



## Gate 2 Introduction

Catarina Braz

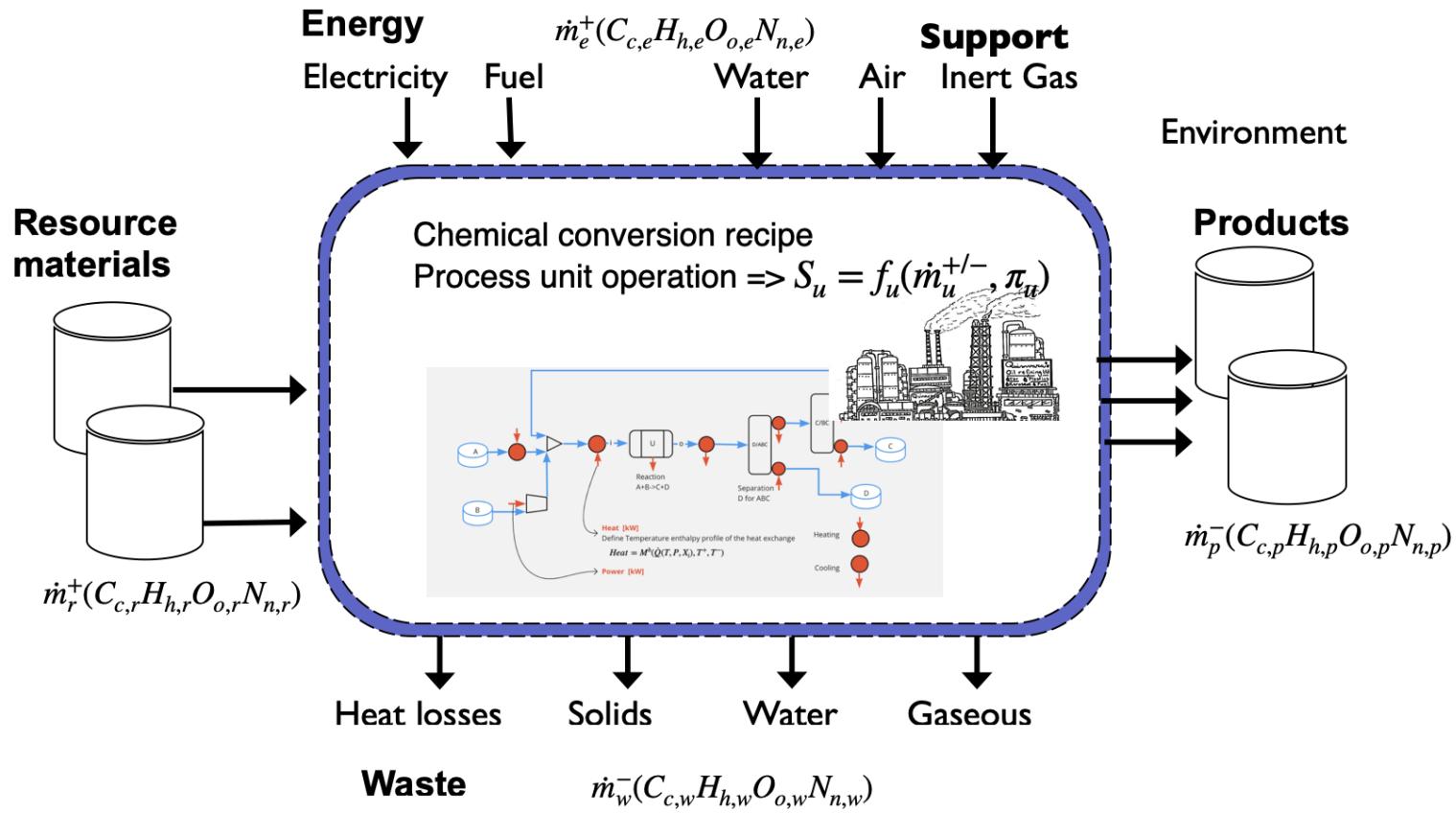
Lausanne – 17.03.2025

- 08:30 - 09:00 Quiz 1
- 09:10 - 09:40 (Catarina) Gate 2 introduction
- 09:50 - 10:50 (Meire) Aspen tutorial 3 part I: Biomass Gasification
- 11:00 - 16:00 Teamwork: Gate 2

# Guidelines for the first report review

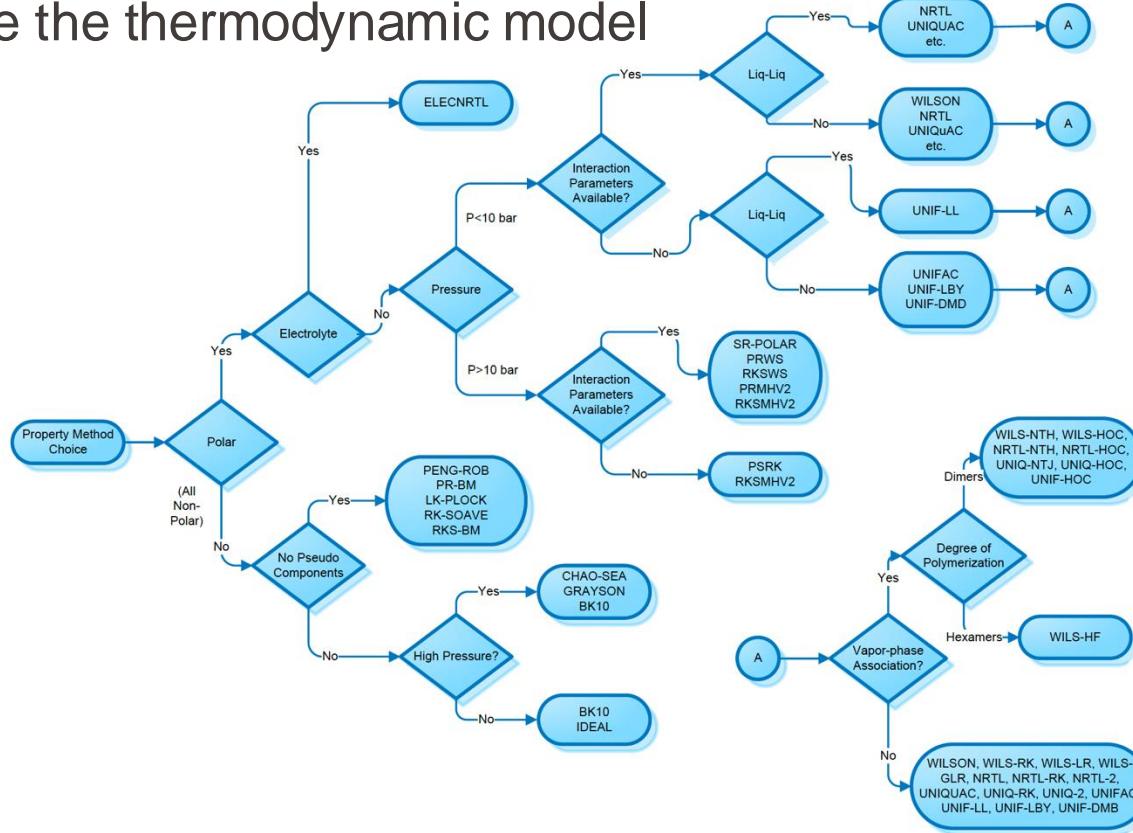
- **Deadline:** March 30
- **Report assigned:** ← You will be informed today
- **Report repository:** [link](#) ← Will be added today
- **Page limit:** 2 – 4 pages
- **Table of contents:**
  - **Summary:** Summarize the work reported in the progress report based on your understanding after reading the report.
  - **Background of the project:** Did the authors present relevant background and motivation for their project work? You can include your suggestions on this.
  - **Goals:** Did the authors clearly state the objectives of their project work? You can also provide some advice.
  - **State of the art:** Did the authors perform a comprehensive state-of-the-art review concerning the project goals? Discuss product specifications, properties, market identification, and renewable and sustainability perspectives. Please make some suggestions.
  - **Process selection:** Did the authors explain the criteria and rating/grading procedure used to make the process selection? The Reviewer can make comments or perform critical analysis on engineering decisions, assumptions, choices, and conclusions presented in the report.
  - **Recommendation:** Based on the information in the project report, give some suggestions for further improvement. These suggestions could include using new technologies, minimising and valorising waste, reducing energy consumption and environmental footprint, etc.
  - **Presentation:** Please provide comments/suggestions on the quality of the report (e.g., clarity, structure, language, etc.).

- Be constructive and respectful
- Give recommendations and hints that help the authors improving the quality and the readability of the report



## Step 1: Define the thermodynamic properties package

- Choose the thermodynamic model



## Step 1: Define the thermodynamic properties package

- Choose the thermodynamic model
- Find or fit the thermodynamic models' parameters
- Validate the values used by the thermodynamic package
  - Try to find experimental VL equilibrium values

## Step 2: Select the process unit operations and choose the appropriate models and operation conditions

- Some useful sources of information:
  - G. Towler, R. Sinnott, *Chemical Engineering Design*, 2021, Elsevier Science
  - R. Turton, J.A. Shaeiwitz, D. Bhattacharyya, W.B. Whiting, *Analysis, Synthesis, and Design of Chemical Processes*, 2018, Pearson Education
  - R. Smith, *Chemical Process Design and Integration*, 2005,
  - J.R. Couper, W.R. Penney, J.R. Fair, S.M. Walas, *Chemical Process Equipment Selection and Design*, 2012, Elsevier Science
  - Stephen M. Hall, *Branan's Rules of Thumb for Chemical Engineers*, 2017, Elsevier Science

## Step 3: Build the flowsheet simulation of your process

### Tips and best practices for planning and building a simulation

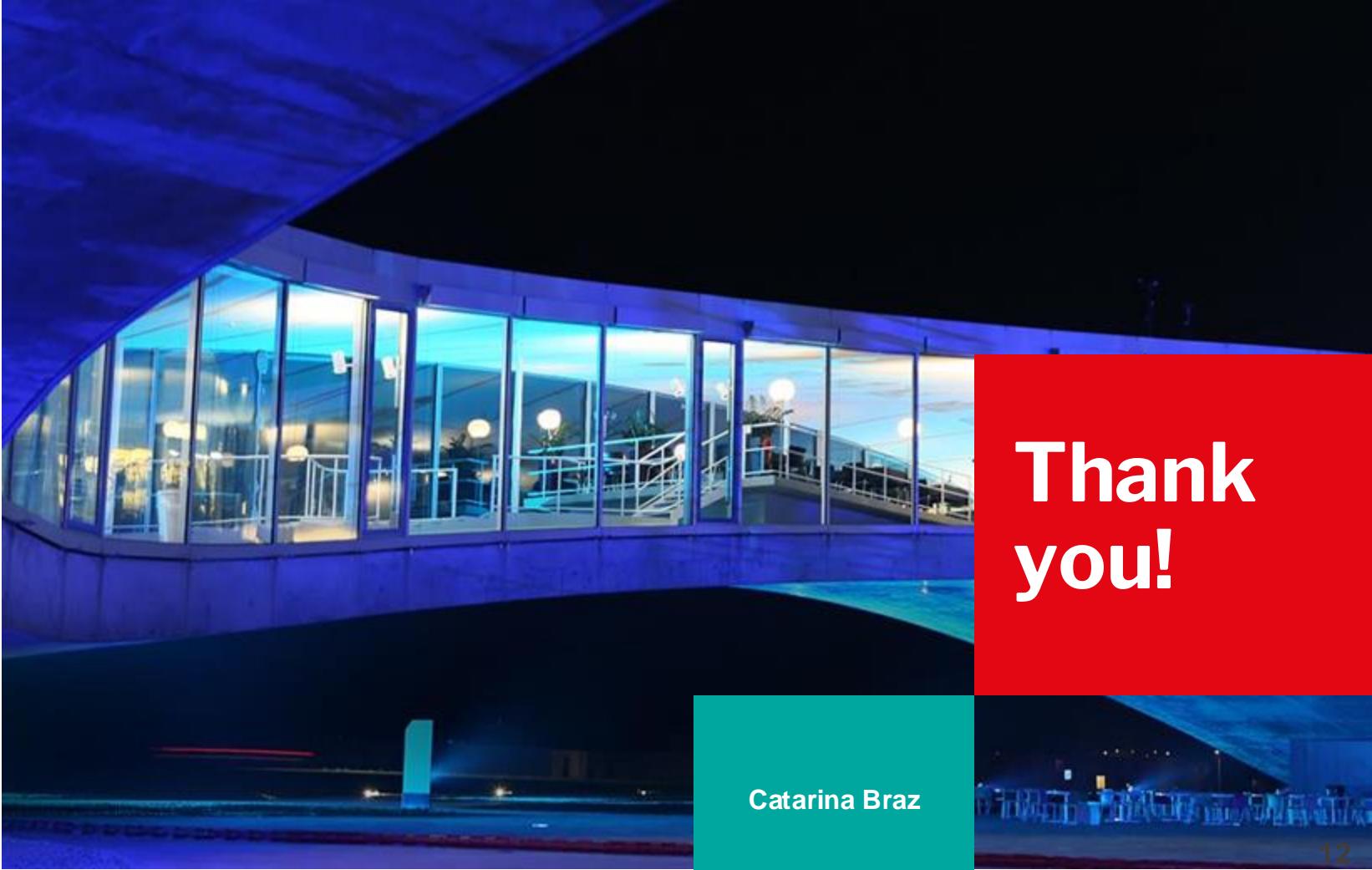
- Establish clear and specific goals for the simulation.
- Sketch out the process on paper to ensure that there are no obvious flaws and that the goals are achievable. Do simple calculations and indicate rough flows and temperatures on the sketch to help visualise the problem.
- **Scrutinise the input data and confirm it is the best available information.**
- Identify major chemicals in the process. If process streams need to be aerated, include atmospheric air (air in Aspen is a refrigeration fluid; it needs to be defined as N<sub>2</sub> and O<sub>2</sub>).
- Obtain plant data if a plant exists or lab data if the process is being developed. If possible, avoid allowing the program to estimate properties by entering data for proprietary materials.
- **Start small, stay focused. Building a model slowly makes it easier to isolate problem areas.**
- **Avoid connecting recycle streams until the simulation has been refined. Instead, use separate feed and product streams.**
- **Set the engineering units and be careful that all input data are in consistent units.**
- Make notes and document the steps taken to develop the simulation.

## Step 4: Calculate the size of the main process equipment and determine the performance indicators

- Based on sizing models in the literature, calculate the size based on the operating conditions and equipment-specific dimensions
  - Choose the material
  - Investigate the operating pressures and temperatures
- Using the results of the simulation model, calculate:
  - Mass conversion efficiency
  - Chemical efficiency
  - Products, co-products and waste
  - Energy consumption as heat and power

## What is expected in Gate 2 chapter/presentation:

- The appropriate thermodynamic property calculations
- The process flowsheet
- The choice of the appropriate process equipment to realise the identified process unit operation
- The definition of the assumptions and the remaining degrees of freedom
- The choice of the operating conditions or operating condition ranges
- Simulation of the mass and energy flows in the system as well as the inputs and outputs of the process.
- Sizes and cost estimation of the main process equipment.
- Performance indicators



Catarina Braz