
-Ideal gas: $PV = nRT$
-Non-ideal behavior
 Van der Waals equation of state (EOS)

$$P = \frac{RT}{\nu - b} - \frac{a}{\nu^2}$$

ν: molar specific volume (= V/n)
a: (positive constant) net intermolecular attractive forces
b: finite volume of the molecules

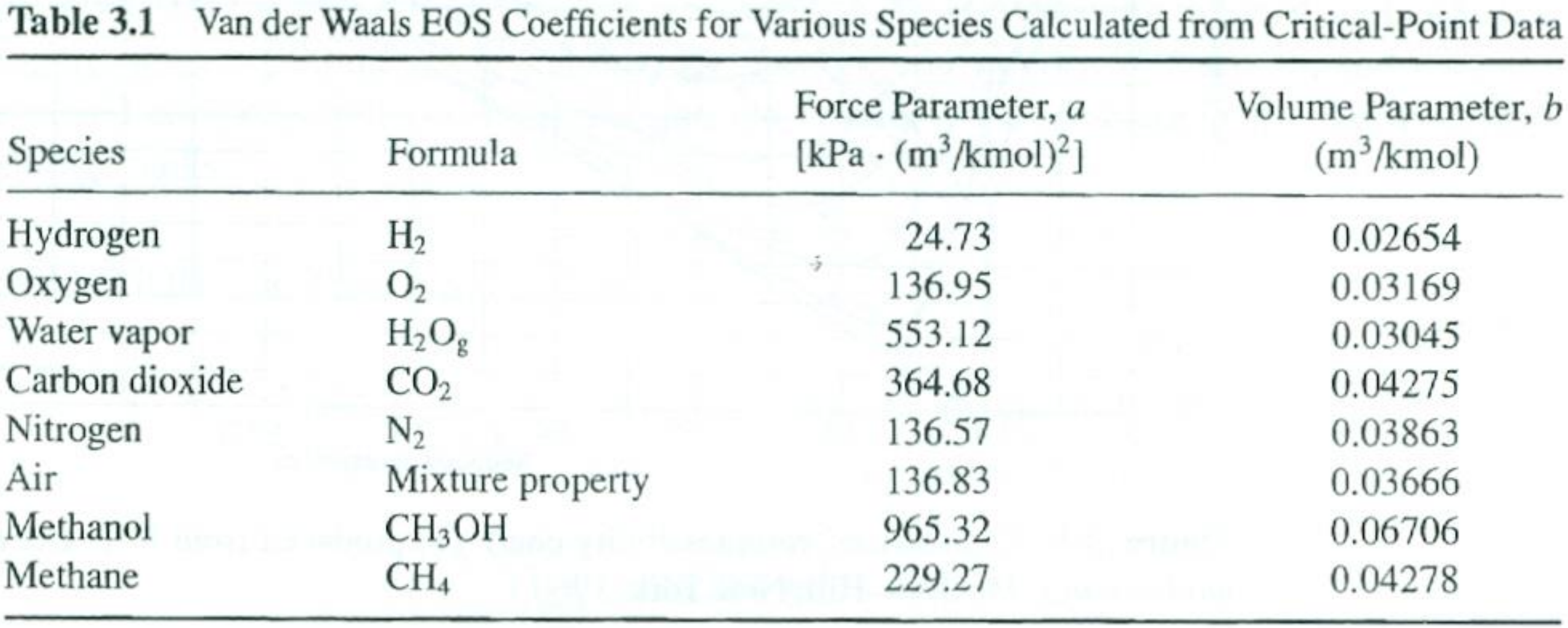


Table 3.1 Van der Waals EOS Coefficients for Various Species Calculated from Critical-Point Data

Species	Formula	Force Parameter, *a* [kPa · (m^3/kmol)^2]	Volume Parameter, *b* (m^3/kmol)
Hydrogen	H_2	24.73	0.02654
Oxygen	O_2	136.95	0.03169
Water vapor	H_2O_g	553.12	0.03045
Carbon dioxide	CO_2	364.68	0.04275
Nitrogen	N_2	136.57	0.03863
Air	Mixture property	136.83	0.03666
Methanol	CH_3OH	965.32	0.06706
Methane	CH_4	229.27	0.04278

A variety of other equation of state (EOS)

Compressibility factor $z = \frac{PV}{nRT}$

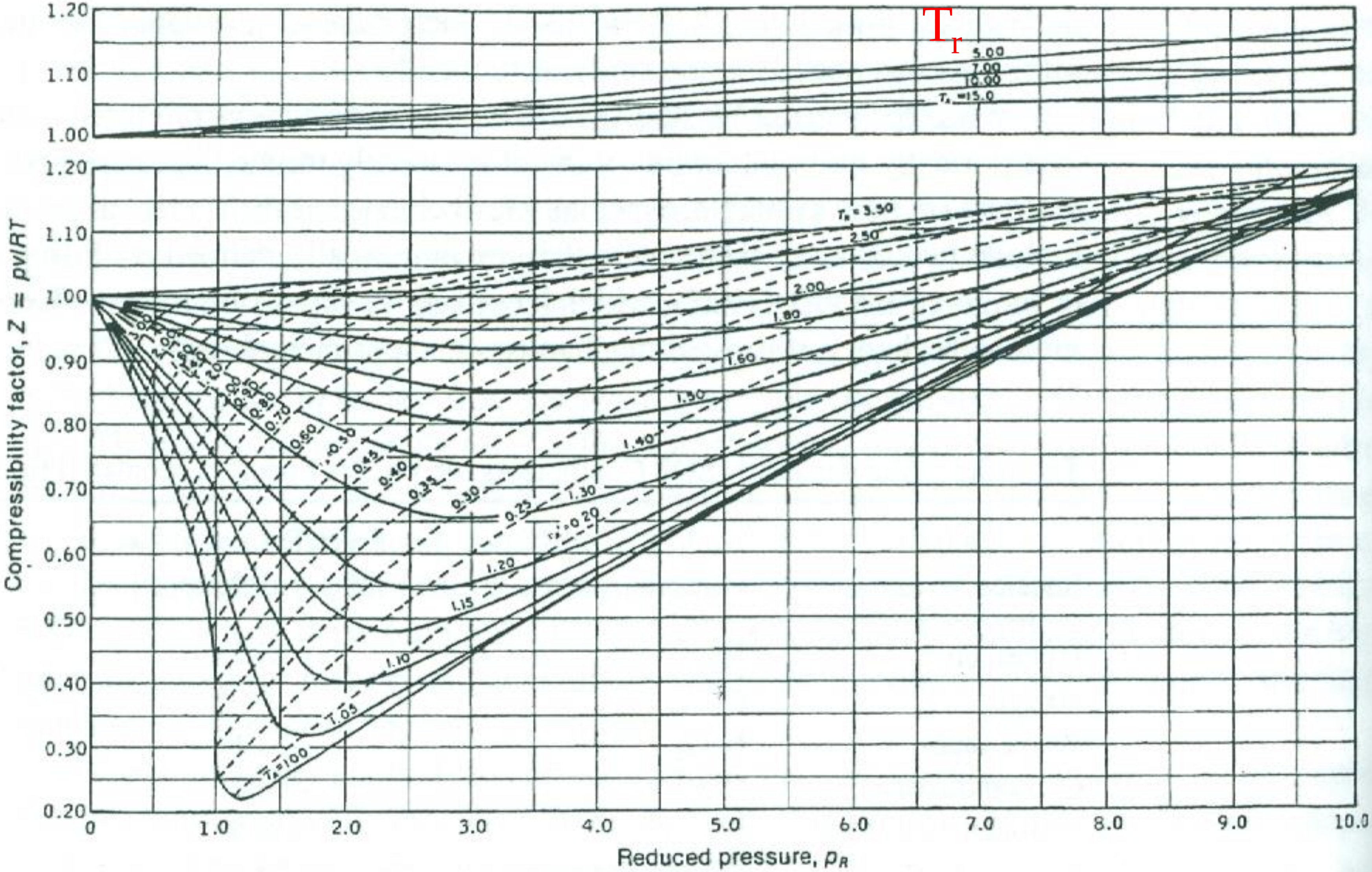


Figure 3.3 Generalized compressibility chart. (Reproduced from E. F. Obert, *Concepts of Thermodynamics*, McGraw-Hill, New York, 1960.)

Reduced pressure $P_r = P/P_c$, P_c: critical P $T_r = T/T_c$

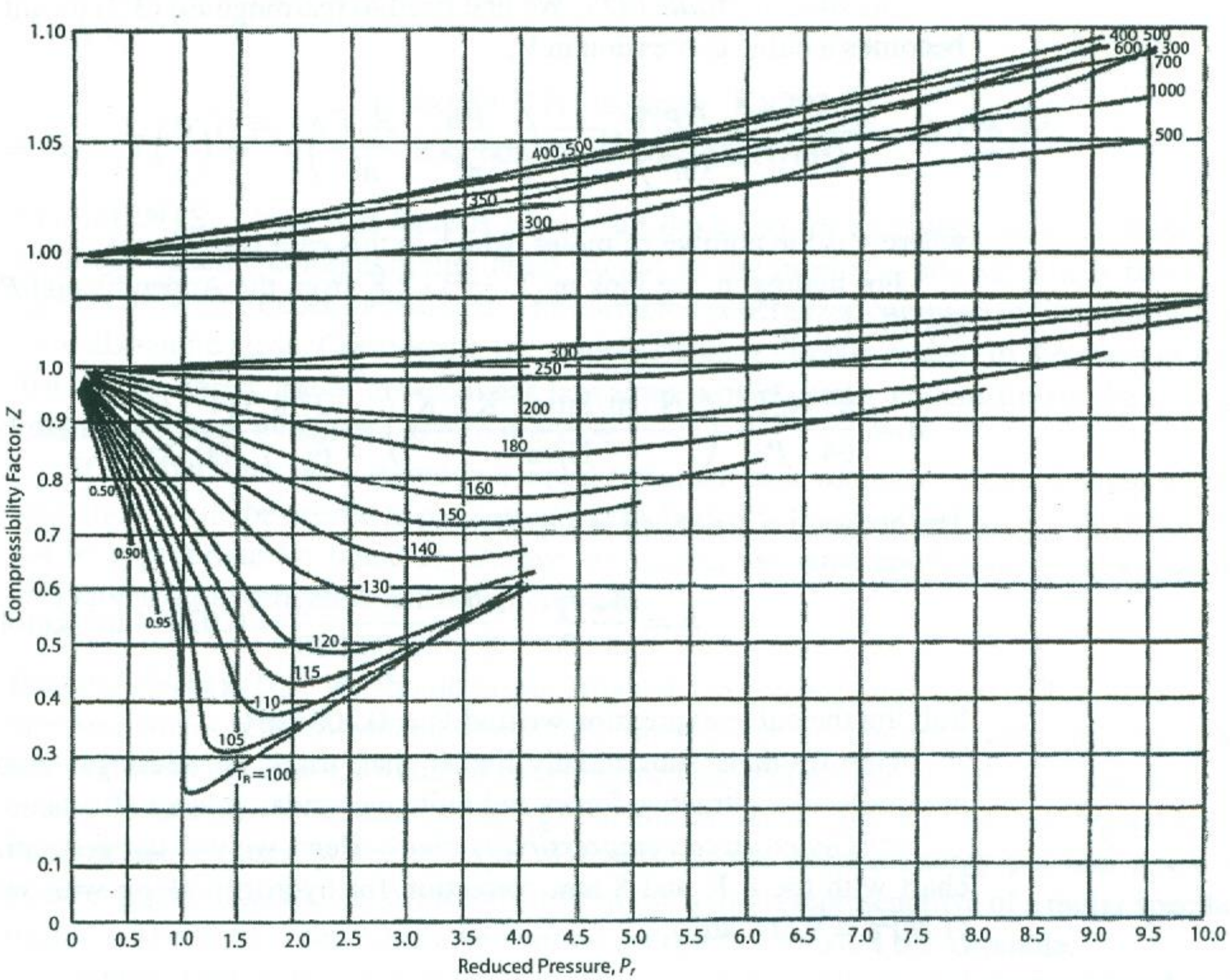


Figure 3.4 Experimentally measured hydrogen compressibility chart. (Reproduced with permission from [3]. Copyright American Chemical Society.)

Example 3.1 Hydrogen Storage Volume

Consider a hydrogen tank storage system for a fuel cell automobile. Seven kilograms of hydrogen gas compressed to 68 Mpa (approximately 10,000 psig) and stored at 20°C is required to provide a driving range of about 480km (approximately 300 miles). Using the ideal gas law, the van der Waals EOS, and the generalized compressibility chart, determine the interior volume required for the hydrogen storage tanks.

For van der Waals EOS, use Table 3.1

-Internal energy (U): total thermal energy stored in a system (cf. In textbook, U (kJ), u (kJ/kg), ū (kJ/kmol))

$$dE = dKE + dPE + dU = \delta Q - \delta W$$

Kinetic E Potential E

Internal energy: (i) translational motion of molecules (ii) vibrational motion (iii) rotational motion of molecules (iv) atomic level storage: inter or intramolecular forces, nuclear spin states

-Enthalpy (H): a measure of the energy stored in a flowing fluid

$$H = U + \frac{P}{\rho} = U + P\nu$$

ν: molar specific volume (= V/n), ρ: density

→ internal energy + flow work (energy required for flow of the fluid across the control volume boundary)

$$ħ = \bar{u} + Pν$$

For an ideal gas, $ħ = \bar{u} + RT$

-Constant pressure specific heat (c_p): the rate of change of enthalpy with temperature at constant pressure

$$C_p(T, P) = \frac{\partial ħ}{\partial T}$$

-Constant volume specific heat (c_v): the rate of change of enthalpy with temperature at constant volume

$$C_v(T, P) = \frac{\partial ħ}{\partial T}$$

T changes → rot & vib mode change → internal E change → specific hear change

Same energy input to two substances: substance with larger specific heat → lower increase in temperature

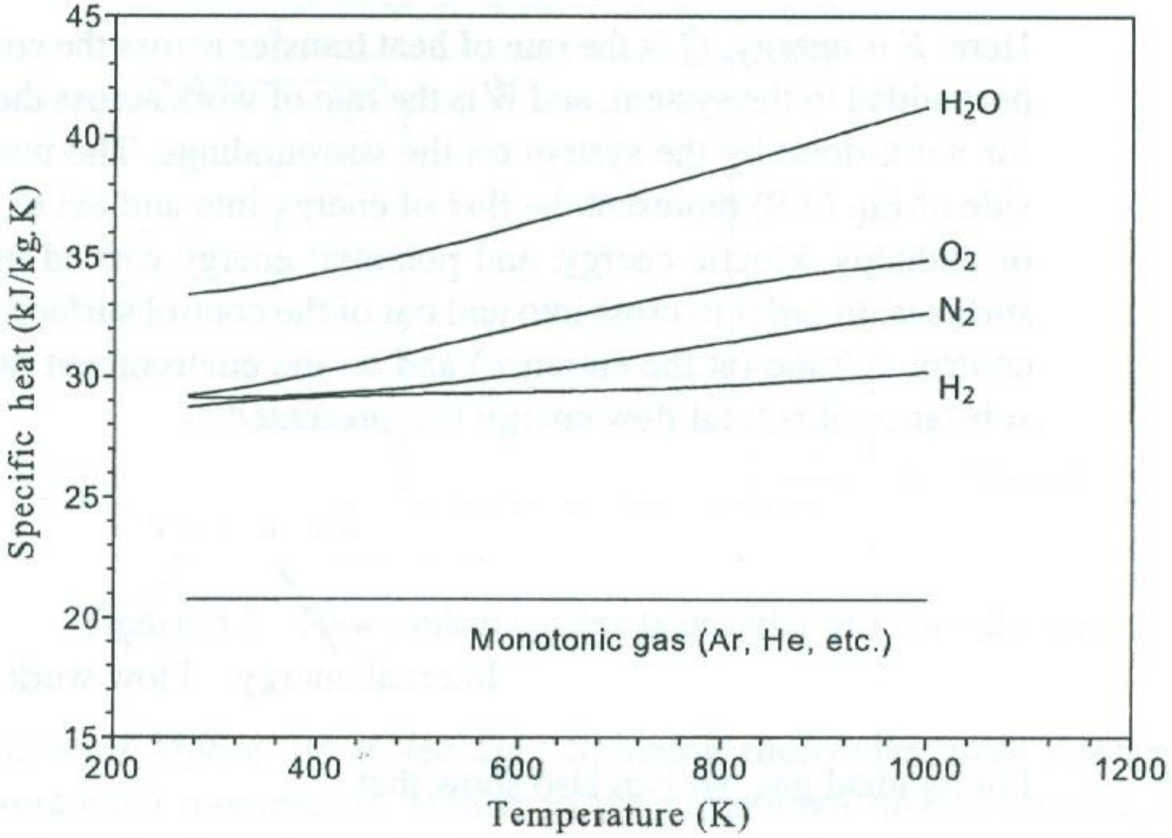


Figure 3.6 Specific heat as function of temperature for several species.

H_2O (high vib & rot) vs. He (no vib & rot)

-Gas-phase specific heat

- Most cases in fuel cells → ideal gas model is valid over the operating range
- Specific heat of an ideal gas is solely a function of temperature (insignificant dependence on pressure)

$$c_p(T) = \frac{d\hbar}{dT} \qquad\qquad c_v(T) = \frac{d\bar{u}}{dT}$$

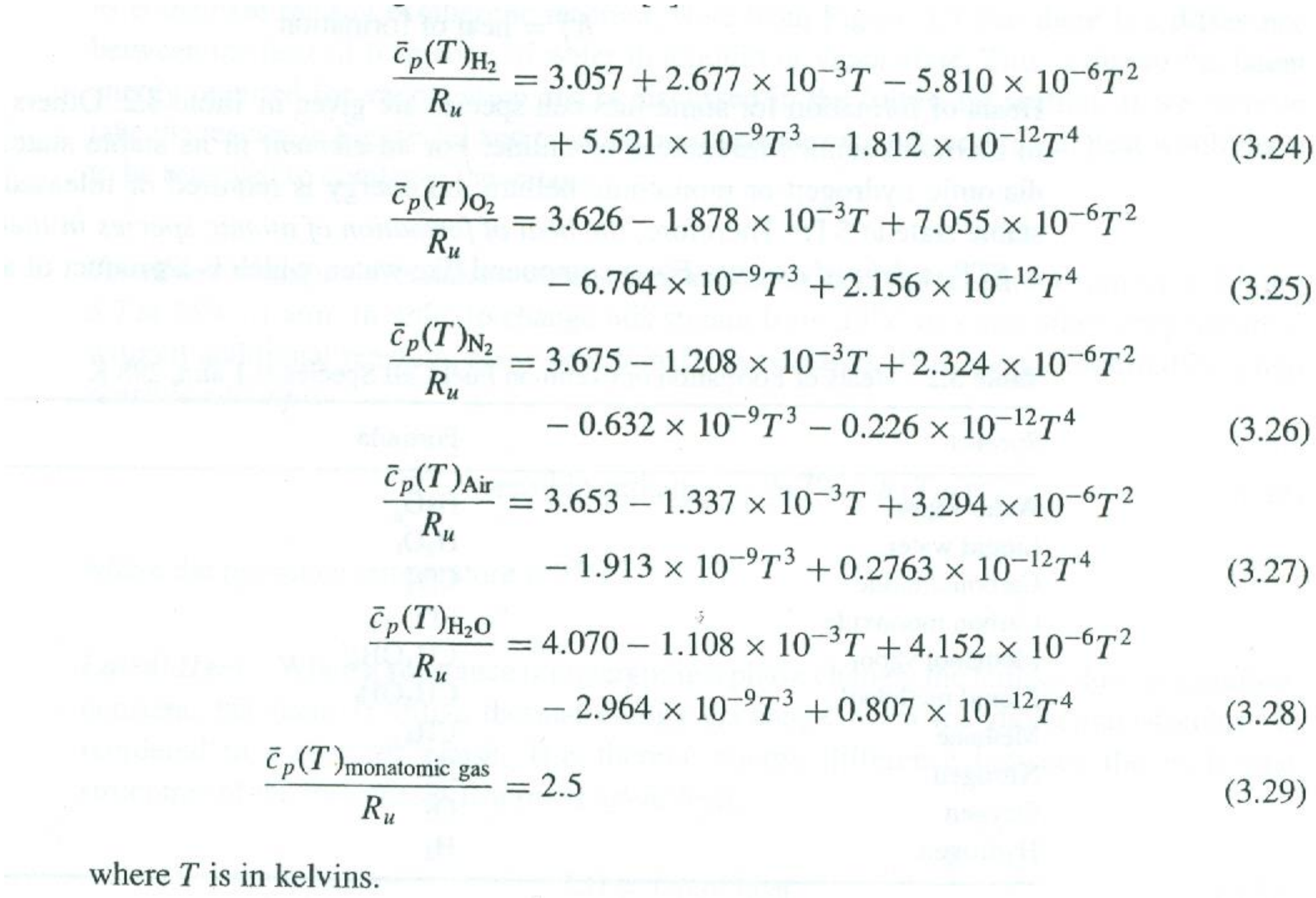
- Enthalpy change between two temperature states of nonreacting substance is known as “sensible enthalpy”

Assume constant $c_p(T)$,

- As shown Fig. 3.6, average T should be chosen to minimize inaccuracies → acceptable in FC since they tend to operate over a narrow T range

- More accurate ones,

- Polynomial expression (valid FC range of 300-1000K)



$$\frac{\bar{c}_p(T)_{H_2}}{R_u} = 3.057 + 2.677 \times 10^{-3}T - 5.810 \times 10^{-6}T^2 + 5.521 \times 10^{-9}T^3 - 1.812 \times 10^{-12}T^4 \quad (3.24)$$

$$\frac{\bar{c}_p(T)_{O_2}}{R_u} = 3.626 - 1.878 \times 10^{-3}T + 7.055 \times 10^{-6}T^2 - 6.764 \times 10^{-9}T^3 + 2.156 \times 10^{-12}T^4 \quad (3.25)$$

$$\frac{\bar{c}_p(T)_{N_2}}{R_u} = 3.675 - 1.208 \times 10^{-3}T + 2.324 \times 10^{-6}T^2 - 0.632 \times 10^{-9}T^3 - 0.226 \times 10^{-12}T^4 \quad (3.26)$$

$$\frac{\bar{c}_p(T)_{\mathrm{Air}}}{R_u} = 3.653 - 1.337 \times 10^{-3}T + 3.294 \times 10^{-6}T^2 - 1.913 \times 10^{-9}T^3 + 0.2763 \times 10^{-12}T^4 \quad (3.27)$$

$$\frac{\bar{c}_p(T)_{H_2O}}{R_u} = 4.070 - 1.108 \times 10^{-3}T + 4.152 \times 10^{-6}T^2 - 2.964 \times 10^{-9}T^3 + 0.807 \times 10^{-12}T^4 \quad (3.28)$$

$$\frac{\bar{c}_p(T)_{\text{monatomic gas}}}{R_u} = 2.5 \quad (3.29)$$

where T is in kelvins.

-Liquid-and solid-phase specific heat: density is constant

→

- No distinction between $c_p(T)$ and $c_v(T)$

e.g. Generally considered constant with T

mass specific heat of liquid water at 25℃ = 4.179 kJ/kg·K

at 100℃ = 4.218 kJ/kg·K

→ 1% higher

2. Heat of formation, sensible enthalpy, and latent heat

-Enthalpy of formation (or heat of formation): enthalpy at standard T and P (STP, 298K, 1atm), h_f°

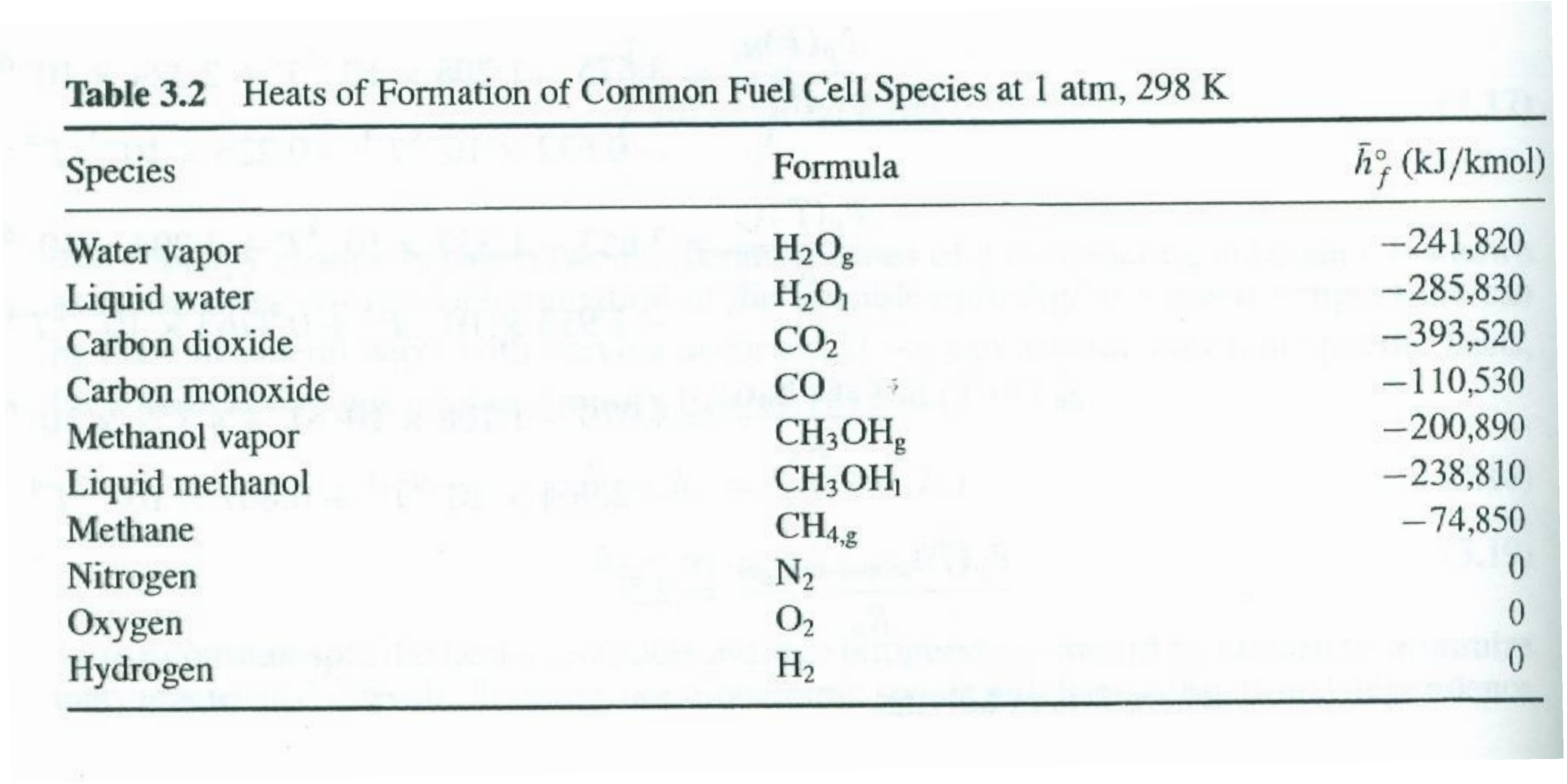


Table 3.2 Heats of Formation of Common Fuel Cell Species at 1 atm, 298 K

Species	Formula	$\bar{h}_f^{\circ}$ (kJ/kmol)
Water vapor	H_2O_g	−241,820
Liquid water	H_2O_l	−285,830
Carbon dioxide	CO_2	−393,520
Carbon monoxide	CO	−110,530
Methanol vapor	CH_3OH_g	−200,890
Liquid methanol	CH_3OH_l	−238,810
Methane	$CH_{4,g}$	−74,850
Nitrogen	N_2	0
Oxygen	O_2	0
Hydrogen	H_2	0

For an element (atomic species) in its stable state (e.g. H_2, He) → no energy is required or released to achieve a stable state at STP → $h_f^\circ = 0$

For water → product of exothermic reaction between O_2 and H_2

Energy is released → lower than the initial reactants → “negative” (exothermic reaction)

If liquid H_2O product → additional heat would have to be removed to condense the vapor

-Sensible enthalpy

Water vapor steam at 25℃, 1atm → to change other T without additional reaction, some heat transfer is required → this energy required is called “sensible enthalpy”

-Latent heat

- Substance under a phase change → no T change (T const), but still thermal energy exchange when the molecular structure is reordered to different phase → this thermal energy difference between the molecular structures of the two phases “latent heat (LH)”
- Consider a droplet evaporating at ambient pressure
  b.p. = 100℃ → energy required “latent heat of vaporization”, h_{lv}
  for water, h_{lv} = 2257 kJ/kg,
  enthalpy of condensation($v \rightarrow l$): -2257 kJ/kg

water freezing: energy release 334 kJ/kg ( )

melting, sublimation…

Example 3.2 Latent Heat of Vaporization

Consider a 1-mg droplet of liquid water at l atm pressure. Determine the sensible enthalpy required to heat the droplet from 25 to 100◦C, and the total energy required for complete vaporization.

-Total enthalpy

- Enthalpy at some state A = enthalpy of formation + sensible enthalpy + latent heat for any phase change

$$h_A = h_f^\circ + h_s + LH$$

→ at any T, the enthalpy is h_f° to arrive at STP plus h_s to heat (or cool) the substance to depart from STP plus LH to achieve the phase state at the given T

Example 3.3 Determination of Enthalpy of a Single Species

Determine the enthalpy per unit mass of water vapor at 600 K, 1 atm.

3. Determination of change in enthalpy for nonreacting species and mixtures

Preheated H_2 in SOFC intake from 300 to 600 K

Example 3.4 Calculation of Enthalpy for Nonreacting Species
Consider water vapor entering a SOFC. Determine the molar and mass specific enthalpy change required to heat the water vapor from a 298 K inlet temperature to 1073 K using
(a) constant specific heats at an average temperature and (b) evaluation of the integration of the proper polynomial expression for the specific heat.

-Nonreacting ideal gas mixture calculation

- In fuel cell, many cases are mixtures

→ for example, air (nitrogen + oxygen), partial pressure, $P_i = y_i P$

P: total mixture pressure, y_i: mole fraction of constituent i

$$y_i = n_i/n_{total} =$$

n_i: # of moles of species i,

& : molar flow rates of species i and the mixture

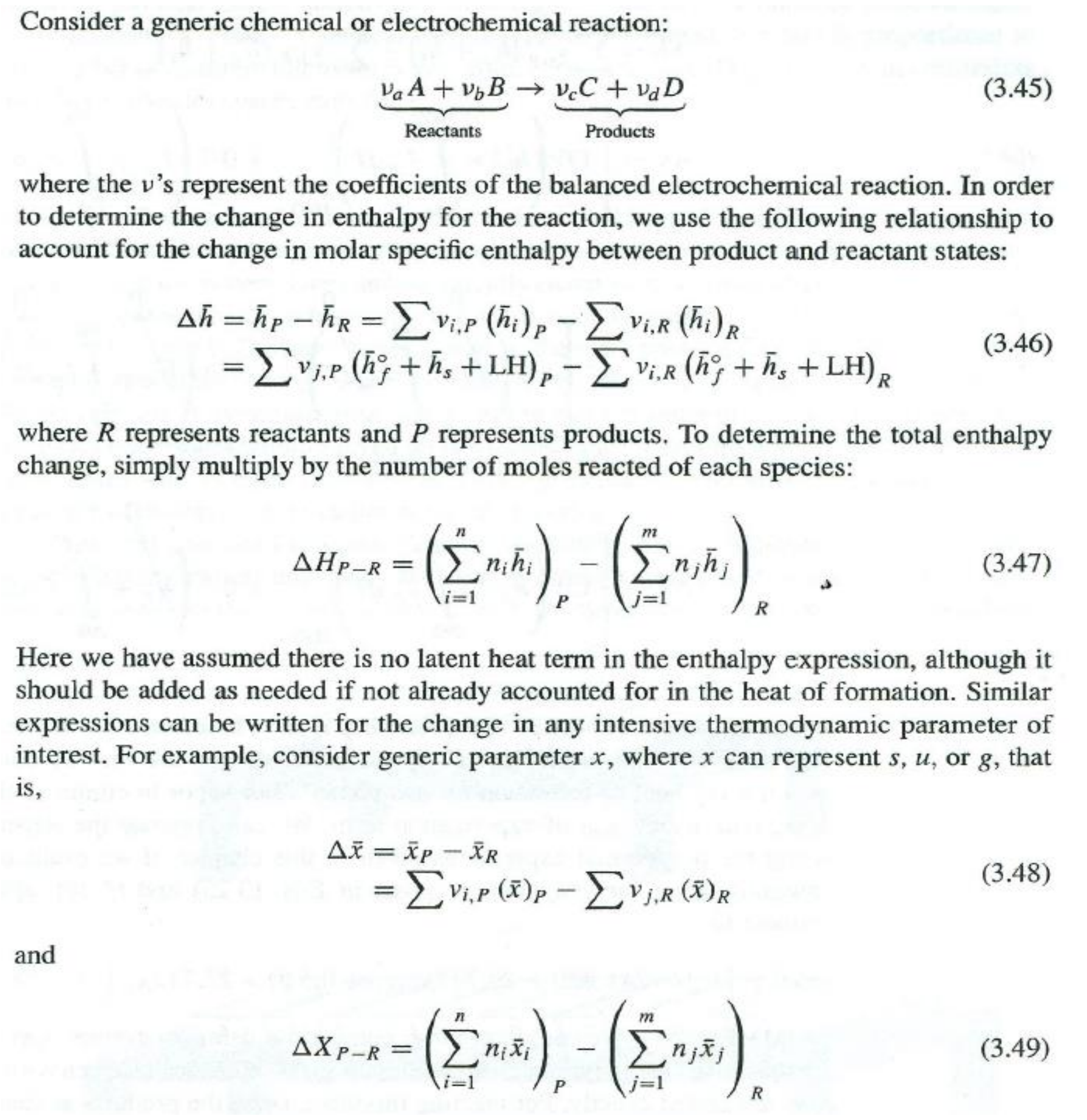
$$\sum P_i = P \text{ and } \sum y_i = 1,$$

: molar intensive thermodynamic parameter (e.g. enthalpy…)

Example 3.5 Determination of Nonreacting Ideal Gas Mixture Properties
Given a mixture of air (21% oxygen and 79% nitrogen by volume) at 2 atm pressure and 350 K, find
(a) the partial pressures of each species and (b) the mixture molar specific heat.

Example 3.6 Change in Properties for a Nonreacting Ideal Gas Mixture
Find the change in absolute enthalpy for a 3-kg mixture of air (21% O_2, 79% N_2 by volume) heated from 400 to 600 K.

4. Determination of change in enthalpy for reacting species and mixtures



Consider a generic chemical or electrochemical reaction:

$$\underbrace{\nu_a A + \nu_b B}_{\text{Reactants}} \rightarrow \underbrace{\nu_c C + \nu_d D}_{\text{Products}} \tag{3.45}$$

where the ν's represent the coefficients of the balanced electrochemical reaction. In order to determine the change in enthalpy for the reaction, we use the following relationship to account for the change in molar specific enthalpy between product and reactant states:

$$\begin{aligned}\Delta\bar{h} = \bar{h}_P - \bar{h}_R &= \sum v_{i,P}\left(\bar{h}_i\right)_P - \sum v_{i,R}\left(\bar{h}_i\right)_R \\ &= \sum v_{j,P}\left(\bar{h}_f^\circ + \bar{h}_s + \mathrm{LH}\right)_P - \sum v_{i,R}\left(\bar{h}_f^\circ + \bar{h}_s + \mathrm{LH}\right)_R\end{aligned} \tag{3.46}$$

where R represents reactants and P represents products. To determine the total enthalpy change, simply multiply by the number of moles reacted of each species:

$$\Delta H_{P-R} = \left(\sum_{i=1}^{n} n_i \bar{h}_i\right)_P - \left(\sum_{j=1}^{m} n_j \bar{h}_j\right)_R \tag{3.47}$$

Here we have assumed there is no latent heat term in the enthalpy expression, although it should be added as needed if not already accounted for in the heat of formation. Similar expressions can be written for the change in any intensive thermodynamic parameter of interest. For example, consider generic parameter x, where x can represent s, u, or g, that is,

$$\begin{aligned}\Delta\bar{x} &= \bar{x}_P - \bar{x}_R \\ &= \sum v_{i,P}\left(\bar{x}\right)_P - \sum v_{j,R}\left(\bar{x}\right)_R\end{aligned} \tag{3.48}$$

and

$$\Delta X_{P-R} = \left(\sum_{i=1}^{n} n_i \bar{x}_i\right)_P - \left(\sum_{j=1}^{m} n_j \bar{x}_j\right)_R \tag{3.49}$$

Example 3.7 Change in Enthalpy for Reacting Gas-Phase Mixture

Find the change in enthalpy per mole of hydrogen for combustion of a 50% hydrogen–50% oxygen mixture (by mole) at 298 K. The final product is water vapor and oxygen at 1000 K.

-Entropy (S): randomness

$$S = k_B \ln\Omega$$

k_B: Boltzmann’s constant ($1.3807 \times 10_{-23}$ J/K)
Ω: # of thermodynamically available quantum microstates

1st law,

-Determination of entropy for ideal gas

Using ideal gas law

Entropy change can be broken down into T-dependent and P-dependent portions

-Determination of entropy for nonreacting liquids & solids (pressure dependence of entropy negligible, c_p constant over T)

-Determination of entropy for ideal gas

Using ideal gas law

Entropy change can be broken down into T-dependent and P-dependent portions

-Determination of entropy for nonreacting liquids & solids (pressure dependence of entropy negligible, c_p constant over T)

-Determination of change in entropy for nonreacting gas mixture
Using ideal gas law

-Determination of change in entropy for reacting gas mixture

-Gibbs function (G): a measure of the mixture work possible at a given state from a const T & P reversible process

$$G \equiv H - TS$$

$$dG = dH - TdS - SdT$$

- For 1st law for simple compressible system at const T & P with only compression work

Gibbs function of a system will always be minimized in a spontaneous process ($dG < 0$)

When the Gibbs energy reaches a local minimum, where the change is zero (dG = 0), the reaction stops and local thermodynamic equilibrium is achieved

- Gibbs free energy ≡ Gibbs function
- Absolute molar intensive Gibbs free energy at given T & P

- Change between two states

- g_f° (Gibbs energy of formation) is calculated based on 298K,1atm zero for stable species in their natural state
- For reacting mixtures,

5. Psychrometrics(습공기 선도): Thermodynamics of moist air mixtures

-The study of nonreacting moist air mixtures

-critical to understand the water balance in low T polymer electrolyte fuel cell (PEFC(or PEMFC))

- In PEFC, water balance is critical to maintain proper electrolyte conductivity while avoiding electrode flooding

Air + vapor, $P = P_a + P_v = y_a P + y_v P$

For humidified anode fuel mixture of CO_2, CO, H_2, H_2O vapor,

$$P = P_{CO2} + P_{H2} + P_{CO} + P_v$$

Humidity ratio, $w = m_v/m_{dry} =$

↓

mass of moisture per mass of dry mixture → rate of moisture mass flow per dry mass flow

- Considering the mixture as an ideal gas

$$w = m_v/m_{dry} =$$

- For air, MW_{dry} = 28.85 kg/kmol

  $w = m_v/m_{dry} =$

P: total pressure, P_v: water partial pressure, P_a: air partial pressure

- Humidity ratio in pure hydrogen humidified stream

  $w = m_v/m_{dry} =$

- Relative humidity: the ratio of actual water vapor pressure(P_v) to the saturation water vapor pressure(P_{sat}). e.g. weather forecast

  $RH = P_v/P_{sat}(T)$, (RH =1 when $P_v = P_{sat}$)

Saturation pressure-temperature for water (Fig.3.12)

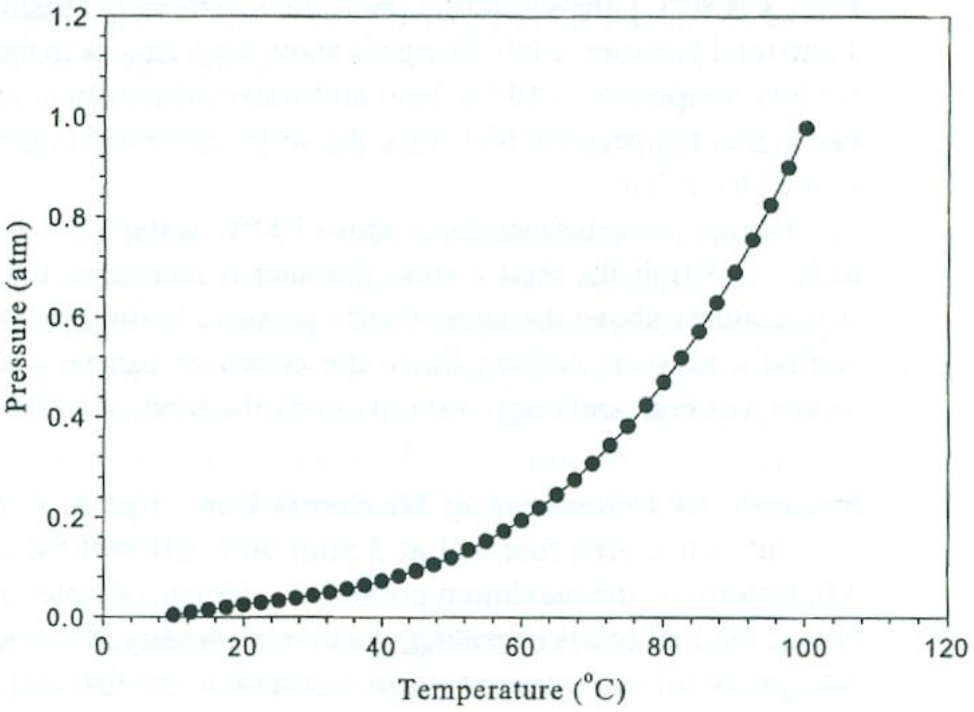


Figure 3.12 Saturation pressure versus temperature for water.

Example 3.8 Calculation of Maximum Water Uptake in a Flow

Given a flow inlet to a 5-cm^2 active area fuel cell at 3 atm, 50% RH at 80◦C, and an anode stoichiometry of 3.0. Determine the maximum possible molar rate of water uptake from the incoming anode flow if the fuel cell is operating at a current density of 0.8 A/cm^2. You can assume the flow rate, pressure, and temperature are constant in the fuel cell.

6. Thermodynamic efficiency of a fuel cell

-FC: conversion of chemical energy into electrical energy

-**Thermodynamic efficiency of FC**

$$\eta_{th} = \frac{\text{actual electrical work}}{\text{maximum available work}}$$

-**Maximum electrical work** for a reversible process

1st law, $dU = \delta Q - \delta W$

mechanical expansion work → electrical work

$$\delta W = \delta W_p + \delta W_e = PdV + \delta W_e$$

for a reversible system, 2nd law, $\delta Q = TdS$

differential change in Gibbs free energy for const T, P

$$dG = dH - TdS - \cancel{SdT}$$

differential change in enthalpy for a given reaction

$$dH = dU + PdV + \cancel{VdP}, \qquad dU = TdS - \delta W_e - PdV$$

→ $-dG = \delta W_e$ in reversible system → maximum electrical work

- The change in Gibbs energy is related to the max. conversion of chemical to electrical energy for a given rxn

-Maximum expected voltage (E°)

- electrical work: moving of an electron through a distance

→ energy(work) required to move a given change

$$w_e = nFE = \left(\frac{\text{eq e-}}{\text{mol reactant}}\right)\left(\frac{\text{C}}{\text{eq e-}}\right)\left(\frac{\text{J}}{\text{C}}\right)$$

- Max. possible reversible voltage of an electrochemical cell

$$E^\circ = \frac{-\Delta g}{nF} = \frac{-\Delta G}{nF}$$

-Thermal voltage (E^{oo}): all the potential chemical energy for a rxn goes into electrical work

dU G $= dH - TdS$ → if there were no heat transfer, no entropy change

→ $dG = dH$

$E^{oo} = E_{th} = \frac{-\Delta H}{nF}$ → max. voltage for a reversible, adiabatic system

- Since there is an enthalpy entropy change associated with every real rxn process → this voltage is merely a limit representing the case of all chemical energy converted into electrochemical work, with no heat transfer or change in available microstates (entropy)

-Maximum thermodynamic efficiency

- ratio of max expected voltage(E^o) to thermal voltage(E^{oo}) = max electrical work to total available potential electrical work = max thermodynamic efficiency

$$\eta_{t,max} = \frac{\text{max electrical work}}{\text{max available work}} = \frac{-\Delta G/nF}{-\Delta H/nF} = \frac{E^o}{E^{oo}} = \frac{\Delta H - T\Delta S}{\Delta H} = 1 - \frac{T\Delta S}{\Delta H}$$

Table 3.3

- cf. ideal Carnot cycle heat engine

$$\eta_{t,max} = 1 - \frac{T_L}{T_H}$$

→ FC: non constrained to a Carnot efficiency → does not mean a FC can have unlimited efficiency

Fig. 3.13: ideal heat engine vs. ideal hydrogen FC

Table 3.3 Enthalpy of Formation, Gibbs Energy of Formation, and Entropy Values at 298 K, 1 atm

Species	Molecular Formula	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol · K)
Carbon	C_s	0	0	5.74
Hydrogen	$H_{2,g}$	0	0	130.57
Nitrogen	$N_{2,g}$	0	0	191.50
Oxygen	O_{2g}	0	0	205.03
Carbon monoxide	CO_g	−110,530	−137,150	197.54
Carbon dioxide	$CO_{2,g}$	−393,520	−394,380	213.69
Water vapor	H_2O_g	−241,820	−228,590	188.72
Liquid water	H_2O_l	−285,830	−237,180	69.95
Hydrogen peroxide	$H_2O_{2,g}$	−136,310	−105,600	232.63
Ammonia	$NH_{3,g}$	−46,190	−16,590	192.33
Hydroxyl	OH_g	39,460	34,280	183.75
Methane	$CH_{4,g}$	−74,850	−50,790	186.16
Ethane	$C_2H_{6,g}$	−84,680	−32,890	229.49
Propane	$C_3H_{8,g}$	−103,850	−23,490	269.91
Octane vapor	$C_8H_{18,g}$	−208,450	17,320	463.67
Octane liquid	$C_8H_{18,l}$	−249,910	6,610	360.79
Benzene	$C_6H_{6,g}$	82,930	129,660	269.20
Methanol vapor	CH_3OH_g	−200,890	−162,140	239.70
Methanol liquid	CH_3OH_l	−238,810	−166,290	126.80
Ethanol vapor	$C_2H_5OH_g$	−235,310	−168,570	282.59
Ethanol liquid	$C_2H_5OH_l$	−277,690	−174,890	160.70

Source: From [1].

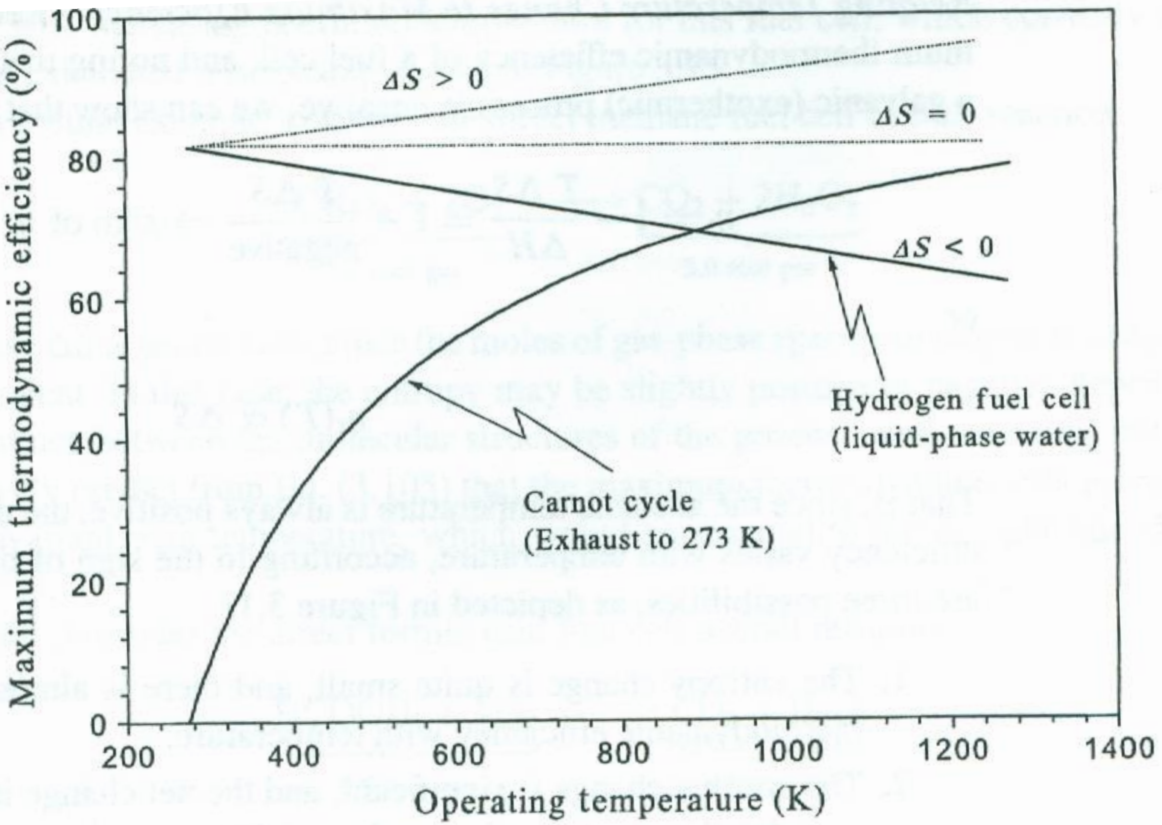


Figure 3.13 Comparison of maximum thermodynamic efficiency for heat engine (Carnot cycle) and fuel cell engine (hydrogen fuel cell, HHV assumed).

- At higher T → heat engine theoretically more efficient (not always efficient for a fuel cell)
- FC shows a decreasing efficiency with T

-Relating T change to max efficiency

$$\eta_t = 1 - \frac{T\Delta S}{\Delta H}$$

-Le chatelier's principles: OCV(open circuit voltage) dependence

- Any change in one of the variables that determines the state of system in equilibrium causes a shift in the position of equilibrium in a direction that tends to counteract the change in the variable under consideration
- In FC, the principle can be applied to a change in T or P on voltage

In hydrogen FC,

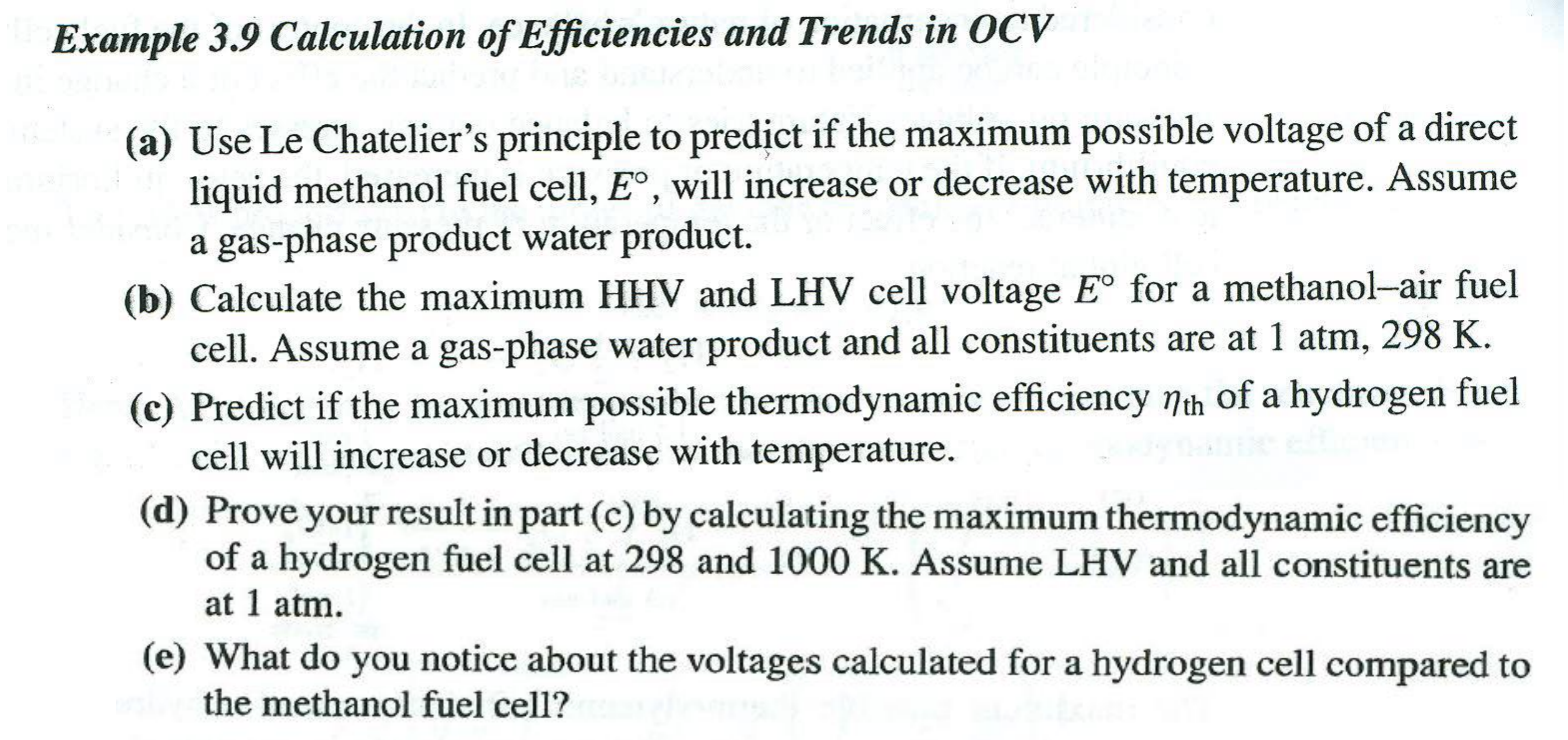
(i) P of reactants↑ → forward rxn(H_2 oxidation)↑ (←gas mole↓)
(ii) P of reactants↓ → reverse rxn↑ → voltage↓

→ Le Chatelier's principle → Nernst equation(OCV) as a function of T & P

-Heating value

For rxn involving water as a product,

- High heating value(HHV, 고위발열량): it is assumed all the product water is in the **liquid** phase
- Low heating value(LHV, 저위발열량): **gas** phase. LHV will result in a lower calculated thermal voltage, since some energy is used for the latent heat of vaporization of the liquid → In practice, the LHV is completely appropriate for high T FC



Example 3.9 Calculation of Efficiencies and Trends in OCV

(a) Use Le Chatelier's principle to predict if the maximum possible voltage of a direct liquid methanol fuel cell, E°, will increase or decrease with temperature. Assume a gas-phase product water product.

(b) Calculate the maximum HHV and LHV cell voltage E° for a methanol–air fuel cell. Assume a gas-phase water product and all constituents are at 1 atm, 298 K.

(c) Predict if the maximum possible thermodynamic efficiency η_{th} of a hydrogen fuel cell will increase or decrease with temperature.

(d) Prove your result in part (c) by calculating the maximum thermodynamic efficiency of a hydrogen fuel cell at 298 and 1000 K. Assume LHV and all constituents are at 1 atm.

(e) What do you notice about the voltages calculated for a hydrogen cell compared to the methanol fuel cell?

7. **Maximum expected OCV: Nernst voltage**

-Thermal voltage(E^{oo}) is function of only T,
reversible voltage(E^{o}) is function of T & P of reactants & products
→ Nernst equation is an expression of the max possible open circuit (zero cell current) voltage as a function of T & P and is an expression of an established thermodynamic equilibrium

$$\nu_A A + \nu_B B \rightarrow \nu_C C + \nu_D D$$

ν: stoichiometric coefficient of balanced electrochemical rxn

In equilibrium, $\Delta G = \Delta G^{o} - RT\,ln[(a_A^{\nu_A} a_B^{\nu_B})/(a_C^{\nu_C} a_D^{\nu_D})]$

a: thermodynamic activity coefficient

To convert to voltage,

$$E(T,P) = \underbrace{\Delta G^{o}/nF}_{\substack{\text{T dependent voltage} \\ \text{evaluated at 1 atm P}}} - \underbrace{(RT/nF)\,ln[(a_A^{\nu_A} a_B^{\nu_B})/(a_C^{\nu_C} a_D^{\nu_D})]}_{\substack{\text{activity dependence} \\ \text{on Nernst voltage}}}$$

-Activity

(i) For concentrated solution → a =1

(ii) For ideal gas, $a = P_i/P^o$, where P_i is partial P, P^o = reference P (1 atm (101,325 Pa))

(iii) For water vapor, partial P of the vapor cannot exceed the saturation P (P_{sat}), which is a function of T. Thus, reference P (P^o) is set to P sat, and $a = P_v/P_{sat}$ (= relative humidity (RH)). For water generating electrode, a = 1

For an ideal gas rxn mixture,

$$E(T,P) = \Delta G^o/nF - (RT/nF)\,ln\{[(P_A/P^o)^{\nu_A}(P_B/P^o)^{\nu_B}]/[(P_C/P^o)^{\nu_C}(P_D/P^o)^{\nu_D}]\}$$

Example 3.10 Nernst Equation for Hydrogen Air Fuel Cell

Given a hydrogen air fuel cell operating at 353 K. Solve for the expected LHV open-circuit voltage if the hydrogen and water vapor mole fractions in the anode are 0.8 and 0.2, respectively, and the oxygen, nitrogen, and water vapor mole fractions in the cathode are 0.15, 0.75, and 0.1, respectively. The cathode and anode pressures are 3 and 2 atm, respectively.

Example 3.11 Thermodynamic Effect of Oxygen Enhancement

Given an H_2–air fuel cell operating at 100◦C with vapor phase water as the product. Determine the approximate expected change in voltage if air is replaced with oxygen, with all else remaining the same.

Example 3.12 Thermodynamic Effect of a Pressure Increase

Given an H_2–air fuel cell operating at 60◦C with vapor-phase water as the product. Determine the approximate expected change in thermodynamic maximum OCV if the cathode pressure is doubled and all else stays the same.

Example 3.13 Expected OCV

Given a H_2–O_2 PEFC with the following properties:

$$H_2 + 1/2O_2 \rightarrow H_2O$$

Anode: y_{H2} =40%, y_{H2O} =20%, y_{O2} =5%, y_{N2} =35%, pressure=4 atm, and $\lambda_a = 1.5$.
Cathode: y_{O2} =20%, y_{H2O} =10%, y_{N2} =70%, pressure=6 atm, and λ_c =2.5.

Find: (a) Maximum expected OCV at 90°C (b) Change in voltage if we take our cathode down to 3 atm, all else the same (c) Ratio of initial to final voltage expected if we boost oxygen mole fraction to 40% and reduce nitrogen fraction to 50% in the cathode

8. Summary