Laboratory of
Computational
Systems
Biotechnology

EPFL

Introduction to Chemical Engineering

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Office hours: Mondays 16h-19h (CH H4 625) or schedule by email

Fridays, 14 - 17h
2025-2026

Course Schedule

Date	Subject
12-Sep	**1. Fundamentals of Material Balances** 1.1. Process definition and classification 1.2. Material balance calculations 1.3. Balances on multiple-unit processes
19-Sep	Exercises
26-Sep	1.4. Chemical reaction stoichiometry 1.5. Balances on reactive Processes
03-Oct	Review on Material Balances
10-Oct	**1.6. Balances on multiple unit reactive processes**
17-Oct	**2. Fundamentals of Energy and Energy Balances** 2.1. Energy balances on closed systems 2.2. Open systems at steady state **3. Balances on Non-Reactive Processes** 3.1. Energy balance calculation 3.2. Changes in Pressure, Temperature, Phases
31-Oct	**4. Balances on Reactive Processes** 4.1. Introduction to the Enthalpy of Reaction 4.2. Heat of Reaction Method 4.3. Heat of Formation Method 4.4 General Procedure to solve energy balance in reactive systems
07-Nov	**Review on Balances on Non-Reactive Processes** Problems: Mass and Energy Balances on non-Reactive Systems
14-Nov	**Midterm Exam: Mass & Energy Balances non-Reactive Systems**
21-Nov	**Review Midterm**

Date	Subject
28-Nov	**Review on Heat of Reaction vs Heat of Formation Methods** **4.5 Hess's Law to compute the Heat of Reaction** **4.6 Heat of Combustion**
05-Dec	**5. Energy balances on mixing processes** **5.1 Distinction between ideal and real solutions** **5.2 Heat of Solution**
12-Dec	Review and Study Session • Summing up with Mass and Energy Balances on Reactive Systems with Recycle

Recommended textbook:
Elementary Principles of Chemical Processes,
Richard M. Felder & Ronald W. Rousseau

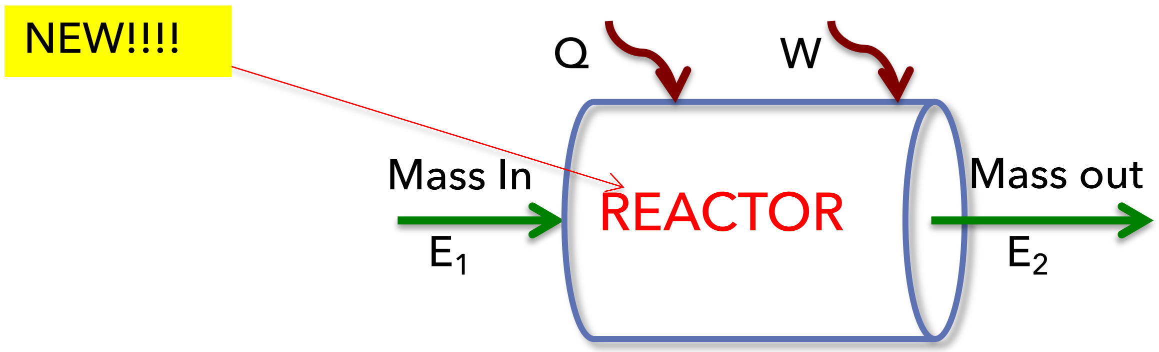
Session VI: Friday 31st October 2025

After studying this session you will be able to:

Understand the term ENTHALPY OF REACTION (ΔH_r). Classification of reactions (sign of ΔH_r)

Introduction to the Enthalpy of Reaction

Recalling: Energy Balance on a Process



law of conservation of energy:

$$E_{\text{accumulated}} = E_{\text{input}} - E_{\text{output}} + E_{\text{gen}} + E_{\text{transferred}}$$

1. What effect do reactions have on the energy balances ?
2. How do we handle the path of species that are generated or consumed ?

NEW: Energy Balance on a Reactive Process

1. What effect do reactions have on the energy balances ?

- Until now (in non-reactive processes):

$$\Delta \dot{H} = \sum_{out} \dot{m}_i \hat{H}_i - \sum_{in} \dot{m}_i \hat{H}_i$$

- NOW (in <u>reactive systems</u>): NEW CALCULATIONS, new terms required to calculate the total ΔH happening in a reactor (since molecular species are being generated or consumed).

2. How do we handle the path of species that are generated or consumed ?

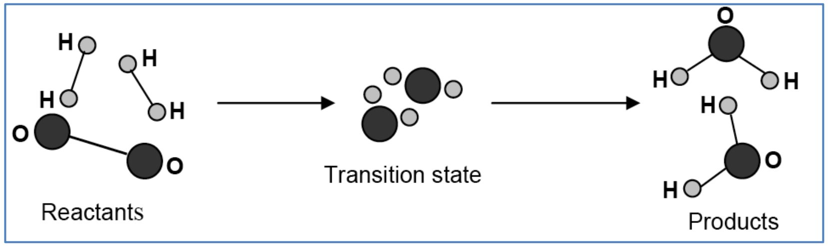
- Until now (in non-reactive processes): we arbitrarily chose a reference state for each specie in the process

- NOW (in <u>reactive systems</u>): not arbitrarily chosen,

But depending on the METHOD used to calculate
ΔH of reaction

1. Understand the Enthalpy of Reaction (ΔH_r)

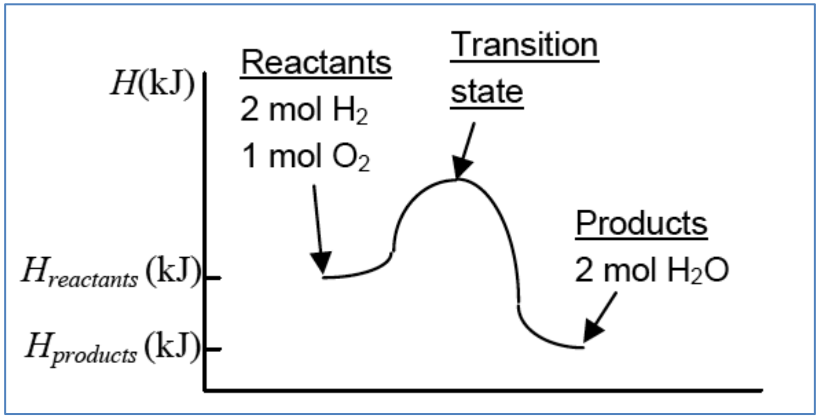
$$2H_2 + O_2 \longrightarrow 2H_2O$$



- One O-O bond and two H-H bonds are broken
- System absorbs energy, U_{system} and H_{system} increase from reactants to transition state
- 4 O-H bonds are formed
- System releases energy, U_{system} and H_{system} decrease from transition state to products.

When a reaction happens:

ENERGY is required to break the reactant chemical bonds



ENERGY is released when the product bonds form

Enthalpy of Reaction (ΔH_r)

- The heat of reaction, $\Delta\hat{H}_r(T,P)$: is the enthalpy change for a process in which stoichiometric ratios of reactants at a given T and P are completely consumed and converted to products at the same T and P.

$$H_{products} - H_{reactants} = \Delta\hat{H}_r(T,P) \ \text{heat of reaction (kJ/mol)}$$

- For stoichiometric quantities of H_2 and O_2 reacting completely at T=25 °C and P=1 atm:

$$2\ \text{mol}\ H_{2\,(g,\ 25\ °C,\ 1\ atm)} + 1\ \text{mol}\ O_{2\,(g,\ 25\ °C,\ 1\ atm)} \longrightarrow 2\ \text{mol}\ H_2O_{\,(l,\ 25\ °C,\ 1\ atm)}$$

$$\Delta\hat{H}°_r = -571.68\ \text{kJ/mol}$$

$\Delta\hat{H}°_r$ is the energy (kJ) that must be transferred to the system to transform 2 mol H_2 and 1 mol O_2 into 2 mol H_2O

BUT WHY

ENTHALPY OF REACTION

AND NOT

INTERNAL ENERGY OF REACTION ?

Classification of reactions…considering the sign of the Enthalpy of Reaction (ΔH_r)

- $\Delta H_r < 0$ ➔ $E_{products} < E_{reactants}$

More energy released by product bond formation than absorbed when reactant bonds break

The reaction is therefore Exothermic

- $\Delta H_r > 0$ ➔ $E_{products} > E_{reactants}$

Less energy released by product bond formation than absorbed when reactant bonds break.

The reaction is therefore Endothermic

Standard Heat of Reaction ($\Delta \hat{H}^{\circ}_r$)

The standard heat of reaction,$\Delta \hat{H}^{\circ}_r$ (kJ/mol), is the heat of the reaction when both the reactants and products are at a specified reference temperature and pressure (usually of 25°C and 1 atm).

The value of $\Delta \hat{H}^{\circ}_r$ is given for a specified phase of the reactants and products and considering that stoichiometric amounts of reactants are completely consumed.

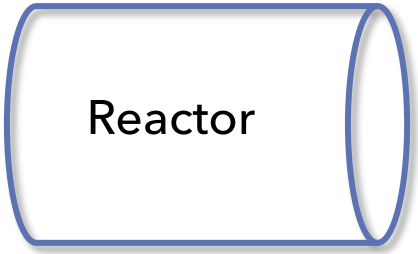
2. Working with the Enthalpy of Reaction (ΔHr)

… to calculate the enthalpy change in a closed system (ΔH)

- If A is a reactant or product of a reaction
  - ν_A is its stoichiometric coefficient
  - $n_{A,r}$ (mol A) is a quantity of A that reacts at 25°C and 1 atm
  - ξ is the extent of reaction

- then the enthalpy change for closed system is

$$\Delta H^\circ_r\ (\mathrm{kJ}) = n_{A,r}(mol\ \ A\ react)\frac{\Delta\hat{H}^\circ_r(kJ/mol)}{|\upsilon_A|} = \xi\Delta\hat{H}^\circ_r$$



$$E_{\text{accumulated}} = \cancel{E}_{\text{input}} - \cancel{E}_{\text{output}} + E_{\text{gen}} \cancel{+E}_{\text{transferred}}$$

$$E_{\text{accumulated}} = E_{\text{gen}} = -\Delta H^\circ_r = -\xi\Delta\hat{H}^\circ_r$$

Working with the Enthalpy of Reaction (ΔHr) … for different STOICHIOMETRY:

So, the enthalpy of <u>a</u> reaction depends on the way that we write the stochiometry in the reaction:

- $2A + B \rightarrow 3C \quad \Delta H_{r1\ (25°C)} = -50\ kJ$
- $4A + 2B \rightarrow 6C \quad \Delta H_{r2\ (25°C)} = -100\ kJ$

The information in both cases is the same, since:

r1: $$\frac{-50\,kJ}{2\,mol\,A\,consumed} = \frac{-50\,kJ}{1\,mol\,B\,consumed} = \frac{-50\,kJ}{3\,mol\,C\,generated}$$

r2: $$\frac{-100\,kJ}{4\,mol\,A\,consumed} = \frac{-100\,kJ}{2\,mol\,B\,consumed} = \frac{-100\,kJ}{6\,mol\,C\,generated}$$

<u>So … REMEMBER: the value of ΔH_r in kJ applies to the stoichiometric quantities defined in the reaction</u>

Working with the Enthalpy of Reaction (ΔHr) … for different PHASES:

Enthalpy of a reaction depends also on the phase of reactants and products:

- ○ $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$ $\Delta\hat{H}_{r1\ (25°C)} = -\ 890.3$ kJ/mol
- ○ $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$ $\Delta\hat{H}_{r2\ (25°C)} = -\ 802.3$ kJ/mol

What is the difference between the values $\Delta\hat{H}_{r1}$ and $\Delta\hat{H}_{r2}$?

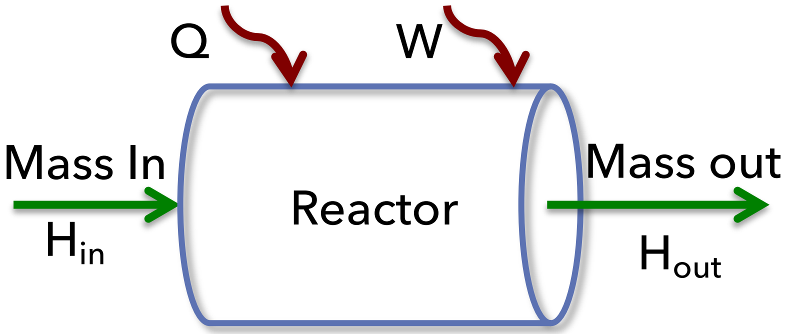
Substracting the reactions r2 – r1:

$$2H_2O(l) \rightarrow 2H_2O(g) \qquad \Delta\hat{H}_{r2\text{-}r1\ (25°C)} = 2\ \Delta\hat{H}_{v\ (25°C)}$$

LOOK OUT!: the fact that ΔH_r is defined for a given phase of A, does not mean that you have the same phase of A in your system…

3. Energy Balances on Reactive Systems

Considering an open, continuous system at steady state:



$$E_{\text{accumulated}} = E_{\text{input}} - E_{\text{output}} + E_{\text{gen}} + E_{\text{transferred}}$$

When reactions occur, the change in enthalpy term in the general energy balance equation is as follows:

$$\cancel{E_{\text{accumulated}}} = \sum \dot{n}_{in}\,\hat{H}_{in} - \sum \dot{n}_{out}\hat{H}_{out} - \xi\Delta\hat{H}_r + \dot{Q} - \cancel{\dot{W}_s}$$

- For single reaction: $0 = \sum \dot{n}_{in}\,\hat{H}_{in} - \sum \dot{n}_{out}\,\hat{H}_{out} - \xi\Delta\hat{H}_r + \dot{Q}$
- For multiple reactions: $0 = \sum \dot{n}_{in}\,\hat{H}_{in} - \sum \dot{n}_{out}\,\hat{H}_{out} - \sum \xi_{r,i}\Delta\hat{H}_{r,i} + \dot{Q}$

Methods used to solve energy balances in Reactive Systems

- There are two (equivalent) methods for solving energy balance in reactive systems

  A. Heat of Reaction Method
  B. Heat of Formation Method

The main goal in both cases is to calculate ΔH:

The difference between the enthalpy of the product stream in the reactor and the enthalpy of the input stream in the reactor

What might imply working with $\Delta\hat{H}_r$

Heat of Reaction Method

A. Heat of Reaction method

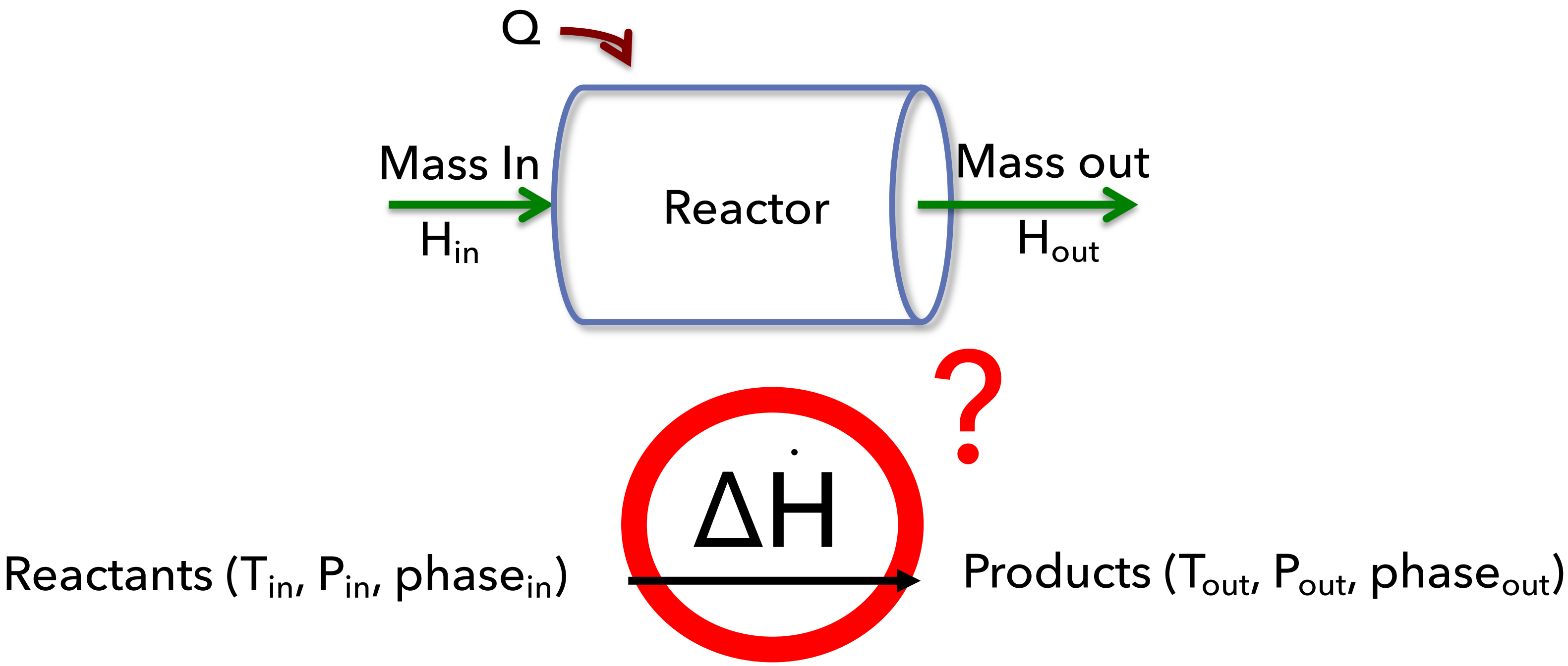
Application:

- The heat of reaction approach is more straightforward if there is only a single reaction for which ΔH°_r is known

Selection of reference condition:

- In this method for all reactants and products, the most convenient choice of reference conditions is that at which the information for the reaction is given
  - Usually the T and P at which the heat of reaction is known is the standard conditions, ΔH°_r (25 °C, 1 atm)

The path to calculate the total enthalpy change in the reactor, ΔH:



Reactants (T_{in}, P_{in}, $phase_{in}$) → Products (T_{out}, P_{out}, $phase_{out}$)

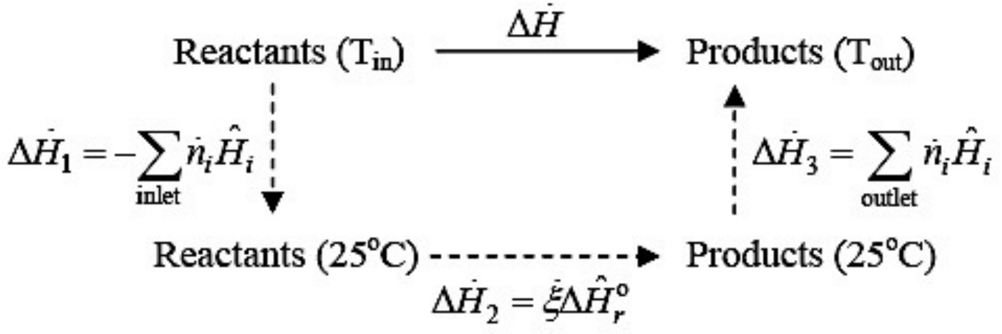
- $\Delta \dot{H}$ is what we really want to know…
- But we do not have this information for the specific conditions and reaction of our process
- WHAT TO DO?

The path to calculate the total enthalpy change in the reactor, ΔH:

(1) bring all reactants from inlet stream conditions to the given (standard) conditions for the heat of reaction ΔH°_r

(2) carry out the reaction under the <u>conditions given for ΔH°_r</u>

(3) bring the products from the standard conditions to the actual conditions in the outlet stream (the conditions at which they leave the reactor)

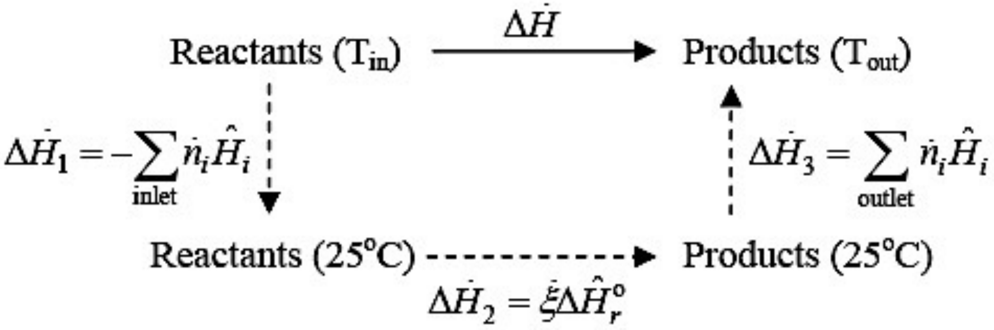


The path to calculate the total enthalpy change in the reactor, ΔH:

(1) bring all reactants from inlet stream conditions to the given (standard) conditions for the heat of reaction $\Delta H°_r$

(2) carry out the reaction under the conditions given for $\Delta H°_r$

(3) bring the products from the standard conditions to the actual conditions in the outlet stream (the conditions at which they leave the reactor)



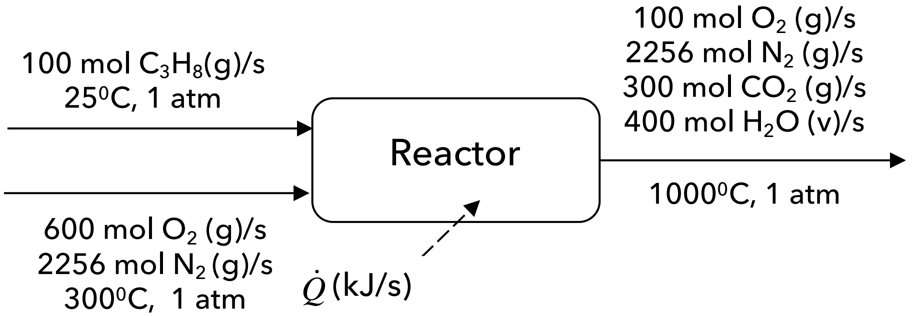
<u>Remember!:</u> We want to know ΔH between the input stream(s) and the output stream(s) – which means that we ALWAYS have to consider the real conditions of the streams in the process to create the paths (define the starting and ending point)

Example

Consider the following reactive process and calculate the heat (kJ/s) that is associated to the mentioned reaction

Given:

$C_3H_8 + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$ $\Delta\hat{H}_r^\circ = -2220$ kJ/mol



100 mol $C_3H_8(g)$/s
25^0C, 1 atm

600 mol O_2 (g)/s
2256 mol N_2 (g)/s
300^0C, 1 atm

Reactor

$\dot{Q}$ (kJ/s)

100 mol O_2 (g)/s
2256 mol N_2 (g)/s
300 mol CO_2 (g)/s
400 mol H_2O (v)/s

1000^0C, 1 atm

0. Understand the process.

Classify it: Open/continuous, single unit, steady-state, reactive

1. Draw and label the flowchart. Reactions: given $\dot{Q}$

2. Method: Heat of reaction method

3. Reference states:

C_3H_8 (g), O_2 (g), N_2 (g), CO_2 (g), H_2O(l) at 25°C et 1 atm

4. Inlet-Outlet Enthalpy table: fill in known and labeled amounts

Substance	$\dot{n}_{in}$ (mol/s)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/s)	$\hat{H}_{out}$(kJ/mol)
C_3H_8	100	0	–	–
O_2	600	$\hat{H}_2$	100	$\hat{H}_4$
N_2	2256	$\hat{H}_3$	2256	$\hat{H}_5$
CO_2	–	–	300	$\hat{H}_6$
H_2O	–	–	400	$\hat{H}_7$

5. Energy Balance Equation:

For open, reactive system at steady state + For the Heat of Reaction Method

$$\cancel{E_{acc}} = E_{in} - E_{out} + E_{gen} + E_{transf} \longrightarrow \cancel{E_{acc}} = \sum \dot{n}_{in}\hat{H}_{in} - \sum \dot{n}_{out}\hat{H}_{out} - \xi\Delta\hat{H}_r + \dot{Q} - \cancel{\dot{W}_s}$$

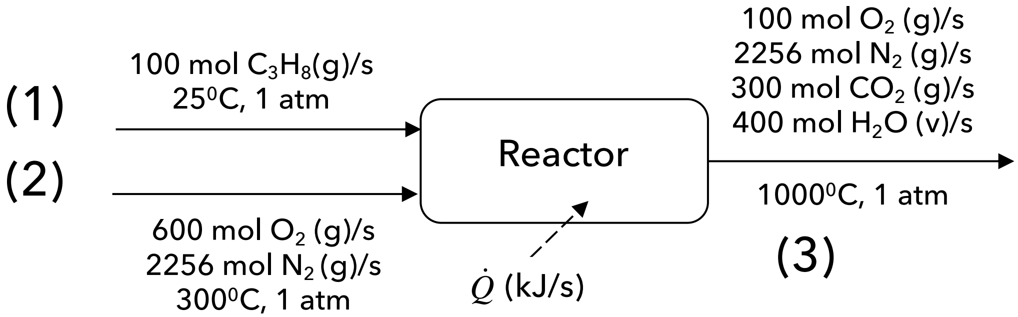
$$\boxed{0 = \sum \dot{n}_{in}\hat{H}_{in} - \sum \dot{n}_{out}\hat{H}_{out} - \xi\Delta\hat{H}_r + \dot{Q}}$$

6. Expressions for specific enthalpies ($\Delta\hat{H}_j$) : from reference state to process state

REFERENCE STATES:

C_3H_8 (g), O_2 (g), N_2 (g), CO_2 (g), H_2O(l)

at 25°C et 1atm



(1)

100 mol C_3H_8(g)/s

25^0C, 1 atm

(2)

600 mol O_2 (g)/s

2256 mol N_2 (g)/s

300^0C, 1 atm

Reactor

$\dot{Q}$ (kJ/s)

100 mol O_2 (g)/s

2256 mol N_2 (g)/s

300 mol CO_2 (g)/s

400 mol H_2O (v)/s

1000^0C, 1 atm

(3)

Stream 1:

$\hat{H}_1 = 0$

Stream 2:

$\hat{H}_2$ = O_2 (g, 25°C, 1atm) → O_2 (g, 300°C, 1atm) = 8.47 kJ/mol (table B.8)

$\hat{H}_3$ = N_2 (g, 25°C, 1atm) → N_2 (g, 300°C, 1atm) = 8.12 kJ/mol

Stream 3:

$\hat{H}_4$ = O_2 (g, 25°C, 1atm) → O_2 (g, 1000°C, 1atm) = 32.47 kJ/mol

$\hat{H}_5$ = N_2 (g, 25°C, 1atm) → N_2 (g, 1000°C, 1atm) = 30.56 kJ/mol

$\hat{H}_6$ = CO_2 (g, 25°C, 1atm) → CO_2 (g, 1000°C, 1atm) = 48.60 kJ/mol

$\hat{H}_7$ = H_2O (l, 25°C, 1atm) → H_2O (g, 1000°C, 1atm) $\int_{25^\circ C}^{100^\circ C} C_{pl}\,dT + \Delta\hat{H}_v + \int_{100^\circ C}^{1000^\circ C} C_{pv}\,dT = 81.71\ kJ/mol$

Substance	n_{in} (mol/s)	$\hat{H}_{in}$ (kJ/mol)	n_{out} (mol/s)	$\hat{H}_{out}$ (kJ/mol)
C_3H_8	100	0	-	-
O_2	600	8,47	100	32,47
N_2	2256	8,12	2256	30,56
CO_2	-	-	300	48,60
H_2O	-	-	400	81,71

6. (Cont) Expression for the term of enthalpy of reaction

$$\dot{\xi} = \frac{|(\dot{n}_{C_3H_8})_{out} - (\dot{n}_{C_3H_8})_{in}|}{|\upsilon_{C_3H_8}|} = \frac{|0-100|}{1} = 100 \ mol/s$$

With $\Delta\hat{H}_r^\circ = -2220$ kJ/mol

7. Solve the Energy Balance Equation

$$0 = \sum \dot{n}_{in} \hat{H}_{in} - \sum \dot{n}_{out} \hat{H}_{out} - \xi\Delta\hat{H}_r + \dot{Q}$$

$$\Rightarrow \dot{Q} = -1.26 \times 10^5 \text{ kJ/s}$$

Heat of Formation Method

B. Heat of Formation method

Application:

- Problems that have multiple reactions occurring simultaneously
- Or if ΔH°_r is not known

It is recommended to use the heat of formation method

CONCEPTS: Formation reaction and standard heat of formation ($\Delta \hat{H}^\circ_f$)

- Formation reaction: A reaction in which a compound is formed from its elemental constituents as they occur in nature
- Standard heat of formation ($\Delta \hat{H}^\circ_f$): the enthalpy change associated with the formation of 1 mol of the compound at a reference temperature and pressure (usually 25°C and 1 atm)

Example: formation reaction of liquid benzene

$$6\ C(s) + 3\ H_2(g) \rightarrow C_6H_6(l) \qquad (\Delta \hat{H}^\circ_f)_{C6H6(l)} = +48{,}66\ \text{kJ/mol}$$

The standard heat of formation is reported in the physical property tables! (Table B.1)

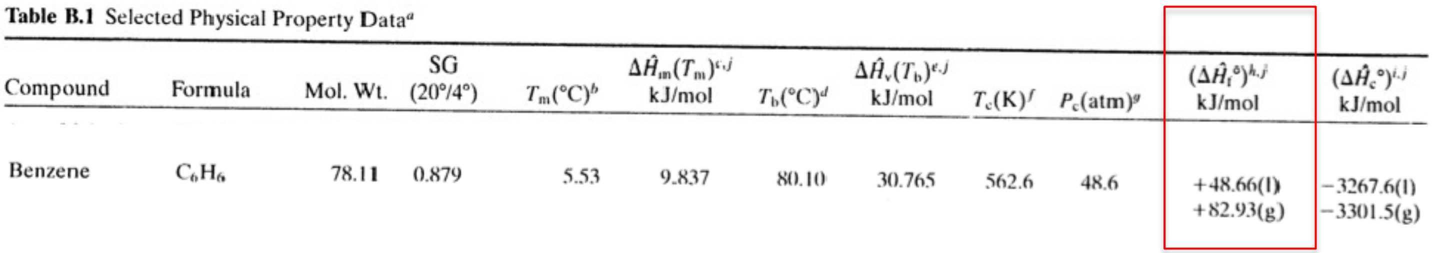


Table B.1 Selected Physical Property Data[a]

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]	$(\Delta\hat{H}_f^\circ)$[h,j] kJ/mol	$(\Delta\hat{H}_c^\circ)$[i,j] kJ/mol
Benzene	C_6H_6	78.11	0.879	5.53	9.837	80.10	30.765	562.6	48.6	+48.66(l) +82.93(g)	−3267.6(l) −3301.5(g)

In Table B.1 the heat of formation is given at 25˚C and 1 atm

The standard heat of formation of the elemental species [C(s), H2(g), O2(g),...] is zero!

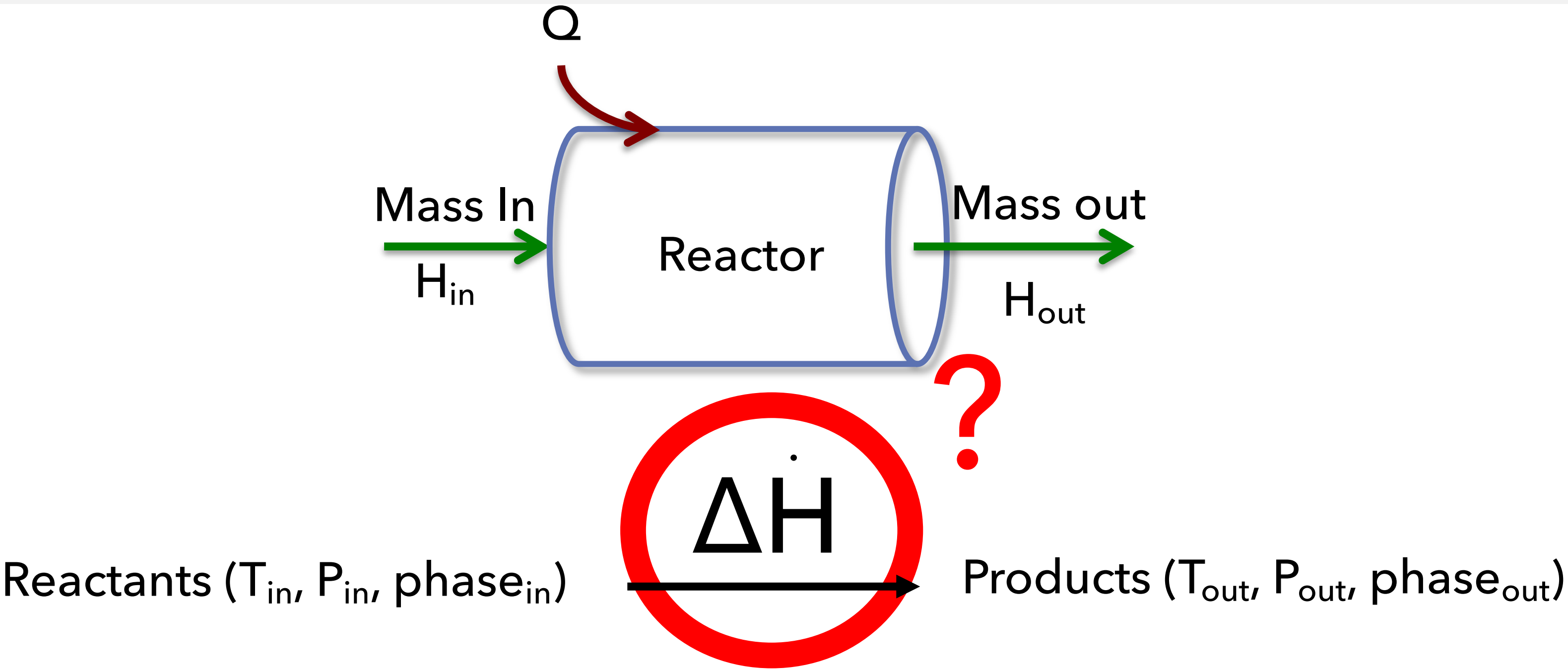
Selection of reference conditions:

- The reference conditions refer to the elemental species forming the reactants and products
- at standard conditions (25°C, 1 atm)
- in the phase in which they appear in the heat of formation

Construct the inlet-outlet enthalpy table:

- We need to find the specific enthalpies for all molecular species in the input and output stream conditions

The path to calculate the total enthalpy change in the reactor, ΔH:



Q

Mass In

H_{in}

Reactor

Mass out

H_{out}

?

$\Delta\dot{H}$

Reactants (T_{in}, P_{in}, $phase_{in}$)

Products (T_{out}, P_{out}, $phase_{out}$)

The problem is the same: calculate ΔH

WHAT ARE WE DOING DIFFERENTLY?

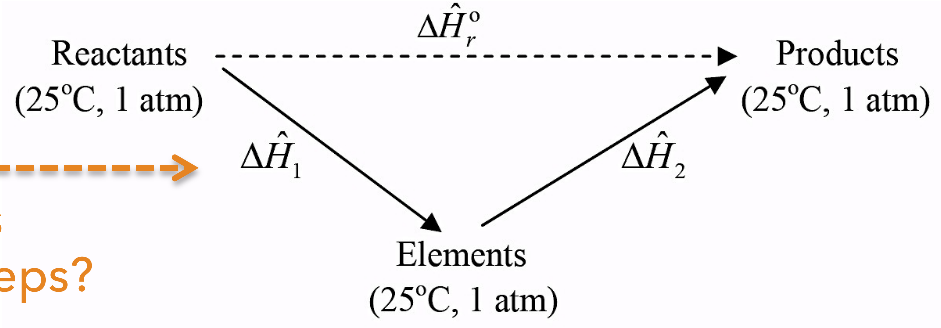
The path to calculate the total enthalpy change in the reactor, ΔH:

(1) Bring the reactants from the inlet stream conditions to 25 °C and 1 atm

(2) Decompose the reactants into elemental species at 25 °C and 1 atm

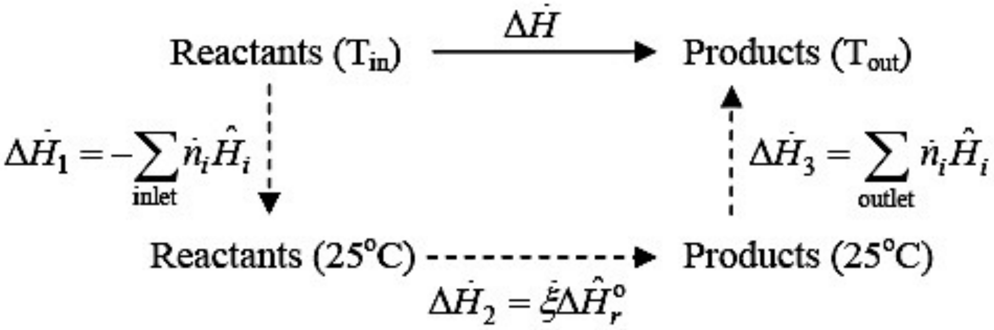
(3) Formation of the products from the elemental species at 25 °C and 1 atm

(4) Bring the products from 25 °C and 1 atm to the outlet stream conditions

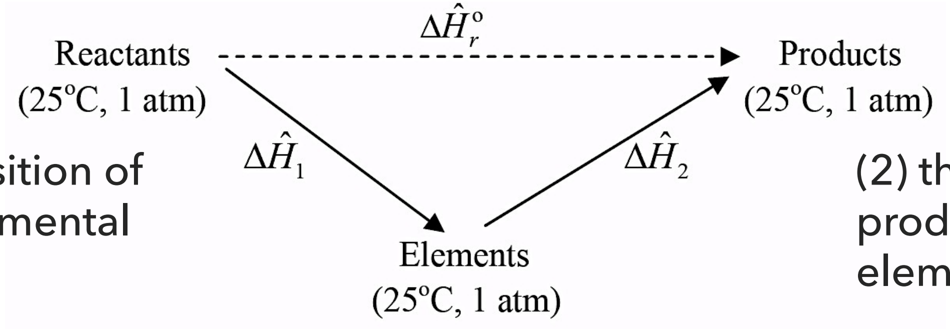


Which are the heats involved in these steps?

Compared with the Heat of Reaction method:



Heats involved in:



(1) the decomposition of reactants into elemental species

(2) the formation of products from the elemental species

HEATS OF FORMATION!

since enthalpy is a state function

$$\Delta\hat{H}_1 = -\sum_{in} |\upsilon_i| \Delta\hat{H}^\circ_{fi}$$

$$\Delta\hat{H}_2 = \sum_{out} |\upsilon_i| \Delta\hat{H}^\circ_{fi}$$

$$\Delta\hat{H}^\circ_r = \Delta\hat{H}_1 + \Delta\hat{H}_2$$

$$\Delta\hat{H}^\circ_r = \sum_{out} |\upsilon_i| \Delta\hat{H}^\circ_{fi} - \sum_{in} |\upsilon_i| \Delta\hat{H}^\circ_{fi}$$

Heat of Reaction method vs. Heat of Formation method

Will the final answer change?

- No. You will obtain the same answer for a reactive energy balance problem regardless of whether you chose to do a heat of formation or a heat of reaction balance

Which one to choose?

- Your choice of method will be dictated by convenience

(much like your choice of atomic balance vs. molecular species balance for reactive mass balances)

General Procedure to solve energy balance in reactive systems

General procedure:
Solving Energy Balance in Reactive Systems

0. Understand the process!

1. Draw and label the flow chart. Include all known phases, temperatures, pressures in the labeling, as well as heat and (if there is any) work. Write the reactions and balance them (stoichiometry)!
2. Decide whether you want to use heat of reaction or heat of formation method
3. Choose a reference state based on the method you have chosen

   For reacting species: Choose reference state (phase, T and P) for each specie in the process given the state for which the heat of reaction/heat of formation is known Heat of reaction method: the reference are the species themselves at 25°C and 1 atm Heat of formation method: the <u>reference are the elemental species</u> in their naturally occurring states at 25°C and 1 atm
4. Prepare an inlet-outlet enthalpy table

To fill with flow rates and specific enthalpies for each of the species in the process.

If a species is at its reference state, its specific enthalpy is zero.

General procedure:
Solving Energy Balance in Reactive Systems

5. Write the Energy Balance equation for your system

Include the heat of reaction term if molecular species were chosen as references, omit it if elemental species were chosen

6. Write expressions for all of the specific enthalpies defined in the energy balance equation by calculating the enthalpy change for each specie to go from its reference state to the process state

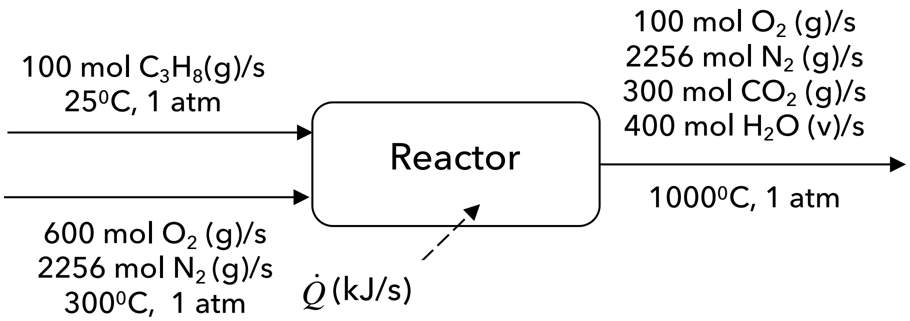
7. Solve all equations!

Example

Consider the following reactive process and calculate the heat (kJ/s) that is associated to the mentioned reaction

Given:

$C_3H_8 + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l) \qquad \Delta\hat{H}_r^\circ = -2220$ kJ/mol



0. Understand the process.

Classify it: Open/continuous, single unit, steady-state, reactive

1. Draw and label the flowchart. Reactions: given $\dot{Q}$

2. Method: Heat of formation method

3. Reference states:

C(s), H_2(g), O_2(g), N_2(g) at 25°C and 1atm

4. Inlet-Outlet Enthalpy table: fill in known and labeled amounts

Substance	$\dot{n}_{in}$ (mol/s)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/s)	$\hat{H}_{out}$(kJ/mol)
C_3H_8	100	$\hat{H}_1$	–	–
O_2	600	$\hat{H}_2$	100	$\hat{H}_4$
N_2	2256	$\hat{H}_3$	2256	$\hat{H}_5$
CO_2	–	–	300	$\hat{H}_6$
H_2O	–	–	400	$\hat{H}_7$

5. Energy Balance Equation:

For open, reactive system at steaty state + For the Heat of Formation Method

$$\cancel{E_{acc}} = E_{in} - E_{out} + \cancel{E_{gen}} + E_{transf}$$

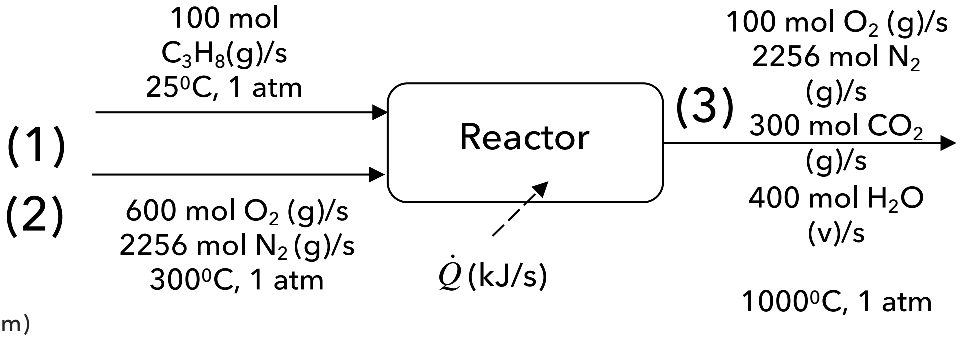
$$\longrightarrow E_{acc} = \sum_{in} \dot{n}_j \Delta\hat{H}°_{f,j} + \sum_{in} \dot{n}_j \Delta\hat{H}_j - \sum_{out} \dot{n}_j \Delta\hat{H}°_{f,j} - \sum_{out} \dot{n}_j \Delta\hat{H}_j + \dot{Q} - \cancel{\dot{W}_s}$$

$$\boxed{0 = \sum_{in} \dot{n}_j \Delta\hat{H}°_{f,j} + \sum_{in} \dot{n}_j \Delta\hat{H}_j - \sum_{out} \dot{n}_j \Delta\hat{H}°_{f,j} - \sum_{out} \dot{n}_j \Delta\hat{H}_j + \dot{Q}}$$

6. Expressions for specific enthalpies ($\hat{H}_{in}$ or $\hat{H}_{out}$) : from reference state to process state

REFERENCE STATES:

$C(s)$, $H_2(g)$, $O_2(g)$, $N_2(g)$ at 25°C and 1atm



(1) 100 mol $C_3H_8(g)$/s 25⁰C, 1 atm

(2) 600 mol O_2 (g)/s 2256 mol N_2 (g)/s 300⁰C, 1 atm

Reactor

$\dot{Q}$ (kJ/s)

(3) 100 mol O_2 (g)/s 2256 mol N_2 (g)/s 300 mol CO_2 (g)/s 400 mol H_2O (v)/s 1000⁰C, 1 atm

Stream 1:

$\hat{H}_1 = (\Delta\hat{H}°_f)_{C3H8(g)}$ = -103.8 kJ/mol (table B.1)

$\hat{H}_1$: $3\ C(s)_{(25°C,\ 1atm)} + 4\ H_2(g)_{(25°C,\ 1atm)} \rightarrow C_3H_8(g)_{\ (25°C,\ 1atm)}$

$$\boxed{\sum_{in} \Delta\hat{H}°_{f,j} + \sum_{in} \Delta\hat{H}_j}$$

Stream 2:

$\hat{H}_2$ = O_2 (g, 25°C, 1atm) → O_2 (g, 300°C, 1atm) = 8.47 kJ/mol (table B.8)

$\hat{H}_3$ = N_2 (g, 25°C, 1atm) → N_2 (g, 300°C, 1atm) = 8.12 kJ/mol

$$\boxed{\sum_{out} \Delta\hat{H}°_{f,j} + \sum_{out} \Delta\hat{H}_j}$$

Stream 3:

$\hat{H}_4$ = O_2 (g, 25°C, 1atm) → O_2 (g, 1000°C, 1atm) = 32.47 kJ/mol

$\hat{H}_5$ = N_2 (g, 25°C, 1atm) → N_2 (g, 1000°C, 1atm) = 30.56 kJ/mol

$\hat{H}_6$ = $C+O_2$ (s+g, 25°C, 1atm) → CO_2 (g, 25°C, 1atm) → CO_2 (g, 1000°C, 1atm) = - 344.9 kJ/mol

$\hat{H}_7$ = $H_2+0{,}5O_2$ (g, 25°C, 1atm) → H_2O (l, 25°C, 1atm) → H_2O (g, 1000°C, 1atm) = - 204,1kJ/mol

Substance	n_{in} (mol/s)	$\hat{H}_{in}$ (kJ/mol)	n_{out} (mol/s)	$\hat{H}_{out}$ (kJ/mol)
C_3H_8	100	-103,8	-	-
O_2	600	8,47	100	32,47
N_2	2256	8,12	2256	30,56
CO_2	-	-	300	-344,9
H_2O	-	-	400	-204,1

6. (Cont) Expression for the term of enthalpy of reaction ? :

NO!

7. Solve the Energy Balance Equation

$$0 = \sum_{in} \dot{n}_j \Delta\hat{H}^\circ_{f,j} + \sum_{in} \dot{n}_j \Delta\hat{H}_j - \sum_{out} \dot{n}_j \Delta\hat{H}^\circ_{f,j} - \sum_{out} \dot{n}_j \Delta\hat{H}_j + \dot{Q}$$

$$\Rightarrow \dot{Q} = -1.26 \times 10^5 \text{ kJ/s}$$

Recalling: Heat of Reaction method

6. (Cont) Expression for the term of enthalpy of reaction

$$\dot{\xi} = \frac{|(\dot{n}_{C_3H_8})_{out} - (\dot{n}_{C_3H_8})_{in}|}{|\upsilon_{C_3H_8}|} = \frac{|0 - 100|}{1} = 100 \ mol/s$$

With $\Delta \hat{H}_r^\circ = -2220$ kJ/mol

7. Solve the Energy Balance Equation

$$0 = \sum \dot{n}_{in} \widehat{H}_{in} - \sum \dot{n}_{out} \widehat{H}_{out} - \xi \Delta \widehat{H}_r + \dot{Q}$$

$$\Rightarrow \dot{Q} = -1.26 \times 10^5 \text{ kJ/s}$$