A NOVEL SEMI-RIGOROUS MODEL FOR BIOMASS PYROLYSIS AND GASIFICATION

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Outlines

1 **Introduction**

Where is gasification?

2 **State of the art**

How is gasification modelled?

3 **Case study**

Terrawatt plant case study

4 **Results**

Main KPIs and other comments

5 **Conclusions**

Achievements & future works

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1.Introduction

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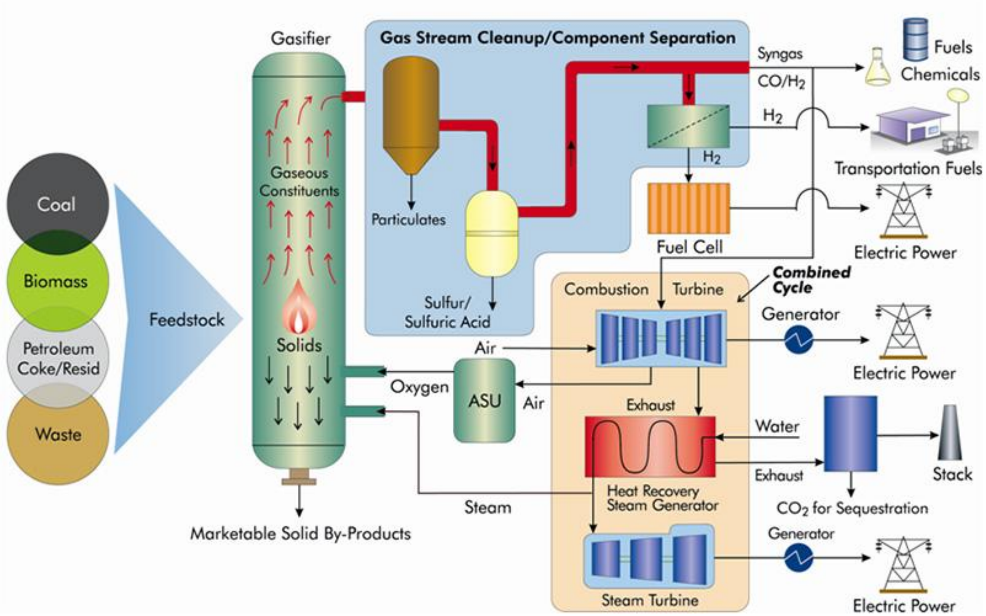
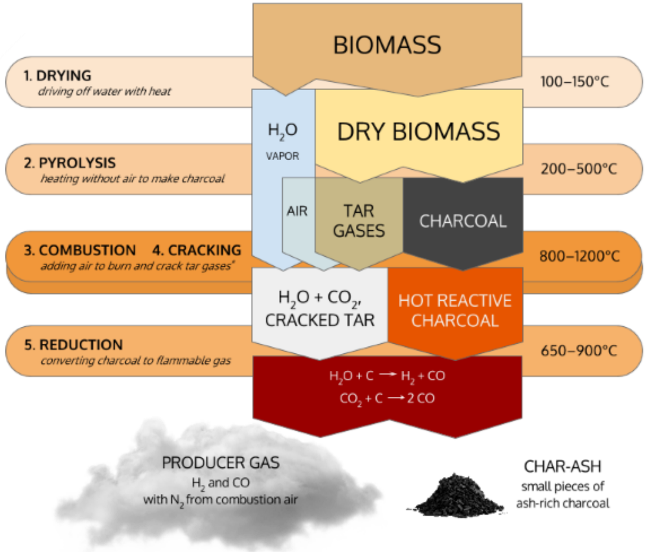
Gasification is interesting…



Source: NETL gasification introduction

… but rather complex



* tar cracking is the breakdown of tar into H_2, CO, and other flammable gases by exposure to high temperatures.

- **Multistep**
- **Hundred thousands of species**
- **Complex chemistry**
- **Heavily dependent on the feedstock and operating conditions**

2.State-of-the-art

How is gasification modelled?

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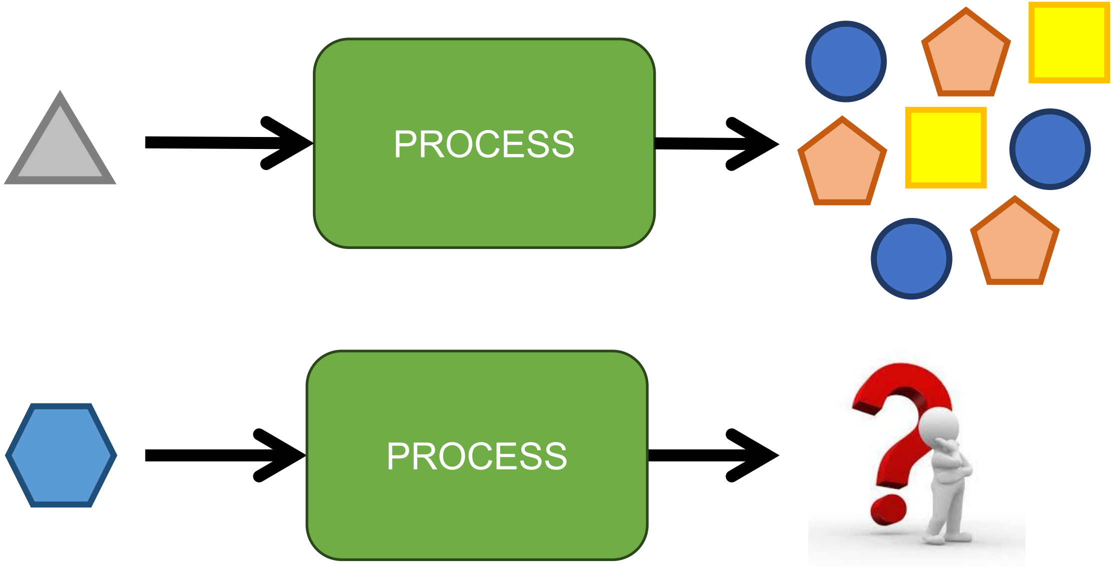
How do bioprocesses work?

- Current models in flowsheet simulators are **too simplified**
- Models developed and tuned for **one operation point**
- Often solely based on **estimated yields**

What happens if the feed or the operating conditions change?



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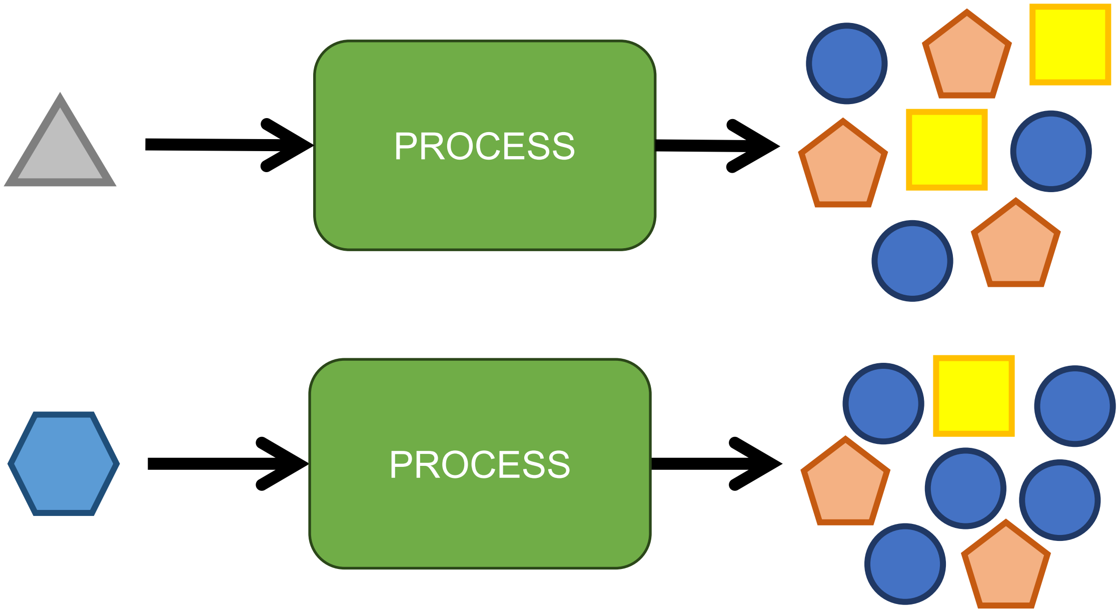
Source: IEA

Why do we need rigorous models?

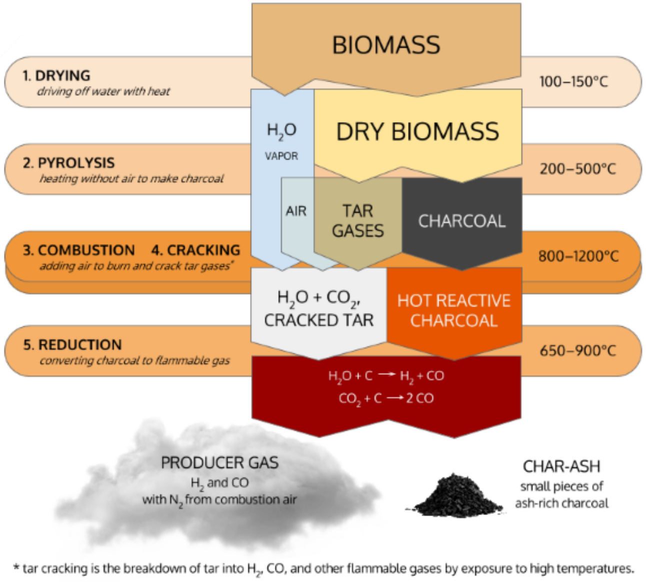
Only **rigorous models** allow for:

- describing a **wider range of feedstocks** without extensive measurements to re-tune the yield-based model
- **designing and sizing** the unit

"make it as simple as possible but not simpler"

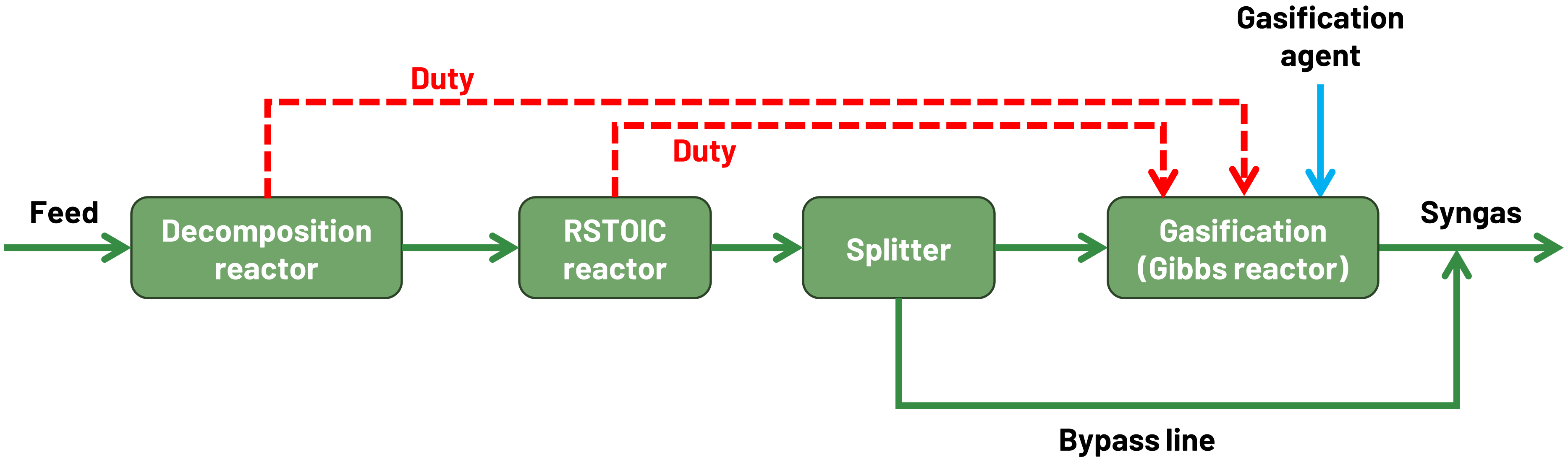


This is the process

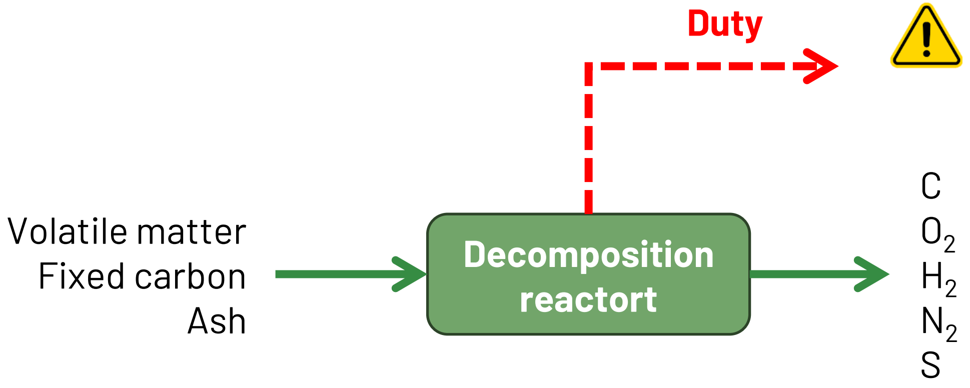


What is done normally in commercial process simulators?

How is it modelled? (I)



How is it modelled? (2)



Duty estimated to close energy balance: it is fictitious

Ultimate analysis → "Elemental" analysis

This chemical process does not exist in pyrolysis/gasification

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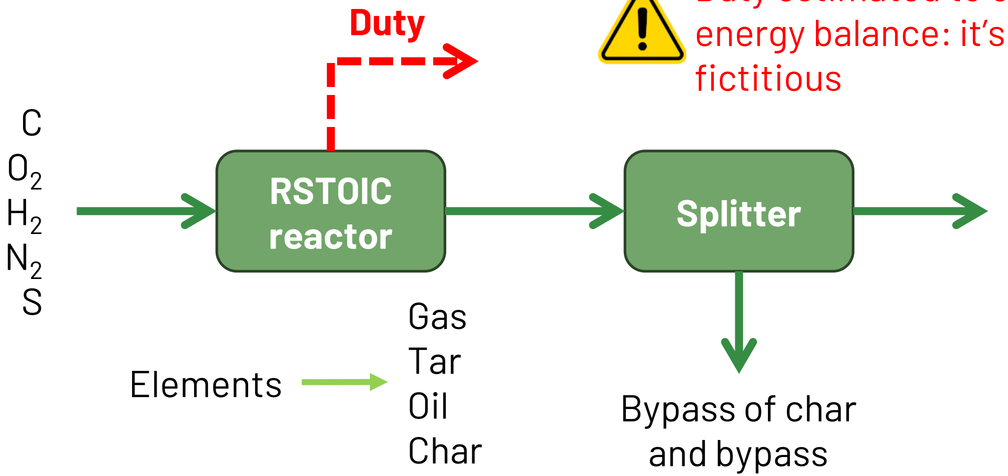
How is it modelled? (3)



Duty estimated to close energy balance: it's fictitious

RSTOIC distributes of the atoms into the pyrolysis cuts based on yield measured with specific biomass and operating conditions

Splitter is designed to match char production and methane yield at the outlet of the gasification chamber

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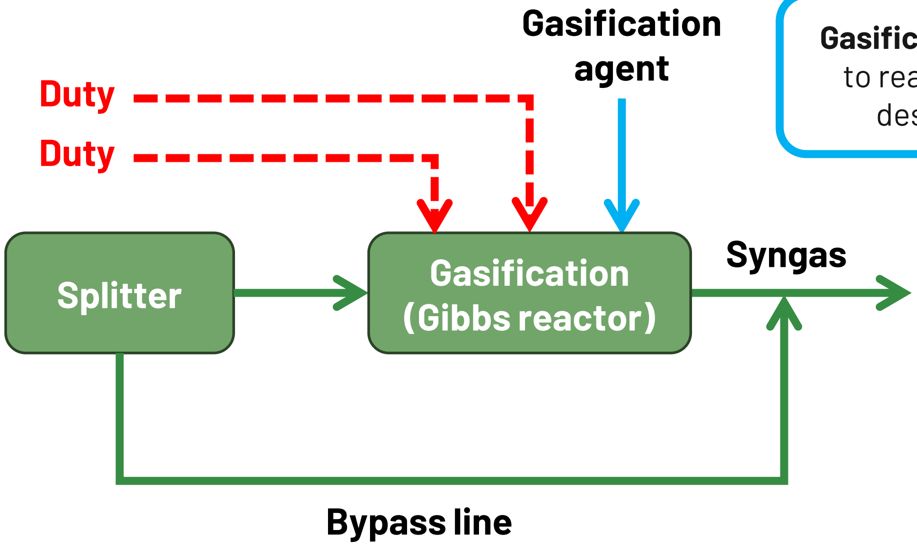
How is it modelled? (4)



Gasification agent is manipulated to reach adiabatic condition or desire outlet temperature

Gibbs reactor (TMD equilibrium) predicts complete gasification of char

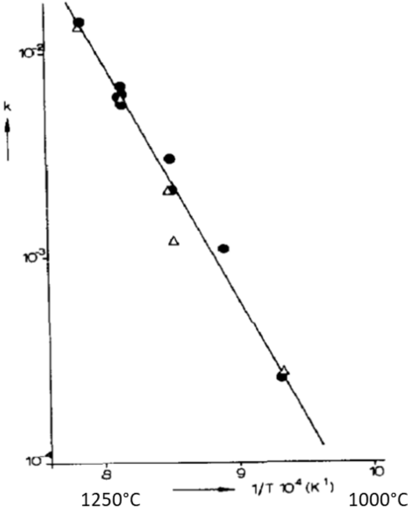
Bypass line arbitrarily remove "species" from the reaction environment just to "match" and adjust the final bio-syngas composition to the expected one

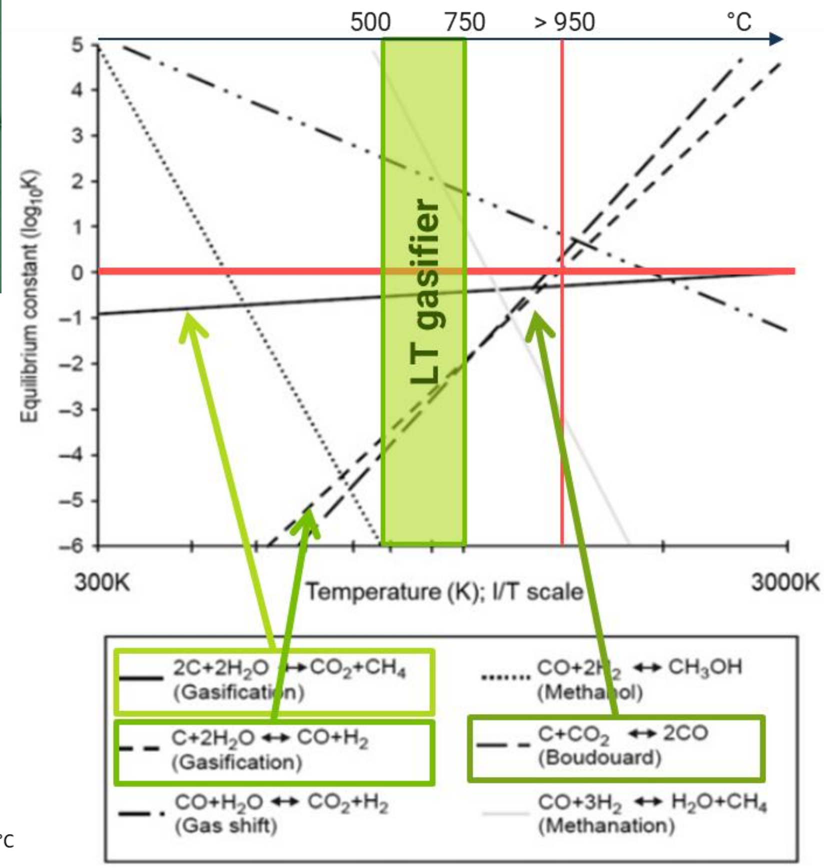
What about char gasification?

For **T < 1000°C char is inert** to gasification and the **reactions are slow…**

KINETIC control though thermodynamic is correct

Basu, 2010, Biomass Gasification and Pyrolysis – Practical Design, Academic Press, 117-165
Groeneveld, M.J., van Swaaij, W.P.M., 1980. Chemical Engineering Science, 35, 1-2, 307-313.





Takeaway on commercial solutions

⚠ Modelling does **not represent the actual chemistry** of what is occurring in the gasification process

⚠ Heat balance is based on **fictitious duties**

⚠ **Even evidence is not fulfilled** (thermodynamic vs kinetic)

⚠ **Missing generality**: what happens to RSTOIC/splitter if you change the feed and/or operating conditions?

⚠ RSTOIC distribute atoms into the products, but this aspect is highly dependent on feedstock quality (kind, size etc) and operational window!

Houston, we have (a big) problem

3.Case study

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SEMPRE-BIO project

SEMPRE-BIO

SEcuring doMestic PRoduction of cost-Effective BIOmethane

- SEMPRE-BIO aims at **demonstrating novel and cost-effective bio-CH_4 production solutions** to support the circular economy and **reduce dependence on fossil fuels**
- Biomethane production tested in **3 demo plants** across Europe accounting for **different feedstocks**

CETAQUA WATER TECHNOLOGY CENTRE · Biogas-E platform voor anaerobe vergisting · Naturgy · Cryo Inox · inveniam · UNIVERSITEIT GENT · terrawatt · Aigües de Barcelona · Innolab Lab 4 Biomass · DBFZ · NV De Zwanebloem · Beta UVIC UNIVERSITAT DE VIC UNIVERSITAT CENTRAL DE CATALUNYA · TMB · ProPuls · DTU · SINTEF

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Case studies

Aigües de Barcelona, Barcelona, Spain

Terrawatt, Marmagne, France

Direct biomethanation of bio-gas/syngas

De zwanebloem, De Panne, Belgium

Biogas upgrade and bio-CH_4 Liquefaction

Source: SEMPRE-BIO webpage

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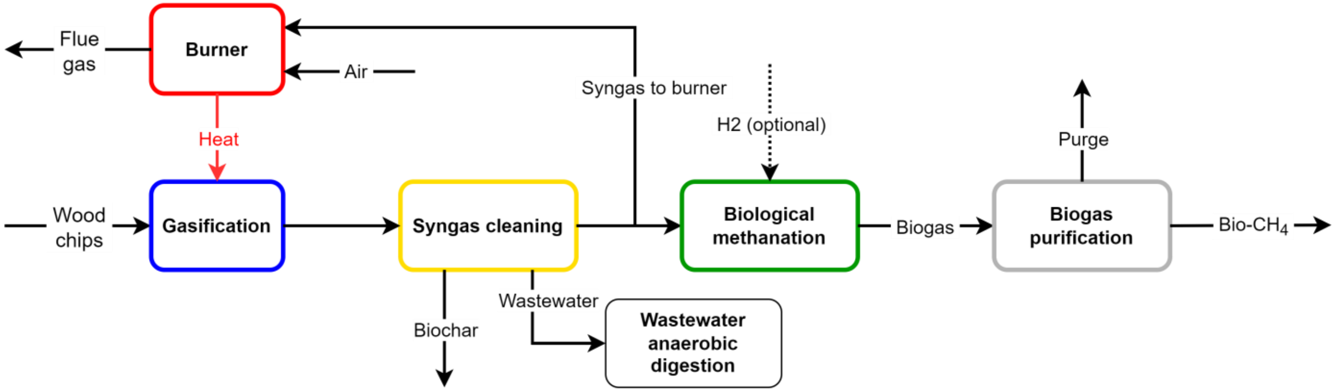
Block Flow Diagram

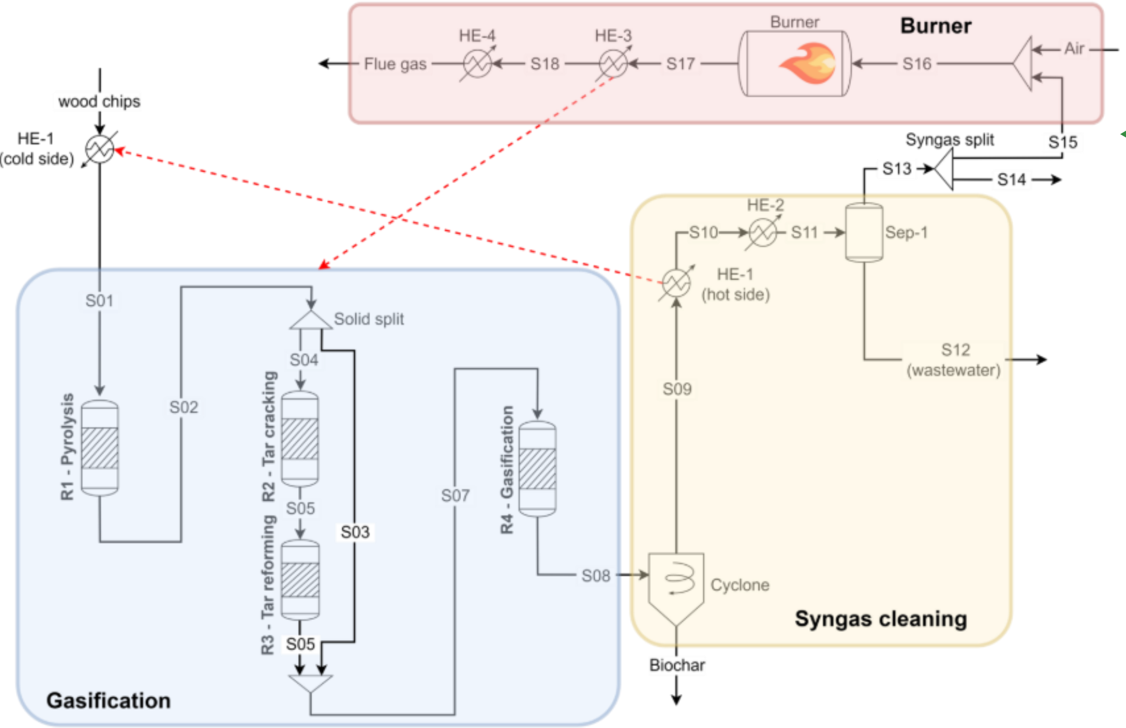
- **Biomass gasification** followed by **biomethanation** of syngas

- Simulation in **COFE V3.6**, license-free simulation software by AmsterChem



Technology provider: terrawatt

Process Flow Diagram

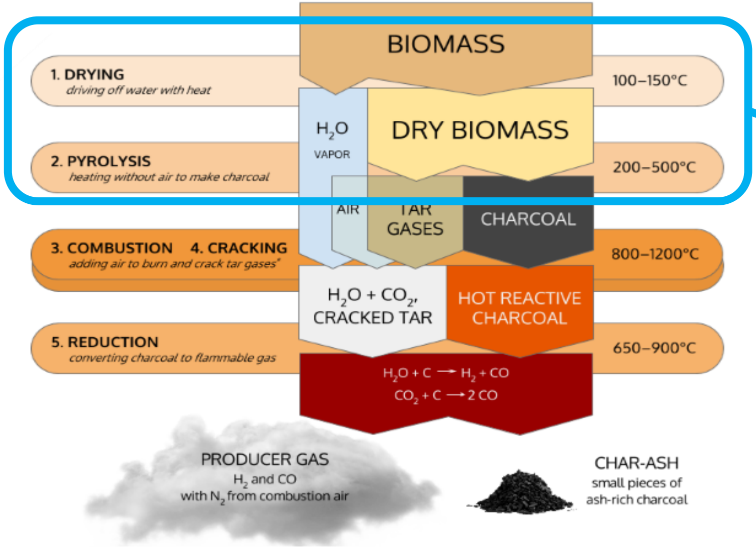


Bio-syngas split is the key to reach adiabatic operation!

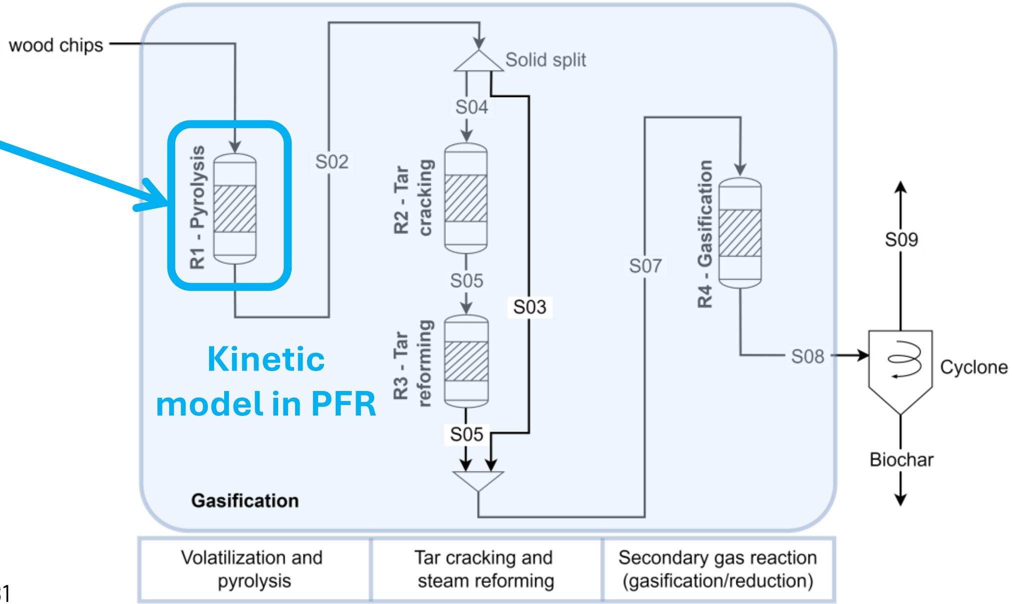
... but we need a good gasification model to

- predict the biosyngas composition → heating value
- hence estimate the split fraction
- overall yield/efficiency of the system

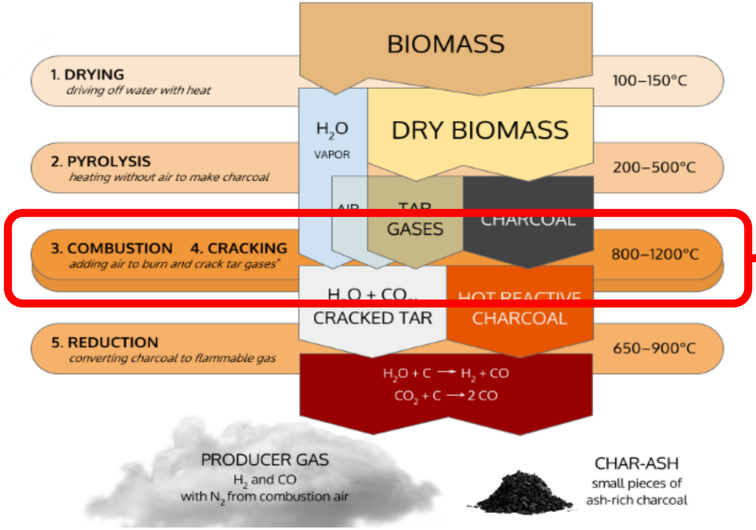
Biomass gasification



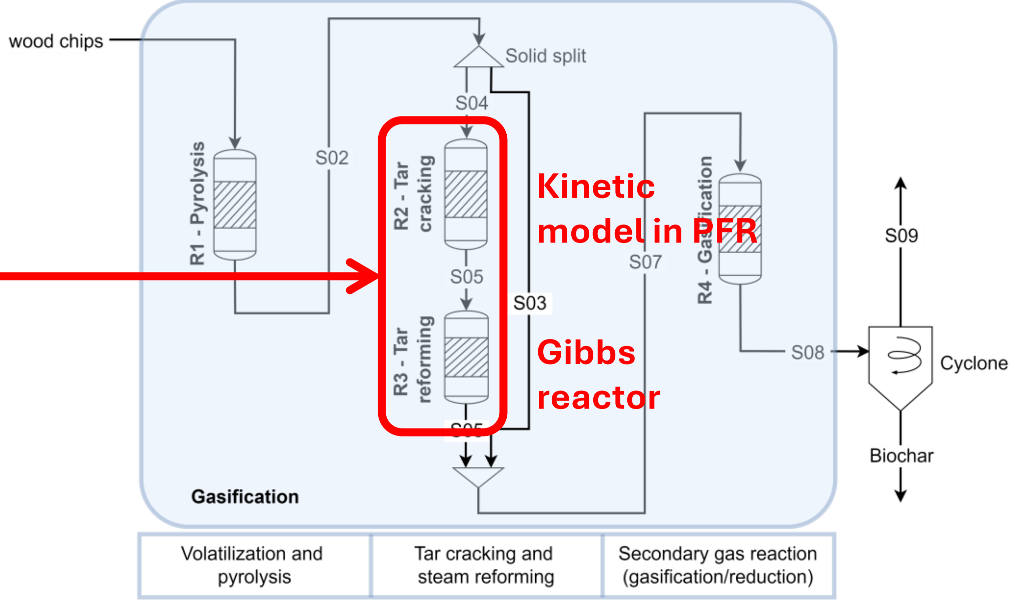
Ranzi et al, 2017. ACS Sustainable Chemistry & Engineering 5, 4, 2867–2881



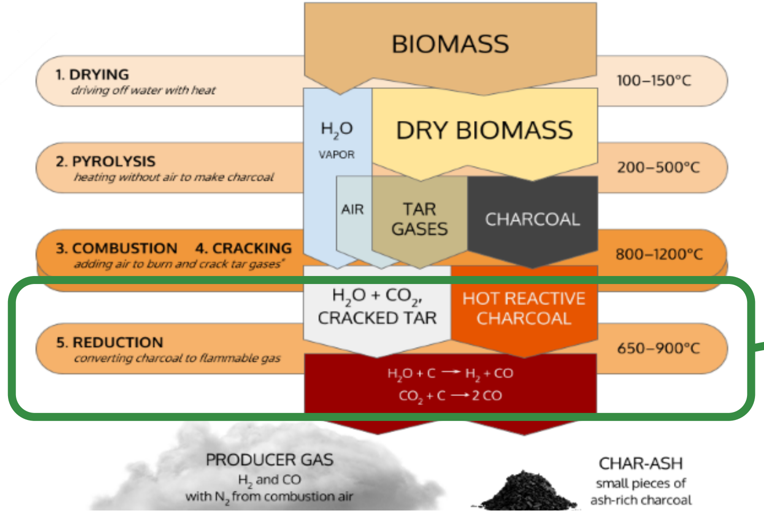
Biomass gasification

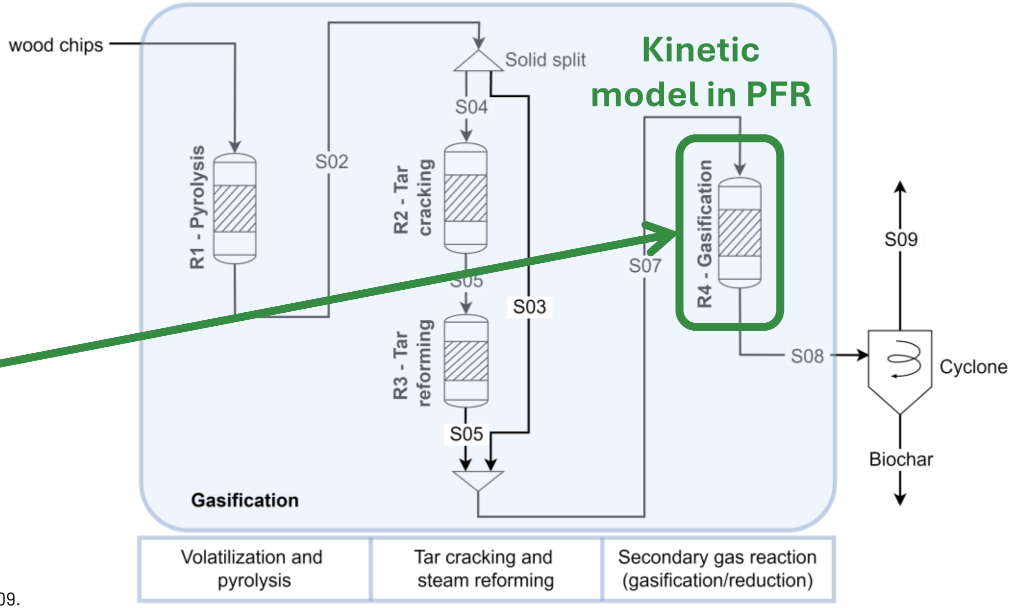


Chen et al., 2021. Chemical Engineering Journal, 417, 127923
Chaurasia, A., 2016. Energy, 116, 1, 1065-1076.



Biomass gasification





Chaurasia, A., 2016. Energy, 116, 1, 1065-1076.
Groeneveld, M.J., van Swaaij, W.P.M., 1980. Chemical Engineering Science, 35, 1-2, 307-313.
Gómez-Barea, A., Leckner, B., 2010. Progress in Energy and Combustion Science, 36, 4, 444-509.

4. Results

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Data source

- The proposed semi-rigorous model has been compared to experimental **data collected from an existing gasifier**, whose owner and technology supplier are sensitive.

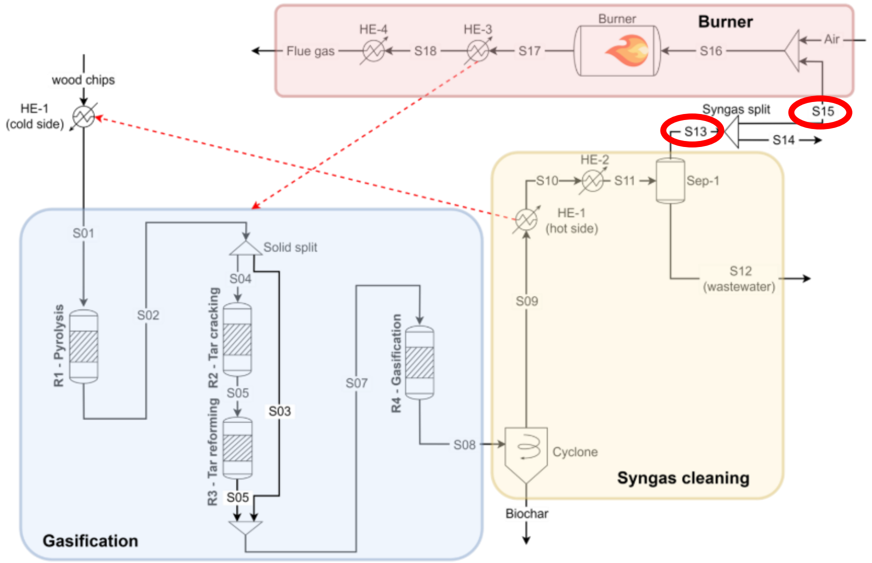
- The facility considered has an analogous layout and size of the unit designed for TERRAWATT and commissioned in Bourges.

Process KPIs

Dry comp [vol%]	Order to magnitude	Absolute error (magnitude)	Relative error (%)
CO	10^1 %	0.1%	-2.0%
CO_2	10^1 %	0.1%	+3.4%
H_2	10^1 %	1.0%	+4.5%
CH_4	10^0 %	1.0%	-25%
Residue tar	10^{-1} %	0.1%	-12%
$C_{1\text{-}3}$ hydrocarbons	10^1 %	1.0%	-9%
Char production (kg/h)	10^1 (kg/h)	1.0 (kg/h)	-5%

Other KPIs

- Estimated **pyrolysis specific energy demand** is **1.78 MJ/kg$_{\text{dry biomass}}$** in line with experimental data for several kind of woody biomass (Daugaard and Brown, 2003, Energy & Fuels)
- Both **LHV** (13.5 MJ/Nm$^3_{\text{syngas}}$) and **HHV** (13.7 MJ/Nm$^3_{\text{syngas}}$) of produced syngas are **aligned** (10-15 MJ/Nm$^3_{\text{syngas}}$) **with industrial data** for a **similar gasification plant** in Sweden (Larson et al, 2021, Fuel Processing Technology)
- Estimated bio-syngas fraction is to be burnt (S15) is around 35% of S13 (in line with pilot data)



5.Conclusions

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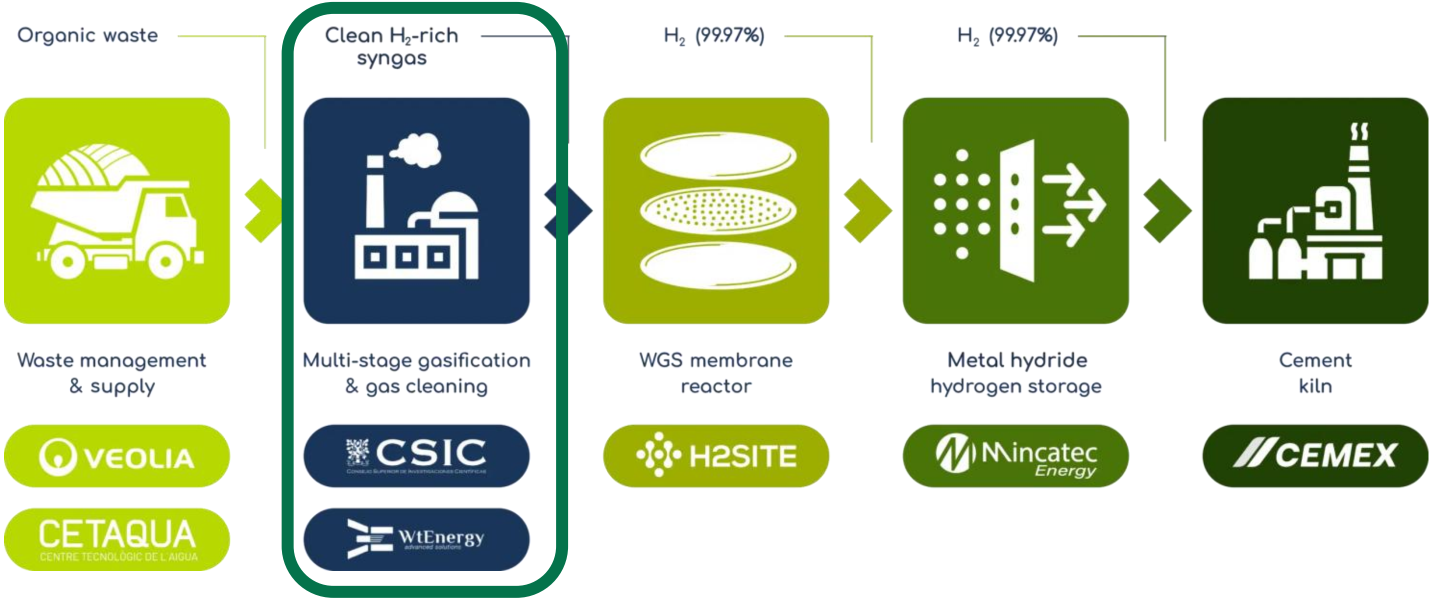
COCO COFE	Aspen PLUS
Physics and chemistry background	**Limited theoretical background**
True reactive steps are simulated	**Non-real steps are also included**
General model	**Feedstock and operating conditions dependent**
Flexibility: can handle variations in the feedstock and operating window	**Not flexible** unless RSTOIC mass balance is re-tuned for different conditions
Kinetic model: preliminary sizing of units	**Yield model**: fulfil only energy & material balance
Computational-intensive	**Lower numerical effort**
Need for **more details** (including thermodynamic properties) for **unconventional species**	Only **conventional species** are considered

Long-term plan

- Wrap up everything into a **single custom module (CAPE-open etc)**
- **Validate** the approach **over experimental data** within different projects using **different types of biomass**
- **Extend the approach** to other feedstocks as the literature will propose "rigorous" models to be adopted

Other application for gasification



Picture credits: HYIELD Project webpage

A novel multi-stage steam gasification and syngas purification demonstration plant for waste to hydrogen conversion

Total granted funding
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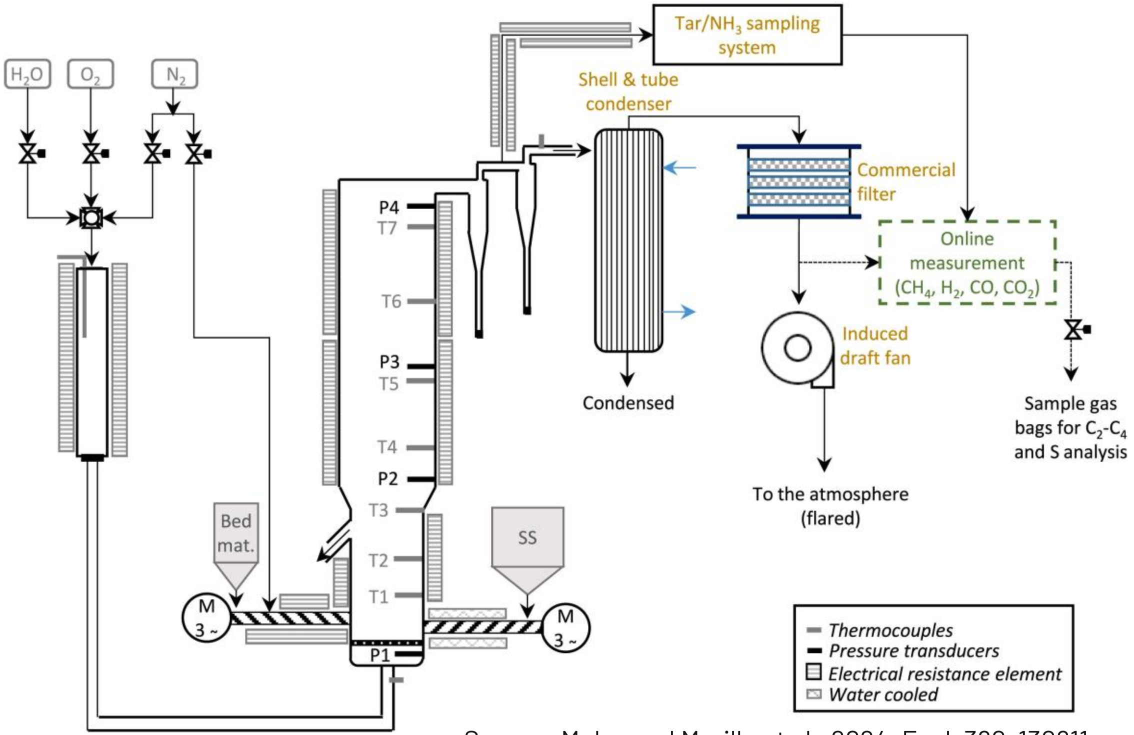
Pilot data

IBC-CSIC 30 kW_{th} BFB gasification pilot

- The gasification model will be **validated** on **exp data** collected from the **30 kW_{th} pilot plant** at IBC-CSIC

- **Different operating points** will be tested by changing temperature, SC, and ER to screen a wide domain to **industrially relevant conditions**



Source: Moles and Murillo et al., 2024, Fuel, 360, 130611

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Presentation Title: *Process Design and Comparison of Three Innovative Technologies for Biomethane Production and/or Purification and Upgrading from Biomass and Biological Wastes*

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Thank you for your kind attention!
I am pleased to answer any questions!

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