UNIVERSITI SAINS MALAYSIA

First Semester Examination
2009/2010 Academic Session

November 2009

EKC 336 – Chemical Reaction Engineering
[Kejuruteraan Tindakbalas Kimia]

Duration : 3 hours
[Masa : 3 jam]

Please check that this examination paper consists of NINE pages of printed material and THREE pages of Appendix before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi SEMBILAN muka surat yang bercetak dan TIGA muka surat Lampiran sebelum anda memulakan peperiksaan ini.]

Instruction: Answer **FOUR (4)** questions. Answer any **TWO (2)** questions from Section A. Answer any **TWO (2)** questions from Section B. All questions carry the same marks.

*[**Arahan:** Jawab **EMPAT** (4) soalan. Jawab **DUA** (2) soalan dari Bahagian A. Jawab **DUA** (2) soalan dari Bahagian B. Semua soalan membawa jumlah markah yang sama.]*

In the event of any discrepancies, the English version shall be used.

[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah diguna pakai].

Section A: Answer any TWO questions.
Bahagian A: Jawab mana-mana DUA soalan.

1. [a] What are the advantages of plug flow reactor?
Apakah kelebihan reaktor aliran palam?

[2 marks/markah]

[b] The gas phase decomposition A→2C ($k = 0.001\ s^{-1}$) is carried out in a plug flow reactor at 300°C and 10 atm. Reactor feed rate is at 1 mol/s, and contains 75 mol% inert. Determine the length of 1 inch diameter pipe needed to reach 99% conversion. Comment on the practicality of your design.

Penguraian fasa gas A→2C ($k = 0.001\ s^{-1}$) dilalukan dalam reaktor aliran palam pada suhu 300°C dan tekanan 10 atm. Kadar suapan reaktor adalah 1 mol/s, dan mengandungi bahan lengai 75% mol. Tentukan panjang yang diperlukan bagi paip yang berdiameter 1 inci bagi mencapai penukaran 99%. Berikan komen sama ada rekabentuk anda praktikal atau tidak.

[8 marks/markah]

[c] The gas-phase reaction A → B + 2C is being carried out batchwise in a vessel at 550°C and 2.5 atm. The reactor is initially charged with a gas mixture of 20% A in inert.

Tindakbalas fasa gas A→ B + 2C dijalankan dalam bekas secara kelompok pada suhu 550°C dan tekanan 2.5 atm. Reaktor pada mulanya disuap dengan campuran gas yang terdiri daripada 20% A dan selebihnya bahan lengai.

[i] Build a stoichiometric table showing concentrations at any conversion, X.

Bina jadual stoikiometri yang menunjukkan kepekatan pada mana-mana penukaran, X.

[ii] Determine the amount of time required to achieve 85% conversion, if the reaction is elementary, the reactor is isothermal, and the rate constant is $0.5\ hr^{-1}$.

Tentukan jumlah masa yang diperlukan untuk mencapai penukaran 85%, sekiranya tindakbalas tersebut adalah asas, reaktor pada keadaan sesuhu dan pemalar kadar adalah 0.5 jam^{-1}.

[10 marks/markah]

[d] Starting with the general mole balance, develop the design equation for a continuous stirred tank reactor. Clearly state each assumption you make, simplify the equation in term of space time by assuming a liquid-phase elementary isomerization reaction of reactant A.
Bermula dengan imbangan mol umum, bina persamaan rekabentuk bagi reaktor tangki pengaduk berterusan. Nyatakan dengan jelas setiap anggapan yang dibuat, permudahkan persamaan dalam bentuk masa ruang dengan beranggapan tindakbalas pengisomeran asas fasa-cecair bagi bahan tindak balas A.

[5 marks/markah]

...3/-

2. [a] The homogeneous gas decomposition of phosphine, $4PH_3(g) \rightarrow P_4(g) + 6H_2(g)$, occurs at 649°C with a rate constant of 10 hr^{-1}. What is the size of plug flow reactor operating at 649°C and 460 kPa to achieve 80% conversion of a feed consisting of 40 mol/hr of pure phosphine?

Penguraian homogen gas fosfin, $4PH_3(g) \rightarrow P_4(g) + 6 H_2(g)$, berlaku pada suhu 649°C dengan pemalar kadar sebanyak 10 jam^{-1}. Apakah saiz reaktor aliran palam yang beroperasi pada suhu 649°C dan tekanan 460 kPa yang diperlukan untuk mencapai penukaran 80% suapan yang terdiri daripada 40 mol/jam fosfin tulen?

[8 marks/markah]

[b] Prepare a stoichiometric table as a function of conversion A showing the effluent concentrations of all species of a gas-phase plug flow reactor for the reaction $A \rightarrow B + 2C$. The reactor feed contains 50 mole % inert.

Sediakan jadual stoikiometri dalam fungsi penukaran A yang menunjukkan kepekatan keluar bagi semua spesis untuk reaktor aliran palam fasa-gas bagi tindakbalas $A \rightarrow B + 2C$. Suapan reaktor terdiri daripada 50 mol % bahan lengai.

[9 marks/markah]

[c] How long should a 50 L batch reactor be operated at 550 K to achieve 95% conversion of A for the elementary gas phase reaction $A + B_2 \rightarrow C$ ($k = 0.125$ $dm^3/mol \cdot s$) if the reactor is charged with only the reactants ($y_{A0} = 0.4$)? What is the final pressure of the vessel at 95% conversion? Assume an initial pressure of 8.2 atm.

Berapa lamakah masa yang diperlukan bagi reaktor kelompok 50 L yang beroperasi pada suhu 550 K bagi mencapai penukaran A sebanyak 95 % bagi tindakbalas asas fasa gas $A + B_2 \rightarrow C$ ($k = 0.125$ $dm^3/mol \cdot s$) sekiranya reaktor disuap dengan bahan tindakbalas ($y_{A0} = 0.4$)? Apakah tekanan akhir reaktor pada tahap penukaran 95%? Anggapkan tekanan awal adalah 8.2 atm.

[8 marks/markah]

3. [a] The photochemical decay of aqueous bromine was studied, with the following results:

Kesusutan fotokimia bagi bromin akues telah dikaji, dan keputusannya adalah seperti berikut:

Time (min) *Masa (min)*	C (Br, ppm) *Kepekatan (Br, ppm)*
10	2.45
20	1.74
30	1.23
40	0.88
50	0.62
60	0.44

[i] Determine the reaction order and specific reaction rate.
Tentukan tertib tindakbalas dan kadar tindakbalas tentu.

[ii] At the steady state condition, calculate the required rate of bromine injected (in pounds) into a 25,000 gallon body of water illuminated by the sunlight to maintain a sterilizing level of 1 ppm bromine.

Pada keadaan mantap, kirakan bromin yang perlu disuntik (dalam paun) ke dalam 25,000 gelen air yang dicahayakan oleh matahari bagi mengekalkan paras pensterilan dengan kepekatan bromin sebanyak 1 ppm.

1 gallon = 3.75 litre
1 pound = 454 g

1 gelen = 3.75 liter
1 paun = 454 g

[11 marks/markah]

[b] The feed to a reactor producing diphenyl is pure benzene in the gas phase at a total pressure of 5 atm and 760°C. The specific reaction rate is 1800 $ft^3/(lbmol \cdot s)$ and the equilibrium constant is estimated to be 0.3. The reactor volume is 1500 dm^3. At an equilibrium reaction one mole of diphenyl and hydrogen gas are produced. What is the equilibrium conversion?

Suapan reaktor yang menghasilkan difernil adalah merupakan benzena tulen dalam fasa gas dengan jumlah tekanan 5 atm dan suhu 760°C. Kadar tindakbalas tentu adalah 1800 kaki^3/(lbmol·s) dan pemalar keseimbangan dianggarkan sebanyak 0.3. Isipadu reaktor adalah 1500 dm^3. Tindakbalas adalah tindakbalas keseimbangan yang menghasilkan 1 mol difernil dan 1 mol gas hidrogen. Apakah penukar keseimbangan?

$$-r_A = k_A\left(C_A^2 - \frac{C_A C_B}{K_{eq}}\right)$$

1 ft^3= 0.0283 m^3
1 dm^3 = 0.001 m^3
1 lb = 0.454 kg

1 kaki^3= 0.0283 m^3
1 dm^3 = 0.001 m^3
1 lb = 0.454 kg

[7 marks/markah]

[c] The catalytic liquid phase decomposition A → 2C (k = 0.001 L/mol·s) is carried out under atmospheric pressure in a batch reactor. Reactant A is charged at 0.1 mol/L. Determine the duration (in days) needed to reach 99% conversion in a 100 L vessel. How does your answer change for a 10 L vessel?

Penguraian fasa cecair bermangkin A → 2C (k = 0.001 L/mol·s) dijalankan pada tekanan atmosfera dalam reaktor kelompok. Bahan tindakbalas A disuap pada 0.1 mol/L. Tentukan tempoh (dalam hari) yang diperlukan untuk mencapai 99% penukaran dalam reaktor 100 L. Bagaimana jawapan anda berubah bagi reaktor 10 L?

[7 marks/markah]

Section B : Answer any TWO questions.
Bahagian B : Jawab mana-mana DUA soalan.

4. [a] The rate law for formation of phosgene, from chlorine, and carbon monoxide, is given as :

Hukum kadar bagi pembentukan fosgen daripada klorin dan karbon monoksida diberikan seperti berikut:

$$r_{COCl_2} = kC_{CO}C_{Cl_2}^{1.5}$$

Suggest a mechanism for this reaction that is consistent with this rate law and draw the reaction path way. [Hint: Cl formed from the dissociation of Cl_2 is one of the two active intermediates.]

Cadangkan satu mekanisma bagi tindakbalas ini yang konsisten dengan hukum kadar dan lakarkan laluan tindakbalas tersebut. [Panduan: Cl yang terbentuk daripada penceraian Cl_2 merupakan satu daripada dua perantaraan aktif.]

[10 marks/markah]

[b] The following reversible, elementary, liquid phase reaction occurs in a CSTR:
Tindakbalas asas, berbalik, fasa cecair yang berikut berlaku dalam sebuah CSTR:

$$A \overset{k}{\leftrightarrow} B$$

The entering flow rate is 10 dm^3/s with a concentration of 2 M of A and the feed temperature is 300 K. What is the reactor volume required in order to achieve 90% of the equilibrium conversion in a CSTR operated adiabatically?

Kadar aliran suapan ialah 10 dm^3/s dengan kepekatan 2 M bahan A dan suhu suapan adalah 300 K. Apakah isipadu reaktor yang diperlukan untuk mencapai 90% penukaran keseimbangan dalam sebuah CSTR yang beroperasi secara adiabatik?

Additional information:
Specific heat capacities: $C_{pA} = C_{pB} = 60$ cal/mol/K
Heat of reaction: $\Delta H^o_{rxn} = -10{,}000$ cal/mol A

Maklumat tambahan:
Haba muatan tentu: $C_{pA} = C_{pB} = 60$ cal/mol/K
Haba tindakbalas: $\Delta H^{o}_{rxn} = -10{,}000$ cal/mol A

Specific rate constant k and equilibrium rate constant K_e is given in Figure Q.4.[a] and Figure Q.4.[b].

Pemalar kadar tentu k dan pemalar kadar kesimbangan K_e diberikan dalam Rajah S.4.[a]dan Rajah S.4.[b].

Adiabatic energy balance:
Imbangan tenaga adiabatik:

$$X = \frac{\sum \Theta_i C_{P_i} (T - T_{i0})}{-[\Delta H^{o}_{Rx}(T_R) + \Delta C_P (T - T_R)]}$$

[15 marks/markah]

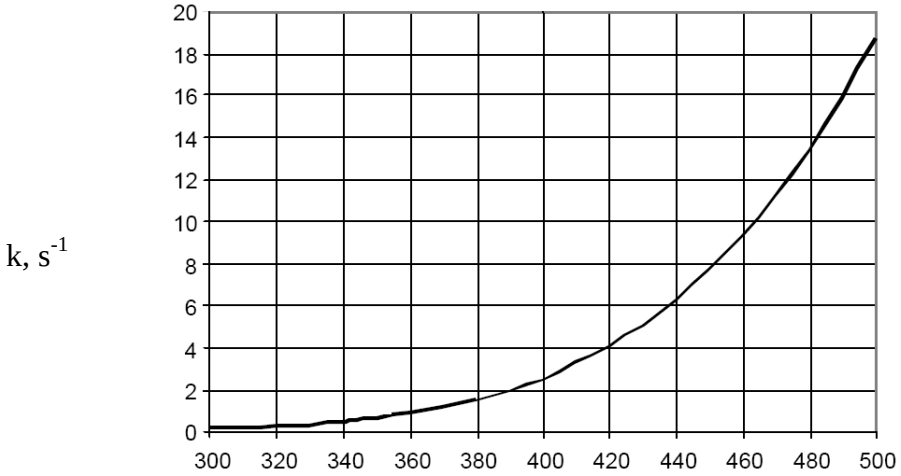

Figure Q.4.[a]
Rajah S.4.[a]

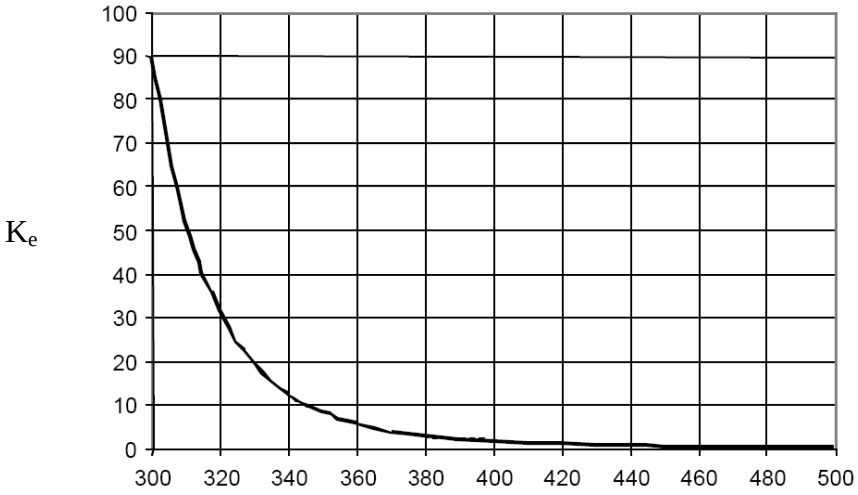

Figure Q.4.[b]
Rajah S.4.[b]

5. [a] Select the reactor schemes that will maximize the selectivity (S) of the desired product, (D) for the following parallel reactions:

Pilih skema reaktor yang dapat memaksimakan kememilihan (S) produk yang dikehendaki (D) bagi tindakbalas selari yang berikut:

$A + B \rightarrow D$: $r_D = k_1 C_A^{0.2} C_B^{2.2}$

$A + B \rightarrow U_1$: $r_{U1} = k_2 C_A^{1.5} C_B^{0.5}$

$A \rightarrow U_2$: $r_{U2} = k_3 C_A$

What is the effect if the overall reaction is highly exothermic?
Apakah kesannya jika tindakbalas keseluruhannya adalah sangat eksotermik?

[7 marks/markah]

[b] Consider the following gas-phase reaction where A is cracked into B and C:
Pertimbangkan tindakbalas fasa gas yang berikut di mana A dipecahkan kepada B dan C:

$A \rightarrow B + C$

The reaction is first order with respect to A and that the specific reaction rate can be expressed by

Tindakbalas tersebut adalah tertib pertama bagi A dan kadar tindakbalas tentu boleh ditentukan dengan

$$\ln k = 34.34 - \frac{34{,}222}{T}$$

...8/-

Where k is in reciprocal seconds and T is in kelvin. It is required to feed 7850 kg of A per hr to a tubular reactor. The reactor consists of 1000 of 1-inch tubes. The reactor is surrounded by a heat exchanger where the heat transfer coefficient is 110 J/m^2.s.K, and the temperature of the heating medium, T_a, is constant at 1150 K. The inlet temperature and pressure are at 1035 K and 162 kPa, respectively. (Given: Molecular weight of A = 58 g/mol)

Di mana, k dalam unit per saat dan T dalam unit Kelvin. Sebanyak 7850 kg A per jam perlu disuapkan ke dalam sebuah reaktor tiub. Reaktor tersebut mengandungi 1000 tiub berdiameter 1 inci. Reaktor tersebut dikelilingi sebuah penukar haba dengan pekali pemindahan haba sebanyak 110 J/m^2.s.K, dan suhu pemanas, T_a adalah malar pada 1150 K. Suhu dan tekanan suapan adalah masing-masing 1035 K dan 162 kPa. (Diberi berat molekul A = 58 g/mol).

[i] Derive the equations to determine the conversion of A and the temperature as a function of the length of the reactor.

Terbitkan persamaan bagi menentukan penukaran A dan suhu dalam fungsi panjang reaktor.

[13 marks/markah]

[ii] The profile of temperature and conversion are plotted as in Figure Q.5. Discuss the profiles.

Profil suhu dan penukaran A diplotkan dalam Rajah S.5. Bincangkan profil tersebut.

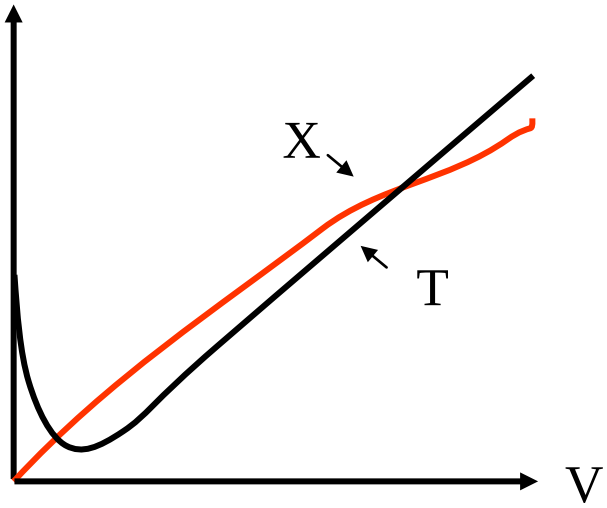

Figure Q.5.
Rajah S.5.

[5 marks/markah]

6. [a] Consider the reactions as below:
Pertimbangkan tindakbalas yang berikut:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

with k_1 = 0.15 s^{-1} and k_2 = 0.30 s^{-1} with C_{AO}= 2.5 mol/dm^3. Determine the space velocity, τ that the reaction need to be carried out in a CSTR in order to obtain the optimal concentration of C. What is the optimal concentration of C?

dengan k_1 = 0.15 s^{-1} dan k_2 = 0.30 s^{-1} dengan C_{AO}= 2.5 mol/dm^3. Tentukan halaju ruang τ bagi tindakbalas tersebut yang perlu dijalankan dalam sebuah CSTR untuk mendapat kepekatan C yang optimal. Apakah kepekatan optimal C?

[7 marks/markah]

[b] The flow through a reactor is 10 dm^3/min. A pulse test gave the following measurements at the outlet:

Aliran melalui sebuah reaktor adalah 10 dm^3/min. Satu ujian denyutan memberi ukuran yang berikut pada alur keluar:

t(min)	0	0.4	1.0	2	3	4	5
C ×10^3 g/dm^3	0	1	3.5	7.4	9.4	9.7	9.4

t(min)	6	8	10	15	20	25	30
C ×10^3 g/dm^3	8.2	5.0	2.4	1.2	0.5	0.2	0

[i] Plot the external age distribution *E*(*t*) curve as a function of time.
Plotkan lengkuk taburan usia keluar E(t) dalam fungsi masa.

[ii] What is the mean residence time?
Apakah purata untuk masa mastautin?

[iii] What is the fraction of the material which spent longer than 15 min in the reactor?

Apakah pecahan bagi bahan yang tinggal dalam reaktor melebihi 15 min?

[18 marks/markah]

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Appendix

Useful differential equations:

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}(u/v) = \frac{(v\frac{du}{dx} - u\frac{dv}{dx})}{v^2}$$

Numerical Evaluation of Integrals:

1. Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] \text{ when } h = x_1 - x_0$$

2. Simpson's three-eights rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

Where $h = \frac{x_3 - x_0}{3}$; $x_1 = x_0 + h$; $x_2 = x_0 + 2h$;

3. Simpson's quadrature formula

$$\int_{x_0}^{x_4} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)]$$

Where $h = \frac{x_4 - x_0}{4}$

4. For N+1 points, where (N/3) is an integer,

$$\int_{x_0}^{x_N} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + \cdots + 3f(x_{N-1}) + f(x_N)]$$

Where $h = \frac{x_N - x_0}{N}$

5. For N+1 points, where N is even,

$$\int_{x_0}^{x_N} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{N-1}) + f(x_N)]$$

Where $h = \frac{x_N - x_0}{N}$

...2/-

Ideal gas constant

$$R = \frac{8.314\ \text{kPa} \cdot .\text{dm}^3}{\text{mol.K}} \qquad R = \frac{1.987\ \text{Btu}}{\text{Ib mol} \cdot^{o} \text{R}}$$

$$R = \frac{0.73\ \text{ft}^3 \cdot .\text{atm}}{\text{Ib mol} \cdot^{o} \text{R}} \qquad R = \frac{8.3144\ \text{J}}{\text{mol.K}}$$

$$R = \frac{0.082\ \text{dm}^3 \cdot .\text{atm}}{\text{mol.K}} = \frac{0.082\ \text{m}^3 \cdot .\text{atm}}{\text{kmol.K}} \qquad R = \frac{1.987\text{cal}}{\text{mol} \cdot \text{K}}$$

Useful Integrals in Reactor Design

$$\int_0^x \frac{dx}{1-x} = ln\frac{1}{1-x} \qquad (A-1)$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x} \qquad (A-2)$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon} ln(1+\varepsilon x) \qquad (A-3)$$

$$\int_0^x \frac{1+\varepsilon x}{1-x} dx = (1+\varepsilon) ln\frac{1}{1-x} - \varepsilon x \qquad (A-4)$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2} dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon ln\frac{1}{1-x} \qquad (A-5)$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2} dx = 2\varepsilon(1+\varepsilon) ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x} \qquad (A-6)$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1} ln\frac{\Theta_B - x}{\Theta_B(1-x)} \quad \Theta B \neq 1 \qquad (A-7)$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{-2}{2ax+b} + \frac{2}{b} \quad for\ b^2 = 4ac \qquad (A-8)$$

$$\int_0^x \frac{dx}{ax^2+bx+c} = \frac{1}{a(p-q)} ln\left(\frac{q}{p}\cdot\frac{x-p}{x-q}\right) \quad for\ b^2 > 4ac \qquad (A-9)$$

$$\int_0^W (1-\alpha W)^{1/2} dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right] \qquad (A-10)$$

$$\int_0^\infty \left(e^{-kt}\right)\delta(t-\tau) dt = e^{-k\tau} \qquad (A-11)$$

Simpson's five-point formula

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) \qquad h = \frac{X_4 - X_0}{4}$$