APPENDIX M

SAMPLE CALCULATIONS OF TRANSPORT PROPERTIES

Sample No. 052642000

	Feed		Product	
	gm-mol/hr	mol %	gm-mol/hr	mol %
H_2	0.6705	21.9570	0.5700	19.1917
CO	0.8330	27.2784	0.7848	26.4262
C_2H_4	0.4685	15.3420	0.4533	15.2644
CO_2	0.6946	22.7462	0.7085	23.8570
CH_4	0.3871	12.6764	0.4316	14.5342
C_2H_6	0.0	0.0	0.0216	0.7266
Total	3.0537		2.9698	

Reaction temperature: T = 507.04 °K,

Reaction pressure: P = 10.53 atm,

Average molecular weight of product: M = 25.1208 $\frac{gm}{mol}$,

Net reactant conversion: 8.3092 %

The viscosity calculations were based on the method described in the book of Reid et al. [180] and all data were obtained from the same source.

Critical Properties and Lennard-Jones Potentials [180]

Component	Critical Temperature T_c (°K)	Critical Pressure P_c (atm)	Critical Volume V_c (cc/mol)	Critical Compressibility Z_c	$\frac{\epsilon}{k}$ (°K)	σ (Å)
H_2	33.2	12.8	65.0	0.305	59.7	2.827
CO	132.9	34.5	93.1	0.295	91.7	3.690
C_2H_4	282.4	49.7	129.0	0.276	224.7	4.163
CO_2	304.2	72.8	94.0	0.274	195.2	3.941
CH_4	190.6	45.4	99.0	0.288	148.6	3.758
C_2H_6	305.4	48.2	148.0	0.285	215.7	4.443

For pure nonpolor gas at low pressure, the viscosity, μ, can be calculated by Chapman-Enskog equation [180]:

$$\mu = 26.69\left(\frac{\sqrt{MT}}{\sigma^2 \Omega_v}\right) \quad \text{in } \mu P \qquad \text{(M.1)}$$

Here, an empirical equation proposed by Nuefeld et al. [180] is used to evaluate

$$\Omega_v = \frac{A}{T^{*B}} + \frac{C}{e^{DT^*}} + \frac{E}{e^{FT^*}} \qquad \text{(M.2)}$$

where $T^* = \left(\frac{k}{\varepsilon}\right)T$, (M.3)

$A = 1.16145$,

$B = 0.14874$,

$C = 0.52487$,

$D = 0.77320$,

$E = 2.16178$,

and $F = 2.43787$.

The viscosities of individual component gases were calculated and are listed below:

Component	T^*	Ω_v	μ (μP)
H_2	8.49313	0.84565	126.26215
CO	5.52933	0.90791	257.29460
C_2H_4	2.25652	1.12955	162.61069
CO_2	2.59754	1.08200	237.24999
CH_4	3.41211	1.00570	169.48480
C_2H_6	2.35067	1.11506	149.72145

Foa a gas mixture at low pressure, the viscosity, μ_m, can be estimated using the mixing rule below [180]:

$$\mu_m = \sum_{i=1}^{n} \frac{y_i \mu_i}{\sum_{j=1}^{n} y_j \phi_{ij}} \qquad (M.4)$$

Here, Wilke's approximation is used to evaluate ϕ_{ij},

$$\phi_{ij} = \frac{[1 + (\frac{\mu_i}{\mu_j})^{\frac{1}{2}}(\frac{M_j}{M_i})^{\frac{1}{4}}]^2}{[8(1 + \frac{M_i}{M_j})]^{\frac{1}{2}}} \qquad (M.5)$$

or,

$$\phi_{ji} = \frac{\mu_j M_i}{\mu_i M_j} \phi_{ij} \qquad (M.6)$$

and y_i is the mole fraction of component i.

All values of ϕ_{ij} were calculated and are summarized in the table below:

j \ i	H_2	CO	C_2H_4	CO_2	CH_4	C_2H_6
H_2	---	0.27717	0.23073	0.19760	0.33731	0.21404
CO	1.88978	---	0.80490	0.76090	1.05333	0.75142
C_2H_4	2.49304	1.27557	---	0.95373	1.33281	0.92734
CO_2	2.29571	1.29656	1.02547	---	1.31923	0.95677
CH_4	1.99971	0.91587	0.73127	0.67318	---	0.67813
C_2H_6	2.69238	1.38628	1.07955	1.03589	1.43882	---

The molecular weights of individual components used in the calculations are $M_{H_2} = 2.016$, $M_{CO} = 28.010$, $M_{C_2H_4} = 28.054$, $M_{CO_2} = 44.010$, $M_{CH_4} = 16.043$, and $M_{C_2H_6} = 30.070$.

The viscosity of the product mixture can now be calculated as $\mu_m = 218.77690$ µP.

To correct the viscosity of a gas mixture at high pressure, following empirical equation of Dean and Stiel will be used.

$$(\mu_m - \mu_m^\circ)\xi_m = 1.08\left(e^{1.439\rho_{r_m}} - e^{-1.11\rho_{r_m}^{1.858}}\right) \quad \text{(M.7)}$$

where μ_m is the high-pressure mixture viscosity, in μP,

μ_m° is the low-pressure mixture viscosity, in μP,

ρ_{r_m} is the pseudo reduced mixture density, $\frac{\rho_m}{\rho_{c_m}}$ (M.8)

ρ_m is the mixture density, in g-mol/cm^3,

ρ_{c_m} is the pseudo critical mixture density, in g-mol/cm^3,

$$\rho_{c_m} = \frac{P_{c_m}}{Z_{c_m} R T_{c_m}} \quad \text{(M.9)}$$

and,

$$\xi_m = \frac{T_{c_m}^{1/6}}{M_m^{1/2} P_{c_m}^{2/3}} \quad \text{(M.10)}$$

Using Prausnitz and Gunn combination rules, following equations can be employed to evaluate the pseudocritical properties for the gas mixture:

$$T_{c_m} = \sum_{i=1}^{n} y_i T_{c_i} \tag{M.11}$$

$$V_{c_m} = \sum_{i=1}^{n} y_i V_{c_i} \tag{M.12}$$

$$Z_{c_m} = \sum_{i=1}^{n} y_i Z_{c_i} \tag{M.13}$$

$$P_{c_m} = \frac{Z_{c_m} R T_{c_m}}{V_{c_m}} \tag{M.14}$$

They are: T_{cm} = 187.09295 °K,

V_{cm} = 94.65828 cm^3/gm-mol,

Z_{cm} = 0.28792,

and P_{cm} = 46.68681 atm.

For the mixture gas at 140 psig = 10.5264 atm, and 507.04 °K, the reduced pressure P_{r_m} and temperature T_{r_m} are:

$$P_{r_m} = \frac{10.5264 \text{ atm}}{46.6868 \text{ atm}} = 0.2255, \qquad \text{(M.15)}$$

and

$$T_{r_m} = \frac{507.04 \text{ °K}}{187.09 \text{ °K}} = 2.7101. \qquad \text{(M.16)}$$

From the generalized compressibility chart of Figure 3-1 on pp. 27 of the book of Reid et al. [180], $Z_{c_m} \approx 0.998$, and so the pseudo critical density of the gas mixture can be calculated, $\rho_{c_m} = 0.01056$ g-mol/cm^3 by Eqn. (M.9). Also from Eqn. (M.10), $\xi_m = 0.0368$.

The molar density of the product gas at 507.04 °K and 10.5264 atm can be estimated as below:

$$\rho_m = \frac{10.5264 \text{ atm}}{(0.998)(82.06 \text{ cm}^3\text{-atm/g-mol}\cdot\text{°K})(507.04 \text{ °K})}$$

$$= 0.00025 \frac{\text{g-mol}}{\text{cm}^3} \qquad \text{(M.17)}$$

The pseudo reduced molar density, ρ_{r_m}, is calculated by Eqn. (M.8), $\rho_{r_m} = 0.0237$. Plugging $\mu_m^\circ = 218.7769\ \mu P$, $\xi_m = 0.0368$, and $\rho_{r_m} = 0.0237$ into Eqn. (M.7), the viscosity of the product gas is corrected, $\mu_m = 219.840\ \mu P$.

The kinematic viscosity for the product gas, ν_m, can be calculated as below:

$$\nu_m = \frac{\mu_m}{\rho_m} \qquad \text{(M.18)}$$

$$= \frac{(219.840\ \mu P)\left(\frac{1\ P}{10^6\ \mu P}\right)\left(\frac{1\ \frac{g}{cm\text{-}sec}}{1\ P}\right)}{\left(0.00025\ \frac{g\text{-}mol}{cm^3}\right)\left(25.1208\ \frac{g}{g\text{-}mol}\right)}$$

$$= 0.0350\ \frac{cm^2}{sec}$$

The cross section of the fixed-bed is

$$A = \frac{\pi}{4}\left[\left(0.25 - 0.035\text{x}2\ \text{in}\right)\left(2.54\ \frac{\text{cm}}{\text{in}}\right)\right]^2$$

$$= 0.1642\ \text{cm}^2 \qquad \text{(M.19)}$$

The superficial velocity across the bed is

$$u_{\text{superficial}} = \frac{\left(2.9698\ \frac{\text{g-mol}}{\text{hr}}\right)\left(\frac{1\ \text{hr}}{3600\ \text{s}}\right)}{\left(0.00025\ \frac{\text{g-mol}}{\text{cm}^3}\right)\left(0.1642\ \text{cm}^2\right)}$$

$$= 20.0961\ \text{cm/s} \qquad \text{(M.20)}$$

The interstitual velocity can be calculated by:

$$u_{\text{interstitual}} = \frac{u_{\text{superficial}}}{\text{void fraction}} \qquad \text{(M.21)}$$

$$u_{interstitial} = \frac{20.0961 \frac{cm}{s}}{0.563}$$

$$= 35.6947 \frac{cm}{s}$$

The Reynolds number based on the mean particle diameter (d_p = 0.015 cm) is,

$$Re_p = \frac{d_p u_{inst.}}{\nu_m}$$

$$= \frac{(0.015 \text{ cm})(35.6947 \frac{cm}{s})}{0.0350 \frac{cm^2}{s}}$$

$$= 15.3 \qquad \text{(M.22)}$$

The axial aspect ratio is calculated by:

$$\frac{z}{d_p} = \frac{(2\frac{3}{16}\ \text{in})(2.54\ \frac{\text{cm}}{\text{in}})}{0.015\ \text{cm}}$$

$$= 370.42 \qquad \text{(M.23)}$$

Assume that the effective diffusivity, D_{eff}, obtained in Eqn. (B.21) of Appendix B can be used to approximate the bulk axial diffusivity D_a, then the Peclet number for axial mass transfer can be determined as follow,

$$Pe = \frac{d_p u}{D_a}$$

$$= \frac{(0.015\ \text{cm})(35.6947\ \frac{\text{cm}}{\text{s}})}{0.0016\ \frac{\text{cm}^2}{\text{s}}}$$

$$= 334.64 \qquad \text{(M.24)}$$