EPFL

Process development
Selection Criteria

François Marechal

2025

IPESE
Industrial Process
and Energy Systems
Engineering

Todays : Course schedule

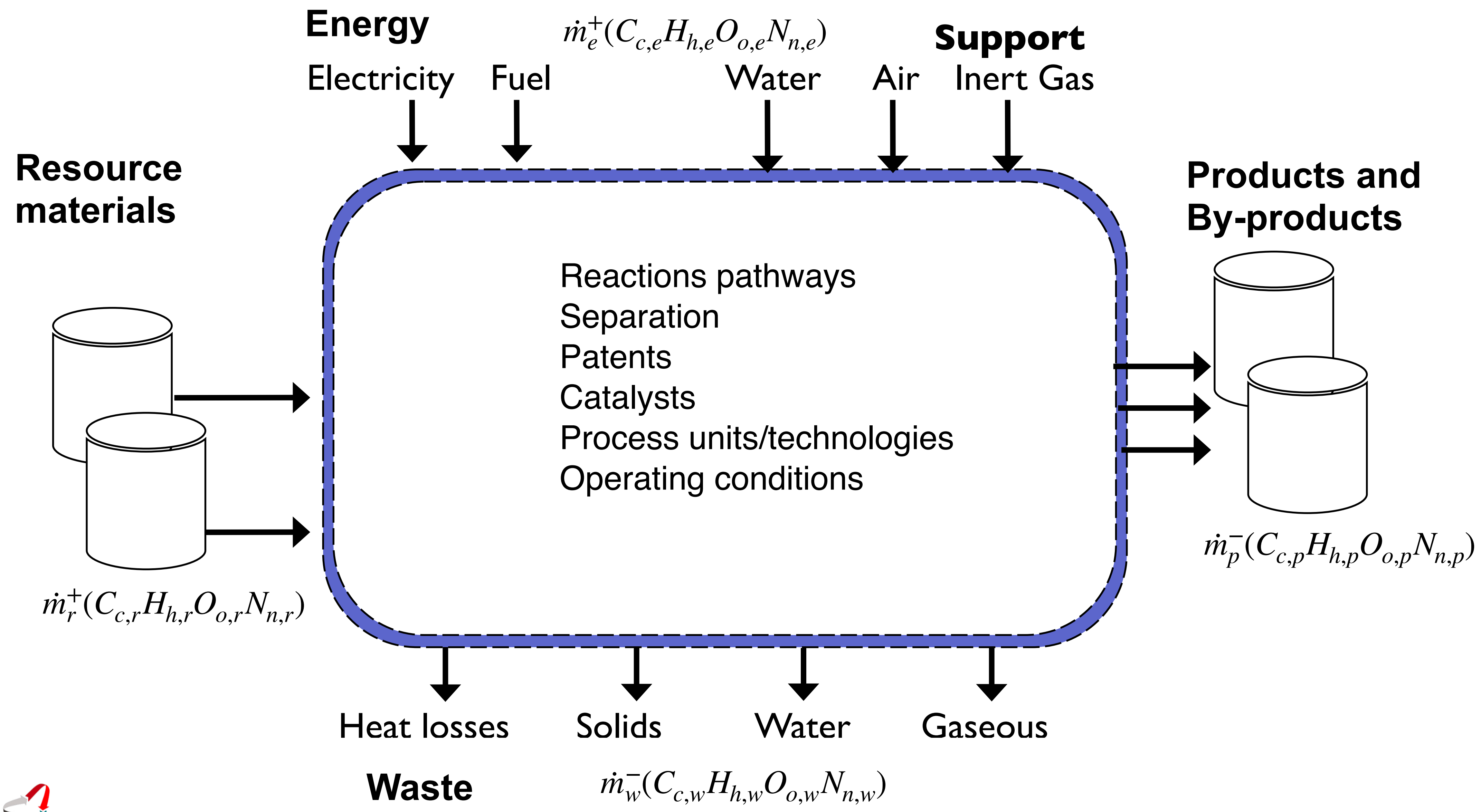
February 24: Selection Criteria

- 08:30 - 09:00 (François) Selection Criteria
- 09:00 - 09:20 (Meire) Process flow diagrams
- 09:30 - 10:30 (Catarina) Aspen Tutorial I: Physical Properties
- 10:40 - 11:10 Quiz 0 (Not graded)

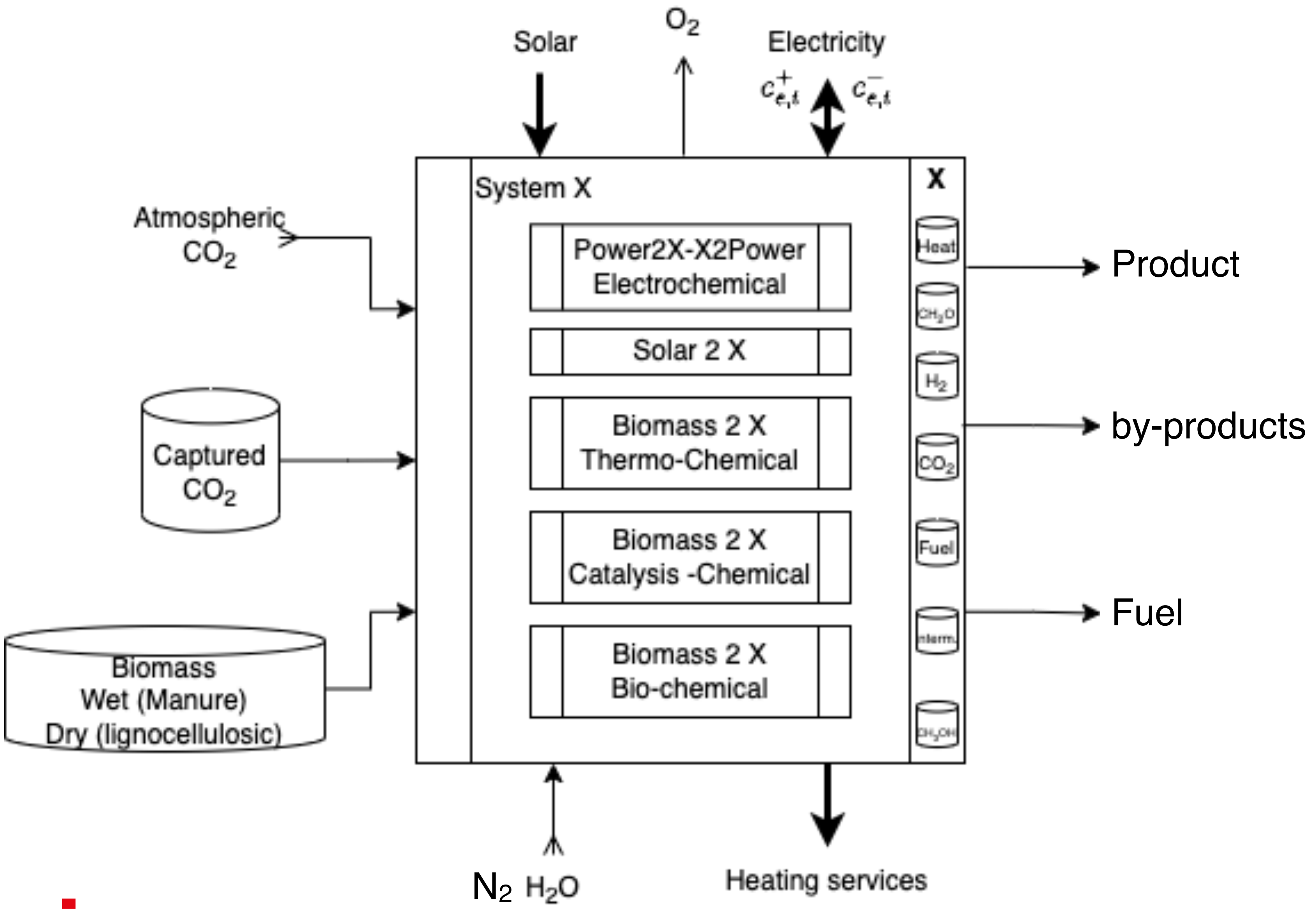
- 11:10 - 16:00 Teamwork
  - Gate 1: Identify and characterise process routes

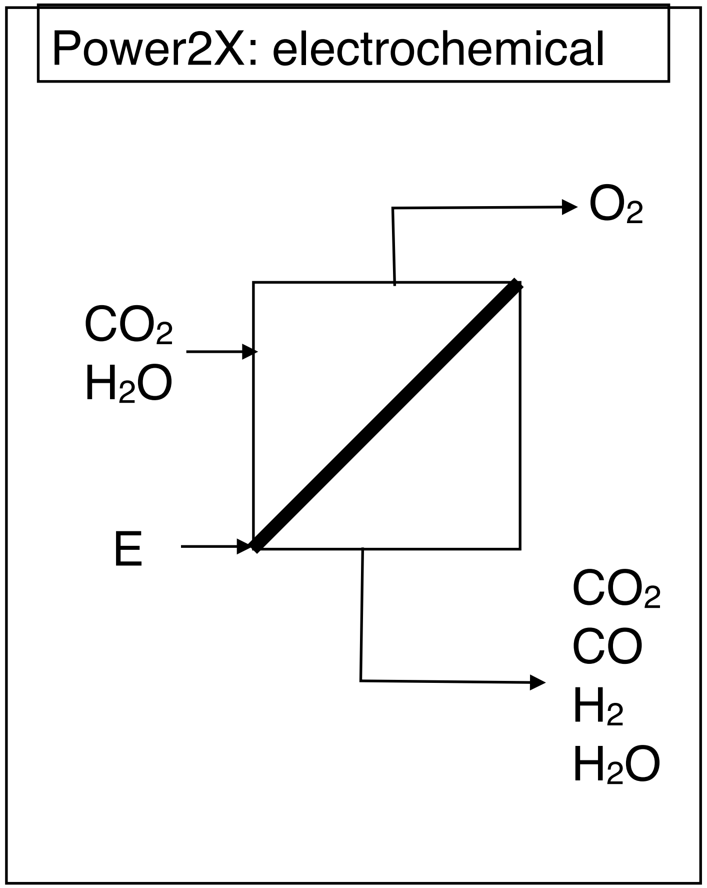
  - Two rooms are available for you CE1 101 and CE1 103

Process Development: Selecting production routes



Towards new resources for chemical products





Gate 1: Products and by-products characterisation

- **Product** and each **By-products (see production routes)**
  - Chemical characterisation
    - Chemical composition
    - Chemical and physical properties
    - Storage and distribution
    - Typical production routes
    - Hazard and safety
    - Environmental impact (scope 1, scope 2 and scope 3 CO2 emissions, …)
  - Markets : today and future
    - Applications
    - Markets :
      - Production volumes [t/year]
      - Locations : EU - US - Asia
      - Value [CHF/t]
      - Typical Process size [t/year]

Gate 1: Chemicals characterisation

- Chemical (CAS) : $C_cH_hO_o\alpha_a$ => Thermodynamic (T_c, P_c, T_{eb}, ω), toxicity, hazard

- Typical State on market : Mass flow : $\dot{M}_i^+ \quad [kg/s]$

  Molar flow : $\dot{N}_i^+ [kmol/s]$

  Composition and specs : $\dot{x}_{i,j} [\%]$

  Distribution/transportation

  Storage : T,P,State and density [m3/t]

- Cost or market value : $c_i \quad [CHF/kg]$
  - Market sizes : quantity and typical production sizes

- Energy : $h[kJ/kmol] = h^0 + \int_{T_0}^{T_{storage}} cp \cdot dT$

  - includes enthalpy of formation and therefore a predefined reference

- Exergy / Gibbs free energy : $e[kJ/kmol] = h^0 - T_0 \cdot s^0$

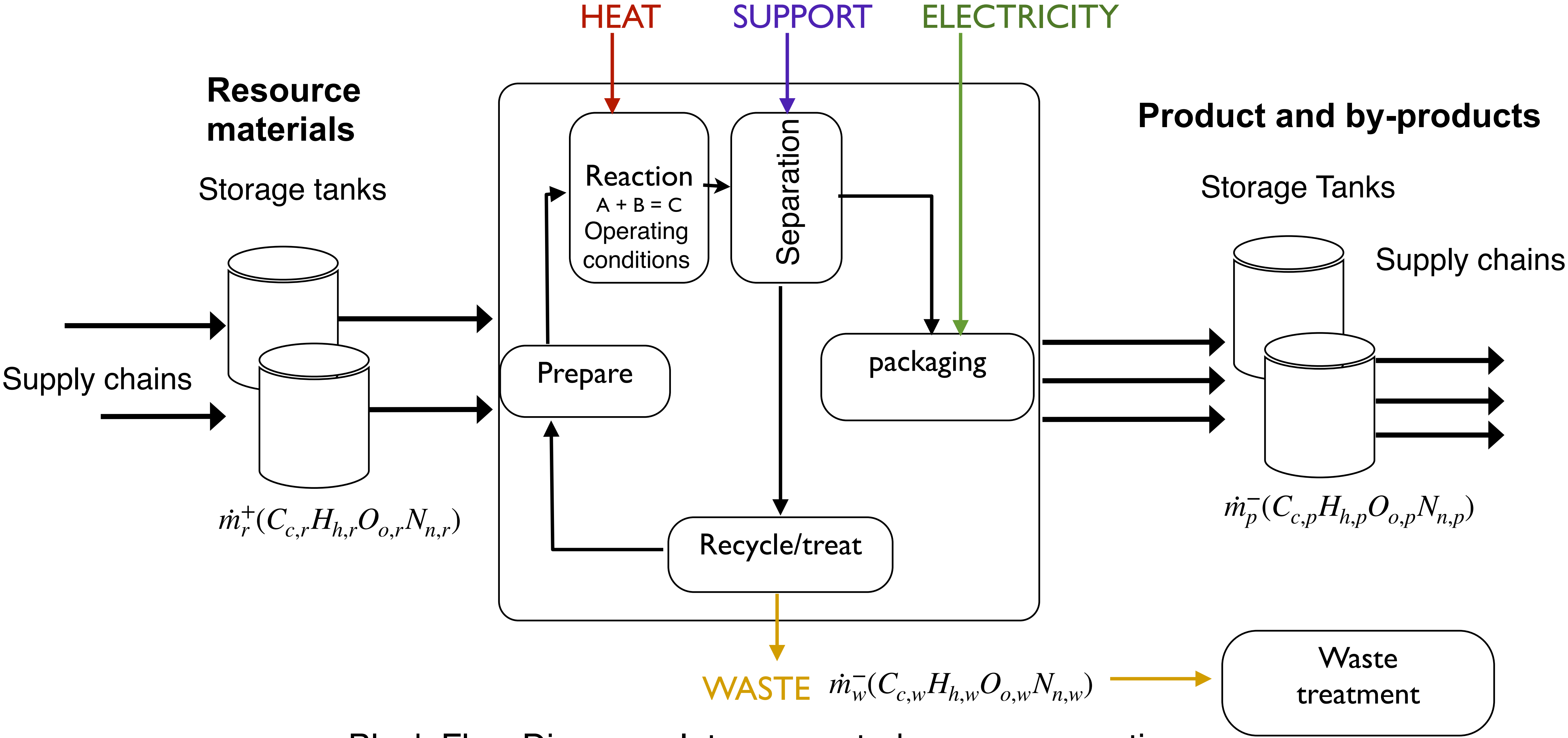
Gate 1: Products, by-products and feedstocks

- Chemical and thermodynamical characterisation
  - [Challenge] : names of products and chemical formula
  - [Challenge] : thermodynamic properties
  - [Challenge] : transportation, storage, safety and hazard properties
- Economical characterisation
  - [Challenge] : present production rates and major producers
  - [Challenge] : markets values, major usage and applications,
  - [Challenge] : future market**s** and applications
- Environmental characterisation
  - [Challenge] : Resources and feedstocks used : cost and availability -> choose the region
  - [Challenge] : Energy consumptions & CO2 emissions (scope 1, 2 and 3)
  - [Challenge] : Environmental impact (LCA)

Gate 1: Production routes

- Make a **literature** search to identify the major production routes:
  - **Raw materials and feed stock** (same approach as for the products)
    - **! should be from CO2 or waste or Biomass resource (not products)**
    - Location, scarcity of raw materials or feedstocks (states, distribution)
    - Environmental impact (impact of sourcing)
  - Other **Resources** needed : e.g. energy, catalysts, solvents, chemicals (!!!)
    - $H_2O, N_2, C_cH_hO_oN_nS_sX \ldots_{x\ldots}$
  - **Process route**
    - Chemical reactions paths
    - Separations paths
    - Operating conditions
      - Temperature, Pressure, Phases :Gas-Liquid-Solid Phases
    - Investment
    - Complexity (number of unit operations)
    - Hazard and operation (HAZOP)
  - **By-products** : => market and future markets
  - **Waste + emissions**
    - Waste treatment techniques
    - End-of-life release in the environment

Gate 1: Process selection → Make a block flow diagram



Block Flow Diagram : Interconnected process operations
Process steps defined by their function in the production route

Helping tool: Mass and Energy Balances

- Accumulation = IN - OUT (steady state Accumulation =0)
  - Irst principle of thermodynamics
- Mass Balance (steady state : No accumulation)

$$\forall a \in atoms : \sum_{i=input} \dot{M}_i^+ \cdot x_{o,a} = \sum_{o=output} \dot{M}_o^- \cdot x_{o,a}$$

- Energy Balance (steady state : No accumulation)

$$\sum_{i=el_{input}} \dot{E}_i^+ + \sum_{i=input} \dot{M}_i^+ \cdot h_i = \sum_{o=el_{output}} \dot{E}_o^- + \sum_{o=output} \dot{M}_o^- \cdot h_o + \sum_{l=losses} \dot{Q}_l^-$$

- Exergy Balance

Exergy losses

$$\dot{L} = \sum_{i=el_{input}} \dot{E}_i^+ + \sum_{i=input} \dot{M}_i^+ \cdot k_i - (\sum_{o=el_{output}} \dot{E}_o^- + \sum_{o=output} \dot{M}_o^- \cdot k_o)$$

$$k_i = h_i(T_i, Pi, x_i) - T_0 \cdot s_i(T_i, Pi, x_i)$$

Mass Balance and Energy Balances: Important to note

- **Mass balance**
  - No mass losses but by-products to market, emissions & waste
  - Chemical reactions (not complete + side reactions)
  - Enabling chemicals (to be considered as resources in the market)
  - Supply chains and storage
- **Energy Balance**
  - Energy is conserved but can be lost in the environment
  - Enthalpy includes the energy of formation (chemical reactions)
  - Lower Heating Value is the energy of formation of a fuel
  - Losses ≠ Ignorance (i.e. not the error of the energy balance)
  - Energy flows to the environment to be characterised

- Mass flows : $$\sum_{o=output \notin products} \dot{M}_o^- \cdot h_o$$

- Heat $$\sum_{l=losses} \dot{Q}_l^-$$

Gate 1: selection criteria

- **Thermodynamic**
  - Heat of reaction
  - Gibbs free energy of reaction or exergy
  - Materials flows: atomic balances and flows,
  - Energy flows: energy balance and flows
- **Economic**
  - Products, energy and feedstock costs
  - Investment
  - Production support chemicals
- **Environmental**
  - Supply chains : feedstocks - energy - waste
  - Life cycle impact assessment (LCA)
  - CO_2 emissions (scope 1, 2 and 3)
- **Hazard and operation**
- **Complexity**

Gate 1: selection criteria

- How to choose/compare processes ?
  1. Make a list of criteria
  2. Define a metric for each criteria
     1. Define a KPI (Key Performance Indicator) : a quantity that qualifies the criteria for each process options
     2. Associate a Grade to each KPI ($Grade(KPI_{c,p})$)
        1. e.g. 1 to 5 to compare the processes
        2. Grades can be associated to quantities or to quality (low-high)
  3. Define weights (relative importance of the criteria)
     1. Consensus in the group
  4. Compare the processes in a matrix

Metrics: key performance indicators

- Thermodynamic
  - Atom economy $\frac{\sum_p^{products}\sum_a^{atoms}\dot{n}_{a_p}}{\sum_f^{feedstocks}\sum_a^{atoms}\dot{n}_{a_f}}$ $[kmol_{a,p}/kmol_{a,f}]$!!! different atoms !!!
  - Specific energy $[MJ/kg_{product}]$
    - ! comparing different sources of energy ! electricity vs fuel
  - Gibbs free energy : $G = \frac{\sum_{out}(\dot{m}_{out}h_{out} - T_0\dot{m}_{out}s_{out}) - \sum_{in}(\dot{m}_{in}h_{in} - T_0\dot{m}_{in}s_{in})}{\dot{m}_p}$ $[MJ/kg_{product}]$
- Economic
  - Operating expenditure : OPEX [CHF/year] or $[CHF/kg_{product}]$
  - Capital expenditure : CAPEX [CHF/year] or $[CHF/kg_{product}]$
  - Footprint : $[m_{land}^2]$
- Environmental
  - Global warming potential $[kg_{CO_2^{eq}}/kg_{product}]$
  - Resource depletion $[kg_{resources}/kg_{product}]$

Example of KPI for a given product P

- OPEX [CHF/ CHF product] : $\dfrac{\int_{t_0}^{t_f} \left(\sum_{F=1}^{n_F} \dot{M}_F^{+}(t) c_F^{+}(t) + E^{+}(t) c_e^{+} - E^{-}(t) c_e^{-} - \dot{M}_{P^-}^{-}(t) c_{P^-}^{-}(t) \right) dt}{\int_{t_0}^{t_f} \left(\sum_{P=1}^{n_P} \dot{M}_P^{-}(t) c_P^{-}(t) \right) dt}$

- CAPEX [CHF/kg product(s)] : $\dfrac{\sum_e I_e}{\int_{t_0}^{t_f} \left(\sum_{P=1}^{n_P} \dot{M}_P^{-}(t) \right) dt}$ or [CHF/CHF products] $\dfrac{\sum_e I_e}{\int_{t_0}^{t_f} \left(\sum_{P=1}^{n_P} \dot{M}_P^{-}(t) \cdot c_p^{-} \right) dt}$

- Specific Cost [CHF/kg product]: $\dfrac{\int_{t_0}^{t_f} \left(\sum_{F=1}^{n_F} \dot{M}_F^{+}(t) c_F^{+}(t) + E^{+}(t) c_e^{+} - E^{-}(t) c_e^{-} - \dot{M}_{P^-}^{-}(t) c_{P^-}^{-}(t) \right) dt + \frac{1}{\tau} \sum_e I_e}{\int_{t_0}^{t_f} \left(\sum_{P=1}^{n_P} \dot{M}_P^{-}(t) \right) dt}$

  Annualisation

- Energy used [kJ/kg] ? : $\dfrac{\int_{t_0}^{t_f} \left(\sum_{F=1}^{n_F} \dot{M}_F^{+}(t) lhv_F + E^{+}(t) - E^{-}(t) \right) dt}{\int_{t_0}^{t_f} \left(\sum_{P=1}^{n_P} \dot{M}_P^{-}(t) \right) dt}$

Gate 1: process selection

- Define a list of selection criteria :
  - $Grade(KPI_{c,p})$: rank of the key performance indicator for criteria c of process p
  - w_c : importance of criteria c in selection
- Make a selection matrix : choose $p \mid \max_p (C_p = \sum_c w_c \cdot Grade(KPI_{c,p}))$

	Weight w_c	Process 1	Process 2	Process 3
Reference		[1,2]	[2,3]	[3,4]
Criteria 1 : Atom economy	0.2	$Grade(KPI_{c,p})$	$\cdots$	
Criteria 2 : Energy	0.3	$\vdots$		
Criteria 3 : Economy	0.3			
Criteria 4 : HAZOP	0.1			
Criteria 5 : complexity	0.1			
Total		$\sum w_c \cdot Grade(KPI_{c,1})$		

AGIR for gate 1: selecting process routes

Analyse: define the goals and the criteria

Generate: collect the information, define the KPI

Interpret: define the grading system, define the relative weights, negotiate importance

Report: make a matrix and explain your choices