

LAMPIRAN

REAKTOR (R-01)

Fungsi : Mereaksikan 6508.9364 kg/jam toluene dengan 1057.0068 kg/jam amoniak menjadi 6343.9521 kg/jam benzonitrile.

Bentuk : Reaktor Katalitik Fixed Bed

Fasa : Gas

Tekanan : 3 atm.

Suhu : 325 – 347 °C

Katalis : V-Ti-O

Kondisi di atas diambil dari majalah **Ind. Eng. Chem. Res.** , 1987, 26 , 804-810, dengan Judul “ *Kinetic and Mechanistic Analysis of Toluene Amoxidation to Benzonitrile on Vanadium – Titanium – Oxides*”.

1. Uraian proses

Reaksi amoksidasi toluene menjadi benzonitrile adalah reaksi non reversible yang menggunakan katalis V-Ti-O dengan penyangga asbestos. Reaksi terjadi pada padatan katalis sedangkan reaktan masuk reaktor pada fase gas. Kondisi operasi reaktor ini adalah adiabatik, suhu gas didalam reaktor 325 - 350 °C dan tekanan 3 atm. Karena panas reaksinya tidak terlalu besar, maka reaksi dijalankan pada kondisi adiabatik sehingga tidak diperlukan media pendingin. Konversi toluene menjadi benzonitrile cukup tinggi yaitu sekitar 85 %, tetapi karena masih ada sebagian toluene yang belum bereaksi maka diperlukan recycle toluene dari hasil atas menara distilasi. Perbandingan mol toluene dengan amoniak adalah 1 : 1,5 (Ind. Eng. Chem. Res. , 1987). Katalisator yang digunakan adalah V-Ti-O (Vanadium-Titanium-Oxides) yang ter-*coating* pada asbestos berbentuk bola. (Ind. Eng. Chem. Res. , 1987).

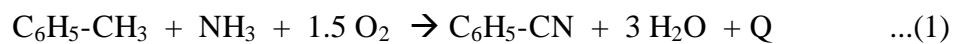
Pada perhitungan reaktor ini diperlukan:

1. Persamaan diferensial yang mewakili Neraca Massa dan Panas.
2. Sifat-sifat fisis dan kimia fluida dan katalis.
3. Lay out Reaktor

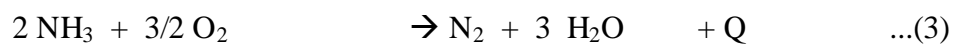
2. Reaksi

Reaksi kimia yang terjadi pada amonolisis toluene dengan adanya oksigen disamping terjadi reaksi utama, juga terjadi reaksi samping. Reaksi yang terjadi adalah sebagai berikut:

a. Reaksi Utama (Pembentukan Benzonitrile)



b. Reaksi samping



Atau dapat disederhanakan :

a. Reaksi Utama



b. Reaksi Samping



dengan :

A : Toluene

E : Air

B : Amoniak

F : Carbon dioksida

C : Oksigen

G : Nitrogen

D : Benzonitrile

H : N – Heptan

Maka pada saat konversi X_1 , X_2 dan X_3 :

$$F_A = F_{A0} \cdot (1 - X_1 - X_2) \quad \dots(7)$$

$$F_B = F_{B0} \cdot (1 - X_3) - F_{A0} \cdot X_1 \quad \dots(8)$$

$$F_C = F_{C0} - 1,5.F_{A0}.(X_1 - 6.X_2) - 0,75.F_{B0}.X_3 \quad \dots(9)$$

$$F_D = F_{D0} + F_{A0}.X_1 \quad \dots(10)$$

$$F_E = F_{E0} + F_{A0}.X_1(3.X_1 + 4.X_2) + 1,5.F_{B0}.X_3 \quad \dots(11)$$

$$F_F = F_{F0} + 7.F_{A0}.X_2 \quad \dots(12)$$

$$F_G = F_{G0} + 0,5.F_{B0}.X_3 \quad \dots(13)$$

$$F_H = F_{H0} \quad \dots(14)$$

Persamaan kinetika untuk reaksi diatas :

$$(-r_1) = \frac{k.PC_7H_8}{1 + K C_7H_8.PC_7H_8 + K_{NH_3}.PNH_3} \quad \dots(15)$$

$$(-r_2) = \frac{k'.PC_7H_8}{1 + K C_7H_8.PC_7H_8 + K_{NH_3}.PNH_3} \quad \dots(16)$$

$$(-r_3) = \frac{k''.PC_7H_8}{1 + K' NH_3.PNH_3} \quad \dots(17)$$

▪ **Data Kinetika**

Parameter	Suhu (K)			Ea Kcal/gmol
	583	598	612	
k , mol/m ³ /det/atm	482.2	613.3	759.5	11.1
k' , mol/m ³ /det/atm	358.5	504.6	683.7	15.8
k'' , mol/m ³ /det/atm	22.1	27.9	34.2	10.6
K C₇H₈ , 1/atm	350	254.6	191.9	
K NH₃ , 1/atm	37.6	29.7	24.1	
K' NH₃ , 1/atm	5.15	3.85	3.08	

(Sumber : Ind. Eng. Chem. Res. , 1987)

▪ **Faktor Tumbukan (A)**

Parameter (Faktor Tumbukan)	Suhu (°C)			A rata-rata
	310	325	339	
A, mol/m ³ /det/atm	6.99E+06	6.99E+06	6.99E+06	6.99E+06
A', mol/m ³ /det/atm	3.01E+08	3.00E+08	3.00E+08	3.00E+08
A'', mol/m ³ /det/atm	2.08E+05	2.09E+05	2.09E+05	2.09E+05

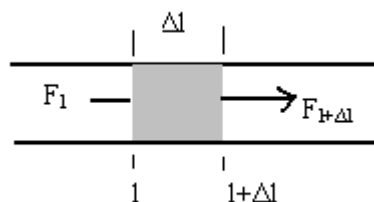
(Sumber : Ind. Eng. Chem. Res. , 1987)

3. Penyusunan Persamaan Matematis

▪ **Neraca Massa**

Asumsi :

1. Aliran reaktan sepanjang reaktor dianggap *plug flow*
 2. Gradien konsentrasi arah aksial diabaikan
 3. *Steady state*
1. Neraca massa Benzonitrile pada elemen volume



Rate of Input – Rate of Output + Rate of Reaction = Rate of Accumulation

$$F_D|_l - F_D|_{l+\Delta l} - (-r_1).A.\varepsilon.\Delta l = 0 \quad \dots(18)$$

$$F_D|_l - F_D|_{l+\Delta l} = (-r_1).A.\varepsilon.\Delta l \quad \dots(19)$$

$$\frac{F_D|_l - F_D|_{l+\Delta l}}{\Delta l} = (-r_1).A.\varepsilon \quad \dots(20)$$

$$\lim \Delta l \rightarrow 0$$

$$F_D|_l - F_D|_{l+\Delta l} = (-r_1).A.\varepsilon \quad \dots(21)$$

$$\frac{dF_D}{dL} = (-r_1). \frac{\pi}{4}.D^2 .\varepsilon \quad \dots(22)$$

$$F_D = F_{D0} + F_{A0}.X_1 \quad \dots(23)$$

$$F_{A0} \frac{dX_1}{dL} = (-r_1). \frac{\pi}{4}.D^2 .\varepsilon \quad \dots(24)$$

$$\frac{dX_1}{dL} = \frac{(-r_1). \pi .D^2 .\varepsilon}{4.F_{A0}} \quad \dots(25)$$

2. Neraca massa karbon dioksida pada elemen volume

$$F_F|_l - F_F|_{l+\Delta l} - (-r_2).A.\varepsilon.\Delta l = 0 \quad \dots(26)$$

$$F_F|_l - F_F|_{l+\Delta l} = (-r_2).A.\varepsilon.\Delta l \quad \dots(27)$$

$$\frac{F_F|_l - F_F|_{l+\Delta l}}{\Delta l} = (-r_2).A.\varepsilon \quad \dots(28)$$

$\lim \Delta l \rightarrow 0$

$$\frac{dF_F}{dL} = (-r_2). \frac{\pi}{4}.D^2 .\varepsilon \quad \dots(29)$$

$$F_F = F_{F0} + 7.F_{A0}.X_2 \quad \dots(30)$$

$$7.F_{A0} \frac{dX_2}{dL} = (-r_2). \frac{\pi}{4}.D^2 .\varepsilon \quad \dots(31)$$

$$\frac{dX_2}{dL} = \frac{(-r_2). \pi .D^2 .\varepsilon}{28.F_{A0}} \quad \dots(32)$$

3. Neraca massa nitrogen pada elemen volume

$$F_G|_l - F_G|_{l+\Delta l} - (-r_3).A.\varepsilon.\Delta l = 0 \quad \dots(33)$$

$$F_G|_l - F_G|_{l+\Delta l} = (-r_3).A.\varepsilon.\Delta l \quad \dots(34)$$

$$\frac{F_G|_l - F_G|_{l+\Delta l}}{\Delta l} = (-r_3).A.\varepsilon \quad \dots(35)$$

$$\lim \Delta l \rightarrow 0$$

$$\frac{dF_G}{dL} = (-r_3). \frac{\pi}{4}. D^2 . \varepsilon \quad \dots(36)$$

$$F_G = F_{G0} + 0,5.F_{B0}.X_3 \quad \dots(37)$$

$$0,5.F_{B0} \frac{dX_3}{dL} = (-r_3). \frac{\pi}{4}. D^2 . \varepsilon \quad \dots(38)$$

$$\frac{dX_3}{dL} = \frac{(-r_3). \pi . D^2 . \varepsilon}{2.F_{B0}} \quad \dots(39)$$

▪ Neraca Panas

Neraca panas pada elemen volume :

Rate of heat input – Rate of heat output = Rate of heat accumulation

$$H|_l - H|_{l+\Delta l} = 0 \quad \dots(40)$$

$$\frac{H|_{l+\Delta l} - H|_l}{\Delta l} = 0 \quad \dots(41)$$

$$\lim \Delta l \rightarrow 0$$

$$\frac{dH}{dL} = 0 \quad \dots(42)$$

$$H = \sum F_i.C_{p_i}.(T - T_{ref}) + F_D.\Delta H_{R1} + F_F.\Delta H_{R2} + F_G.\Delta H_{R3} \quad \dots(43)$$

Maka; persamaan (43) didiferensialkan, didapatkan :

$$dH = \sum F_i.C_{p_i}.dT + F_{A0}.\Delta H_{R1}.dX_1 + 7.F_{A0}.\Delta H_{R2}.dX_2 + 0,5.F_{B0}.\Delta H_{R3}.dX_3 \dots(44)$$

Persamaan (44) dimasukkan ke persamaan (42) didapatkan :

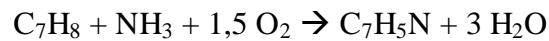
$$\begin{aligned} \frac{dH}{dL} = \Sigma F_i \cdot C_{p_i} \cdot \frac{dT}{dL} + F_{A0} \cdot \left[\Delta H_{R1} \cdot \frac{dX_1}{dL} + 7 \cdot \Delta H_{R2} \cdot \frac{dX_2}{dL} \right] \\ + 0,5 \cdot F_{B0} \Delta H_{R3} \frac{dX_3}{dL} = 0 \end{aligned} \quad \dots(45)$$

atau,

$$\frac{dT}{dL} = \frac{F_{A0} \cdot \left[\Delta H_{R1} \cdot \frac{dX_1}{dL} + 7 \cdot \Delta H_{R2} \cdot \frac{dX_2}{dL} \right] + 0,5 \cdot F_{B0} \Delta H_{R3} \frac{dX_3}{dL}}{\Sigma F_i \cdot C_{p_i}} \quad \dots(46)$$

4. Panas Reaksi (ΔH_R)

a. Reaksi 1 : Pembentukan Benzonitril



$$\Delta H_R = \Delta H_{R0} + \int_{T_0}^T \Delta C_p dT \quad \dots(47)$$

Diambil $T_0 = 25 \text{ }^\circ\text{C}$, fasa gas. Pada $25 \text{ }^\circ\text{C} = 298,15 \text{ K}$; panas pembentukan komponen-komponen di atas adalah :

$$\Delta H_f^0 C_7H_8 = 11,95 \cdot 10^3 \text{ kcal/kgmol}^{-1}$$

$$\Delta H_f^0 NH_3 = -10,92 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_f^0 O_2 = 0$$

$$\Delta H_f^0 C_7H_5N = 52,3 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_f^0 H_2O = -57,8 \cdot 10^3 \text{ kcal/kgmol}$$

$$\begin{aligned} \Delta H_{R1}^0 &= \Delta H_f^0 C_7H_5N + 3 \Delta H_f^0 H_2O - \Delta H_f^0 C_7H_8 - \Delta H_f^0 NH_3 - \Delta H_f^0 O_2 \quad .(48) \\ &= [52,3 + 3 \cdot (-57,8) - 11,95 - (-10,92) - 0] \cdot 10^3 \\ &= -122,13 \cdot 10^3 \text{ kcal/kgmol} \end{aligned}$$

¹ Reid, et. al, 'Properties of Gases and Liquids', 3 ed

$$\int_{T=248,15K}^T \Delta C_p dT = \int_{T_0}^T \Delta a dT + \int_{T_0}^T \Delta b T dT + \int_{T_0}^T \Delta c T^2 dT + \int_{T_0}^T \Delta d T^3 dT \quad \dots(49)$$

dari perhitungan di muka untuk reaksi 1 di atas maka harga Δa , Δb , Δc , dan Δd

$$\Delta a = 6,1045$$

$$\Delta b = 0,0102$$

$$\Delta c = -4,2533 \cdot 10^{-5}$$

$$\Delta d = 2,4559 \cdot 10^{-8}$$

Sehingga :

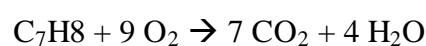
$$\int_{T_0}^T \Delta C_p dT = 6,1045 (T - 298,15) + \frac{0,0102}{2} (T^2 - 298,15^2) - \frac{4,2533 \cdot 10^{-5}}{3} (T^3 - 298,15^3) + \frac{2,4559 \cdot 10^{-8}}{4} (T^4 - 298,15^4) \quad \dots(50)$$

$$\int_{T_0}^T \Delta C_p dT = -1946,171 + 6,1045 T + 5,1 \cdot 10^{-3} T^2 - 1,4178 \cdot 10^{-5} T^3 + 6,13975 \cdot 10^{-9} T^4 \quad \dots(51)$$

ΔH_{R1}^0 dan persamaan (51) dimasukkan ke persamaan (47) :

$$\Delta H_{R1} = -1,240762 \cdot 10^5 + 6,1045 T + 5,1 \cdot 10^{-3} T^2 - 1,4178 \cdot 10^{-5} T^3 + 6,13975 \cdot 10^{-9} T^4 \quad \dots(52)$$

b. Reaksi 2 : Pembentukan CO₂



$$\Delta H_f^0 C_7H_8 = 11,95 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_f^\circ \text{CO}_2 = -94,05 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_f^\circ \text{H}_2\text{O} = -57,8 \text{ kcal/gmol} = -57,8 \cdot 10^3 \text{ kcal/kgmol}$$

$$\begin{aligned} \Delta H_{R2}^\circ &= 4 \Delta H_f^\circ \text{H}_2\text{O} + 7 \Delta H_f^\circ \text{CO}_2 - [\Delta H_f^\circ \text{C}_7\text{H}_8 + 9 \Delta H_f^\circ \text{O}_2] \quad \dots(53) \\ &= [4(-57,8) + 7(-94,05) - [(11,95 - 9)] \cdot 10^3] \\ &= -901,5 \cdot 10^3 \text{ kcal/kgmol} \end{aligned}$$

$$\Delta = 7 \text{ CO}_2 + 4 \text{ H}_2\text{O} - \text{C}_7\text{H}_8 - 9 \text{ O}_2$$

$$\Delta a = 7(4,729) + 4(7,701) - (-5,816) - 9(6,713) = 9,306$$

$$\Delta b = 7(1,754 \cdot 10^{-2}) + 4(4,595 \cdot 10^{-6}) - (0,1224) - 9(-0,879 \cdot 10^{-6}) = 2,2259 \cdot 10^{-3}$$

$$\Delta c = 7(-1,338 \cdot 10^{-9}) + 4(2,52 \cdot 10^{-6}) - (-6,604 \cdot 10^{-5}) - 9(4,4,17 \cdot 10^{-8}) = -5,507 \cdot 10^{-5}$$

$$\begin{aligned} \Delta d &= 7(4,097 \cdot 10^{-9}) + 4(-0,859 \cdot 10^{-9}) - (1,173 \cdot 10^{-8}) - 9(-2,544 \cdot 10^{-9}) \\ &= 3,6409 \cdot 10^{-8} \end{aligned}$$

Maka :

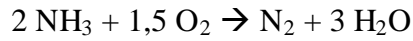
$$\begin{aligned} \int_{T_0=248,15}^T \Delta C_p dT &= 9,306(T - 298,15) + \frac{2,2259 \cdot 10^3}{2} (T^2 - 298,15^2) \\ &\quad - \frac{5,507 \cdot 10^{-5}}{3} (T^3 - 298,15^3) + \frac{3,6409 \cdot 10^{-8}}{4} (T^4 - 298,15^4) \end{aligned}$$

$$\begin{aligned} \int_{T_0}^T \Delta C_p dT &= -2458,9268 + 9,306 T + 1,11295 \cdot 10^{-3} T^2 - 1,8357 \cdot 10^3 \\ &\quad + 9,10225 \cdot 10^{-9} T^4 \quad \dots(54) \end{aligned}$$

ΔH_{R1}^0 dan persamaan (54) masuk ke persamaan (47) didapatkan :

$$\begin{aligned} \Delta H_{R2} &= -903958,9268 + 9,306 T + 1,1129 \cdot 10^{-3} T^2 - 1,8357 \cdot 10^{-5} T^3 \\ &\quad + 9,10225 \cdot 10^{-9} T^4 \quad \dots(55) \end{aligned}$$

c. Panas Reaksi 3 : Pembentukan Nitrogen



$$\Delta H_f^\circ \text{NH}_3 = -10,92 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_f^\circ \text{N}_2 = \Delta H_{fo} \text{O}_2 = 0$$

$$\Delta H_f^\circ \text{H}_2\text{O} = -57,8 \cdot 10^3 \text{ kcal/kgmol}$$

$$\Delta H_{R3}^0 = 3 \cdot \Delta H_f^\circ \text{H}_2\text{O} + 2 \cdot \Delta H_f^\circ \text{NH}_3 \quad \dots(56)$$

$$= [3 \cdot (-57,8) - 2 \cdot (-10,92)] \cdot 10^3$$

$$= -151,56 \cdot 10^3 \text{ kcal/kgmol}$$

dari data di atas :

$$\Delta a = 7,4275$$

$$\Delta b = -1,0132$$

$$\Delta c = -4,51 \cdot 10^{-7}$$

$$\Delta d = 4,109 \cdot 10^{-9}$$

$$\int_{T_0=248,15}^T \Delta C_p dT = 7,4275 (T - 298,15) + \frac{-1,0132}{2} (T^2 - 298,15^2) -$$

$$\frac{4,51 \cdot 10^{-7}}{3} (T^3 - 298,15^3) + \frac{4,109 \cdot 10^{-9}}{4} (T^4 - 298,15^4)$$

$$\int_{T_0}^T \Delta C_p dT = -1631,9445 + 7,4275 T - 6,6 \cdot 10^{-3} T^2 - 1,5033 \cdot 10^{-7} T^3$$

$$+ 1,02725 \cdot 10^{-9} T^4 \quad \dots(57)$$

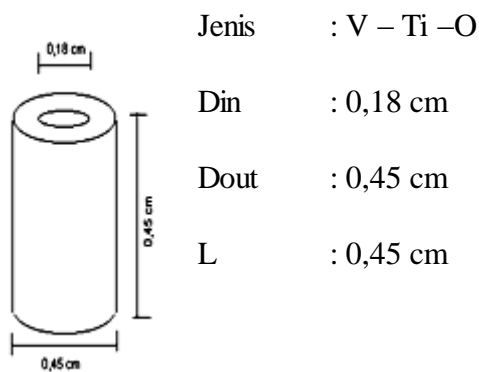
maka,

$$\Delta H_{R3} = \Delta H_{R3}^0 + \int \Delta C_p dT \quad \dots(58)$$

ΔH_{R3}^0 dan persamaan (57) masuk ke persamaan (58) didapatkan :

$$\begin{aligned} \Delta H_{R3} &= -1,53192 \cdot 10^5 + 7,4275 \cdot T - 6,6 \cdot 10^{-3} T^3 - 1,5033 \cdot 10^{-7} T^3 \\ &\quad + 1,02725 \cdot 10^{-9} T^4 \end{aligned} \quad \dots(59)$$

5. Katalisator



Jenis : V – Ti –O

Din : 0,18 cm

Dout : 0,45 cm

L : 0,45 cm

▪ Diameter Equivalen Katalis (Dp)

Bila dinyatakan dalam diameter equivalen yaitu diameter bola yang mempunyai volume yang sama dengan silinder, maka :

$$V_s = \frac{\pi}{4} (D_{out}^2 - D_{in}^2) L \quad \dots(60)$$

Dimana :

V_s = Volume Silinder, cm^3

Din = Diameter dalam katalis, cm

Dout = Diameter luar katalis, cm

L = Panjang katalis, cm

$$V_s = \frac{\pi}{4} (0,45^2 - 0,18^2) \cdot 0,45$$

$$V_s = 0,0601 \text{ cm}^3$$

Untuk diameter bola dinyatakan dalam :

$$V_B = \frac{\pi}{6} Dp^3 \quad \dots(61)$$

Dimana :

$$V_B = \text{Volume Bola, cm}^3$$

$$Dp = \text{Diameter Partikel, cm}$$

Maka,

$$0,0601 = \frac{\pi}{6} Dp^3$$

$$Dp = \left(\frac{6 \cdot 0,0601}{\pi} \right)^{\frac{1}{3}}$$

$$Dp = 0,486 \text{ cm}$$

▪ **Porositas Katalis (ϵ)**

$$\text{Sphericity } (\psi) = \frac{\text{Luas area bola}}{\text{Luas area katalis}} \quad \dots(62)$$

$$\text{Luas area bola} = \pi \cdot Dp^3 \quad \dots(63)$$

$$= \pi (0,486)^2$$

$$= 0,7418 \text{ cm}^2$$

$$\text{Luas area katalis} = \pi \cdot L (D_{in} + D_{out}) + 2 \cdot \frac{\pi(D_{out}^2 - D_{in}^2)}{4} \quad \dots(64)$$

$$= \pi \cdot 0,45 (0,18 + 0,45) + 2 \cdot \frac{\pi(0,45^2 - 0,18^2)}{4}$$

$$= 1,1572 \text{ cm}^2$$

Jadi,

$$\text{Sphericity } (\psi) = \frac{0,7418 \text{ cm}^2}{1,1572 \text{ cm}^2}$$

$$= 0,6409$$

Dari Fig. 223 Brown didapatkan :

$$\text{Porositas } (\varepsilon) = 0,48$$

6. Viskositas dan Berat Molekul Gas

Viskositas masing-masing gas dihitung dengan persamaan :

$$\mu = a + bT + cT^2 \quad \dots(65)$$

dimana :

μ = Viskositas gas, kg/m.jam

a, b, c = konstanta

T = Suhu, K

Tabel 1. Konstanta untuk masing-masing komponen

Senyawa	BM	a	b	c
Toluene	92,141	0,008885373	5,15271E-05	-2,57873E-08
Amoniak	17,031	-0,01398411	0,000187172	-7,0007E-08
Air	18,015	0,0228351	0,000166776	-3,86307E-08
Benzonitrile	103,124	0,01396038	0,000164608	-6,9923E-08
N-Heptana	100,25	-0,0122036	0,000316765	3,19519E-08
Oksigen	31,999	-0,002261805	0,000192142	-3,87181E-08
Nitrogen	28,013	0,01156783	0,000186341	-5,74518E-08
C. Dioksida	44,01	-0,000325824	0,000198823	-5,627E-08

(Sumber : Reid, "Properties of Gases and Liquids")

Hasil perhitungan lengkap disajikan dalam Tabel.2

Tabel 2. Hasil perhitungan untuk masing-masing komponen

Senyawa	BM	kgmol/jam	kg/jam		y_i	μ_i (kg/m.jam)	$y_i \cdot B_{mi}$	$y_i \cdot B_{mi}^{1/2}$	$y_i \cdot B_{mi}^{1/2} \cdot \mu_i$
Nitrogen	28.013	1104.5801	30942.6030	1.0000	0.6970	0.1025	19.5237	3.6888	0.3780
Oksigen	31.999	293.6226	9395.6285	0.2658	0.1853	0.0988	5.9283	1.0480	0.1036
C. Dioksida	44.01	0.0000	0.0000	0.0000	0.0000	0.0985	0.0000	0.0000	0.0000
Amoniak	17.031	110.1085	1875.2572	0.0997	0.0695	0.0729	1.1832	0.2867	0.0209
N-Heptana	100.25	1.0470	104.9643	0.0009	0.0007	0.1887	0.0662	0.0066	0.0012
Air	18.015	1.8094	32.5955	0.0016	0.0011	0.1088	0.0206	0.0048	0.0005
Toluene	92.141	73.4056	6763.6692	0.0665	0.0463	0.0305	4.2676	0.4446	0.0136
Benzonitrile	103.124	0.2989	30.8208	0.0003	0.0002	0.0874	0.0194	0.0019	0.0002
Total		1584.8720	49145.5385		1.0000		31.0092	5.4815	0.5180

Viskositas campuran gas dihitung dengan persamaan :

$$\mu_{\text{camp}} = \frac{\sum y_i \cdot \mu_i \cdot B_{mi}^{0.5}}{\sum y_i \cdot B_{mi}^{0.5}} \quad \dots(66)$$

$$= \frac{0,5180}{5,4815}$$

$$= 0,094 \text{ kg/m.jam}$$

$$= 2.6248 \cdot 10^{-5} \text{ kg/m.dtk}$$

Sedangkan berat molekul rata-rata campuran gas adalah :

$$BM_{\text{avg}} = \sum y_i \cdot B_{mi} \quad \dots(67)$$

dimana :

y_i = fraksi mol komponen i

BM_i = berat molekul komponen i

Jadi,

$$B_{mavg} = 31.0092 \text{ kg/kgmol}$$

7. Densitas Campuran Gas

Jiak gas dianggap mengikuti hukum gas ideal :

$$PV = nRT \quad \dots(68)$$

$$PV = \frac{M}{BM} RT$$

$$M = \frac{P.V.BM}{R.T}$$

$$\rho = \frac{M}{V} = \frac{P.BM}{R.T}$$

$$\rho_{\text{camp}} = \frac{P.BM_{\text{avg}}}{R.T} \quad \dots(69)$$

dimana :

P = tekanan total, atm

BM_{avg} = berat molekul rata-rata gas, kg/kmol

R = konstanta gas ideal, m³.atm/kgmol.K

T = suhu, K

Jadi,

$$\begin{aligned} \rho_{\text{camp}} &= \frac{3 \text{ atm} \cdot 31.0092 \text{ kg} / \text{kgmol}}{0,08206 \frac{\text{atm} \cdot \text{m}^3}{\text{kgmol} \cdot \text{K}} \cdot 598 \text{ K}} \\ &= 1,8952 \text{ kg/m}^3 \end{aligned}$$

8. Menghitung Diameter Reaktor

$$Re = \frac{\rho \cdot v \cdot D}{\mu} \quad \dots(70)$$

Dimana :

- Re = reynold number
- v = kecepatan gas, m/dtk
- D = diameter reaktor, m
- μ = viskositas gas, kg/m.dtk

Bilangan reynold dalam partikel :

$$\text{Rep} = \frac{\rho_{camp}.v.Dp}{\mu_{camp}} \quad \dots(71)$$

Asumsi, Rep = 300 (Brown)

$$300 = \frac{1,8952 \text{ kg/m}^3 .v.0,00486 \text{ m}}{2,6248.10^{-5} \text{ kg/m.dtk}}$$

$$v = 0,8548 \text{ m/dtk}$$

Bilangan reynold dalam reaktor :

$$\text{Ret} = \frac{\rho_{camp}.v.D}{\mu_{camp}} \quad \dots(72)$$

Asumsi, Ret = 200000 (Brown)

$$200000 = \frac{1,8952 \text{ kg/m}^3 .0,8548 \text{ m/dtk}.D}{2,6248.10^{-5} \text{ kg/m.dtk}}$$

$$D = 3,2403 \text{ m}$$

9. Panjang Bed Katalis

Dari perhitungan diperoleh panjang bed katalis = 11,7 m.

10. Mechanical Design Reaktor

▪ Tebal Shell

Bahan : Carbon stainless steel SA - 285 grade C

Ukuran:

* Diameter dalam Shell (IDS) = 3,2402 m = 127,5688 in = 10,6307 ft

* Jari - jari dalam Shell (ri) = 1,6201 m = 63,7844 in

Poperasi = 3 atm

Faktor keamanan diambil 20 %

Pdesign = 3,6 atm = 52,9054 psia

Suhu operasi = 325 °C = 617 °F

Untuk T = 617 °F, maka dari Tabel 13.1 Brownell&Young diperoleh harga :

max allowable stress (f) = 13750 psi

max efisiensi sambungan (E) = 0,8

faktor korosi (C) = 0,125 in

Maka nilai tebal Shell dicari dengan persamaan:

$$ts = \frac{P * ri}{f * E - 0,6 * P} + C \quad \dots(73)$$

ts = 0,4327 in

Dipilih tebal plate standard = 7/16 in (Brownell&Young)

Diameter luar shell (ODS) = IDS + 2.ts
= 128,4438 in

Dipilih ODS = 130 in (Brownell&Young)

▪ Head and Bottom

Bentuk : *Torispherical dished head*

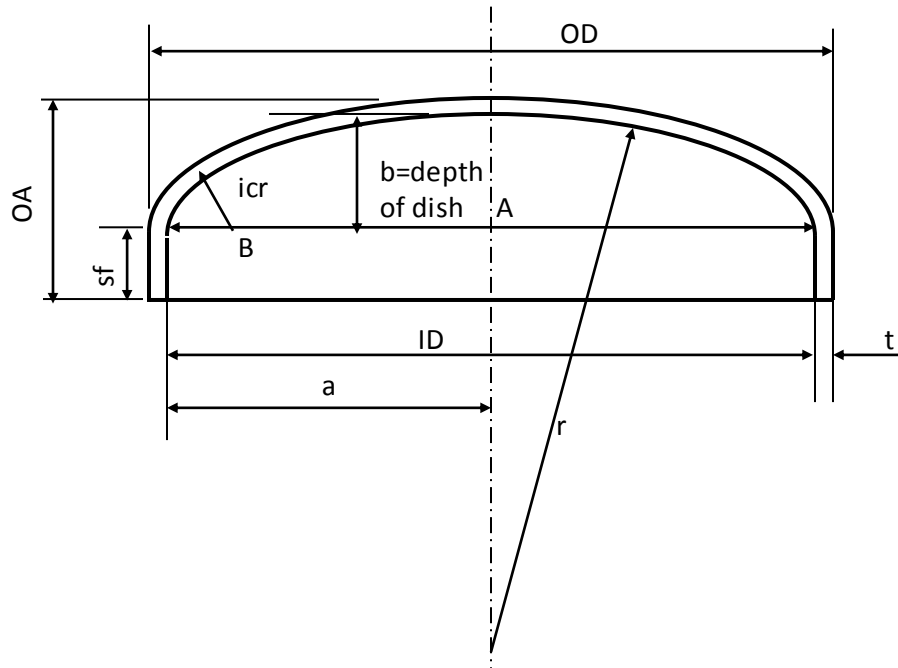
Dipilih bentuk ini karena *torispherical dished head* cocok untuk tekanan rendah (P = 15 – 200 psi).

Persamaan untuk mencari tebal head dan Bottom :

$$th = \frac{0,885.P.IDS}{f.E - 0,1.P} + C \quad \dots(74)$$

$$th = 0,6683 \text{ in}$$

Dipilih tebal plate standard = 3/4 in (Brownell& Young)



$$r = IDS = 130 \text{ in}$$

$$icr = 7,65 \text{ in}$$

$$icr/OD = 5,89 \%$$

dari tabel 5.11 Brownell & Young, diperoleh harga :

$$sf = 3 \text{ in}$$

$$a = IDS/2 = 63,7844 \text{ in}$$

$$AB = a - icr = 56,1303 \text{ in}$$

$$BC = r - icr = 119,9147 \text{ in}$$

$$AC = (BC^2 - AB^2)^{0.5} = 105,9666 \text{ in}$$

$$b = r - AC = 21,6022 \text{ in}$$

$$\begin{aligned}
 \text{tinggi head (OA)} &= th + b + sf \\
 &= 25,3522 \text{ in} \\
 &= 0,6439 \text{ m}
 \end{aligned}$$

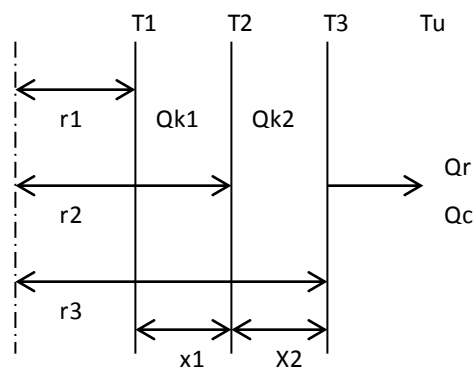
▪ **Tinggi Reaktor**

$$\begin{aligned}
 \text{Tinggi reaktor total} &= \text{Panjang Bed} + 2 \cdot \text{Tinggi head} \\
 &+ 2 \cdot \text{Jarak head-katalis} \\
 &= 536,6865 \text{ in} = 13,6318 \text{ m}
 \end{aligned}$$

▪ **Tebal Isolasi Reaktor**

Asumsi :

1. Perpindahan panas konduksi terjadi dalam keadaan *steady state*
2. Sifat-sifat bahan tidak berubah terhadap suhu



Keterangan :

r_1 = jari-jari dalam reaktor

r_2 = jari-jari luar reaktor

r_3 = jari-jari isolator luar

Q_{k1} = perp. panas konduksi melalui dinding reaktor

Q_{k2} = perp. panas konduksi melalui isolator

Q_c = perp. panas konveksi

Q_r = perp. panas radiasi

T1 = suhu dinding dalam reaktor

T2 = suhu dinding luar reaktor

T3 = suhu isolator luar

Tu = suhu udara luar

x1 = tebal dinding reaktor

x2 = tebal isolator

Bahan isolator yang dipakai adalah asbestos. Asbestos mempunyai konduktivitas thermal cukup rendah, ketahanan terhadap air sangat baik dan maximum tensile strength cukup tinggi. Asbestos dapat digunakan pada rentang suhu antara 33-750°F (Rase and Barrow, 1957).

Sifat-sifat fisis asbestos (Holman, 1988) :

$$k_2 = 0,117 \text{ Btu/j.ft.F}$$

$$\varepsilon = 0,95$$

$$\rho = 36 \text{ lb/ft}^3$$

Carbon steel :

$$k_1 = 21 \text{ Btu/j.ft.F}$$

$$\rho = 490 \text{ lb/ft}^3$$

Konduksi

$$Q_{k1} = \frac{k_1 \cdot A}{x_1} (T_2 - T_1) \quad \dots(75)$$

$$Q_{k2} = \frac{k_2 \cdot A}{x_2} (T_3 - T_2) \quad \dots(76)$$

perpindahan panas secara seri,

$$Q_k = \frac{T_1 - T_{31}}{\frac{x_1}{k_1 \cdot A} + \frac{x_2}{k_2 \cdot A}} \quad \dots(77)$$

Konveksi

$$h_c = 0,19 \cdot (T_3 - T_u)^{1/3} \quad \dots(78)$$

$$h_c = 0,7904 \text{ Btu/j.ft}^2 \cdot \text{F}$$

$$Q_c = h_c \cdot A \cdot (T_3 - T_u) \quad \dots(79)$$

$$Q_c = 38,7804 \text{ Btu/j.ft}^2$$

Radiasi

$$Q_r = \tau \cdot A \cdot \varepsilon \cdot (T_3^4 - T_u^4) \quad \dots(80)$$

$$\zeta = 1,71 \cdot 10^{-9} \text{ Btu/j.ft}^2 \cdot \text{R}^4$$

$$Q_r = 66,9745 \text{ Btu/j.ft}^2$$

$$Q_k = Q_c + Q_r$$

Diperoleh tebal isolasi,

$$x_2 = 0,5275 \text{ ft} = 16,0787 \text{ cm} = 6,3302 \text{ in}$$

▪ Berat Reaktor

$$\text{Berat shell} = 0,25 \cdot \pi \cdot (\text{ODS}^2 - \text{IDS}^2) \cdot (L + 2 \cdot \text{jarak head-katalis}) \cdot \rho_s \quad \dots(81)$$

$$= 67742,2898 \text{ lb}$$

$$\text{Berat head} = 2 \cdot \pi / 24 \cdot (\text{ODS}^3 - \text{IDS}^3) \cdot \rho_s \quad \dots(82)$$

$$= 8976,0590 \text{ lb}$$

$$\text{Berat isolator} = 0,25 \cdot \pi \cdot (\text{ODS}^2 - \text{IDS}^2) \cdot (L + 2 \cdot \text{jarak head-katalis}) \cdot \rho_s \quad \dots(83)$$

$$= 1381,9778 \text{ lb}$$

$$\begin{aligned} \text{Berat gas} &= 0,25 \cdot \pi \cdot (\text{IDS}/12)^2 \cdot (\text{L} + 2 \cdot \text{jarak head-katalis}) \cdot \rho_s \quad \dots(84) \\ &= 425,2464 \text{ lb} \end{aligned}$$

$$\begin{aligned} \text{Berat katalis} &= 0,25 \cdot \pi \cdot (\text{IDS}/12)^2 \cdot \text{L} \cdot \rho_k \cdot (1 - \epsilon) \quad \dots(85) \\ &= 5948,5590 \text{ lb} \end{aligned}$$

Jadi, berat reaktor :

$$\begin{aligned} \text{Berat reaktor} &= 83574,1321 \text{ lb} \\ &= 37908,3906 \text{ kg} \end{aligned}$$

▪ Diameter Nozzle Pemasukan dan Pengeluaran

Untuk menentukan diameter nozel yang berhubungan dari dan ke reaktor digunakan persamaan (Peters&Timmerhouse):

$$\text{Di,opt} = 3,9 \cdot q_f^{0,45} \cdot \rho_f^{0,13} \quad \dots(86)$$

Dengan,

Di,opt = diameter optimum, in

qf = debit fluida, cuft/s

rhof = densitas fluida, lb/cuft

a. Pipa umpan masuk reaktor

Flow rate (Fv) = 1584,8729 kgmol/jam = 49145,5385 kg/jam

Suhu = 598,15 K

Tekanan = 3 atm = 303975 Pa

R = 1,314 atm.ft³/lbmol.K = 0,08206 m³atm/kgmol.K

Komp.	Kgmol/j	x, mol	BM	x.BM
Nitrogen	1104.5801	0.6970	28.013	19.52
Oksigen	293.6226	0.1853	31.999	5.93
C. Dioksida	0.0000	0.0000	44.01	0.00
Amoniak	110.1085	0.0695	17.031	1.18
N-Heptana	1.0470	0.0007	100.25	0.07
Air	1.8094	0.0011	18.015	0.02
Toluene	73.4056	0.0463	92.141	4.27
Benzonitrile	0.2989	0.0002	103.124	0.02
Σ	1584.872	1		31.01

$$\rho_f = \frac{P \cdot BM}{R \cdot T} = 0,1184 \text{ lb/ft}^3 = 1,8953 \text{ kg/m}^3$$

$$Q_f = \frac{\text{Flowrate}}{\rho_f} = 3,3873 \text{ ft}^3/\text{s}$$

$$D_{i,\text{opt}} = 5,1170 \text{ in}$$

Dipilih pipa standar (IPS) :

$$\text{Nominal pipe size} = 6 \text{ in} \quad (\text{Brownell})$$

$$\text{ID} = 5,761 \text{ in}$$

$$\text{Sch. Number} = 80$$

b. Pipa hasil keluar reaktor

$$\text{Flow rate (Fv)} = 1623,8005 \text{ kgmol/jam} = 49145,4301 \text{ kg/jam}$$

$$\text{Suhu} = 620,85 \text{ K}$$

$$\text{Tekanan} = 2,5 \text{ atm} = 253312,5 \text{ Pa}$$

$$R = 1,314 \text{ atm.ft}^3/\text{lbmol.K} = 0,08206 \text{ m}^3\text{atm/kgmol.K}$$

Komp.	Kgmol/j	x, mol	BM	x.BM
Nitrogen	1104.5801	0.6802	28.013	19.0557
Oksigen	126.9228	0.0782	31.999	2.5012
C. Dioksida	58.2334	0.0359	44.01	1.5783
Amoniak	48.8896	0.0301	17.031	0.5128
N-Heptana	1.0470	0.0006	100.25	0.0646
Air	218.7421	0.1347	18.015	2.4268
Toluene	3.8677	0.0024	92.141	0.2195
Benzonitrile	61.5177	0.0379	103.124	3.9069
Jumlah	1623.8005	1		30.2657

$$\rho_f = \frac{P \cdot BM}{R \cdot T} = 0,09278 \text{ lb/ft}^3$$

$$Q_f = \frac{\text{Flowrate}}{\rho_f} = 4,3227 \text{ ft}^3/\text{s}$$

$$D_{i,\text{opt}} = 5,5323 \text{ in}$$

Dipilih pipa standar (IPS) :

$$\text{Nominal pipe size} = 6 \text{ in} \quad (\text{Brownell})$$

$$\text{ID} = 5,761 \text{ in}$$

$$\text{Sch. Number} = 80$$

11. Spesifikasi Reaktor

Fungsi	: Mereaksikan gas amoniak dan toluene menjadi Benzonitrile, dengan bantuan udara.
Jenis	: Fixed Bed catalytic Reaktor
Fasa	: Gas
Bentuk	: Silinder tegak
Suhu masuk	: 325 C
Suhu keluar	: 347 C
Tekanan Udara	: 3 atm absolut
Tebal Bed Katalis	: 11,7 m
Jenis Katalis	: V-Ti-O
Diameter katalis	: 0,0049 m
Konversi Benzonitrile	: 0,8333
Konversi CO ₂	: 0,1133
Konversi Nitrogen	: $1,5969 \cdot 10^{-10}$
Tinggi Reaktor	: 13,6318 m
Diameter shell	: 3,3020 m
Tebal dinding	: 7/16 in
Bahan Konstruksi	: Carbon steel SA-285 grade-C
Tebal isolasi	: 16,0787 cm
Jumlah Reaktor	: 1 buah

