Process Development Introduction

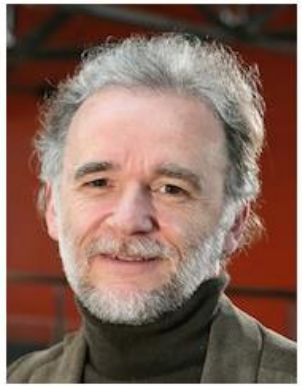
François Maréchal
Catarina Braz
Meire Domingos

Lausanne – 17.02.2025

Teaching team

Lecturers:

- François Maréchal



Adjunct Professor, SCI STI FM Group

francois.marechal@epfl.ch

- Catarina Braz

Scientist, SCI STI FM Group

catarina.braz@epfl.ch

- Meire Domingos

Scientist, SCI STI FM Group

meire.ribeirodomingos@epfl.ch

Teaching team

Teaching Assistants:

Du Wen

du.wen@epfl.ch

Soline Corre

soline.corre@epfl.ch

Arthur Waeber

arthur.waeber@epfl.ch

Marie Jones

marie.jones@epfl.ch

Oktay Boztas

oktay.boztas@epfl.ch

Lorenzo Teodori

lorenzo.teodori@epfl.ch

Gudbjörn Arnarson

gudbjorn.arnarson@epfl.ch

Vibhu Baibhav

vibhu.baibhav@epfl.ch

Danial Tahery

Sanjay Venkatachalam

sanjay.venkatachalam@epfl.ch

Today's schedule

- 08:30 - 09:15 (François+Catarina+Meire) Course introduction
- 09:15 - 09:45 Group formation and project assignment
- 10:00 - 12:00 (Dr. Pouransari) Role of Process Development in Industry: Case Studies from Syngenta
- 13:00 - 16:00 Teamwork: Gate 1

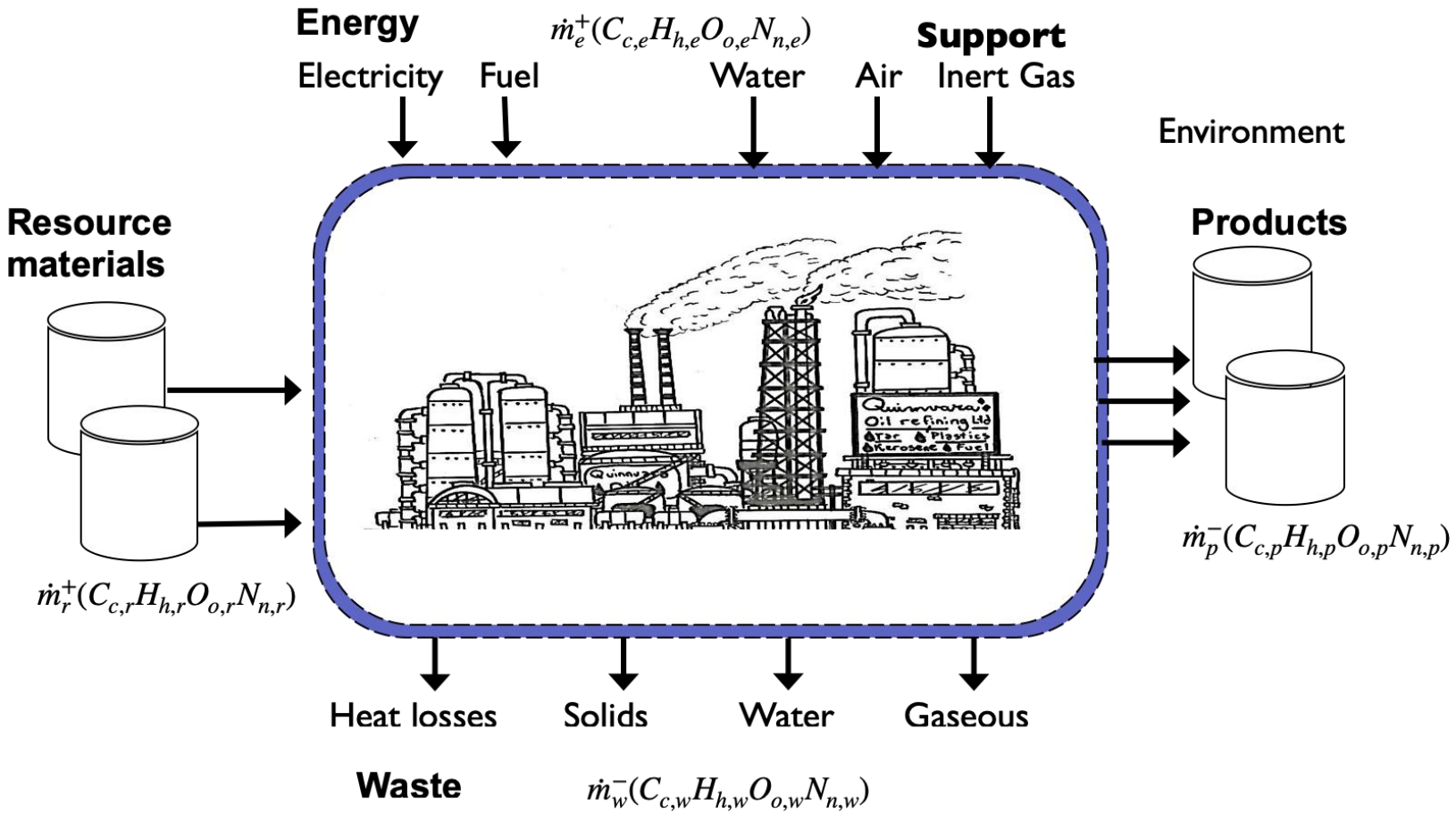
Process Development

- **Your boss:**
  - Develop a process to make one given product
- **His management board**
  - Use renewable energy and go Net-zero emission

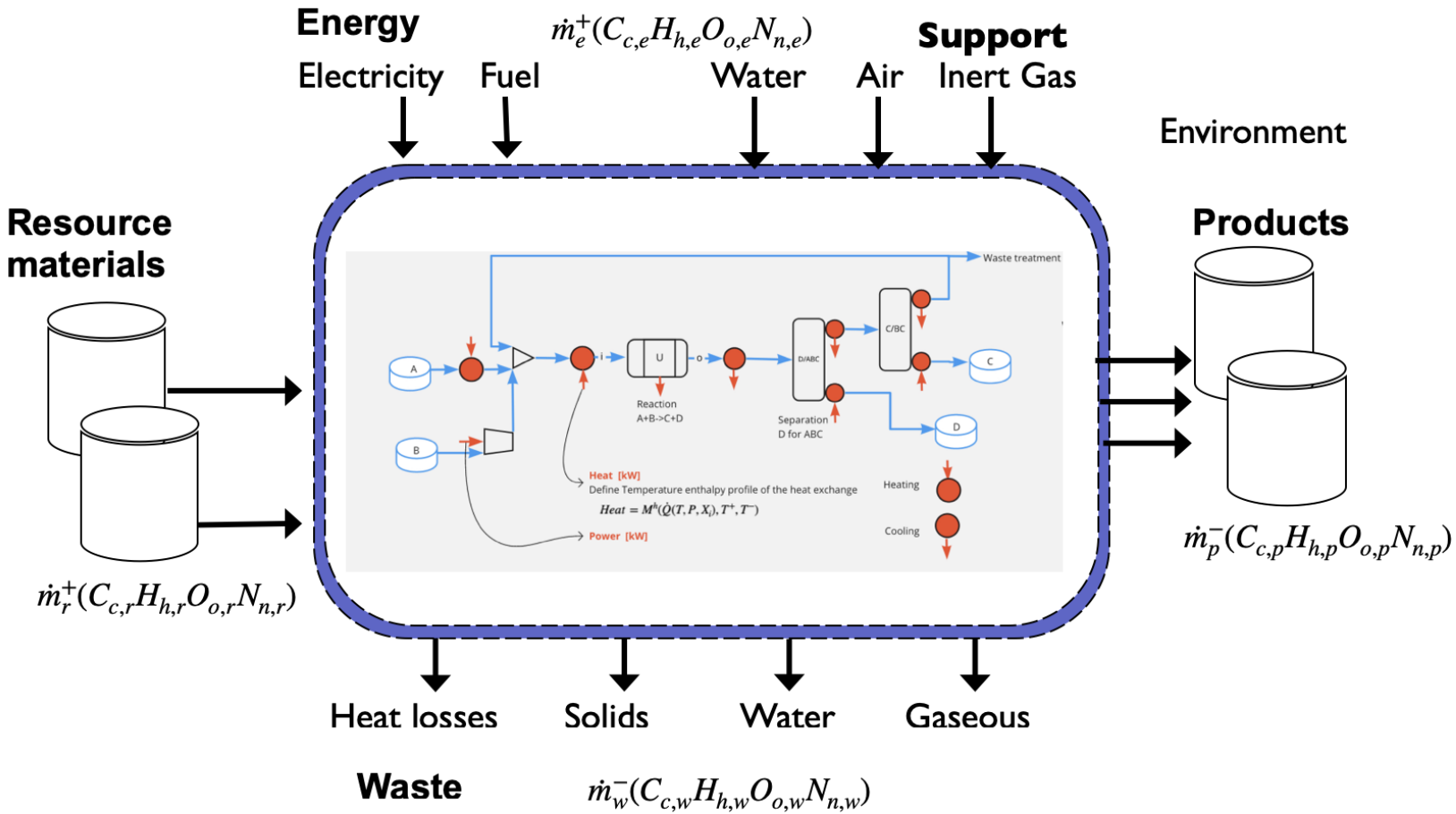
Process Development

- **Your professor:**
  - Activate your **chemical engineering** knowledge to design a chemical process that produces a **chemical product** with a **minimum of resources** and a **minimum environmental impact** and define the required **investment** and the associated profit and impacts.
  - Solve the problem with a methodology and the appropriate tools
  - Learn to work in a **team** and **report** the results
  - Participate in a European Student contest
    - (Link for new edition available soon)

Process Development



Process Development



Process Development

- **Decide:**
  - The process units to buy
    - Type, size and cost
    - Support materials : e.g. catalysts
  - How they are interconnected
    - Piping
  - How they are operated
    - Operating conditions & profiles
  - How they are controlled
  - How do you mitigate risks related to the operation
- **Inform about performances:**
  - Economic
  - Environmental impact
  - Social

Process Development Roadmap

- **Gate 1:** Choose the reaction paths and the resources
- **Gate 2:** Calculate mass and energy flows of the selected process flowsheet
- **Gate 3:** Close the energy balance and optimise the process operating conditions
- **Gate 4:** Size the equipment and assess the cost and risks of the process scheme

Gate 1: Main process options

- Identify the importance of the product in the market as well as its value and impact.
- Define the perspectives for the product application in future markets
- Define the challenges with respect to sustainability of the proposed product and production routes
- Identify the main production routes that are currently used and the potential alternatives
- Define the key performance indicators that can be used to compare the production routes.
- Define the state of the art of the promising production routes
- Propose the key production routes that you are going to further investigate in your project.

Gate 1: Process selection: flows characterisation

- Chemical: $C_c H_h O_o \alpha_a$ => Thermodynamic (T_c, P_c, T_{eb}, ω)
- Toxicity/risks
- State on market:

Mass flow : $\dot{M}_i^+ \quad [kg/s]$

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

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

- Cost or market value: $c_i \quad [CHF/kg]$
- Energy (inc. heat of formation):

$$H_i[kJ/year] = \int_{year} \dot{M}_i^+(t) \cdot h_i(t) dt$$

- Exergy:

$$E_i[kJ/year] = \int_{year} \dot{M}_i^+(t) \cdot k_i(t) dt = \int_{year} \dot{M}_i^+(t) \cdot (h_i(t) - T_0(t) \cdot s_i(t))\, dt$$

- Gibbs free energy

Gate 1: Process selection: Production routes

Make a literature search to identify the major known production routes

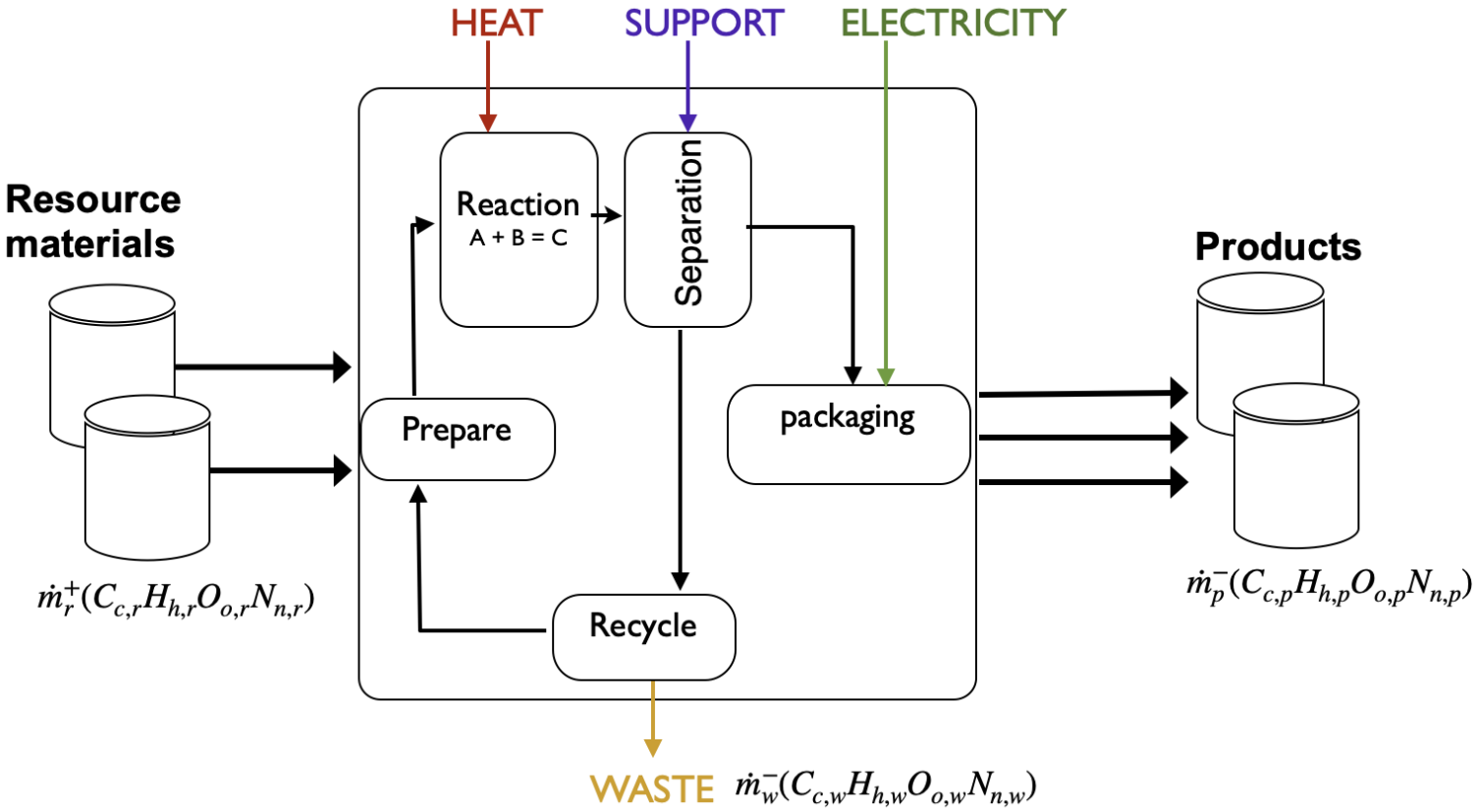
- **Product**: market and future markets
  - Typical production rates (per plant) and annual markets
  - Applications of the product defines the possible markets
- **Raw materials:** from renewable resources in addition to the chemical and economic characterization, define:
  - scarcity of raw materials
  - environmental impact
- **Resources** needed: e.g. energy, catalysts, solvents
  - scarcity of resources
  - environmental impact
- **Process routes**
  - Chemical reaction paths and operating conditions, temperature, pressure
  - Complexity
  - Hazard and operation (HAZOP)
- **By-products** (and potential applications)
- **Waste + emissions**
  - waste treatment techniques
  - end-of-life release in the environment
  - toxicity
  - environmental impact

Gate 1: Process selection: Selecting routes

- Define a list of selection criteria :
  - KPI_c : key performance indicator for criteria c (physical units, method to measure/rank)
  - w_c : importance of criteria c in selection
- Make a selection matrix : choose $o \mid \max_o(C_o = \sum_c w_c \cdot KPI_{c,o})$

	Weight	Process 1	Process 2	Process 3
Reference		[1,2]	[2,3]	[3,4]
Criteria 1 : Atom economy	0.2	$KPI_{1,1}$	…	
Criteria 2 : Energy	0.3	⋮		
Criteria 3 : Economy	0.4			
Criteria 4 : HAZOP	0.1			
Total		$\sum w_c \cdot KPI_{c,1}$		

Gate 1: Process selection: Make a block flow diagram

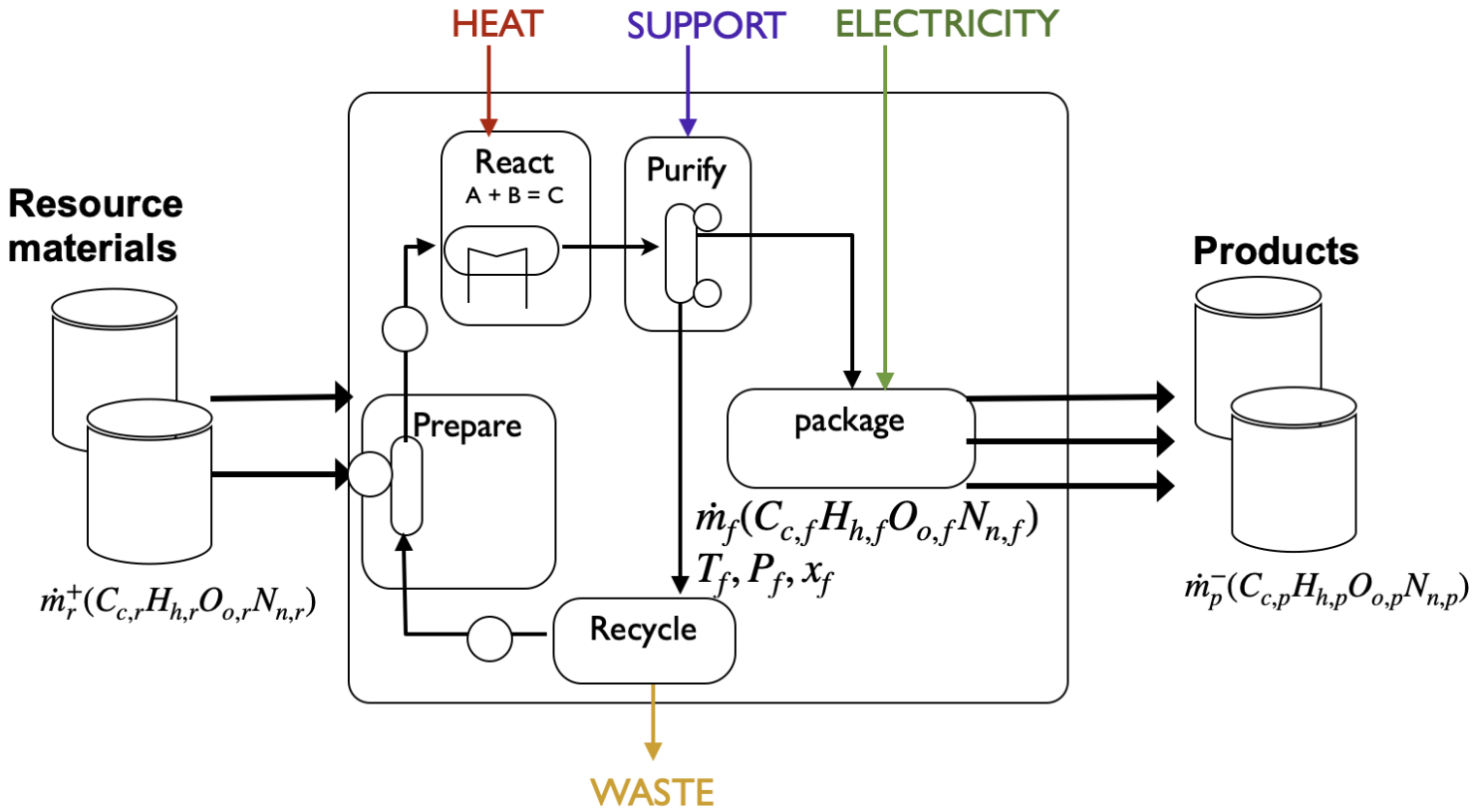


Process steps defined by their function in the production

Block flow diagram

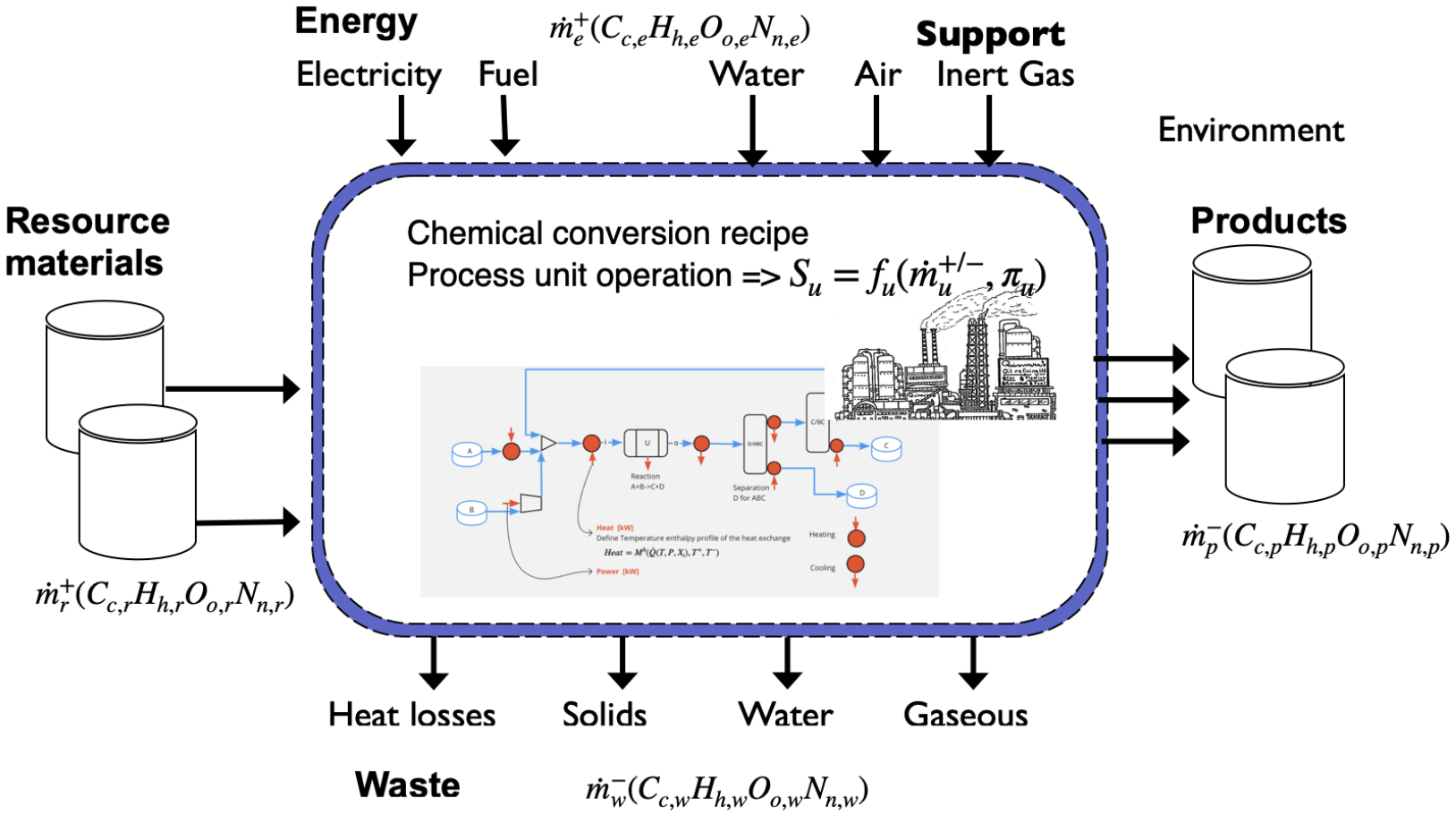
- Verify mass and energy balances
  - atoms are not lost
  - energy is not lost
- Mention states, temperatures and operating pressures
- Do not forget the inlet and outlet states (storage or distribution form)

Gate 2: Process flowsheet simulation

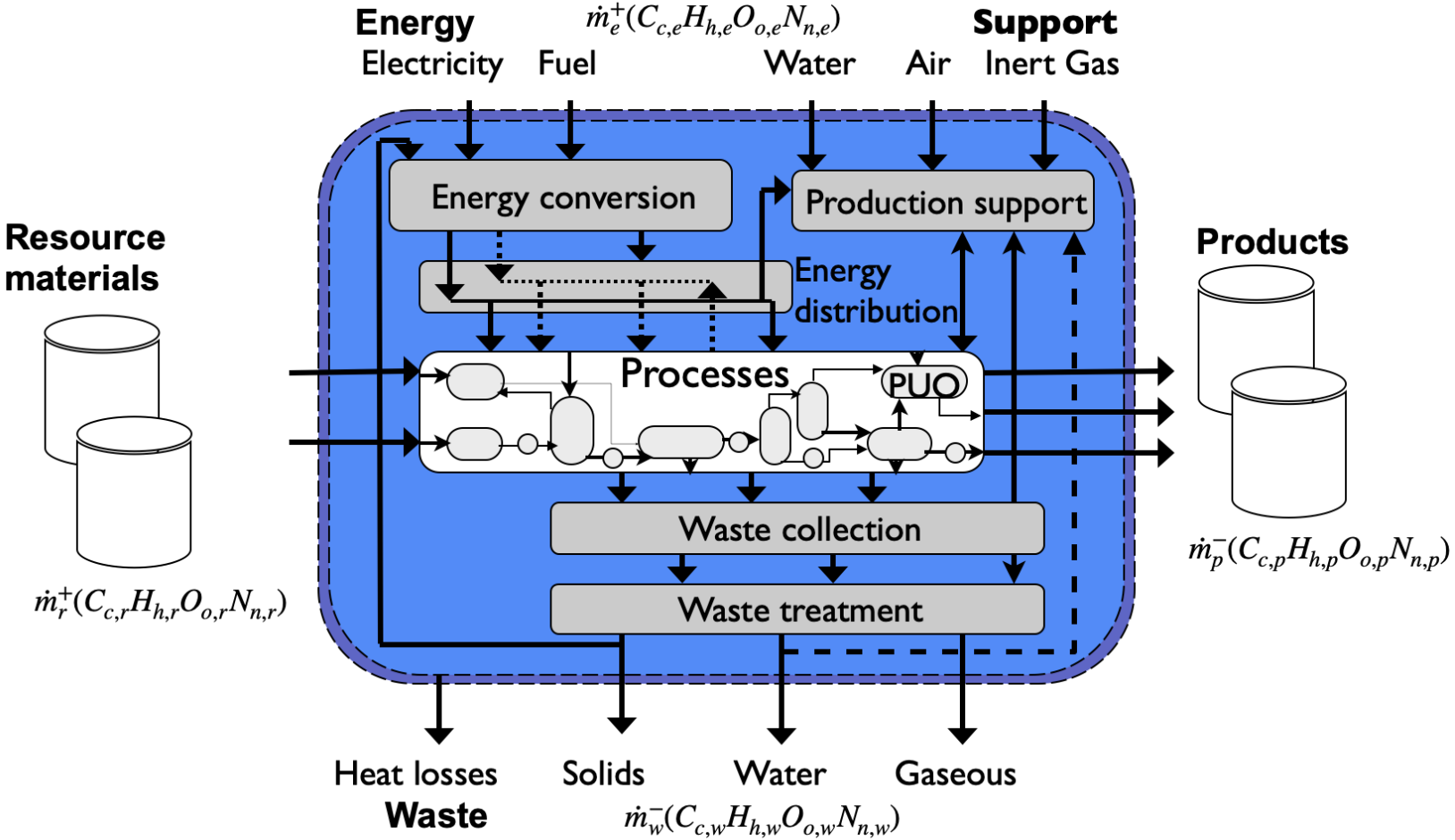


Process unit operation replaced by the equipment to realise the operation
Flows and operating conditions are calculated

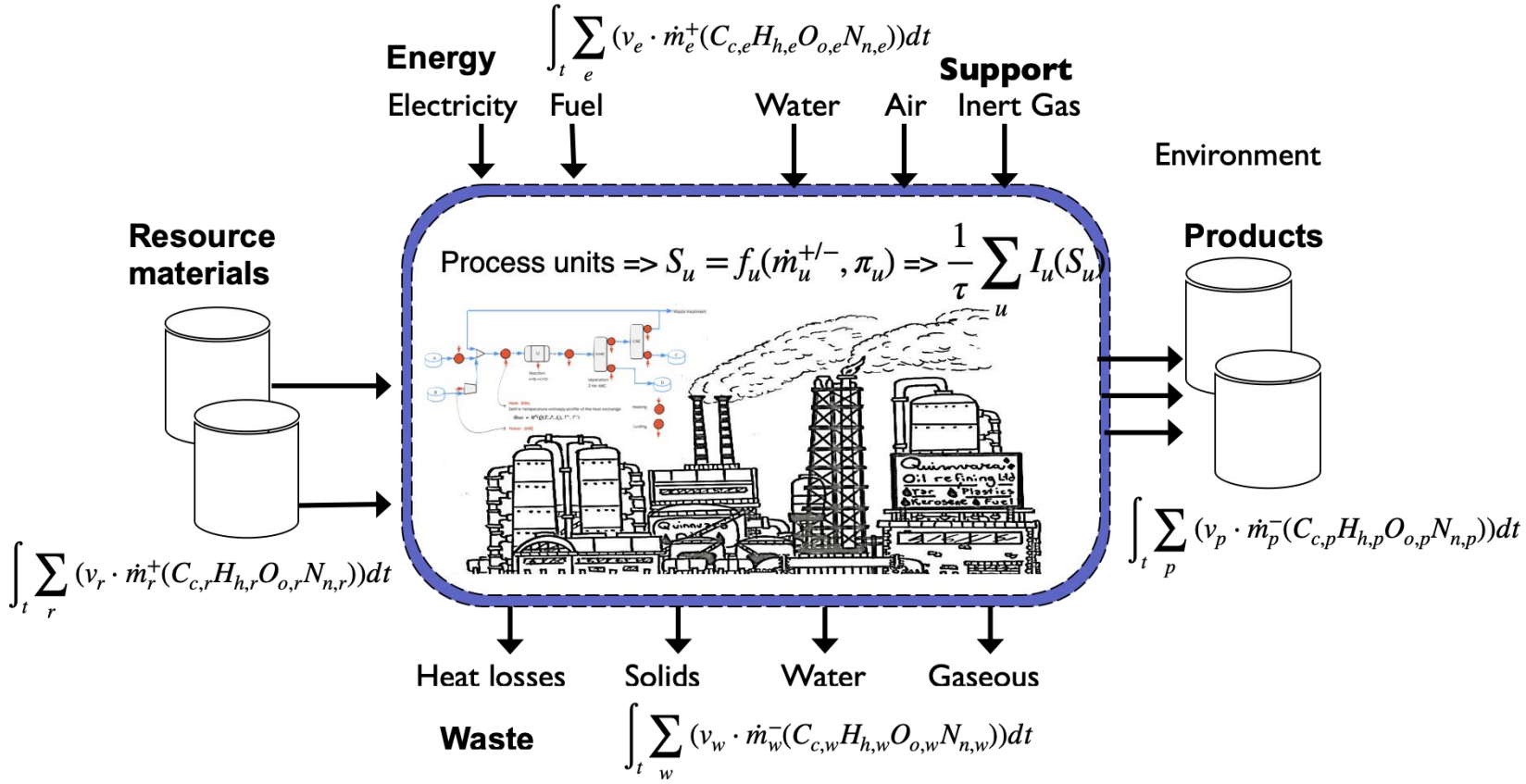
Gate 2: Process flowsheet: unit sizes



Gate 3: Closing the energy balance



Gate 4: Process Assessment



Hazard and Operation

- Evaluate risk of operation
- Mitigate risks
  - Adapt design
- Define control strategies
  - Start-up
  - Shut-down
  - Emergency

AGIR and Project based learning

Analyse

Generate

Interpret

Report

AGIR and Project based learning

Analyse

State the problem and Activate your knowledge

- Read the question
  → We'll show you the way similar problems have been solved
- Activate the computational tools needed
  → Be inspired by the examples
- Describe what you are looking for
  → E.g. define the physical units of what is expected

AGIR and Project based learning

Analyse

Generate

Generate numbers by computer tools

- Program the generation of numbers with comments and reporting
  - → duplicate and adapt the codes
  - → document and report your assumptions
  - → reference the data sources
- Develop process models
  - Structure → define flowsheets and specifications
  - Solve → converge
  - Extract numbers

Programming languages are needed

→ Aspen Plus (flowsheeting tool)

→ Python or R: elementary levels are required for manipulating data/presenting data

AGIR and Project based learning

Analyse
Generate
Interpret the generated results: from numbers to chemical engineering meaning

- Program the interpretation of the generated numbers
  - Graphs
  - Tables
  - Numbers

→ we use Quarto: reproducible science & open source

- Do not forget
  - Physical units
  - Axis titles
  - Captions
  - References

AGIR and Project based learning

Analyse
Generate
Interpret
Report

Generate numbers by computer tools

- Convey the message to people outside your group
- Make a summary of your main results
- Make a documentation to the others
- Add references

Toolbox

Toolbox is a collection of tools that you are going to use to realise the mission. They will be of different types :

- **Theory**: is giving you the theoretical background needed.
  - Lecture notes: in Moodle
  - Q&A in a forum: We will answer your questions
  - Application in group work + discussion with your TA and professors
- **Software tools:** allow you to apply the theory to accomplish the mission. In this section, you will find tutorials, exercises and examples.
- **Reporting**: guidelines and tools to report the realisation of the mission
- **Further readings**: if you would like to develop a deeper knowledge of the mission

Teamwork

The project is realised by a team of 3 students.

It is important to distribute the work and the responsibilities when realising the mission. A good teamwork implements the AGIR steps in a coordinated fashion to be efficient in the task realisation:

- **Coordination**: description of the tasks, validation of the assumptions, work allocation, synthesis of the results and their interpretation
- **Communication**: who is doing what, "what" meaning a sub task with boundary conditions and expected results defined.
- **Validation**: teamwork allows easy validation mechanism, when someone is realising a task, it makes sense to have another teammate making a critical review of the work done.
- **Exchanges:** discussion, critics, validation, support. A team is focused on the results generation and their quality. It is therefore important to have a place to exchange, be open to ideas, and welcome remarks and criticisms of others.

Collaboration platform

- **Mattermost: Discussion with TA**
- **Moodle: agenda + forum**
- **Quarto: report template**
- **Whiteboard: for the summary of the course**

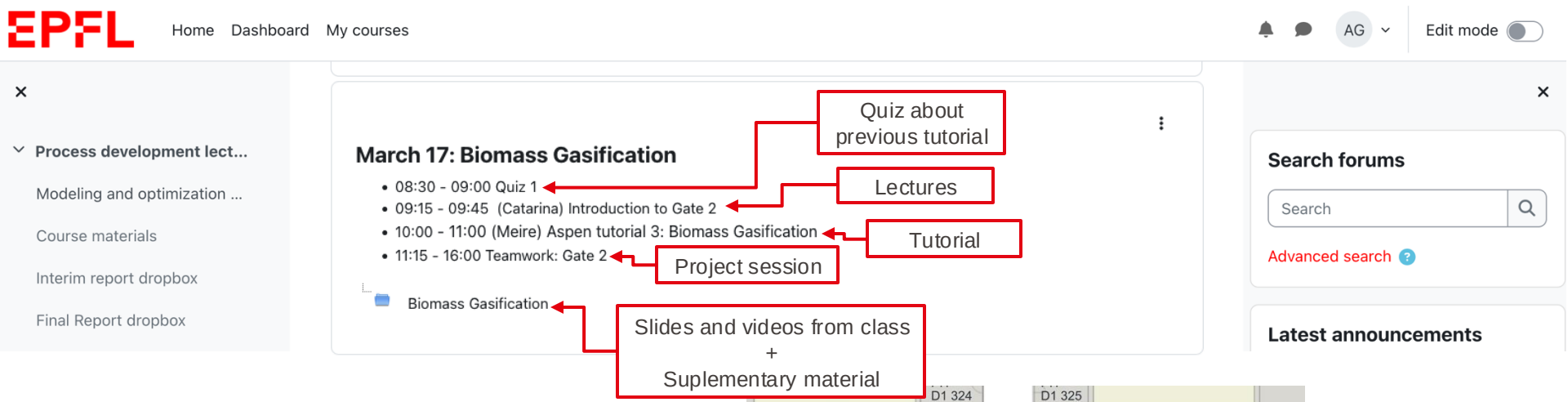
Teaching Assistants

- Teaching assistants will help you realise the missions
  - Guide you in the missions
  - Answer your questions
  - Share their own experience
- One teaching assistant per project + one backup assistant
  - Team & time organisation left to the team
  - Office hours online (to be organised by the team)
- Teaching assistant have their own job!
  - Not a 24-hour hotline.

Course Schedule

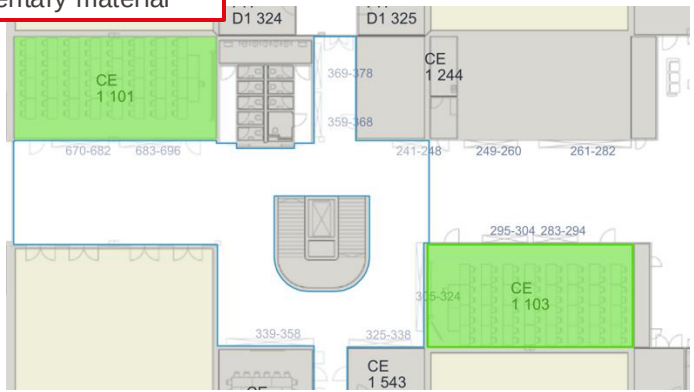
Week nº	Monday	Lecture topic	Lecturer	Tutorial	TA presenter
		Course introduction	Dr N. Pouransari		
1	17.02.2024	"Role of Process Development in Industry: Case Studies from Syngenta"	(Syngenta)		
2	24.02.2024	Selection criteria+Process flow diagrams	François + Meire	Aspen Tutorial 1: Physical properties	Catarina
3	03.03.2024			Aspen Tutorial 2: Biomass simulation	Marie
4	10.03.2024	Gate 1 discussion			
5	17.03.2024	Gate 2 introduction	Catarina	Aspen Tutorial 3: Gasification	Meire
6	24.03.2024			Aspen Tutorial 4: Co-electrolysis	Arthur
7	31.03.2024	Economic Analysis	Catarina	Aspen Tutorial 5: Reactors + Aspen convergence	Arthur
8	07.04.2024			Aspen Tutorial 6: Distilation columns I+II	Catarina
9	14.04.2024	Heat recovery	François	Equipment costing	Wen
10	21.04.2024	Easter break			
11	28.04.2024	Gate 2 discussion			
12	05.05.2024	Gate 3 Introduction+Closing the energy balance	François	ROSMOSE Tutorial I	Soline
13	12.05.2024	Composite curves	François	ROSMOSE Tutorial II	Meire
14	19.05.2024	HAZOP	Bubbi		
15	26.05.2024	Gate 3 + 4 presentation prep.			
16	02.06.2024				
17	09.06.2024	Holiday			
18	16.06.2024	Final Presentation			

Daily Lecture Organization



Afternoon session 13:00 – 16:00:

- Project session
- Extra room in CE1 103



Grade components

1. Tutorial quizzes – 10%
   - Total of 8 quizzes with five questions (points), to get a 6, you need 30 points
2. Gate 1 report review – 20%
   - Deadline for Gate 1 report: 16.03.2025
   - Deadline for review: 30.03.2025
3. Final presentation – 20%
   - Preparation for public presentation: 26.05.2025
   - Public presentation: 16.06.2025
4. Final report – 50%
   - Deadline for final report: 15.06.2025
   - Teamwork individual contribution
     - Peer and self-assessment
     - TA assessment

Grading reports by at least 2 TAs

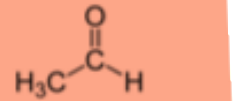
Presentation (30%):		**0.3**
	General appreciation (10%)	0.1
	Content (60%)	
	Process selection and alternatives	0.05
	Sustainability focus clear	0.05
	Process well-described	0.15
	Energy analysis	0.1
	Economic analysis	0.1
	All required elements presented	0.05
	Clear and justified conclusions	0.05
	Mastery of concepts evident	0.05
	Quality of presentation and results (25%)	
	Scientific, and engineering quality	0.1
	Contribution of all group members	0.05
	Clear and appropriate	0.1
	Response to questions (5%):	0.05
	Grade I:	
Report (70%):		**0.7**
	Clarity of report, contents, traceability and completeness (25%):	0.25
	Content (65%)	
	Executive summary	0.075
	References and literature review	0.05
	Process selection	0.05
	Process description	0.05
	Process modeling and assumptions	0.2
	Block and PF diagrams	0.05
	Energy analysis	0.05
	Equipment sizing	0.025
	Economic analysis	0.05
	Conclusions (relevant and justified)	0.05
	Report layout, structure and overall quality (10%):	0.1
	Grade II:	

Gates and missions deadlines

1. **Gate 1:** Process selection (Feb 17 – March 10)
   - March 10: Presentation
2. **Gate 2:** Process flowsheet simulation (March 17 – April 28)
   - April 28: Presentation
3. **Gate 3:** Process Integration (May 5 - May 26)
4. **Gate 4:** Process design assessment (May 6 - May 31)
   - May 26: draft presentation on campus for preparation of public presentation
   - June 16: Public presentation

Proposed projects

1 — Acetaldehyde



TAs
- Lorenzo
- Meire

2 — SAF from Biodiesel

TAs
- Vibhu
- Catarina

3 — SAF from Ethanol

TAs
- Danial
- Meire

4 — Depolymerisation of PET to EG

TAs
- Soline
- Oktay

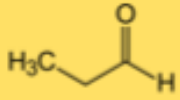
5 — Sustainable liquid fuels from microalgae

TAs
- Bubbi
- Arthur

6 — Syngas derived olefins to SAF

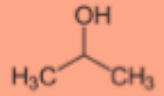
TAs
- Danial
- Catarina

7 — Propionaldehyde



TAs
- Marie
- Sanjay

8 — Isopropanol



TAs
- Wen
- Sanjay

9 — Maritime fuels via aqueous phase reforming

TAs
- Arthur
- Soline

10 — Enzymatic hydrolysis of PET

TAs
- Oktay
- Lorenzo

Groups creation

- Present yourself
  - Your name
  - Where are you from
  - Your background
  - Your passion
  - What do you hate the most

- 1st mission: Choose a name for your start-up company

Thank you!

François Maréchal
Catarina Braz