Neraca energi dengan reaksi kimia

KONSEP

- Dalam reaksi kimia umumnya ada efek panas.
- Terdapat perbedaan kandungan entalpi antara reaktan dengan hasil reaksi.
- Bila hasil-hasil reaksi mempunyai entalpi lebih besar dari pada pereaksinya maka perlu dimasukkan panas pada sistem bereaksi, atau sebaliknya.

$$A + 2B + Q + H_1^o \longrightarrow 2C + D + H_2^O$$

- NM : $A + 2B \longrightarrow 2C + D$
- NP : $Q + H_1^o \longrightarrow H_2^o$

$$Q = H_2^o - H_1^o = \Delta H_R^o$$

ΔH_R^o = panas reaksi pada keadaan standar (25°C, 1 atm)

- ΔH_R^o = positif, maka perlu panas ⟶ REAKSI ENDOTERMIS
- ΔH_R^o = negatif, maka mengeluarkan panas ⟶ REAKSI EKSOTERMIS
- Entalpi reaksi didefinisikan berdasarkan reaksinya (jumlah bahan dalam mol sesuai persamaan reaksinya)

$$CH_4(g) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(l): \quad \Delta\hat{H}_{r1}(25°C) = -890.3\ \text{kJ/mol}$$
$$2\,CH_4(g) + 4\,O_2(g) \longrightarrow 2\,CO_2(g) + 4H_2O(l): \quad \Delta\hat{H}_{r2}(25°C) = -1780.6\ \text{kJ/mol}$$

- Nilai dari panas reaksi tergantung pada keadaan (padat, cair, atau gas) dari senyawa yang terlibat.

$$CH_4(g) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(l): \quad \Delta\hat{H}_r(25°C) = -890.3\ \text{kJ/mol}$$
$$CH_4(g) + 2\,O_2(g) \longrightarrow CO_2(g) + 2\,H_2O(g): \quad \Delta\hat{H}_r(25°C) = -802.3\ \text{kJ/mol}$$

- Panas reaksi standar, ΔH_R^o adalah panas reaksi jika baik reaktan maupun hasil reaksi berada pada keadaan standar (25 ^oC, 1 atm)

- Panas pembentukan standar, ΔH_f^o, adalah perubahan entalpi sehubungan dengan pembentukan 1 mol senyawa dari unsur pembentuknya pada keadaan standar (25 ^oC, 1 atm)
- Panas reaksi standar dapat dihitung dari panas pembentukan standar

$$\Delta \hat{H}_r^\circ = \sum_i \nu_i \Delta \hat{H}_{fi}^\circ = \sum_{\text{products}} |\nu_i| \Delta \hat{H}_{fi}^\circ - \sum_{\text{reactants}} |\nu_i| \Delta \hat{H}_{fi}^\circ$$

- Panas pembakaran standar, ΔH_C^o, adalah panas reaksi pembakaran dengan oksigen yang menghasilkan hasil reaksi tertentu (misal $CO_2(g)$, H_2O (l)) dimana baik reaktan maupun hasil reaksi pada keadaan standar.
- Panas reaksi standar dapat dihitung dengan menggunakan panas pembakaran standar

$$\Delta \hat{H}_r^\circ = -\sum_i \nu_i (\Delta \hat{H}_c^\circ)_i = \sum_{\text{reactants}} |\nu_i| (\Delta \hat{H}_c^\circ)_i - \sum_{\text{products}} |\nu_i| (\Delta \hat{H}_c^\circ)_i$$

example 9.3-1 F-R

Determination of a Heat of Reaction from Heats of Formation

Determine the standard heat of reaction for the combustion of liquid *n*-pentane, assuming $H_2O(l)$ is a combustion product.

$$C_5H_{12}(l) + 8\,O_2(g) \rightarrow 5\,CO_2(g) + 6\,H_2O(l)$$

Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20°/4°)	T_m(°C)[b]	$\Delta\hat{H}_m(T_m)$[c,j] kJ/mol	T_b(°C)[d]	$\Delta\hat{H}_v(T_b)$[e,j] kJ/mol	T_c(K)[f]	P_c(atm)[g]	$(\Delta\hat{H}_f°)$[h,j] kJ/mol	$(\Delta\hat{H}_c°)$[i,j] kJ/mol
Methyl ethyl ketone	C_4H_8O	72.10	0.805	−87.1	—	78.2	32.0	—	—	—	−2436(l)
Naphthalene	$C_{10}H_8$	128.16	1.145	80.0	—	217.8	—	—	—	—	−5157(g)
Nickel	Ni	58.69	8.90	1452	—	2900	—	—	—	0(c)	—
Nitric acid	HNO_3	63.02	1.502	−41.6	10.47	86	30.30	—	—	−173.23(l)	—
										−206.57(aq)	
Nitrobenzene	$C_6H_5O_2N$	123.11	1.203	5.5	—	210.7	—	—	—	—	−3092.8(l)
Nitrogen	N_2	28.02	—	−210.0	0.720	−195.8	5.577	126.20	33.5	0(g)	—
Nitrogen dioxide	NO_2	46.01	—	−9.3	7.335	21.3	14.73	431.0	100.0	+33.8(g)	—
Nitric oxide	NO	30.01	—	−163.6	2.301	−151.8	13.78	179.20	65.0	+90.37(g)	—
Nitrogen pentoxide	N_2O_5	108.02	$1.63^{18°}$	30	—	47	—	—	—	—	—
Nitrogen tetraoxide	N_2O_4	92.0	1.448	−9.5	—	21.1	—	431.0	99.0	+9.3(g)	—
Nitrous oxide	N_2O	44.02	$1.226^{-89°}$	−91.1	—	−88.8	—	309.5	71.70	+81.5(g)	—
n-Nonane	C_9H_{20}	128.25	0.718	−53.8	—	150.6	—	595	23.0	−229.0(l)	−6124.5(l)
										—	−6171.0(g)
n-Octane	C_8H_{18}	114.22	0.703	−57.0	—	125.5	—	568.8	24.5	−249.9(l)	−5470.7(l)
										−208.4(g)	−5512.2(g)
Oxalic acid	$C_2H_2O_4$	90.04	1.90	Decomposes at 186°C				—	—	−826.8(c)	−251.9(s)
Oxygen	O_2	32.00	—	−218.75	0.444	−182.97	6.82	154.4	49.7	0(g)	—
n-Pentane	C_5H_{12}	72.15	$0.63^{18°}$	−129.6	8.393	36.07	25.77	469.80	33.3	−173.0(l)	−3509.5(l)
										−146.4(g)	−3536.1(g)
Isopentane	C_5H_{12}	72.15	$0.62^{19°}$	−160.1	—	27.7	—	461.00	32.9	−179.3(l)	−3507.5(l)
							—			−152.0(g)	−3529.2(g)
1-Pentene	C_5H_{10}	70.13	0.641	−165.2	4.94	29.97		474	39.9	−20.9(g)	−3375.8(g)
Phenol	C_6H_5OH	94.11	$1.071^{25°}$	42.5	11.43	181.4	—	692.1	60.5	−158.1(l)	−3063.5(s)
										−90.8(g)	—
Phosphoric acid	H_3PO_4	98.00	$1.834^{18°}$	42.3	10.54	$(-\frac{1}{2}H_2O$ at 213°C)		—	—	−1281.1(c)	—
										−1278.6(aq, $1H_2O$)	—
Phosphorus (red)	P_4	123.90	2.20	$590^{43\ atm}$	81.17	Ignites in air, 725°C		—	—	−17.6(c)	—
										0(c)	

Sumber :
F-R

Calcium hydroxide	$Ca(OH)_2$	74.10	2.24			($-H_2O$ at 580°C)				−986.59(c)	—
Calcium oxide	CaO	56.08	3.32	2570	50	2850	—	—	—	−635.6(c)	—
Calcium phosphate	$Ca_3(PO_4)_2$	310.19	3.14	1670	—	—	—	—	—	−4138(c)	—
Calcium silicate	$CaSiO_3$	116.17	2.915	1530	48.62	—	—	—	—	−1584(c)	—
Calcium sulfate	$CaSO_4$	136.15	2.96	—	—	—	—	—	—	−1432.7(c) −1450.4(aq)	—
Calcium sulfate (gypsum)	$CaSO_4 \cdot 2H_2O$	172.18	2.32		($-1.5\ H_2O$ at 128°C)		—	—	—	−2021(c)	—
Carbon (graphite)	C	12.010	2.26	3600	46.0	4200	—	—	—	0(c)	−393.51(c)
Carbon dioxide	CO_2	44.01	—	−56.6 at 5.2 atm	8.33	(Sublimes at −78°C)		304.2	72.9	−412.9(l) −393.5(g)	— —
Carbon disulfide	CS_2	76.14	$1.261^{22°/20°}$	−112.1	4.39	46.25	26.8	552.0	78.0	+87.9(l) +115.3(g)	−1075.2(l) 1102.6(g)
Carbon monoxide	CO	28.01	—	−205.1	0.837	−191.5	6.042	133.0	34.5	−110.52(g)	−282.99(g)
Carbon tetrachloride	CCl_4	153.84	1.595	−22.9	2.51	76.7	30.0	556.4	45.0	−139.5(l) −106.7(g)	−352.2(l) −385.0(g)
Chlorine	Cl_2	70.91	—	−101.00	6.406	−34.06	20.4	417.0	76.1	0(g)	—
Chlorobenzene	C_6H_5Cl	112.56	1.107	−45	—	132.10	36.5	632.4	44.6	—	—
Chloroethane	C_2H_5Cl	See ethyl chloride									

Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20°/4°)	T_m(°C)[b]	$\Delta\hat{H}_m(T_m)$[c,j] kJ/mol	T_b(°C)[d]	$\Delta\hat{H}_v(T_b)$[e,j] kJ/mol	T_c(K)[f]	P_c(atm)[g]	$(\Delta\hat{H}_f°)$[h,j] kJ/mol	$(\Delta\hat{H}_c°)$[i,j] kJ/mol
Sodium thiosulfate	$Na_2S_2O_3$	158.11	1.667	—	—	—	—	—	—	−1117.1(c)	—
Sulfur (rhombic)	S_8	256.53	2.07	113	10.04	444.6	83.7	—	—	0(c)	—
Sulfur (monoclinic)	S_8	256.53	1.96	119	14.17	444.6	83.7	—	—	+0.30(c)	—
Sulfur dioxide	SO_2	64.07	—	−75.48	7.402	−10.02	24.91	430.7	77.8	−296.90(g)	—
Sulfur trioxide	SO_3	80.07	—	16.84	25.48	43.3	41.80	491.4	83.8	−395.18(g)	—
Sulfuric acid	H_2SO_4	98.08	$1.834^{18°}$	10.35	9.87	Decomposes at 340°C		—	—	−811.32(l)	—
										−907.51(aq)	—
Toluene	C_7H_8	92.13	0.866	−94.99	6.619	110.62	33.47	593.9	40.3	+12.00(l)	−3909.9(l)
										+50.00(g)	−3947.9(g)
Water	H_2O	18.016	$1.00^{4°}$	0.00	6.0095	100.00	40.656	647.4	218.3	−285.84(l)	—
										−241.83(g)	—
m-Xylene	C_8H_{10}	106.16	0.864	−47.87	11.569	139.10	36.40	619	34.6	−25.42(l)	−4551.9(l)
										+17.24(g)	−4594.5(g)
o-Xylene	C_8H_{10}	106.16	0.880	−25.18	13.598	144.42	36.82	631.5	35.7	−24.44(l)	−4552.9(l)
										+18.99(g)	−4596.3(g)
p-Xylene	C_8H_{10}	106.16	0.861	13.26	17.11	138.35	36.07	618	33.9	−24.43(l)	−4552.91(l)
										17.95(g)	−4595.2(g)
Zinc	Zn	65.38	7.140	419.5	6.674	907	114.77	—	—	0(c)	—

From Equation 9.3-1

$$\Delta\hat{H}_r^\circ = 5(\Delta\hat{H}_f^\circ)_{CO_2(g)} + 6(\Delta\hat{H}_f^\circ)_{H_2O(l)} - (\Delta\hat{H}_f^\circ)_{C_5H_{12}(l)}$$

$$\Downarrow \text{ Heats of formation from Table B.1}$$

$$\Delta\hat{H}_r^\circ = [5(-393.5) + 6(-285.84) - (-173.0)]\ \text{kJ/mol}$$

$$= \boxed{-3509\ \text{kJ/mol}}$$

To verify the formula for $\Delta\hat{H}_r^\circ$, we may write the stoichiometric equations for the formation reactions of the reactants and products:

1. $5\,C(s) + 6\,H_2(g) \rightarrow C_5H_{12}(l)$: $\Delta\hat{H}_{r1}^\circ = (\Delta\hat{H}_f^\circ)_{C_5H_{12}(l)}$
2. $C(s) + O_2(g) \rightarrow CO_2(g)$: $\Delta\hat{H}_{r2}^\circ = (\Delta\hat{H}_f^\circ)_{CO_2(g)}$
3. $H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$: $\Delta\hat{H}_{r3}^\circ = (\Delta\hat{H}_f^\circ)_{H_2O(l)}$

The desired reaction,

4. $C_5H_{12}(l) + 8\,O_2(g) \rightarrow 5\,CO_2(g) + 6\,H_2O(l)$: $\Delta\hat{H}_r^\circ = ?$

may be obtained as $5 \times (2) + 6 \times (3) - (1)$ (*verify*), and the given formula for $\Delta\hat{H}_r^\circ$ then follows from Hess's law.

Example 9.4-1 F-R

Calculation of a Heat of Reaction from Heats of Combustion

Calculate the standard heat of reaction for the dehydrogenation of ethane:

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

From Table B.1,

$$(\Delta \hat{H}_c^\circ)_{C_2H_6} = -1559.9 \text{ kJ/mol}$$
$$(\Delta \hat{H}_c^\circ)_{C_2H_4} = -1411.0 \text{ kJ/mol}$$
$$(\Delta \hat{H}_c^\circ)_{H_2} = -285.84 \text{ kJ/mol}$$

From Equation 9.4-1, therefore,

$$\Delta\hat{H}_r^\circ = (\Delta\hat{H}_c^\circ)_{C_2H_6} - (\Delta\hat{H}_c^\circ)_{C_2H_4} - (\Delta\hat{H}_c^\circ)_{H_2} = \boxed{136.9 \text{ kJ/mol}}$$

As an illustration, let us demonstrate the validity of this formula using Hess's law. The combustion reactions are

1. $C_2H_6 + \frac{7}{2}O_2 \rightarrow 2\,CO_2 + 3\,H_2O$
2. $C_2H_4 + 3\,O_2 \rightarrow 2\,CO_2 + 2\,H_2O$
3. $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

It is easy to show that

4. $C_2H_6 \rightarrow C_2H_4 + H_2$

is obtained as (1) − (2) − (3). (Show it.) The desired result follows from Hess's law.

- Salah satu penggunaan data panas reaksi pembakaran standar adalah untuk mencari panas pembentukan standar senyawa-senyawa yang reaksi pembentukannya tidak terjadi secara alamiah.

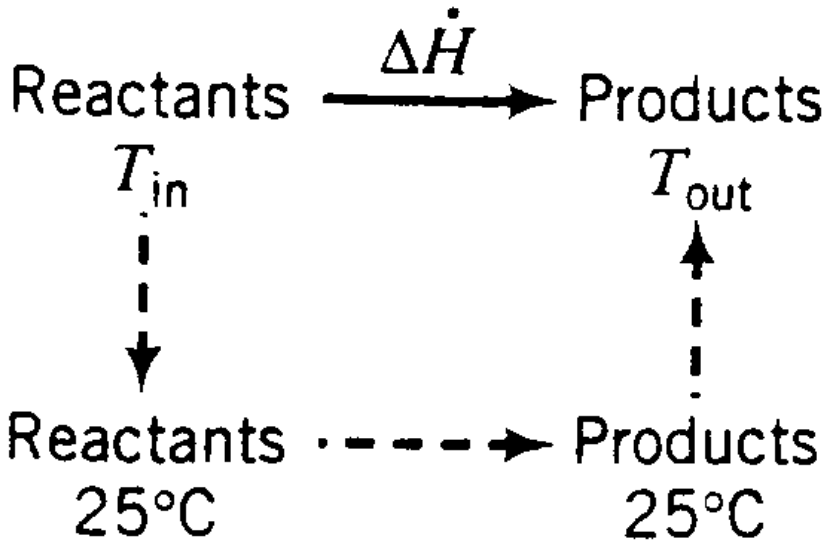
$$\Delta\hat{H}^\circ_r = -\sum_i \nu_i(\Delta\hat{H}^\circ_c)_i = \sum_{\text{reactants}} |\nu_i|(\Delta\hat{H}^\circ_c)_i - \sum_{\text{products}} |\nu_i|(\Delta\hat{H}^\circ_c)_i$$

$$5\,C(s) + 6\,H_2(g) \rightarrow C_5H_{12}(l): \quad \Delta\hat{H}^\circ_f = ?$$

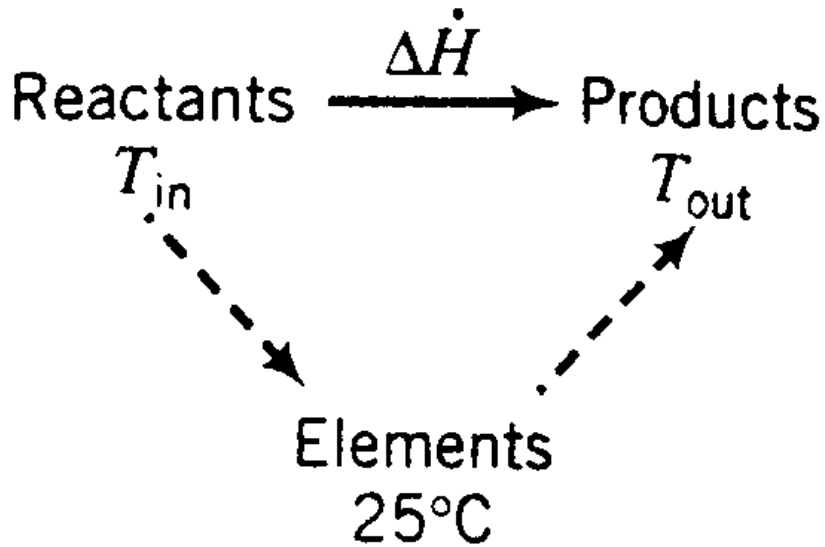
cannot be carried out in a laboratory, but carbon, hydrogen, and pentane can all be burned and their standard heats of combustion determined experimentally. The heat of formation of pentane may then be calculated from Equation 9.4-1 as

$$(\Delta\hat{H}^\circ_f)_{C_5H_{12}(l)} = 5(\Delta\hat{H}^\circ_c)_{C(s)} + 6(\Delta\hat{H}^\circ_c)_{H_2(g)} - (\Delta\hat{H}^\circ_c)_{C_5H_{12}(l)}$$

Pengaruh suhu pada panas reaksi



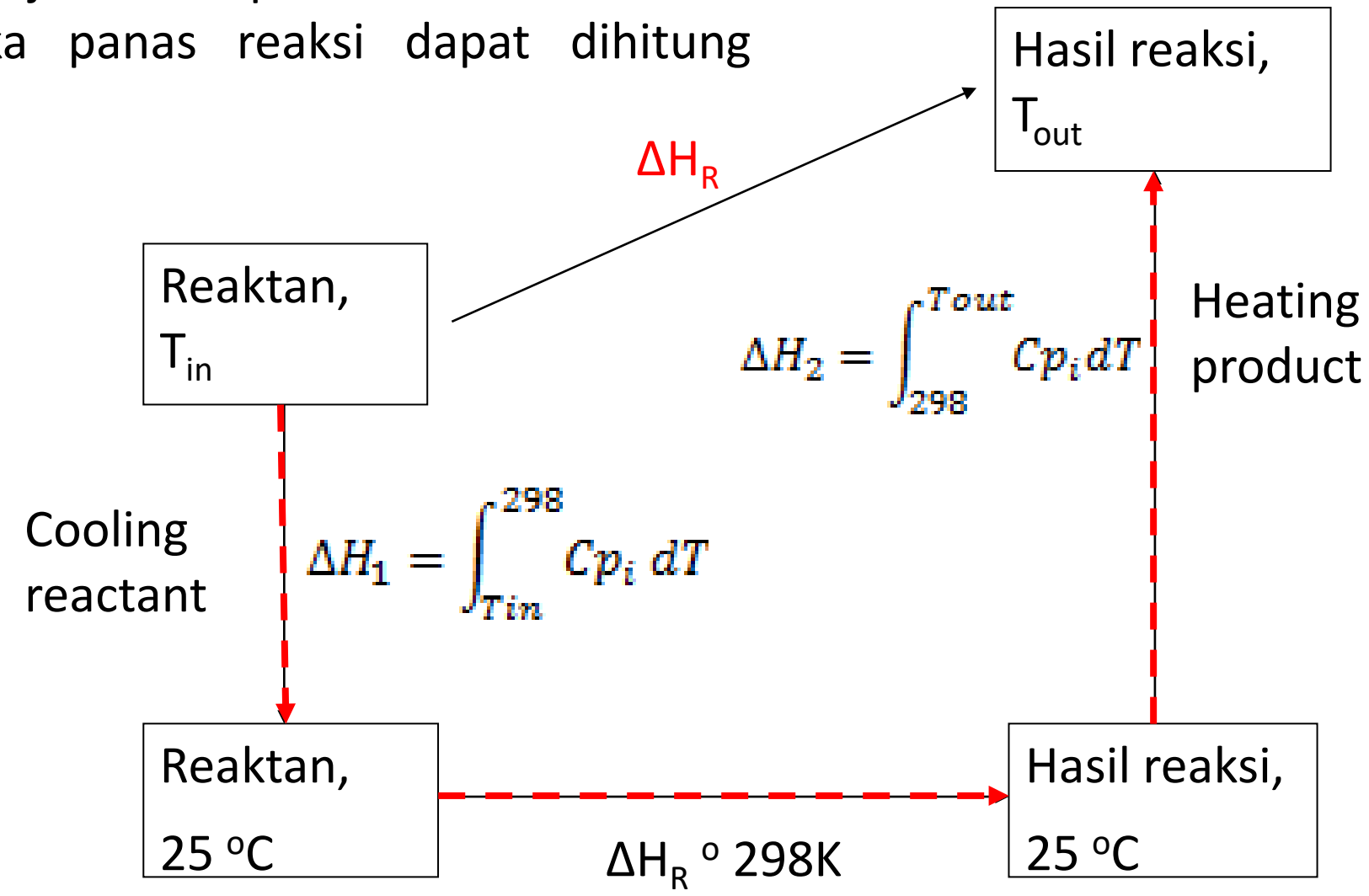
(*a*) Process path for heat of reaction method



(*b*) Process path for heat of formation method

- Suhu hasil reaksi, T_{out} dapat sama atau berbeda dengan suhu reaktan, T_{in}

Jika reaksi dijalankan pada keadaan bukan standar maka panas reaksi dapat dihitung dengan cara :



- $\Delta H_R = \Delta H_1 + \Delta H_R^{o} + \Delta H_2$

Latihan

- Reaksi $4NH_3(g) + 5O_2\ (g) \longrightarrow 4NO(g) + 6H_2O$ dijalankan dalam suatu reaktor. NH_3 dan udara diumpankan pada suhu 750 ^oC. Sejumlah 90% NH_3 bereaksi membentuk NO. Umpan O_2 sebanyak 2,4 kali umpan NH_3 (dalam mol). Jika suhu keluar reaktor tidak boleh melebihi 920 ^oC, berapa panas yang dihasilkan dari reaksi tersebut?

gas	ΔH_{f298}, kal/mol	Cp, a+bT, cal/mol.K
NH_3	-10960	6,7 + 0,006T
O_2	0	8,3 + 0,0002T
NO	21600	8,05 + 0,0002T
H_2O	-57800	7,2 + 0,003T
N_2	0	8,5 + 0,0001T