F.1 Calculations of Vapor Organics Concentration

Calculation of vapor methanol concentration:

From vapor methanol calibration curve: $y = 5 \times 10^{-08}x + 1 \times 10^{-08}$

Where y is the vapor methanol concentration (mol/ml)

x is the peak area (V.s)

To find vapor methanol concentration by using: $y = (5 \times 10^{-08} \times x) + 1 \times 10^{-08}$

Example,

Time (h)	Peak Area (V.s)			
	1	2	3	Average
1.00	5.36	5.72	5.26	5.45

At time 1.00 h; $y = (5 \times 10^{-08} \times 5.45) + 1 \times 10^{-08} = 2.82 \times 10^{-7}$ mol/ml

F.2 Calculations of fluxes

Calculation of flux:

Permeate flux (J) (mol/ m^2.h) is defined as

$$J = \frac{n}{At} \qquad (2.1)$$

where n is the mol of permeate

A is the effective membrane area

t is the time of the experiment

Example,

Effective membrane area = 5.31×10^{-4} m^2

Mol of permeated methanol = 2.82×10^{-7} mol/ml

Dry air flow rate = 50 ml/min

$$J = \frac{2.82 \times 10^{-7} \frac{mol}{ml} \times 50 \frac{ml}{min} \times 60 \frac{min}{h}}{5.31 \times 10^{-4}\ m^2}$$

$$J = 1.593\ mol/(m^2.h)$$

F.2 Calculations of Permeability

F.2.1 Calculation of Permeability for PV:

Permeability of component i (P_i) (mol.m/ m^2.h.kPa) is defined as

$$P_i = \frac{J_i \ l}{(x_i^F \gamma_i P_i^{sat} - y_i^P P^P)} \tag{2.2}$$

where J_i is the permeate flux of component i
l is the membrane thickness
x_i^F is the mole fraction of component i in feed
γ_i is the activity coefficient of component i in feed
P_i^{sat} is the vapor pressure of component i in feed
y_i^P is the mole fraction of component i in permeate
P^P is the permeate total pressure

Activity coefficient (γ_i) calculated from Non-Random Two Liquid model (NRTL) whereas, the variables in this model gets from program Aspen Engineering Suite 2006.

Vapor pressure (P_i^{sat}) calculated from Antoine's equations

F.2.1.1 Calculation of Permeability for single-component:

From **Table G.2.1** Show fluxes and permeability of pure methanol (100 wt %) as a feed for PV

Time (h)	Flux (mol/m^2.h)			Permeability (mol.m/m^2.h.kPa)		
	1	2	3	1	2	3
1.00	1.572	1.673	1.543	1.07E-06	1.14E-06	1.05E-06

Membrane thickness (l) = 46 x 10^{-6} m
Flux (J) = 1.572 mol/ m^2.h
Activity coefficient (γ_i) = 1
Vapor pressure (P^{sat}) = 68.34 kPa
Permeate pressure (P^P) = 0.76 kPa

$$P = \frac{1.572 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{(1 \times 1 \times 68.34 - 0.76)}$$

$$P = 1.07 \times 10^{-6} \text{ mol.m/m}^2\text{.h.kPa}$$

F.2.1.2 Calculation of Permeability for bi-component:

From **Table G.6.1** Show fluxes and permeability of methanol/ethanol (20:80 wt %) mixture as a feed for PV

Fluxes and permeability of methanol

Time (h)	Flux ($mol/m^2.h$)			Permeability ($mol.m/m^2.h.kPa$)		
	1	2	3	1	2	3
1.00	0.163	0.106	0.129	4.16E-07	2.72E-07	3.30E-07

Membrane thickness (l) = 46 x 10^{-6} m
Flux (J) = 0.163 mol/ m^2.h
Activity coefficient (γ_i) = 1.01599 ; from Appendix E
Vapor pressure (P^{sat}) = 68.34 kPa
Permeate pressure (P^P) = 0.060 kPa ; from Appendix C

$$P = \frac{0.163 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{[(0.26 \times 1.01599 \times 68.34) - 0.060]}$$

$$P = 4.16 \times 10^{-7} \text{ mol.m/m}^2\text{.h.kPa}$$

Fluxes and permeability of ethanol

Time (h)	Flux ($mol/m^2.h$)			Permeability ($mol.m/m^2.h.kPa$)		
	1	2	3	1	2	3
1.00	0.001	0.001	0.001	1.68E-09	1.68E-09	1.68E-09

Membrane thickness (l) = 46 x 10^{-6} m
Flux (J) = 0.001 mol/ m^2.h
Activity coefficient (γ_i) = 0.99613 ; from Appendix E
Vapor pressure (P^{sat}) = 37.42 kPa
Permeate pressure (P^P) = 0.021 kPa ; from Appendix C

$$P = \frac{0.001 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{[(0.74 \times 0.99613 \times 37.42) - 0.021]}$$

$$P = 1.68 \times 10^{-9} \text{ mol.m/m}^2\text{.h.kPa}$$

F.2.2 Calculation of Permeability for VP:

Permeability of component i (P_i) (mol.m/m^2.h.kPa) is defined as

$$P_i = \frac{J_i \ l}{(P_i^F - P_i^P)} \qquad (2.3)$$

where J_i is the permeate flux of component *i*
l is the membrane thickness
P_i^F is the partial pressure of component *i* in feed
P_i^P is the partial pressure of component *i* in permeate

F.2.2.1 Calculation of Permeability for single-component:

From **Table G.2.2** Show fluxes and permeability of pure methanol (100 wt %) as a feed for VP

Time (h)	Flux (mol/m^2.h)			Permeability (mol.m/m^2.h.kPa)		
	1	2	3	1	2	3
1.00	1.128	1.196	-	7.67E-07	8.13E-07	-

Membrane thickness (*l*) = 46 x 10^{-6} m
Flux (*J*) = 1.128 mol/ m^2.h
Vapor pressure (P_i^F) = 68.34 kPa
Permeate pressure (P^P) = 0.67 kPa ; from Appendix C

$$P = \frac{1.128 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{(68.34 - 0.67 \text{ kPa})}$$

$$P = 7.67\times10^{-7} \text{ mol.m/m}^2\text{.h.kPa}$$

F.2.2.2 Calculation of Permeability for bi-component:

From **Table G.6.2** Show fluxes and permeability of methanol/ethanol (20:80 wt %) mixture as a feed for VP

Fluxes and permeability of methanol

Time (h)	Flux ($mol/m^2.h$)			Permeability ($mol.m/m^2.h.kPa$)		
	1	2	3	1	2	3
1.00	0.254	0.197	0.189	6.23E-07	4.82E-07	4.63E-07

Membrane thickness (*l*) = 46×10^{-6} m
Flux (*J*) = 0.254 mol/ m^2.h
Partial pressure (P_i^F) = 18.87 kPa ; from Appendix D
Permeate pressure (P^P) = 0.098 kPa ; from Appendix C

$$P = \frac{0.254 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{(18.87 - 0.098)}$$

$$P = 6.23\times10^{-7} \text{ mol.m/m}^2\text{.h.kPa}$$

Fluxes and permeability of ethanol

Time (h)	Flux ($mol/m^2.h$)			Permeability ($mol.m/m^2.h.kPa$)		
	1	2	3	1	2	3
1.00	0.001	0.001	0.001	2.32E-09	2.32E-09	2.32E-09

Membrane thickness (*l*) = 46×10^{-6} m
Flux (*J*) = 0.001 mol/ m^2.h
Partial pressure (P_i^F) = 25.76 kPa ; from Appendix D
Permeate pressure (P^P) = 0.012 kPa ; from Appendix C

$$P = \frac{0.001 \text{ mol/ m}^2\text{.h} \times 46 \times 10^{-6}\text{m}}{(25.76 - 0.012)}$$

$$P = 2.32\times10^{-9} \text{ mol.m/m}^2\text{.h.kPa}$$