Process and metabolic modelling and Multidisciplinary Design Optimization

Álvaro Cabeza, Online webinar, 23 November 2021

Horizon 2020
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Objectives

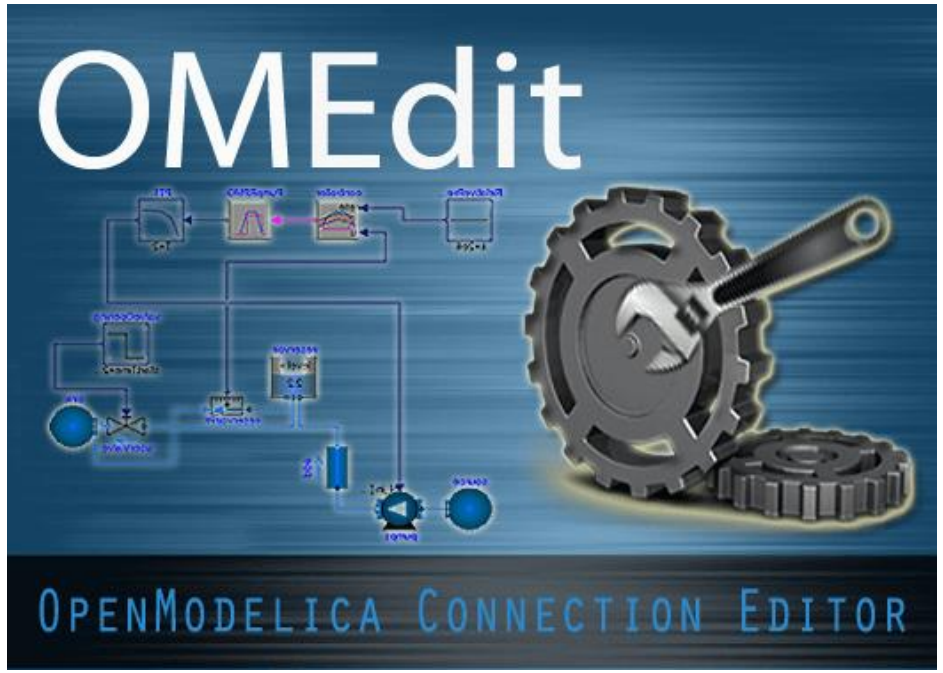
- BioRECO$_2$VER process mathematical modelling
  - Lab system parametrization
  - Industrial scale model (TEA & LCA)

- Parametrized model calibration & validation

- Process optimization (performance improvement)

Modelling and simulation

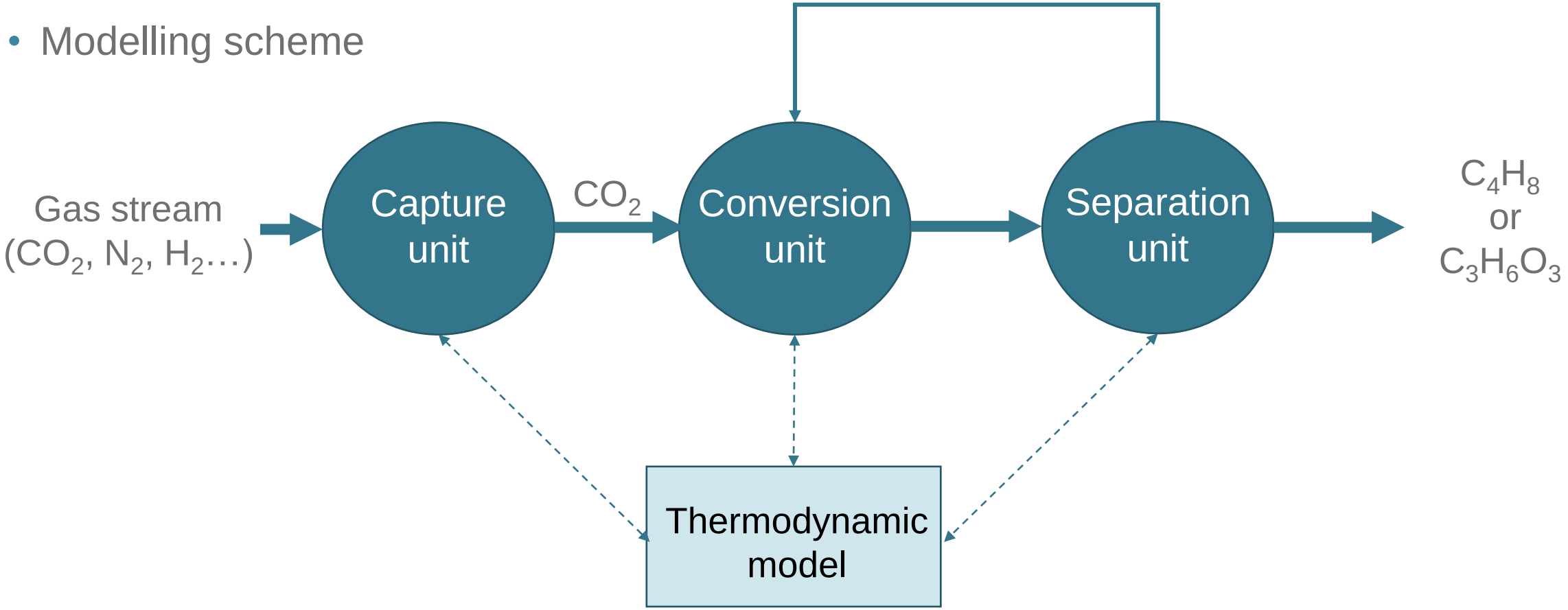
- Model(s) development environment



- **Open source**
- Powerful solvers included
- Direct connection with Python (data retrieval & optimization)
- Programming by “blocks”→ Direct connection to develop a process model

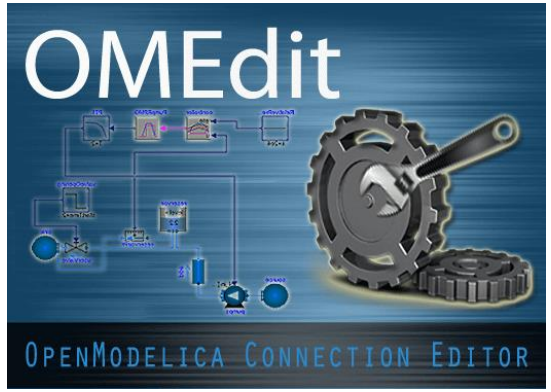
Modelling and simulation

- Modelling scheme



Modelling and simulation

- Model calibration – Calibration tool



Model

Simulation

Objective function(s)

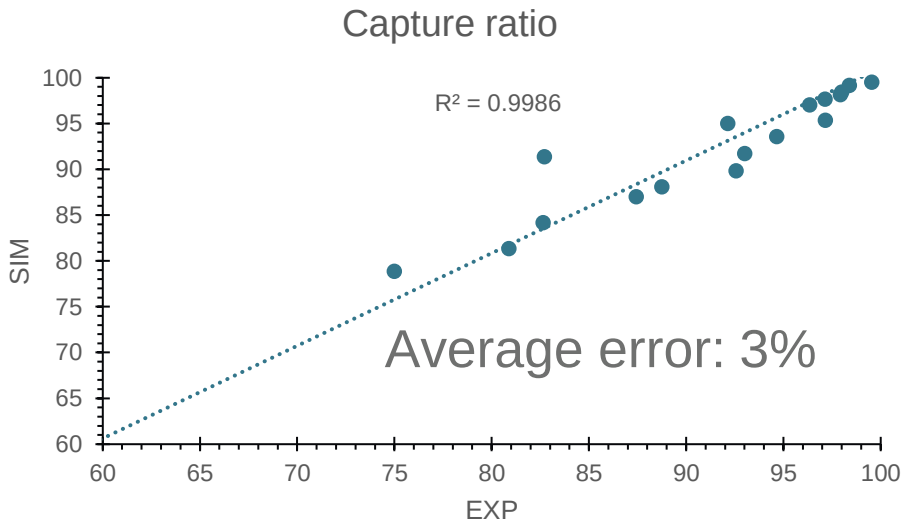
Optimization algorithm(s)

Adjusted parameters (**Partial calibration with experimental data**)

Objective function value (model error)

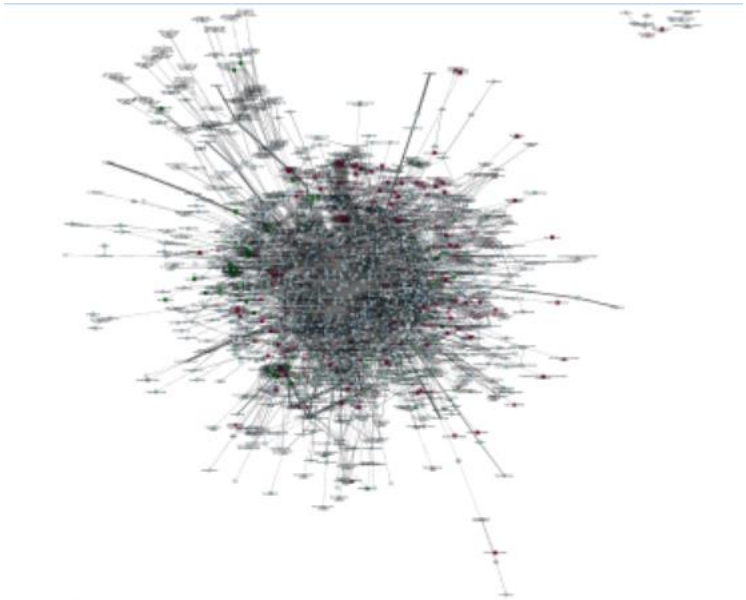
Modelling and simulation

- Model calibration – Results
  - Calibration is a minimization problem
    - Objective function: (Experimental – Simulated)^2
    - Physical sense checked
  - Suitable agreement when data was available
    - Adequate data for capture
      - Example: capture ratio
    - Uncertainty in conversion data
      - Metabolic modelling as a solution → Kinetics

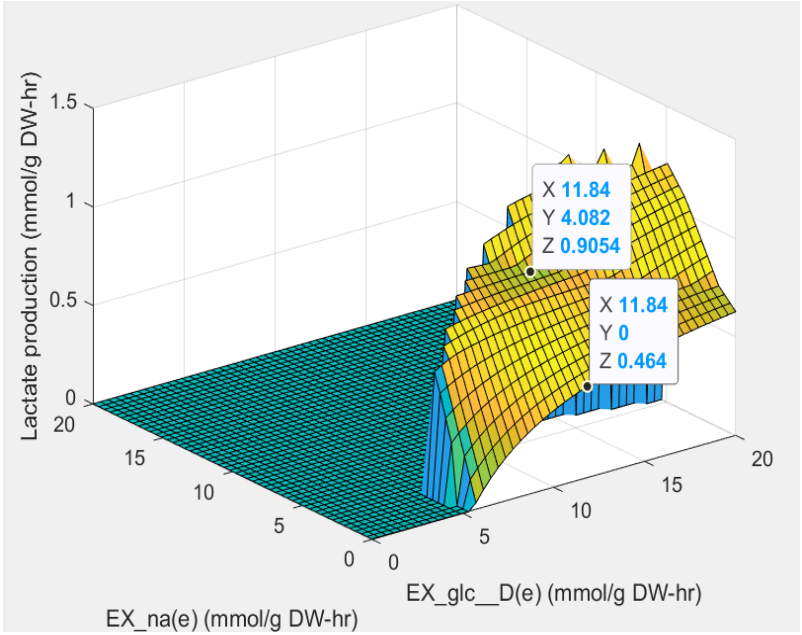


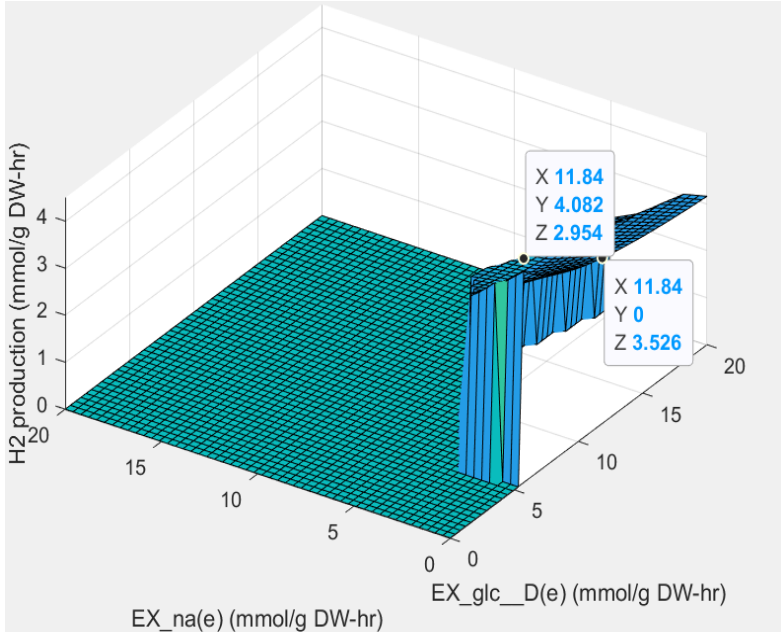
Modelling and simulation

- Model calibration – Results
  - Uncertainty in conversion data
    - Metabolic modelling as a solution → Kinetics



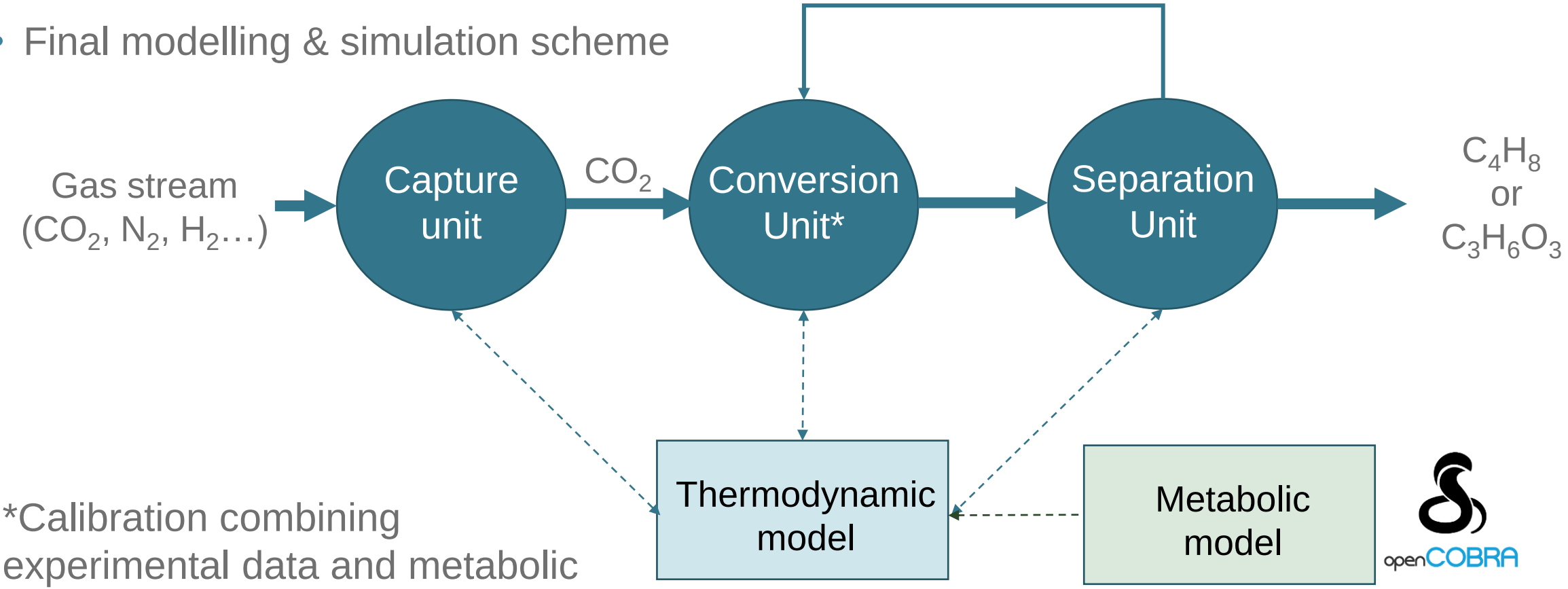
(Gautam and Xu. (2021). Appl Biochem Biotechnol)





Modelling and simulation

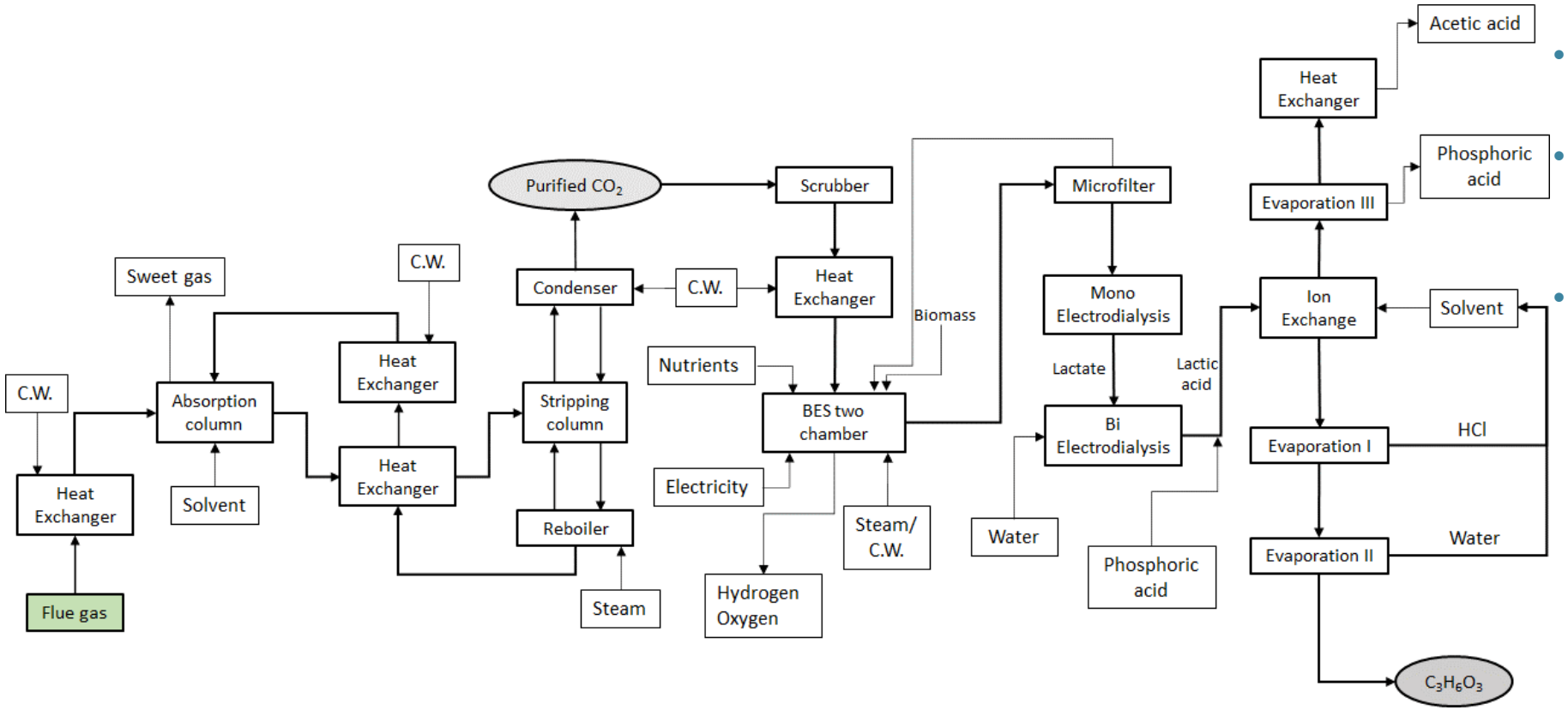
- Final modelling & simulation scheme



*Calibration combining experimental data and metabolic modelling

Modelling and simulation

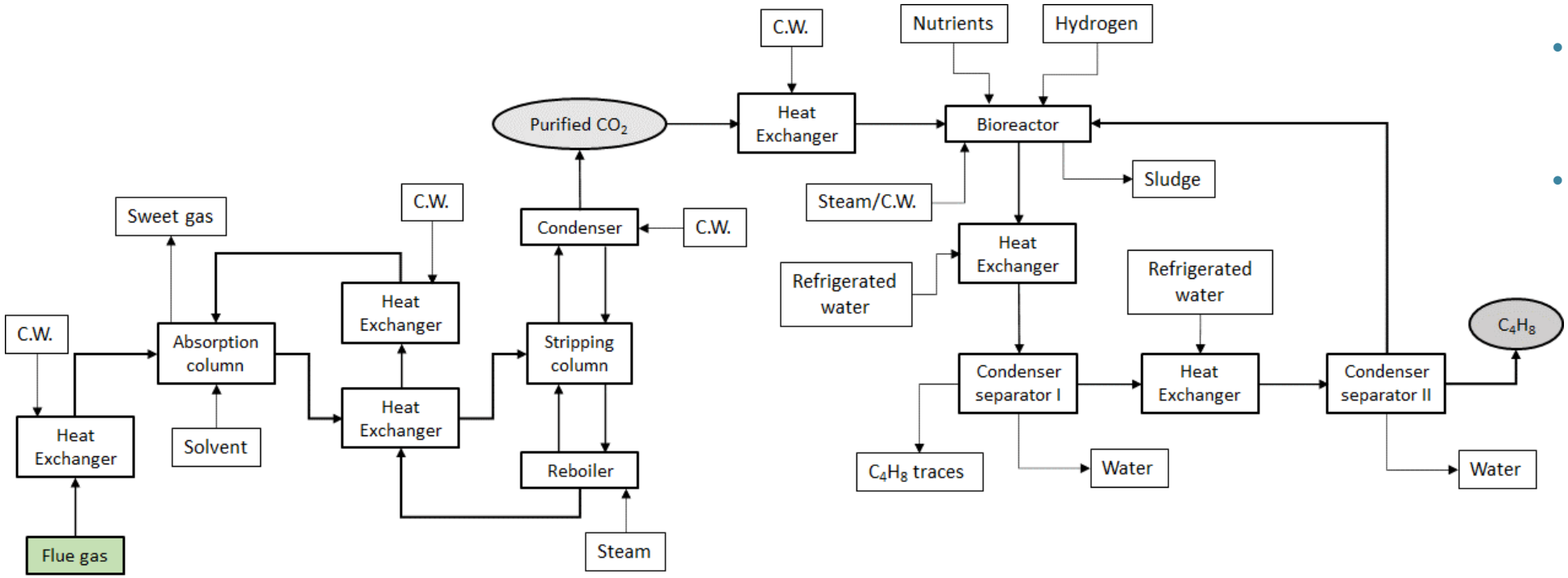
- Scaled up system (250,000 tCO_2/y) – Lactic acid production



- 3 capture units & 8 reactors per capture unit (154 kt_{lact}/y)
- Overall mass & energy balance (including utilities and main chemicals)
- Main equipment (like reactor and capture rig) and auxiliar devices (e. g. pumps and heat exchangers): sizing and performance

Modelling and simulation

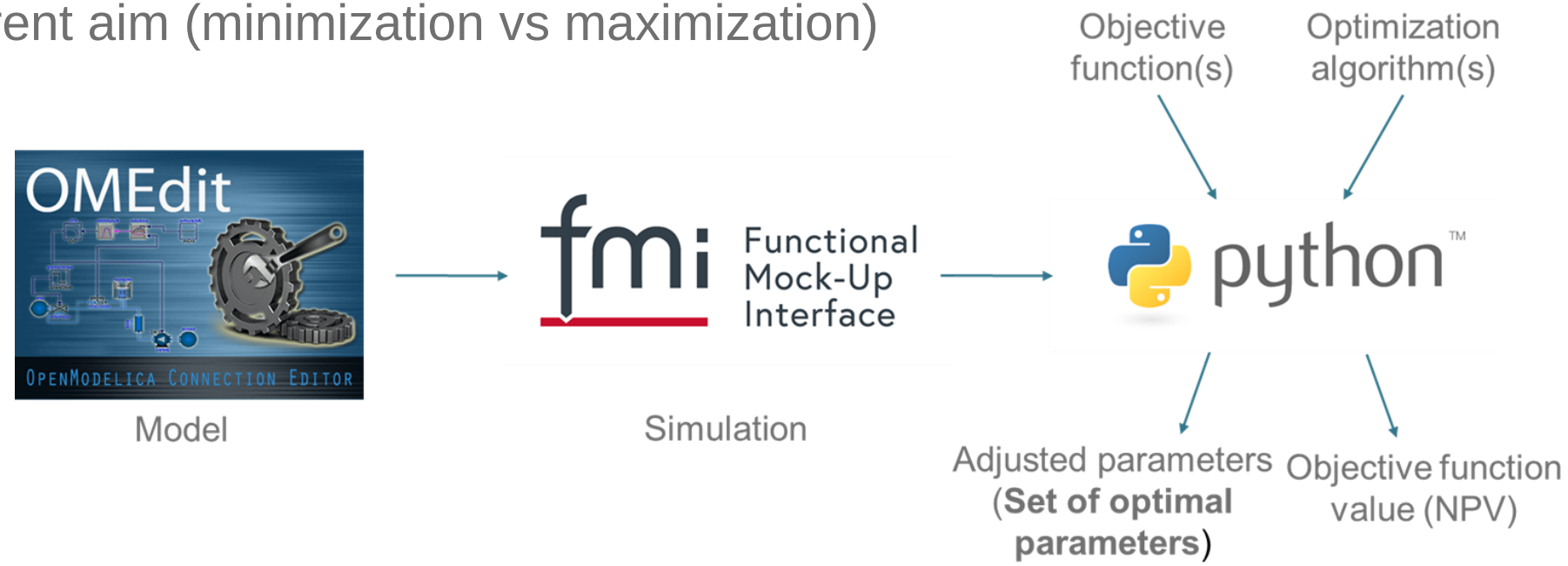
- Scaled up system (250,000 tCO_2/y) – Isobutene production



- 3 capture units & 20 reactors per capture unit (100 kt_{iso}/y)
- Overall mass & energy balance (including utilities and main chemicals)
- Main equipment (like reactor and capture rig) and auxiliar devices (e. g. pumps and heat exchangers): sizing and performance

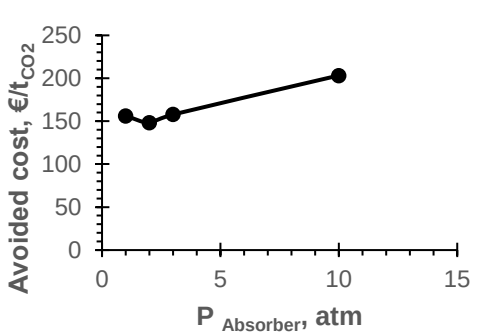
Optimization

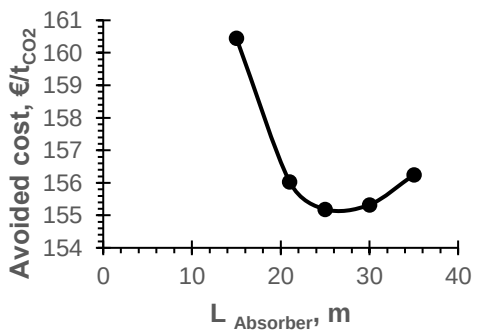
- Optimization - Tool
  - Same tool as the used for calibration
    - Different objective function (performance): Net Present Value
    - Different aim (minimization vs maximization)



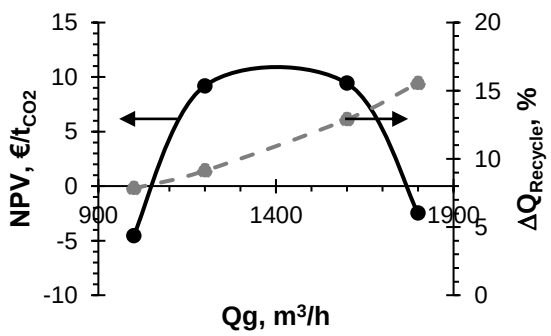
Optimization

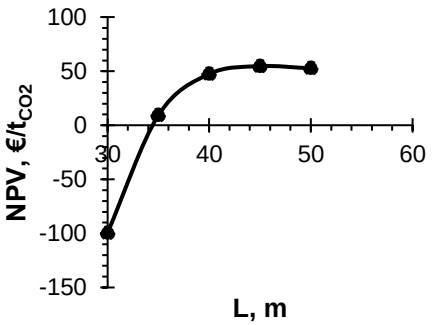
- Optimization – Tool & Results
  - Final optimization strategy: factorial analysis of size (like lengths, diameters) and operational (e. g. temperatures and pressures) variables
    - Examples:





Capture





Isobutene production

Advances beyond the SoA

- Thermodynamics for novel tailored made solvents for CO_2 capture
  - Simulation results like that in commercial simulators

- Comprehensive modelling of bio-electrochemical & biological systems, considering each feasible involved process
  - Physical chemistry (mass transfer & equilibrium)
  - Microbiology (growth and production)
  - Electrochemistry (hydrogen production by water electrolysis)
  - Bio-electrochemistry (hydrogen production using biocathodes)

- Simulation/optimization tool based on open-source environment: OpenModelica & Python
  - The tool allowed to simulate hypothetical scenarios and, showing the way for upscaling the project technology

Conclusions

- For the capture step, the developed tool produces similar results to those produced by commercial simulators
- Suitable calibration when experimental data is available
- Optimization (simplified) performed
- Possibility to simulate hypothetical scenarios and point the objectives to cover in the future work

Thank you for your attention!

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BioRECO2VER

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