

# Introduction to Chemical Engineering

**Teaching by:**

**Vassily Hatzimanikatis** ([vassily.hatzimanikatis@epfl.ch](mailto:vassily.hatzimanikatis@epfl.ch))

**Assistants:**

|               |                                                                      |
|---------------|----------------------------------------------------------------------|
| Denis Joly    | ( <a href="mailto:denis.joly@epfl.ch">denis.joly@epfl.ch</a> )       |
| Konrad Lagoda | ( <a href="mailto:konrad.lagoda@epfl.ch">konrad.lagoda@epfl.ch</a> ) |
| Zi Xuan Ng    | ( <a href="mailto:zixuan.ng@epfl.ch">zixuan.ng@epfl.ch</a> )         |

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

Fridays, 14h15 - 17h00  
2024-2025

# Course Schedule

| Date          | Subject                                                                                                                                                                          |
|---------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 13-Sep        | <b>1. Fundamentals of Material Balances</b><br>1.1. Process definition and classification<br>1.2. Material balance calculations                                                  |
| <b>20-Sep</b> | 1.3. Balances on multiple-unit processes                                                                                                                                         |
| 27-Sep        | <b>Review on Mass Balances (non-reactive)</b>                                                                                                                                    |
| 04-Oct        | 1.4. Chemical reaction stoichiometry<br><b>1.5.1 Balances on reactive processes (part 1)</b>                                                                                     |
| 11-Oct        | <b>1.5.2 Balances on reactive processes (part 2)</b><br><b>1.6. Balances on multiple unit reactive processes</b><br><b>Review on Mass Balances (non-reactive &amp; reactive)</b> |
| 18-Oct        | <b>2. Energy and Energy Balances</b><br>2.1. Energy balances on closed systems<br>2.2. Open systems at steady state                                                              |
| 01-Nov        | <b>3. Balances on Non-Reactive Processes</b><br>3.1. Energy balance calculation<br>3.2. Changes in Pressure, Temperature, Phases<br>3.3. Mixing and Solution                     |
| 08-Nov        | <b>4. Balances on Non-Reactive Processes</b><br>Problems: Mass and Energy Balances on non-Reactive Systems                                                                       |
| 15-Nov        | <b>Midterm Exam: Mass &amp; Energy Balances non-Reactive Systems</b>                                                                                                             |
| 22-Nov        | <b>Review Midterm</b>                                                                                                                                                            |
| 29-Nov        | <b>5. Balances on Reactive Processes</b><br>5.1. Heats of reaction/combustion<br>5.2. Combustion reactions<br>5.3. Enthalpy of reaction<br>5.4. Energy balance calculation       |
| 06-Dec        | <b>6. Energy balances on mixing processes</b><br><b>Review</b>                                                                                                                   |

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

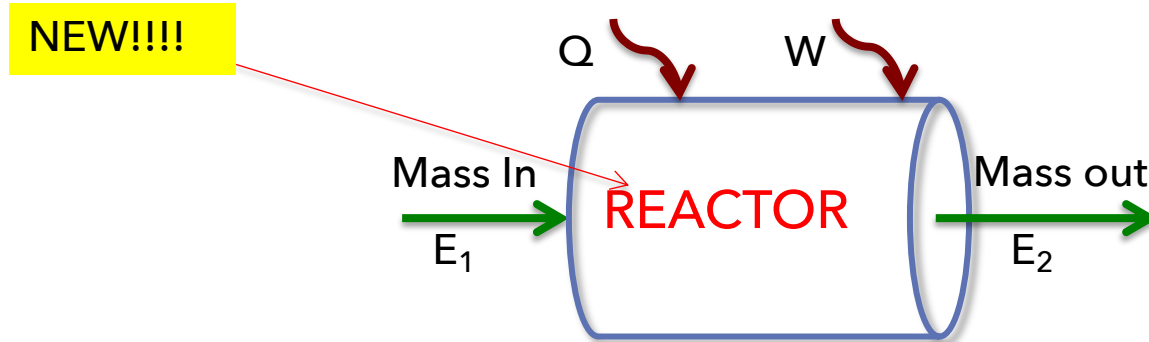
# Session VI: Friday 1<sup>st</sup> November 2024

After studying this session you will be able to:

Understand the term **ENTHALPY OF REACTION** ( $\Delta H_r$ ). Classification of reactions (sign of  $\Delta H_r$ )

# Introduction to Energy Balance on a Reactive Process

# 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 ?

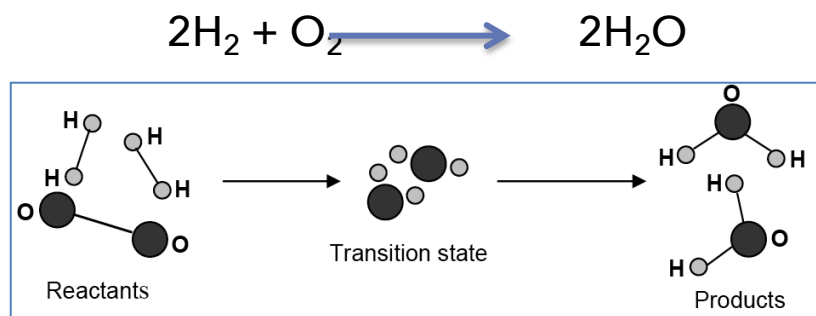
- Until now (in non-reactive processes): 
$$\Delta\dot{H} = \sum_{out} \dot{m}_i \hat{H}_i - \sum_{in} \dot{m}_i \hat{H}_i$$
- NOW (in reactive systems): NEW CALCULATIONS, new terms required to calculate the total  $\Delta H$  happening in a reactor (since molecular species are being generated or consumed).

## 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 reactive systems): not arbitrarily chosen, But depending on the METHOD used to calculate  $\Delta H$  of reaction



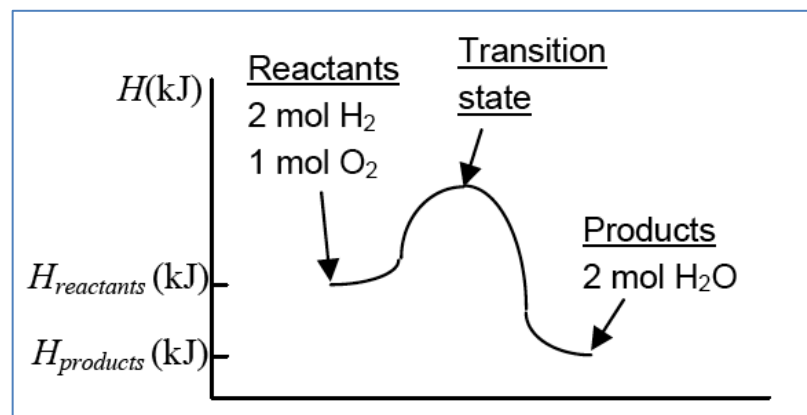
# 1. Understand the Enthalpy of Reaction ( $\Delta H_r$ )



- One O-O bond and two H-H bonds are broken
- System absorbs energy,  $U_{\text{system}}$  and  $H_{\text{system}}$  increase from reactants to transition state
- 4 O-H bonds are formed
- System releases energy,  $U_{\text{system}}$  and  $H_{\text{system}}$  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 ( $\Delta H_r$ )

- 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.

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

- For stoichiometric quantities of  $H_2$  and  $O_2$  reacting completely at  $T=25^\circ\text{C}$  and  $P=1 \text{ atm}$ :



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

$\Delta \hat{H}_r^\circ$  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 ( $\Delta H_r$ )

- $\Delta H_r < 0 \quad \rightarrow \quad E_{\text{products}} < E_{\text{reactants}}$

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

The reaction is therefore Exothermic

- $\Delta H_r > 0 \quad \rightarrow \quad E_{\text{products}} > E_{\text{reactants}}$

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

The reaction is therefore Endothermic

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

The standard heat of reaction,  $\Delta \hat{H}_r^\circ$  (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).

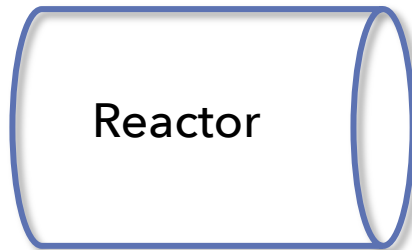
The value of  $\Delta \hat{H}_r^\circ$  is given for a specified phase of the reactants and products and considering that stoichiometric amounts of reactants are completely consumed.

## 2. Working with the Enthalpy of Reaction ( $\Delta H_r$ )

... to calculate the enthalpy change in a closed system ( $\Delta H$ )

- If A is a reactant or product of a reaction
  - $\nu_A$  is its stoichiometric coefficient
  - $n_{A,r}$  (mol A) is a quantity of A that reacts at 25°C and 1 atm
  - $\xi$  is the extent of reaction
- then the enthalpy change for closed system is

$$\Delta H_r^\circ \text{ (kJ)} = n_{A,r} \text{ (mol A react)} \frac{\Delta \hat{H}_r^\circ \text{ (kJ/mol)}}{|\nu_A|} = \xi \Delta \hat{H}_r^\circ$$



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

$$E_{\text{accumulated}} = E_{\text{gen}} = -\Delta H_r^\circ = -\xi \Delta \hat{H}_r^\circ$$

# Working with the Enthalpy of Reaction ( $\Delta H_r$ ) for different STOICHIOMETRY:

So, the enthalpy of a reaction depends on the way that we write the stoichiometry in the reaction:



The information in both cases is the same, since:

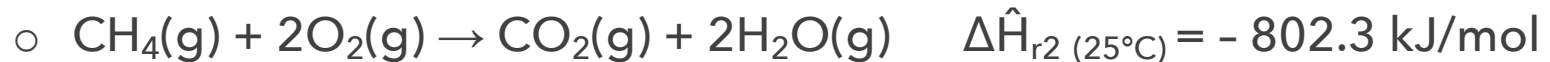
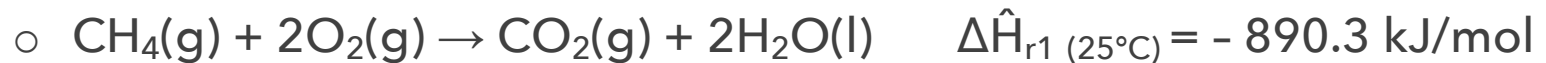
r1: 
$$\frac{-50 \text{ kJ}}{2 \text{ mol } A \text{ consumed}} = \frac{-50 \text{ kJ}}{1 \text{ mol } B \text{ consumed}} = \frac{-50 \text{ kJ}}{3 \text{ mol } C \text{ generated}}$$

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

So ... REMEMBER: the value of  $\Delta H_r$  in kJ applies to the stoichiometric quantities defined in the reaction

# Working with the Enthalpy of Reaction ( $\Delta H_r$ ) for different PHASES:

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



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

Subtracting the reactions  $r2 - r1$ :

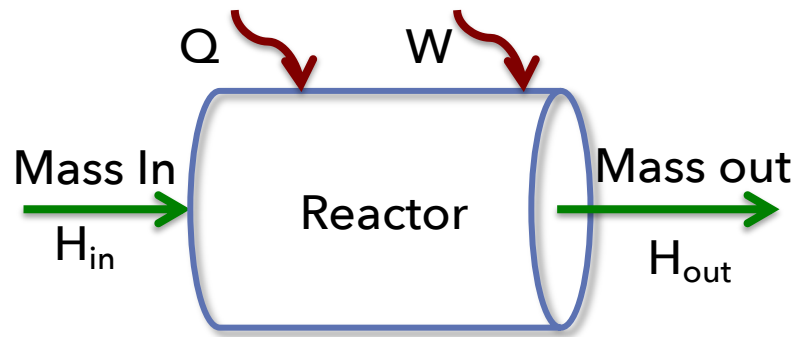


$$\Delta \hat{H}_{r2-r1} (25^\circ\text{C}) = 2 \Delta \hat{H}_v (25^\circ\text{C})$$

**LOOK OUT!**: the fact that  $\Delta H_r$  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:

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

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

# 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  $\Delta H$ :

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  $\Delta \hat{H}_r$

# A. Heat of Reaction method

## Application:

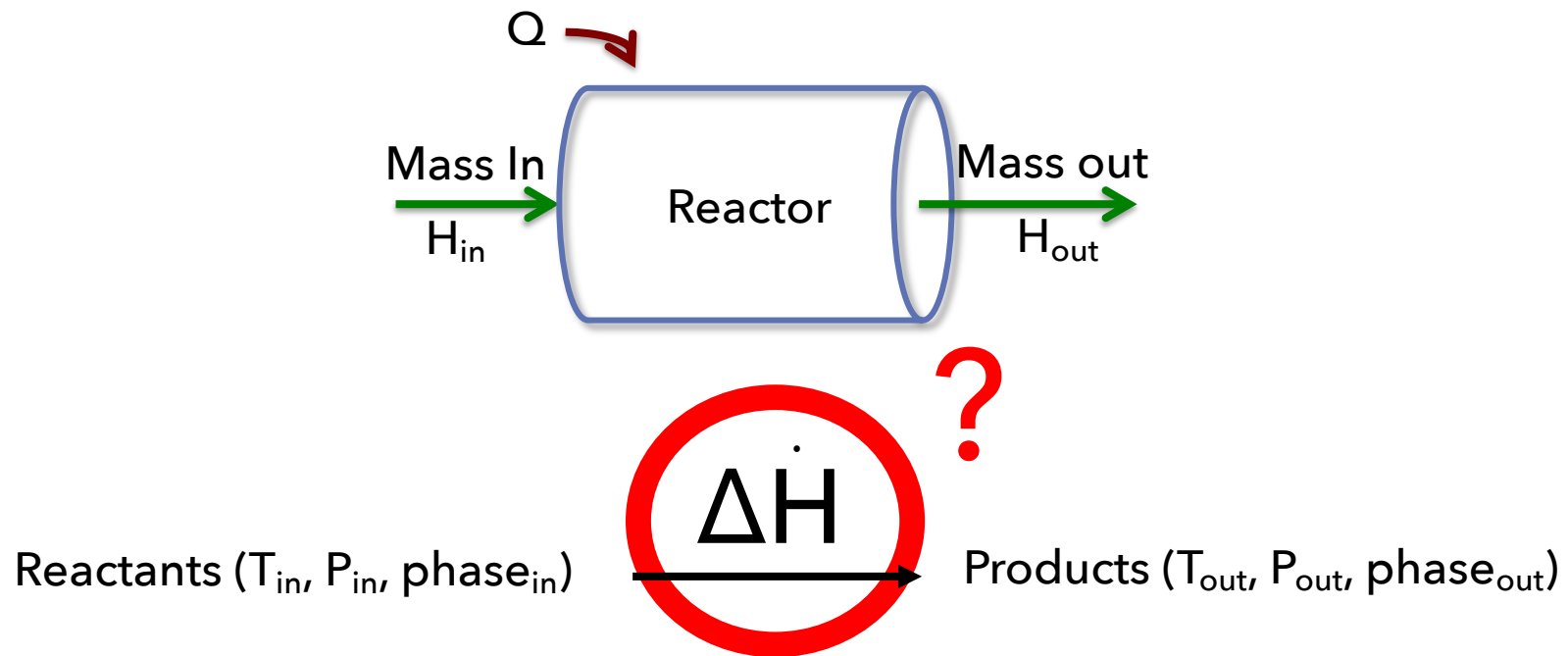
- The heat of reaction approach is more straightforward if there is only a single reaction for which  $\Delta H^\circ_r$  is known

## 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,  $\Delta H^\circ_r$  (25 °C, 1 atm)



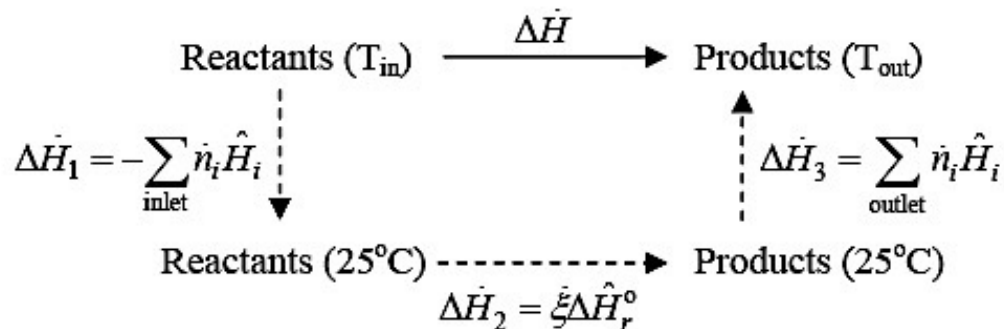
# The path to calculate the total enthalpy change in the reactor, $\Delta H$ :



- $\Delta H$  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?

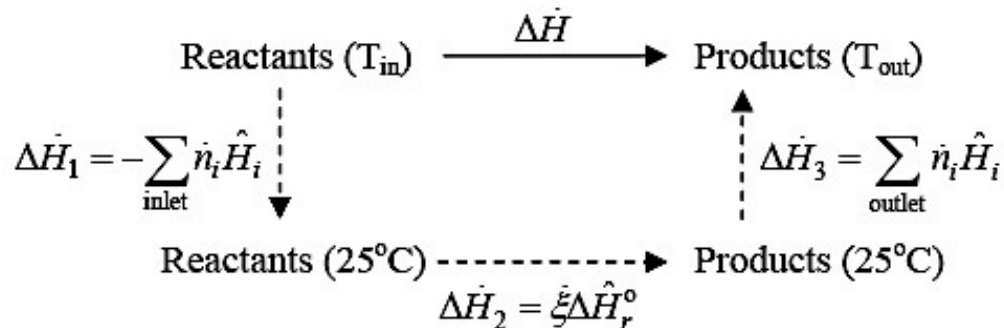
# The path to calculate the total enthalpy change in the reactor, $\Delta H$ :

- (1) bring all reactants from inlet stream conditions to the given (standard) conditions for the heat of reaction  $\Delta H_r^\circ$
- (2) carry out the reaction under the conditions given for  $\Delta H_r^\circ$
- (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, $\Delta H$ :

- (1) bring all reactants from inlet stream conditions to the given (standard) conditions for the heat of reaction  $\Delta H^\circ_r$
- (2) carry out the reaction under the conditions given for  $\Delta H^\circ_r$
- (3) bring the products from the standard conditions to the actual conditions in the outlet stream (the conditions at which they leave the reactor)

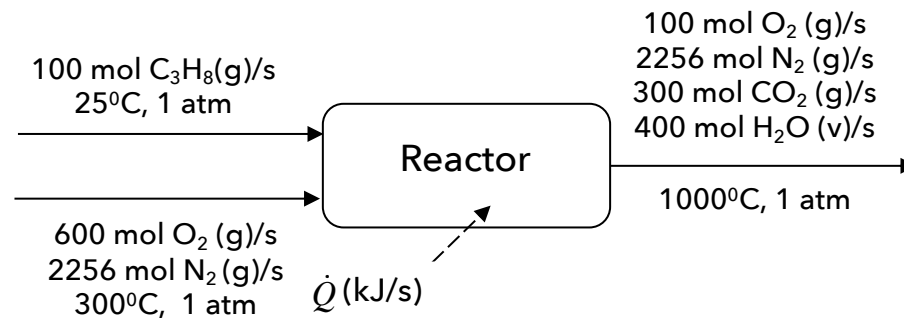
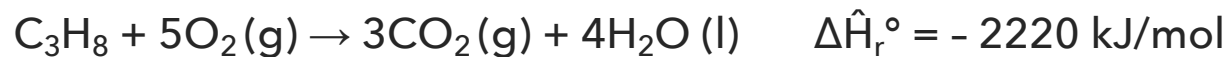


**Remember!:** We want to know  $\Delta H$  between the input stream(s) and the output stream(s) - which means that we ALWAYS have to consider the real conditions of the streams in the process to create the paths (define the starting and ending point)

# Example

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

Given:



0. Understand the process.

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

1. Draw and label the flowchart. Reactions: given

## 2. Method: Heat of reaction method

### 3. Reference states:

$\text{C}_3\text{H}_8$  (g),  $\text{O}_2$  (g),  $\text{N}_2$  (g),  $\text{CO}_2$  (g),  $\text{H}_2\text{O}$  (l) at  $25^\circ\text{C}$  et 1 atm

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

| Substance              | $\dot{n}_{\text{in}}$ (mol/s) | $\hat{H}_{\text{in}}$ (kJ/mol) | $\dot{n}_{\text{out}}$ (mol/s) | $\hat{H}_{\text{out}}$ (kJ/mol) |
|------------------------|-------------------------------|--------------------------------|--------------------------------|---------------------------------|
| $\text{C}_3\text{H}_8$ | 100                           | 0                              | —                              | —                               |
| $\text{O}_2$           | 600                           | $\hat{H}_2$                    | 100                            | $\hat{H}_4$                     |
| $\text{N}_2$           | 2256                          | $\hat{H}_3$                    | 2256                           | $\hat{H}_5$                     |
| $\text{CO}_2$          | —                             | —                              | 300                            | $\hat{H}_6$                     |
| $\text{H}_2\text{O}$   | —                             | —                              | 400                            | $\hat{H}_7$                     |

## 5. Energy Balance Equation:

For open, reactive system at steady state +

For the Heat of Reaction Method

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

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

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

REFERENCE STATES:

$\text{C}_3\text{H}_8(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$ ,  $\text{CO}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{l})$   
at  $25^\circ\text{C}$  et 1 atm

Stream 1:

$$\hat{H}_1 = 0$$

Stream 2:

$$\hat{H}_2 = \text{O}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{O}_2(\text{g}, 300^\circ\text{C}, 1\text{atm}) = 8.47 \text{ kJ/mol (table B.8)}$$

$$\hat{H}_3 = \text{N}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{N}_2(\text{g}, 300^\circ\text{C}, 1\text{atm}) = 8.12 \text{ kJ/mol}$$

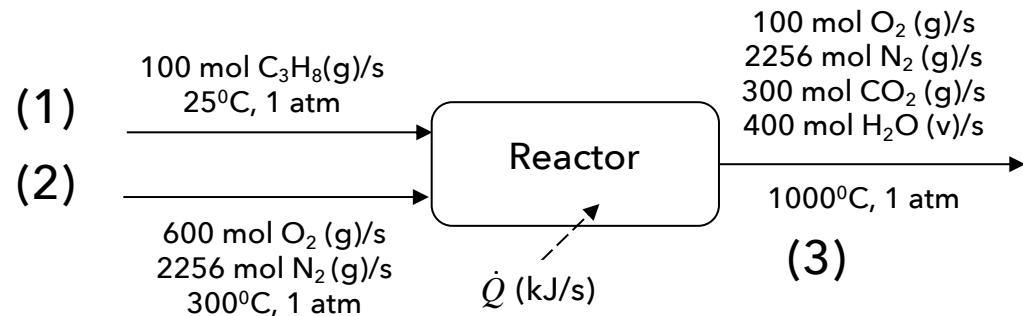
Stream 3:

$$\hat{H}_4 = \text{O}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{O}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = 32.47 \text{ kJ/mol}$$

$$\hat{H}_5 = \text{N}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{N}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = 30.56 \text{ kJ/mol}$$

$$\hat{H}_6 = \text{CO}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{CO}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = 48.60 \text{ kJ/mol}$$

$$\hat{H}_7 = \text{H}_2\text{O}(\text{l}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{H}_2\text{O}(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = \int_{25^\circ\text{C}}^{100^\circ\text{C}} C_{pl} dT + \Delta \hat{H}_v + \int_{100^\circ\text{C}}^{1000^\circ\text{C}} C_{pv} dT = 81.71 \text{ kJ/mol}$$



| Substance | $n_{in}$<br>(mol/s) | $\hat{H}_{in}$<br>(kJ/mol) | $n_{out}$<br>(mol/s) | $\hat{H}_{out}$<br>(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

$$\dot{\xi} = \frac{|(\dot{n}_{\text{C}_3\text{H}_8})_{\text{out}} - (\dot{n}_{\text{C}_3\text{H}_8})_{\text{in}}|}{|v_{\text{C}_3\text{H}_8}|} = \frac{|0 - 100|}{1} = 100 \text{ mol/s}$$

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

7. Solve the Energy Balance Equation

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

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



# B. Heat of Formation method

Application:

- Problems that have multiple reactions occurring simultaneously
- Or if  $\Delta H^\circ_r$  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



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

**Table B.1** Selected Physical Property Data<sup>a</sup>

| Compound | Formula                | Mol. Wt. | SG<br>(20°/4°) | $T_m(^{\circ}\text{C})^b$ | $\Delta\hat{H}_m(T_m)^{e,j}$<br>kJ/mol | $T_b(^{\circ}\text{C})^d$ | $\Delta\hat{H}_v(T_b)^{e,j}$<br>kJ/mol | $T_c(\text{K})^f$ | $P_c(\text{atm})^g$ | $(\Delta\hat{H}_f^{\circ})^{h,j}$<br>kJ/mol | $(\Delta\hat{H}_c^{\circ})^{i,j}$<br>kJ/mol |
|----------|------------------------|----------|----------------|---------------------------|----------------------------------------|---------------------------|----------------------------------------|-------------------|---------------------|---------------------------------------------|---------------------------------------------|
| Benzene  | $\text{C}_6\text{H}_6$ | 78.11    | 0.879          | 5.53                      | 9.837                                  | 80.10                     | 30.765                                 | 562.6             | 48.6                | +48.66(l)<br>+82.93(g)                      | -3267.6(l)<br>-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), H<sub>2</sub>(g), O<sub>2</sub>(g),...] is zero!

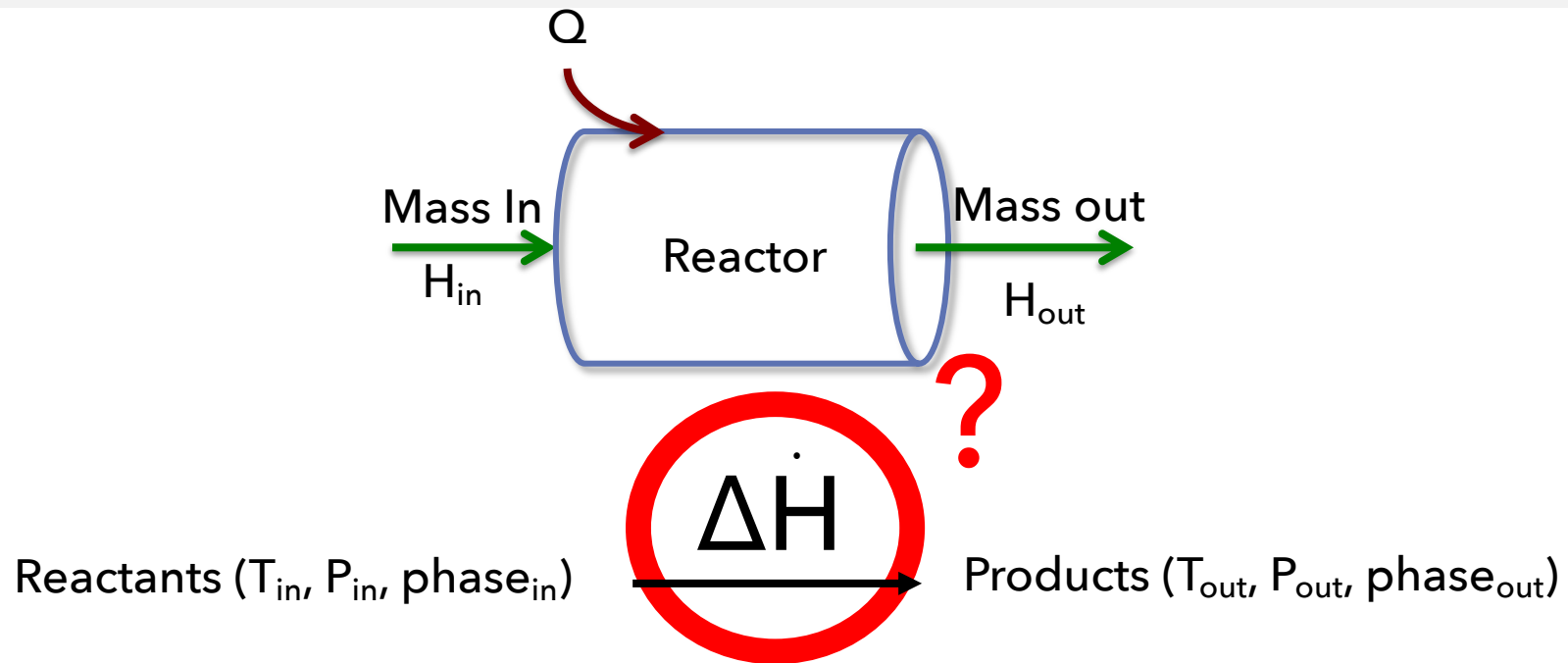
Selection of reference conditions:

- 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, $\Delta H$ :

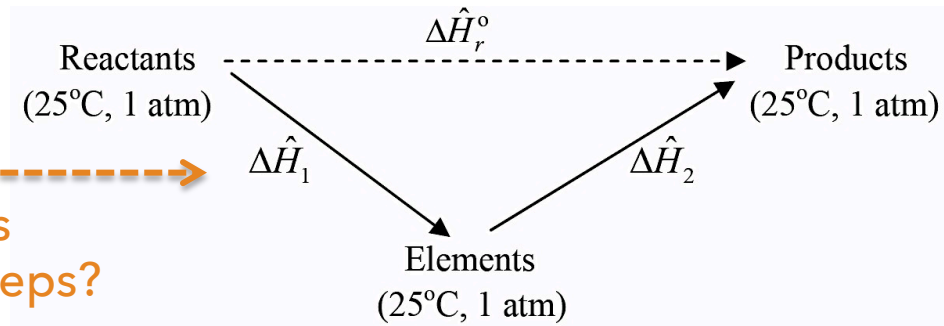


The problem is the same: calculate  $\Delta H$

WHAT ARE WE DOING DIFFERENTLY?

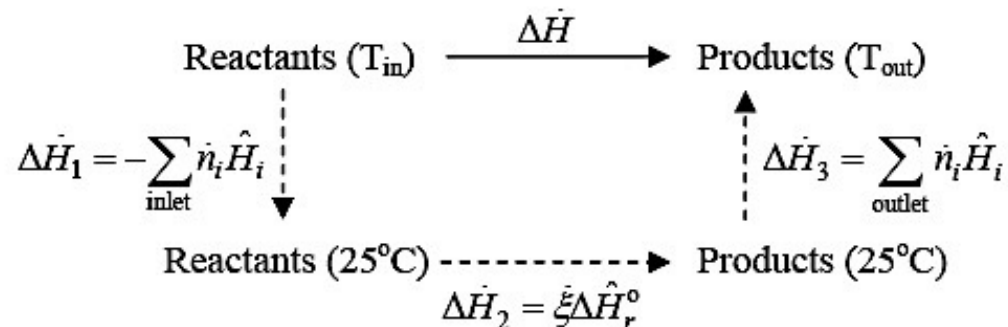
The path to calculate the total enthalpy change in the reactor,  $\Delta H$ :

- (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

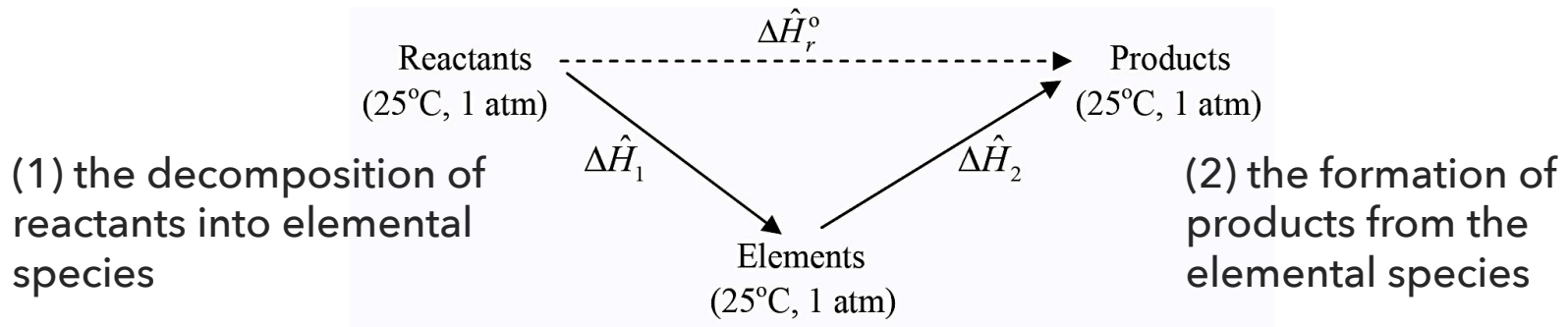


Which are the heats involved in these steps?

Compared with the Heat of Reaction method:



Heats involved in:



## HEATS OF FORMATION!

since enthalpy is a state function

$$\Delta \hat{H}_1 = - \sum_{in} |v_i| \Delta \hat{H}_{fi}^{\circ}$$

$$\Delta \hat{H}_2 = \sum_{out} |v_i| \Delta \hat{H}_{fi}^{\circ}$$

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

$$\Delta \hat{H}_r^{\circ} = \sum_{out} |v_i| \Delta \hat{H}_{fi}^{\circ} - \sum_{in} |v_i| \Delta \hat{H}_{fi}^{\circ}$$

# 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: 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 reference are the elemental species 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

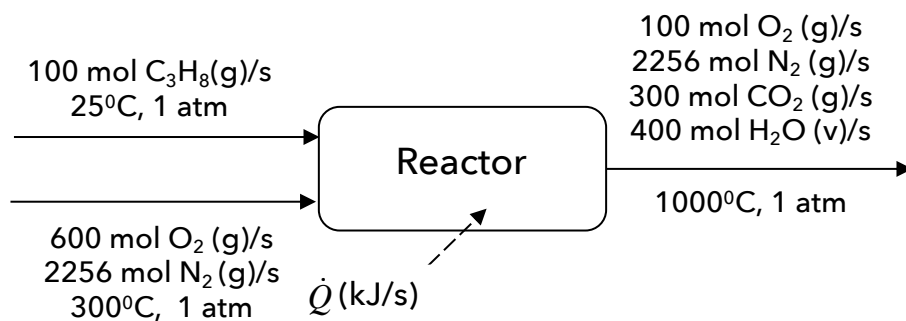
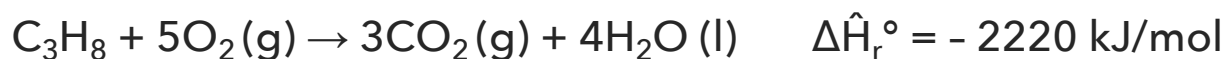
7. Solve all equations!



# Example

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

Given:



0. Understand the process.

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

1. Draw and label the flowchart. Reactions: given

## 2. Method: Heat of formation method

### 3. Reference states:

C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C and 1 atm

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

| Substance                     | $\dot{n}_{\text{in}}$ (mol/s) | $\hat{H}_{\text{in}}$ (kJ/mol) | $\dot{n}_{\text{out}}$ (mol/s) | $\hat{H}_{\text{out}}$ (kJ/mol) |
|-------------------------------|-------------------------------|--------------------------------|--------------------------------|---------------------------------|
| C <sub>3</sub> H <sub>8</sub> | 100                           | $\hat{H}_1$                    | –                              | –                               |
| O <sub>2</sub>                | 600                           | $\hat{H}_2$                    | 100                            | $\hat{H}_4$                     |
| N <sub>2</sub>                | 2256                          | $\hat{H}_3$                    | 2256                           | $\hat{H}_5$                     |
| CO <sub>2</sub>               | –                             | –                              | 300                            | $\hat{H}_6$                     |
| H <sub>2</sub> O              | –                             | –                              | 400                            | $\hat{H}_7$                     |

## 5. Energy Balance Equation:

For open, reactive system at steady state

For the Heat of Formation Method

$$E_{\text{acc}} = E_{\text{in}} - E_{\text{out}} + E_{\text{gen}} + E_{\text{transf}} = \sum_{\text{in}} \dot{n}_j \Delta \hat{H}_{f,j}^{\circ} + \sum_{\text{in}} \dot{n}_j \Delta \hat{H}_j - \sum_{\text{out}} \dot{n}_j \Delta \hat{H}_{f,j}^{\circ} - \sum_{\text{out}} \dot{n}_j \Delta \hat{H}_j + \dot{Q} - \dot{W}_s$$

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

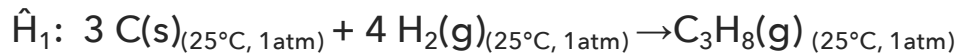
## 6. Expressions for specific enthalpies ( $\hat{H}_{\text{in}}$ or $\hat{H}_{\text{out}}$ ) : from reference state to process state

REFERENCE STATES:

C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C and 1 atm

Stream 1:

$$\hat{H}_1 = (\Delta \hat{H}_f^{\circ})_{\text{C}_3\text{H}_8(\text{g})} = -103.8 \text{ kJ/mol (table B.1)}$$



Stream 2:

$$\hat{H}_2 = \text{O}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{O}_2(\text{g}, 300^\circ\text{C}, 1\text{atm}) = 8.47 \text{ kJ/mol (table B.8)}$$

$$\hat{H}_3 = \text{N}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{N}_2(\text{g}, 300^\circ\text{C}, 1\text{atm}) = 8.12 \text{ kJ/mol}$$

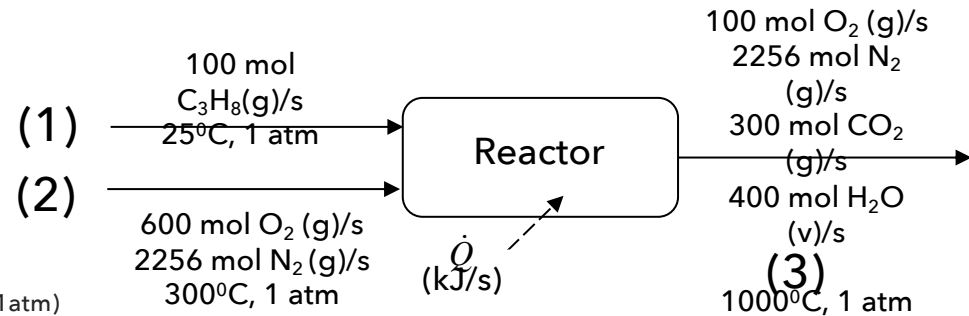
Stream 3:

$$\hat{H}_4 = \text{O}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{O}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = 32.47 \text{ kJ/mol}$$

$$\hat{H}_5 = \text{N}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{N}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = 30.56 \text{ kJ/mol}$$

$$\hat{H}_6 = \text{C} + \text{O}_2(\text{s} + \text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{CO}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{CO}_2(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = -344.9 \text{ kJ/mol}$$

$$\hat{H}_7 = \text{H}_2 + 0.5 \text{ O}_2(\text{g}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{H}_2\text{O}(\text{l}, 25^\circ\text{C}, 1\text{atm}) \rightarrow \text{H}_2\text{O}(\text{g}, 1000^\circ\text{C}, 1\text{atm}) = -204.1 \text{ kJ/mol}$$



$$\sum_{\text{in}} \Delta \hat{H}_{f,j}^{\circ} + \sum_{\text{in}} \Delta \hat{H}_j$$

$$\sum_{\text{out}} \Delta \hat{H}_{f,j}^{\circ} + \sum_{\text{out}} \Delta \hat{H}_j$$

| Substance | $n_{in}$<br>(mol/s) | $\hat{H}_{in}$<br>(kJ/mol) | $n_{out}$<br>(mol/s) | $\hat{H}_{out}$<br>(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

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

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

# Recalling: Heat of Reaction method

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

$$\dot{\xi} = \frac{|\dot{n}_{\text{C}_3\text{H}_8}_{\text{out}} - \dot{n}_{\text{C}_3\text{H}_8}_{\text{in}}|}{|v_{\text{C}_3\text{H}_8}|} = \frac{|0 - 100|}{1} = 100 \text{ mol/s}$$

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

7. Solve the Energy Balance Equation

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

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