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A methodology for best pathway identification of waste recovery

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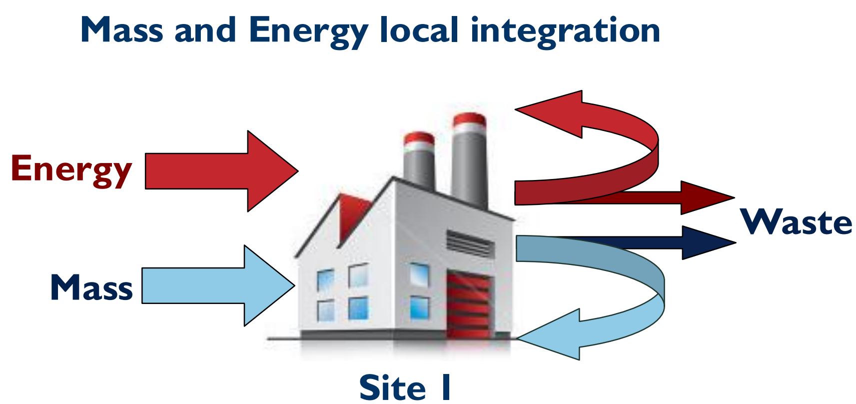
Outline

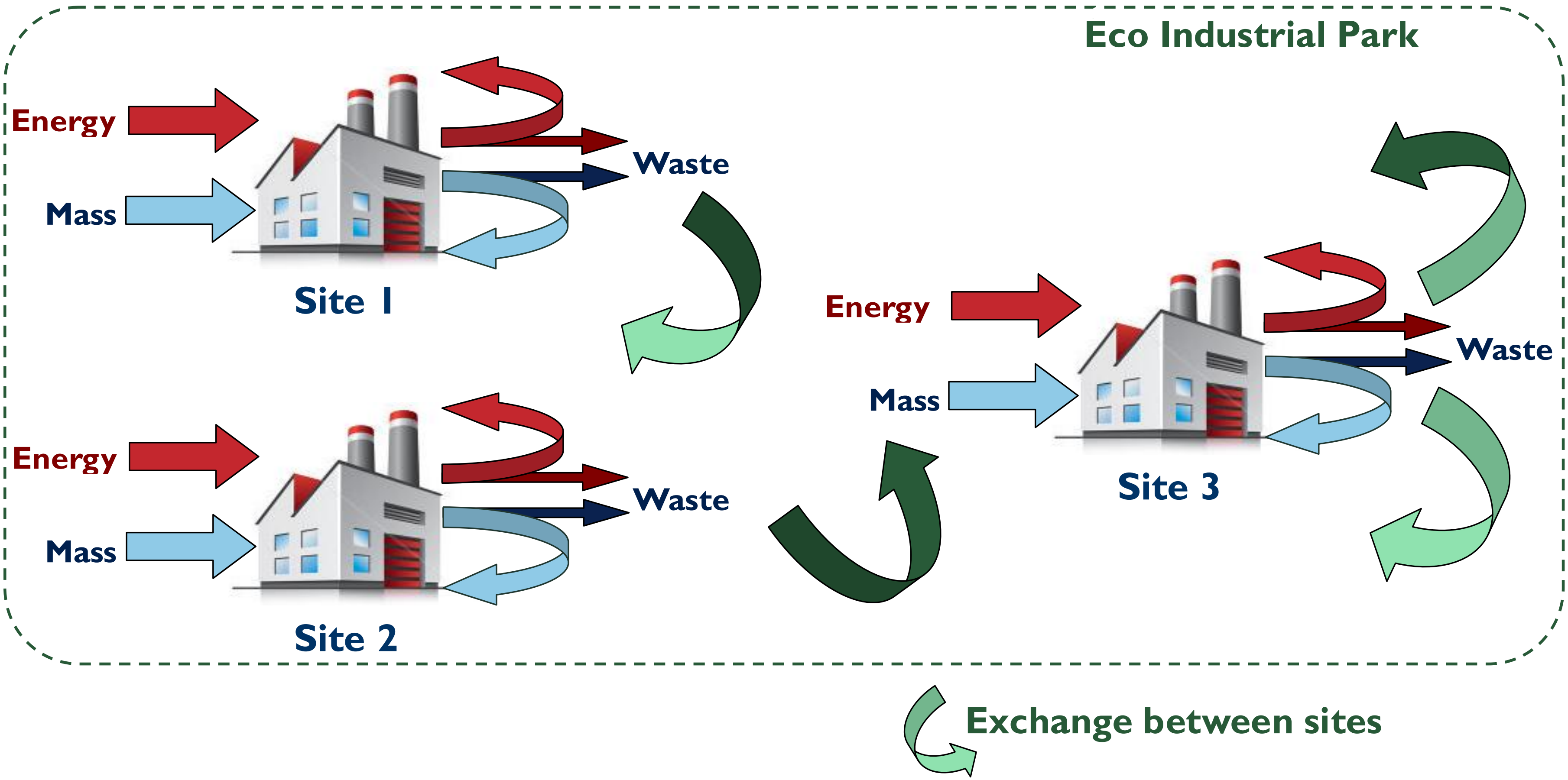
- Introduction
- Proposed Methodology
- Case Study
  - Wood conversion processes
  - Modeling conversion process
  - Simulation results
  - Data extraction
  - Combinatorial paths
- Conclusion and Outlook

Introduction: Context

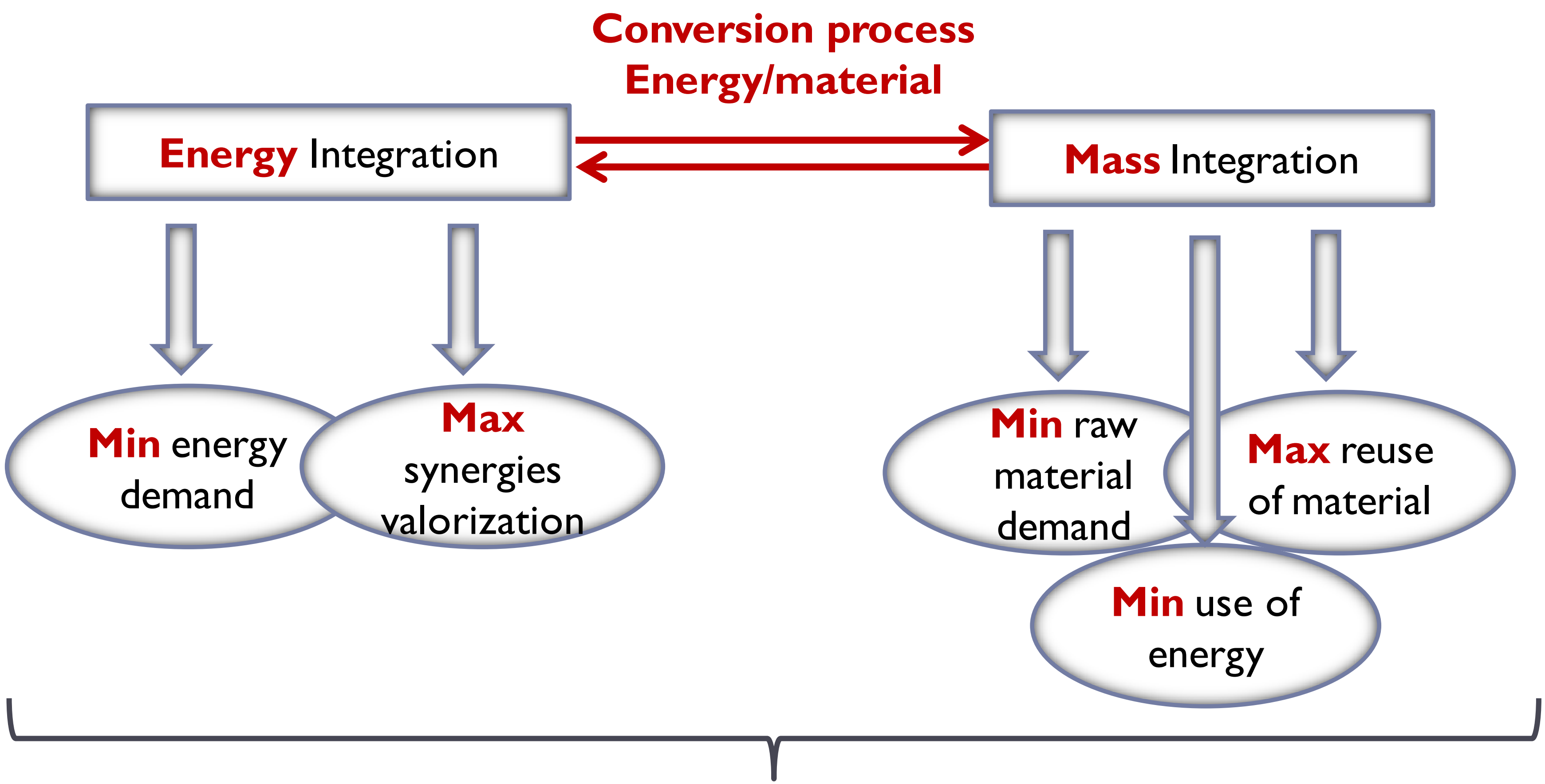


Introduction: Context

Energy and Mass territorial integration



Introduction: Problem

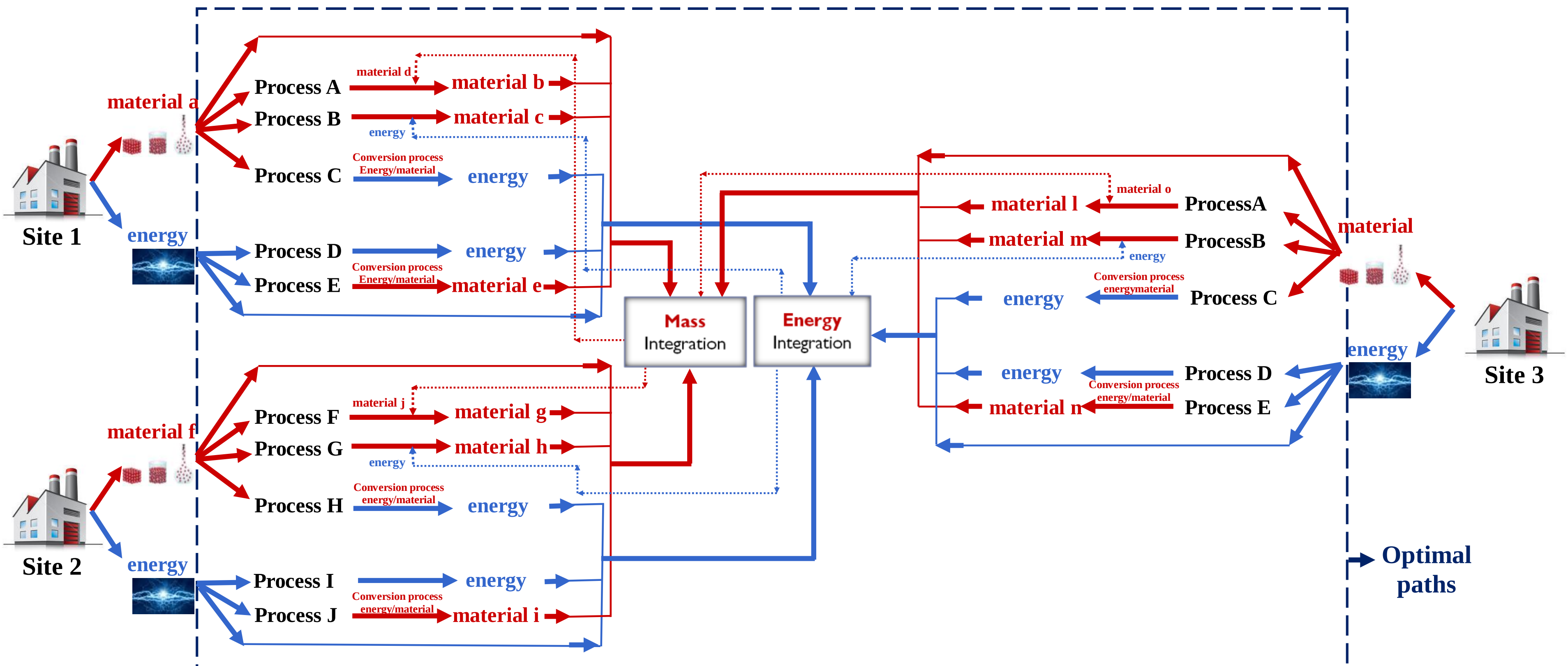


Combine both problems while considering the conversion processes

Introduction: Objective and concept

Systematic methodology for the integration of energy/material conversion processes in the territory.

Methodology Concept

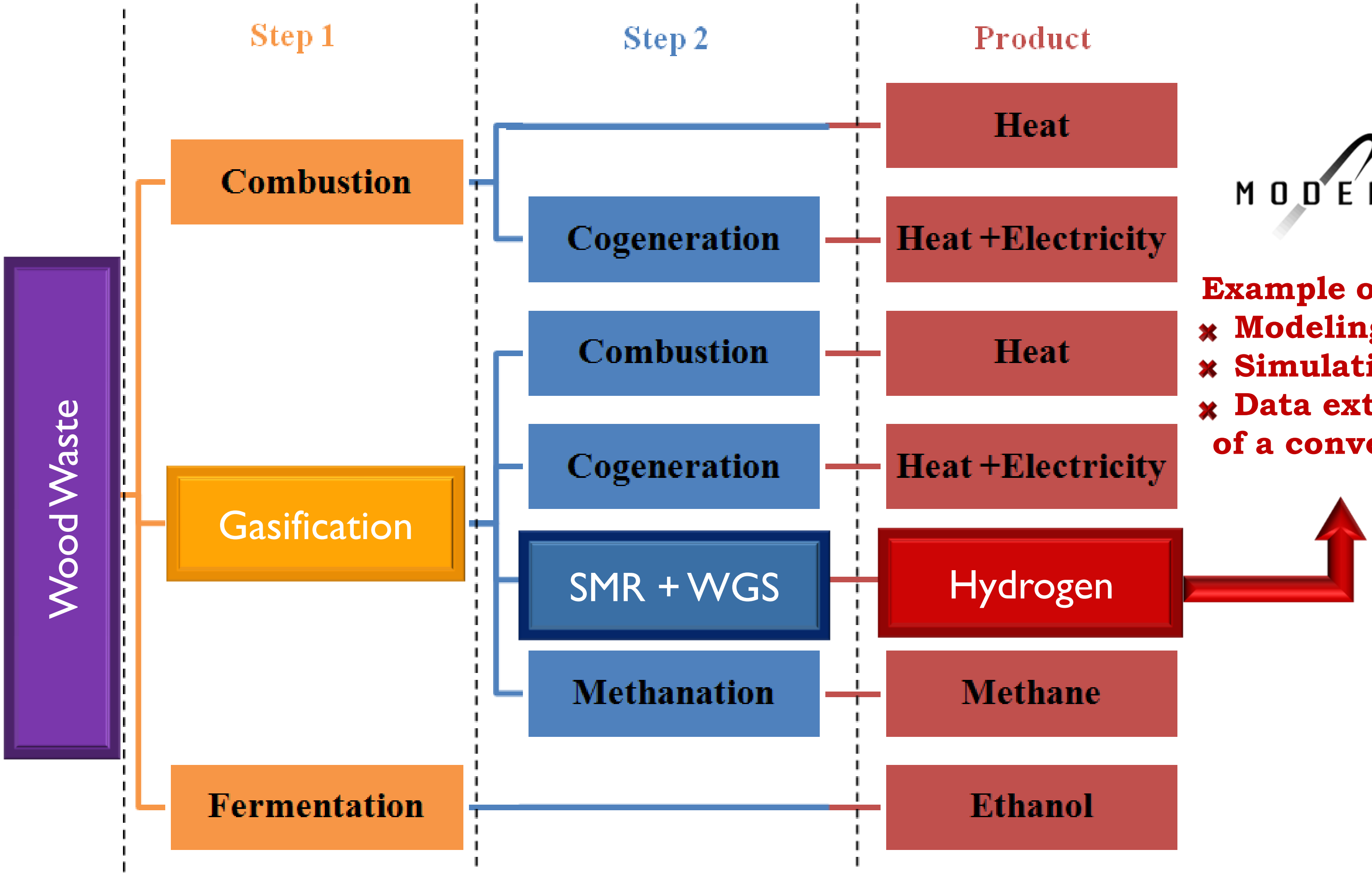


Methodology

Proposed methodology

1. Energy and material flow extraction of each actor of a territory
2. Conduct a territorial energy and mass integration
3. Identification of waste streams
4. Inventory of the conversion processes for each of these streams
5. Combinatorial establishment of possible paths
6. Generating the superstructure scenarios and conducting energy and mass integrations

Case study: Wood conversion processes

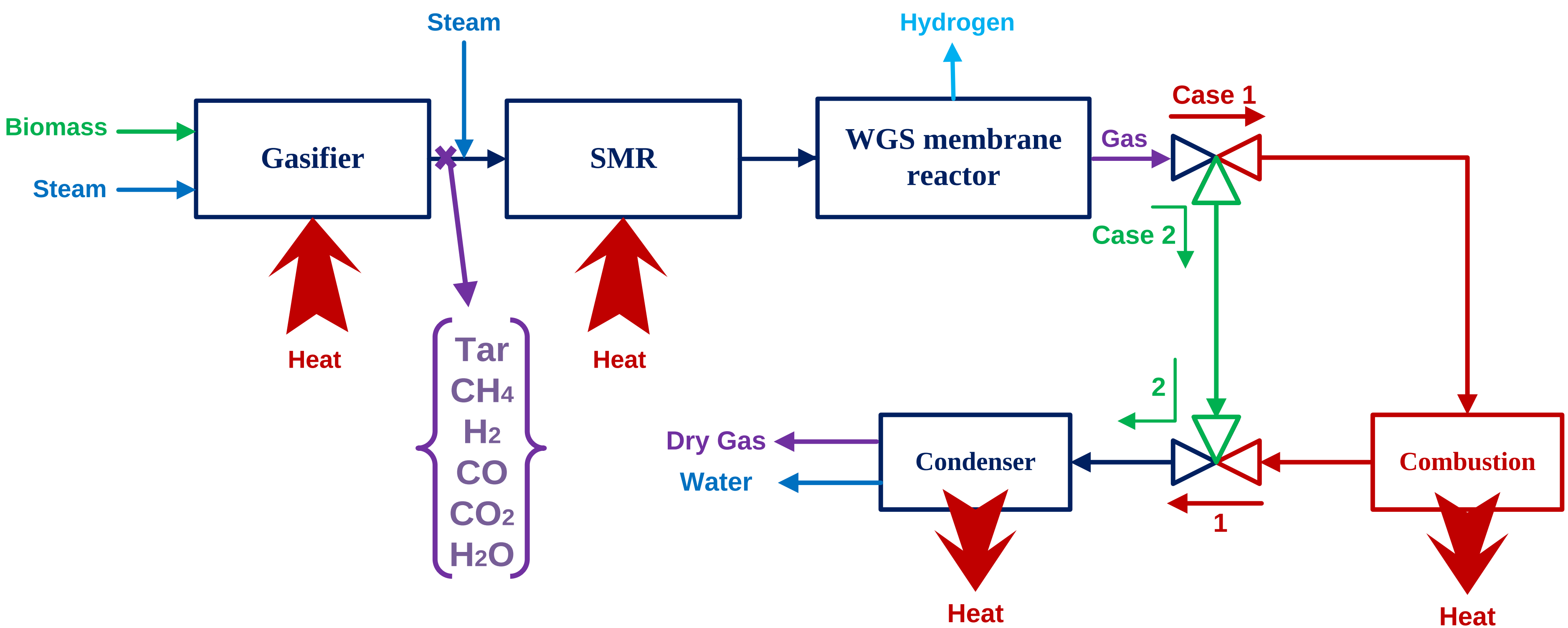


MODELICA

Example of :
- **Modeling**
- **Simulation**
- **Data extraction of a conversion system**

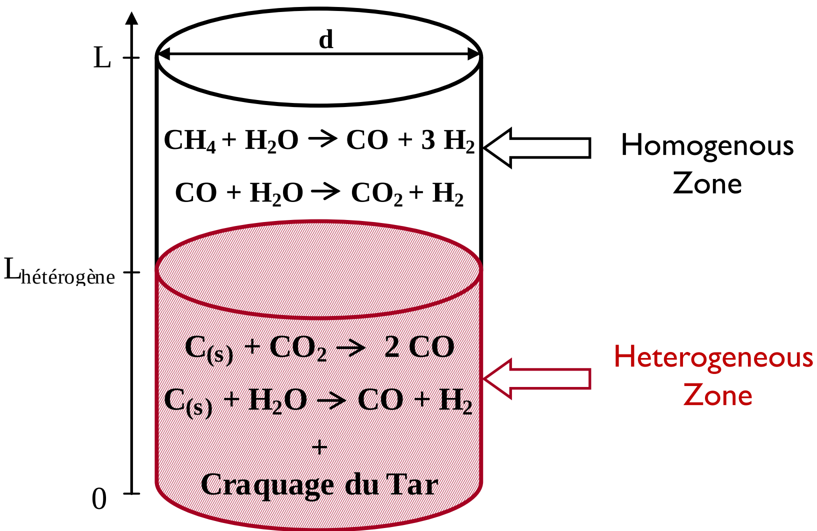
Case Study: Modeling conversion processes

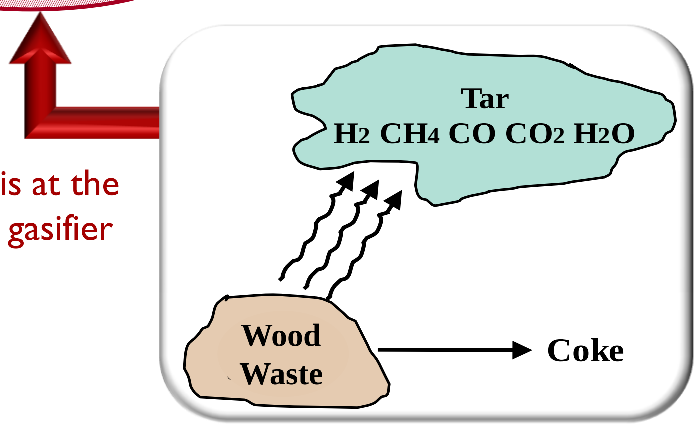
Bloc diagram of Wood to hydrogen conversion system



Case Study: Modeling conversion processes

Gasifier





Biomass pyrolysis at the entrance of the gasifier

Mass balance:

$$\frac{dF_i}{dz} = A \sum_{k=1}^{N_R} \gamma_{ik}\, r_k$$

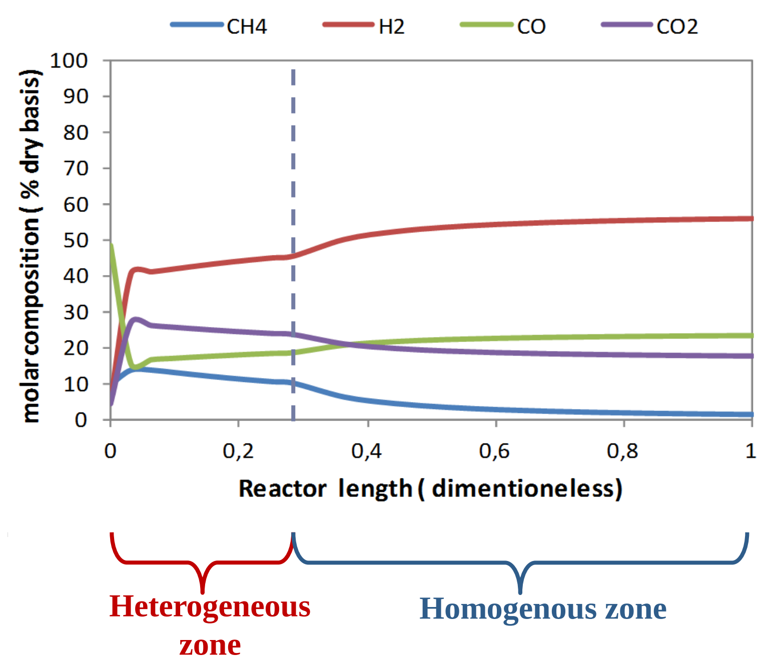
Reaction rate

Energy balance:

Enthalpy of reaction

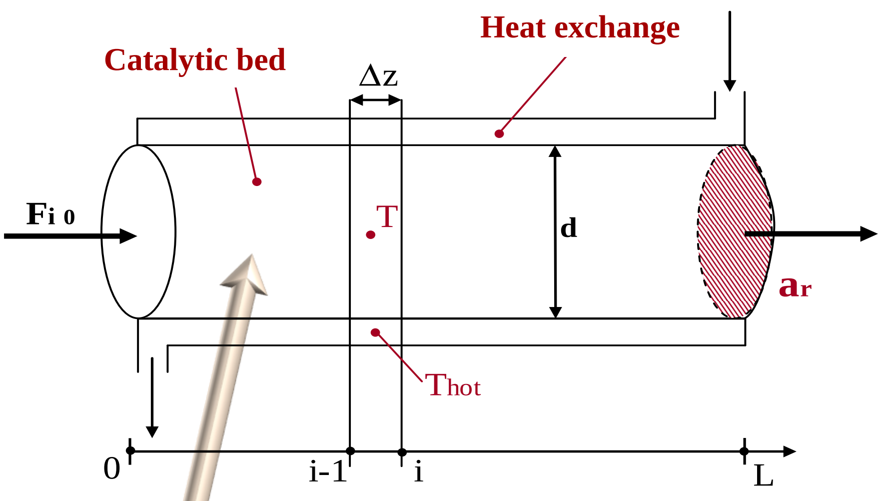
$$\frac{dT}{dz} = \frac{A \sum_{k=1}^{N_R} (-\Delta H_k r_k) - \frac{dQ}{dz}}{\sum_{i=1}^{R} (-F_i C_{p_i})}$$

[W/m]



Case Study: Modeling conversion processes

Steam Methane Reformer



$$CH_4 + 0{,}5CO_2 + 0{,}5H_2O \rightarrow 1{,}5CO + 2{,}5H_2$$

$$C_6H_6 + 3CO_2 + 3H_2O \rightarrow 9CO + 6H_2$$

$$C_{10}H_8 + 5CO_2 + 5H_2O \rightarrow 15CO + 9H_2$$

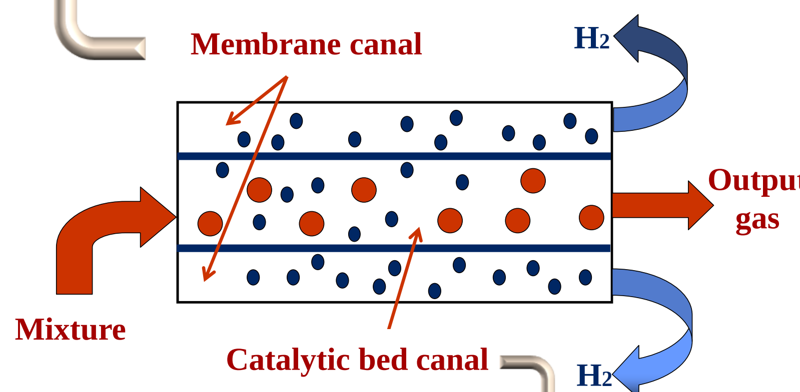
Tar

$$\frac{dX_i}{dz} = \frac{X_i - X_{i-1}}{\Delta z}$$

$$\Delta z = \frac{L}{N}$$

Water Gas Shift membrane reactor

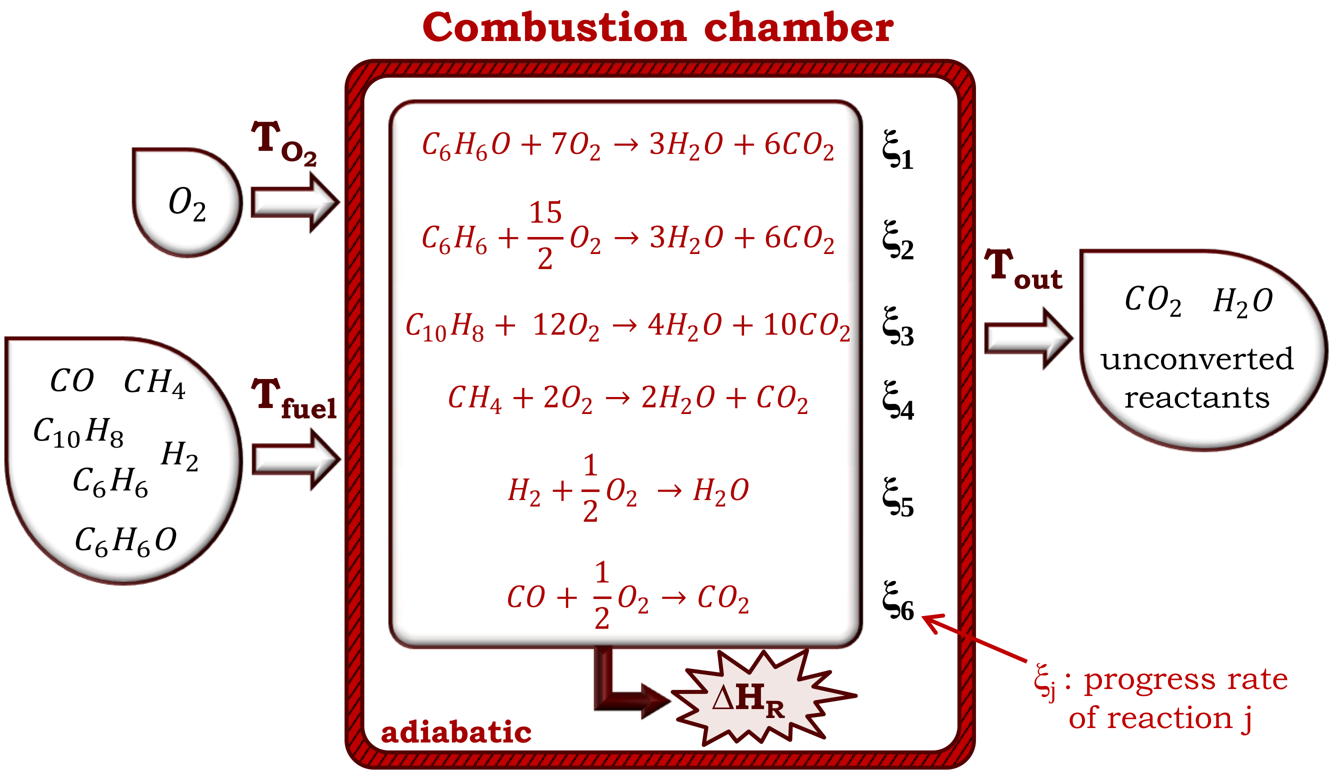
$$\begin{cases} \dfrac{dG_{H_2}}{dw} = a_{H_2} N_{H2} \left(\dfrac{L}{W}\right) \\ \dfrac{dT_{nr}}{dw} = \dfrac{a_{H_2} N_{H2} \Delta H_2 \left(\dfrac{L}{W}\right) + q\left(\dfrac{L}{W}\right)}{\sum_{i=1}^{R}(-G_i C_{p_i})} \end{cases}$$



$$CO + H_2O \rightarrow CO_2 + H_2$$

$$\begin{cases} \dfrac{dF_i}{dw} = \gamma_i(-r_{co}) - j.\, a_{H_2} N_{H2} \left(\dfrac{L}{W}\right) \\ \dfrac{dT_r}{dw} = \dfrac{-\Delta H(-r_{co}) - a_{H_2} N_{H2} \Delta H_{H_2} \left(\dfrac{L}{W}\right) - q\left(\dfrac{L}{W}\right)}{\sum_{i=1}^{R}(-F_i C_{p_i})} \end{cases}$$

Case Study: Modeling conversion processes



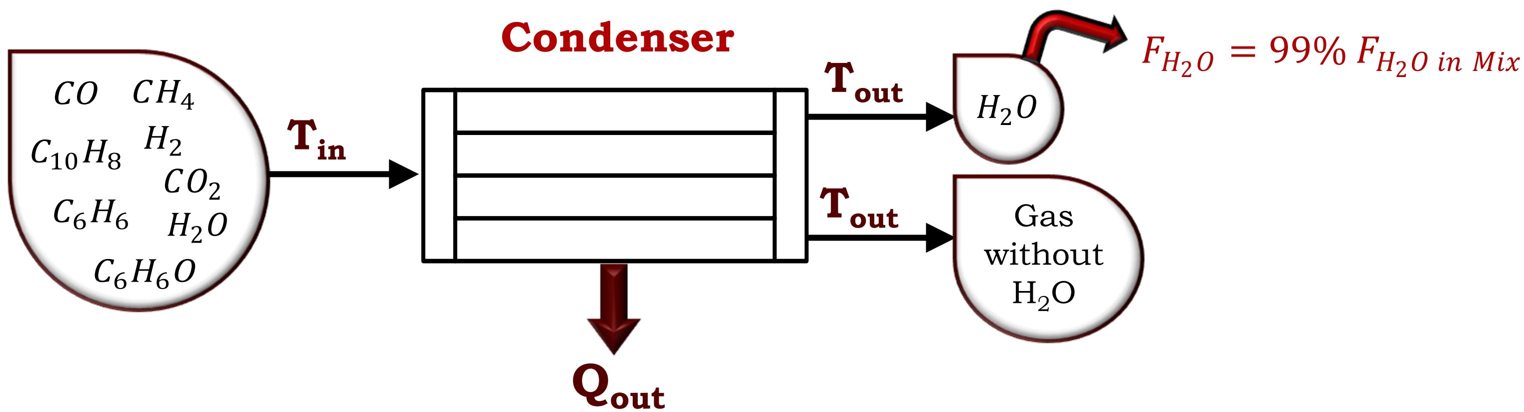
Stoichiometric coefficient

$$
\begin{cases}
F_i = F_{i0} \pm \sum_{j=1}^{6} \upsilon_{ij}\, \xi_j \\
F_{total} = \sum_i F_i \\
x_i = F_i / F_{total} \\
P_i = x_i P_T \\
K_{eq\,j} = \dfrac{\prod_i {P_p}_i^{\gamma_{ij}}}{\prod_i {P_R}_i^{\gamma_{ij}}}
\end{cases}
$$

Reaction j   Component i

$$
\underbrace{Q}_{\text{Adiabatic} \rightarrow Q=0} = \sum_i F_{out_i} h_{out_i}(T_{out}) - F_{fuel} h_{fuel}(T_{fuel}) - F_{O_2} h_{O_2}(T_{O_2}) - \underbrace{(-\Delta H_R)}_{\text{Exothermic } \Delta H_R < 0}
$$

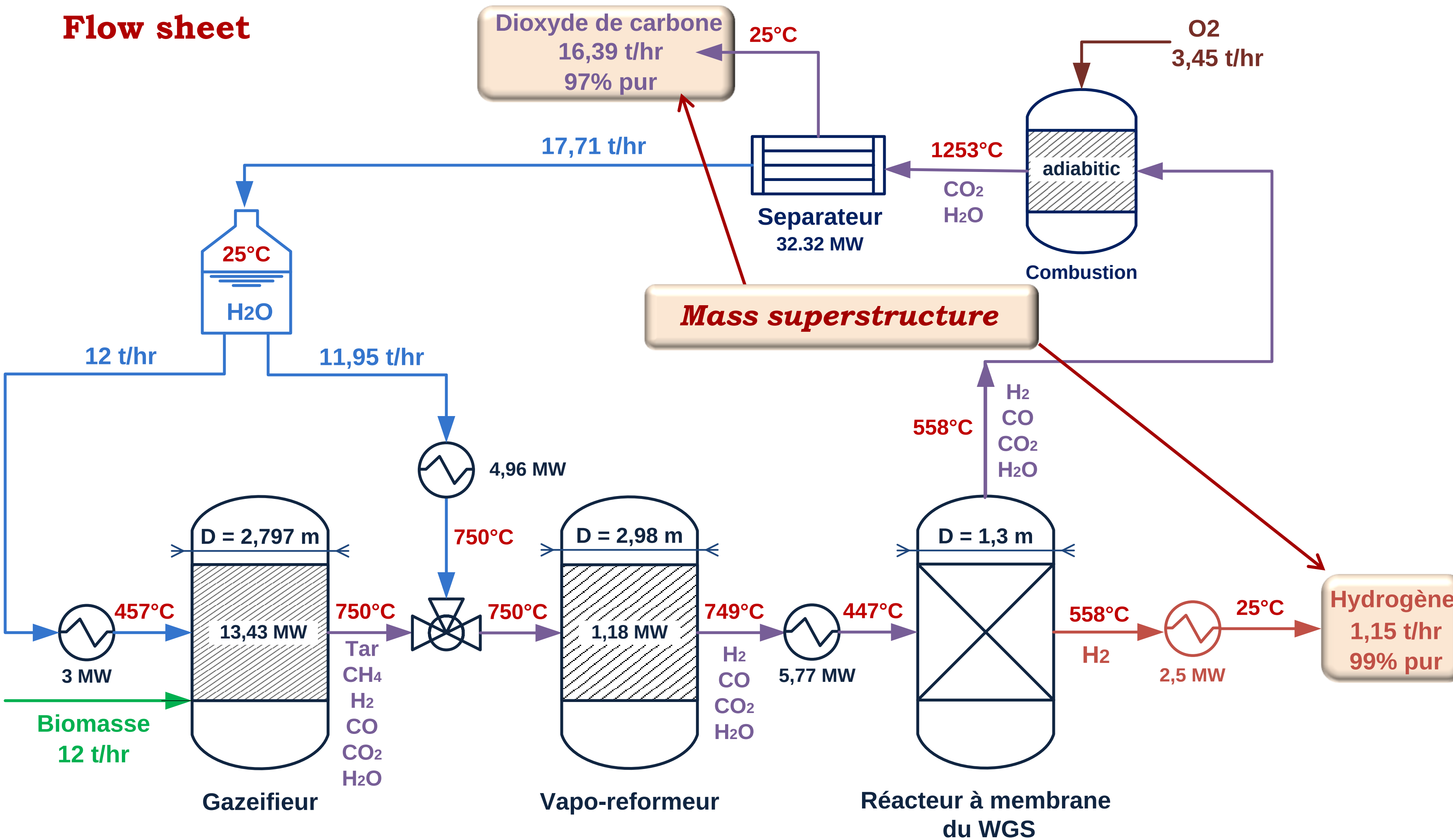
Case Study: Modeling conversion processes



$$Q_{out} = F_{gas_{out}} h_{gas_{out}} (T_{out}) + F_{H_2O} h_{H_2O} (T_{out}) - F_{in} h_{in} (T_{in})$$

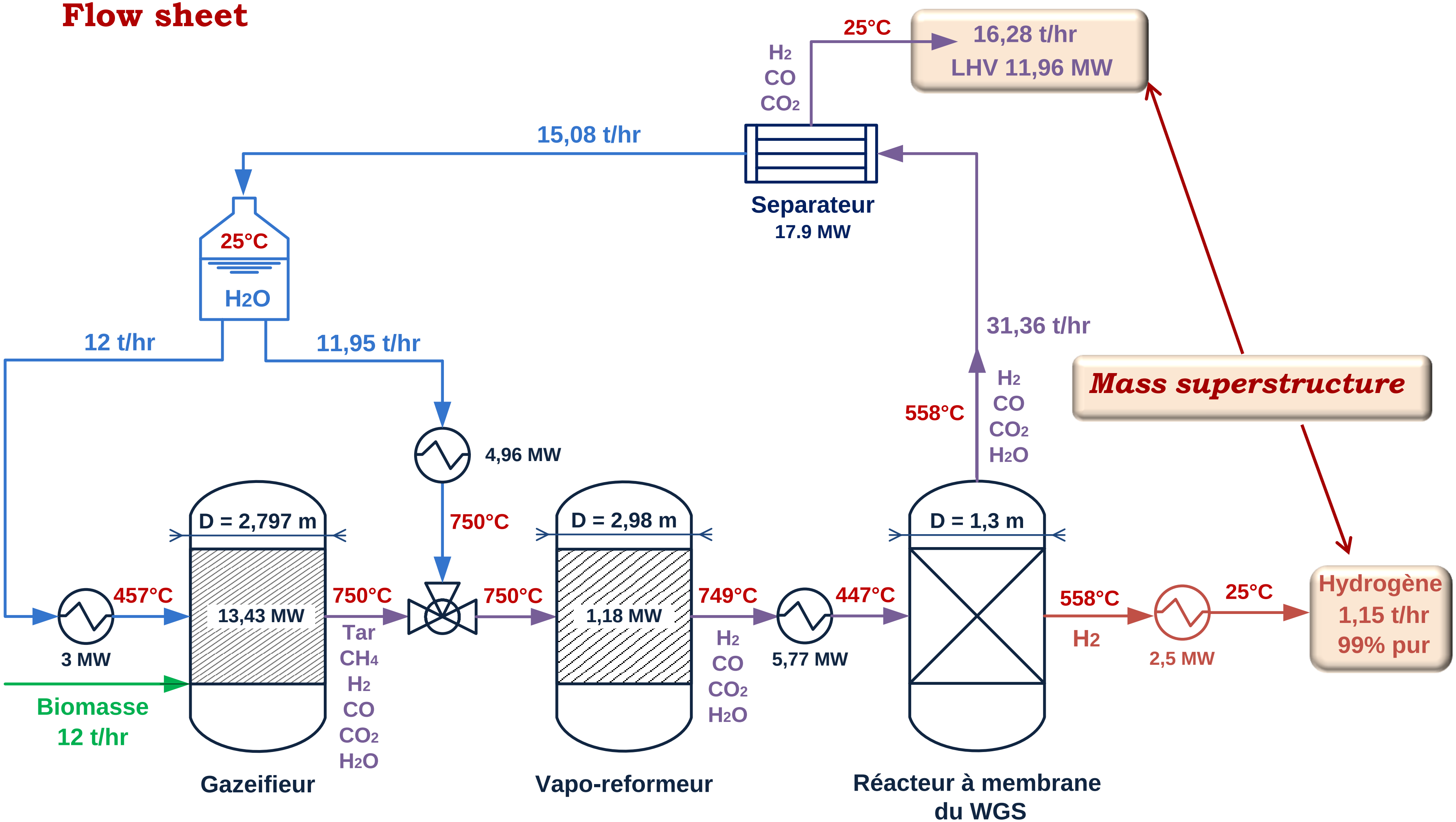
Case Study: Simulation results

Flow sheet



Case Study: Simulation results

Flow sheet



Case Study: Data Extraction

1. Heat flow extraction from the flow sheet of each path

Heat Flux	Tin (°C)	Tout (°C)	Q(MW)
Steam Source	25	456.85	3
Gasifier	456.85	749.85	13.43
Additional water	25	749.85	4.96
Steam Reformer	749.85	750.41	1.21
SR to WGS	750.41	446.85	5.79
Combustion	558.36	1253	adiabatic
Condenser	1253	25	32.32
WGS output hydrogen	558.36	25	2.55

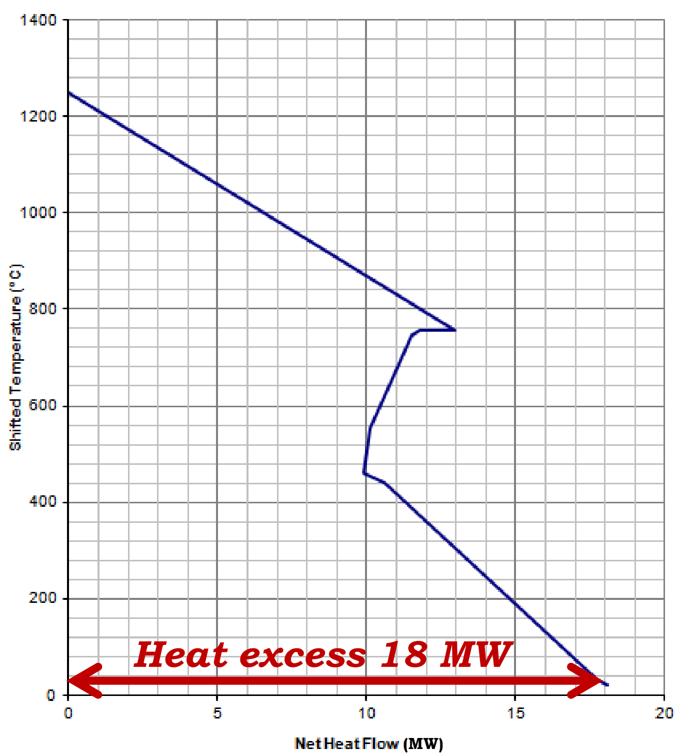
With combustion

Heat Flux	Tin (°C)	Tout (°C)	Q(MW)
Steam Source	25	456.85	3
Gasifier	456.85	749.85	13.43
Additional water	25	749.85	4.96
Steam Reformer	749.85	750.41	1.21
SR to WGS	750.41	446.85	5.79
Condenser	558.36	25	17.9
WGS output hydrogen	558.36	25	2.55

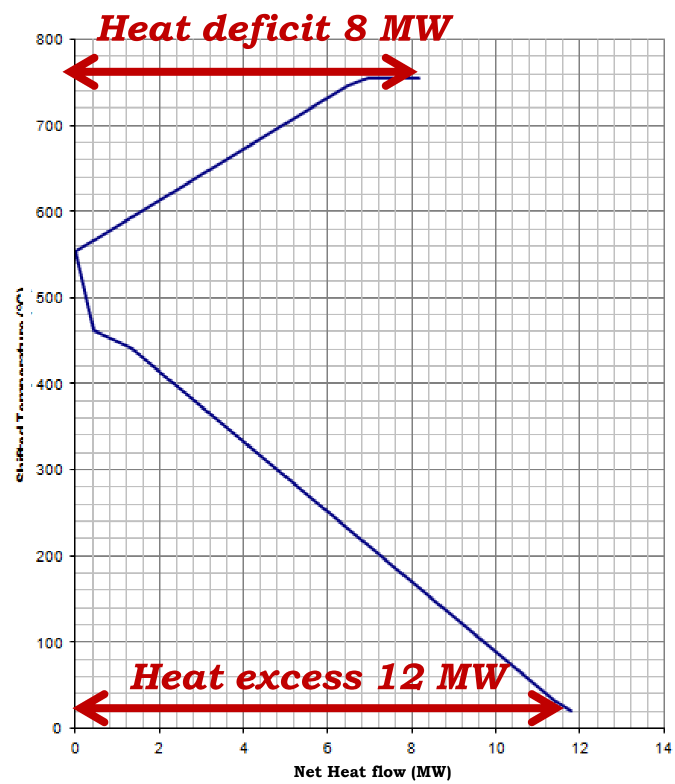
Without combustion

Case Study: Data Extraction

2. Energy superstructure: Grand Composite Curve



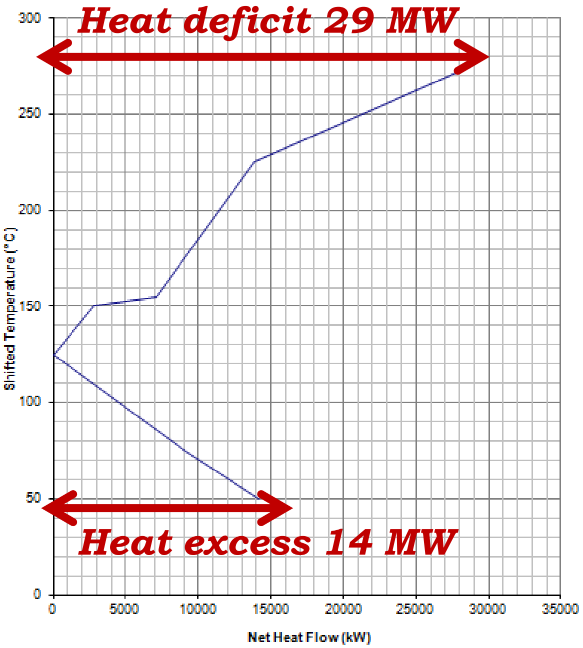
With combustion



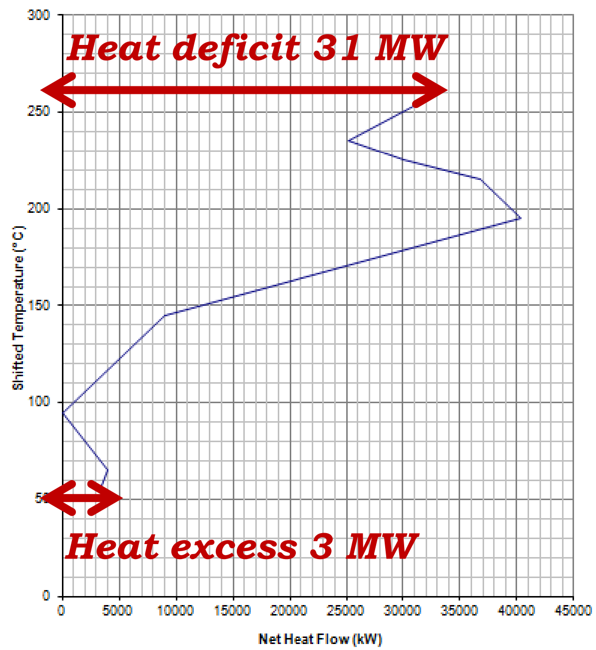
Without combustion

Case Study: Combinatorial paths

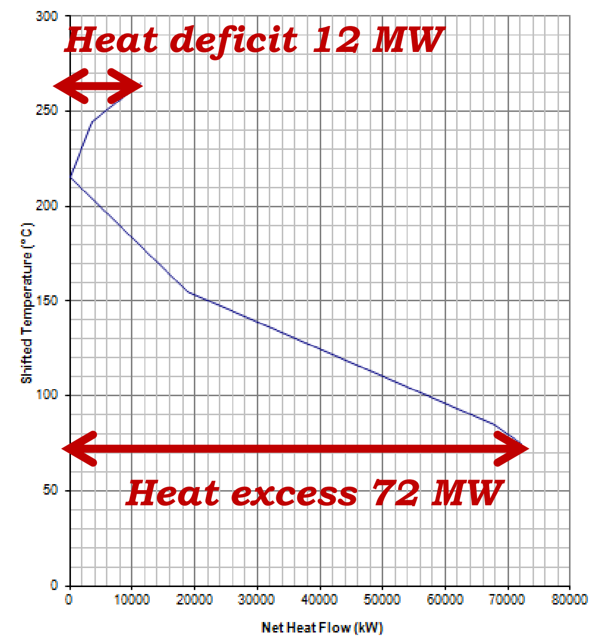
Site 1



Site 2



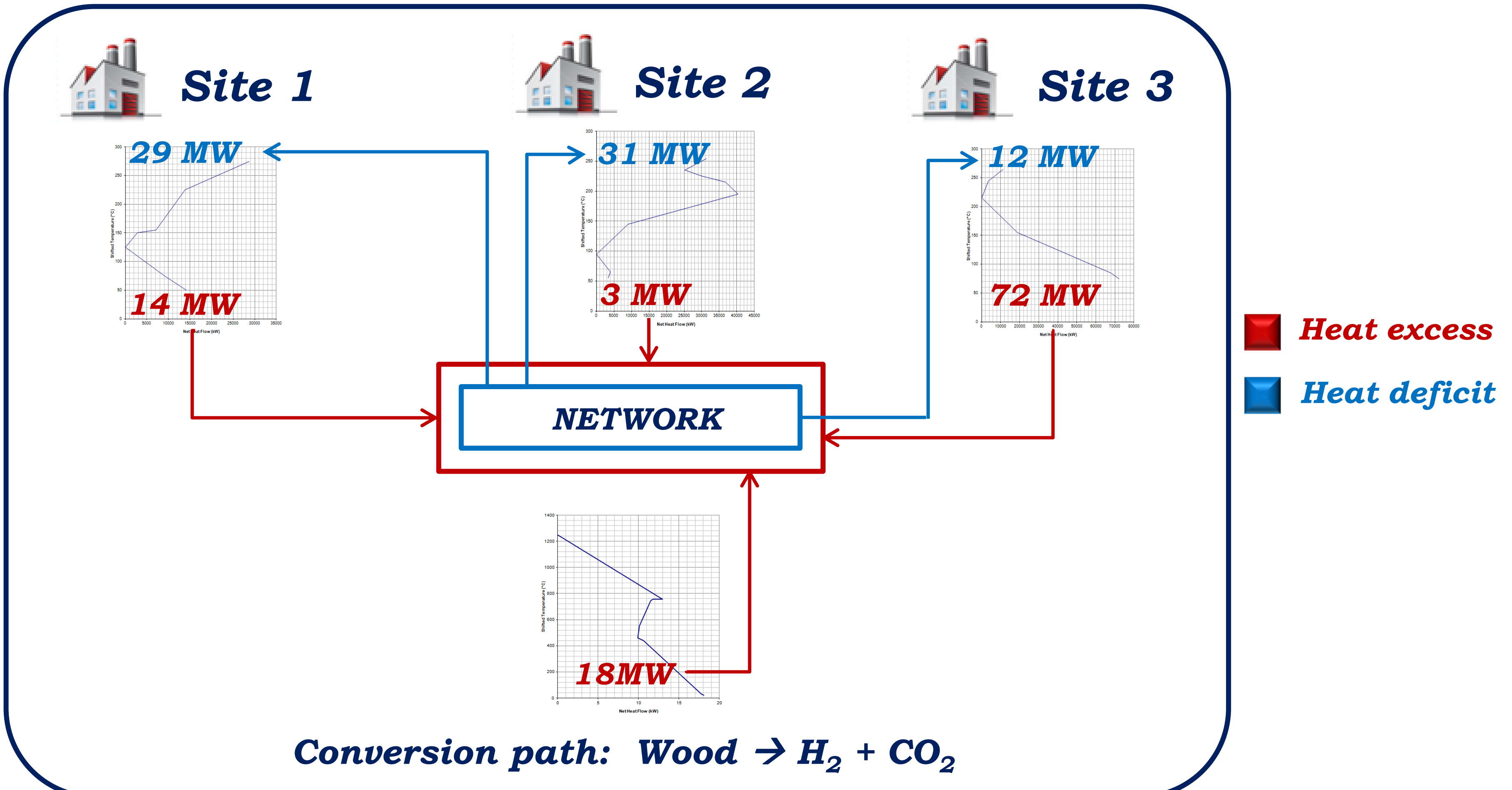
Site 3



\+ **Hydrogen demand**
Carbon Dioxide demand

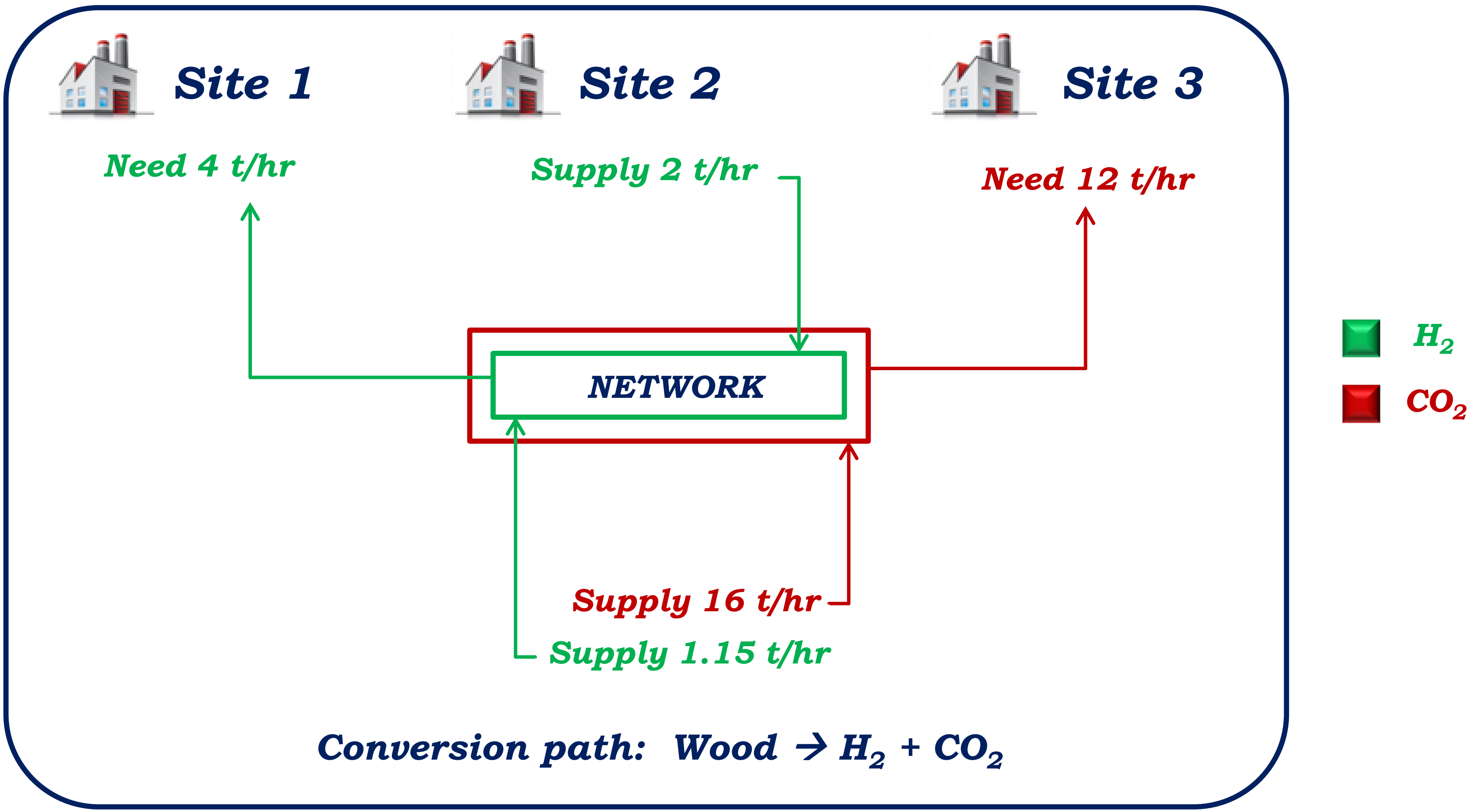
Case Study: Combinatorial paths

Energy superstructure → Energy integration



Case Study: Combinatorial paths

Mass superstructure → Mass integration



Case Study: Combinatorial paths

Option 1

Site 1

Site 2

Site 3

+

Wood → H_2 + CO_2

Option 2

Site 1

Site 2

Site 3

+

Wood → CH_4 + CO_2

. . .

Option n

Site 1

Site 2

Site 3

+

Wood → x

Mass and Energy integration for each option and economic evaluation

Conclusion and Outlook

Conclusion

Proposition of a methodology for the integration of conversion process in the territory for waste valorization

Application of this methodology in a case study:

- Modeling

-Simulation

-Data extraction

Future Work

Obtain total cost for each pathway

Energy and Mass network optimization by modeling the transfer through pipes