Bio4Fuels

Norwegian Centre for Sustainable Bio-Based Fuel and Energy

Bio4Fuels: Efficient and sustainable use of biomass as a renewable feedstock

Filippo Bisotti, Matteo Gilardi, Olaf T. Berglihn,
Theresa Rücker, Torbjørn Pettersen, Bernd Wittgens

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Outlines

- Introduction
  - Why we need to re-think the modelling of bioprocesses
  - Our strategy
  - Hurdles in our strategy

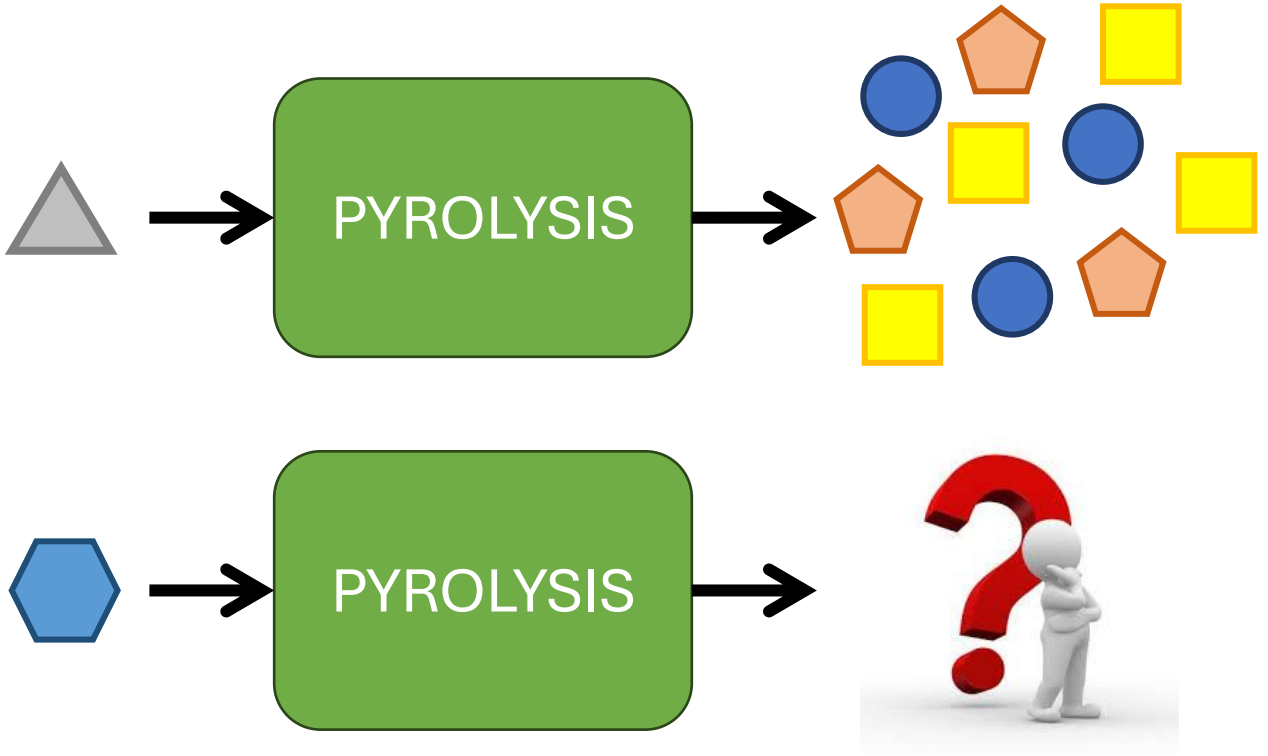
- Case study: Bio4Fuel project – from lab scale to relevant scale biorefinery
  - Our strategy step-by-step
  - Key advantage of the strategy using CAPE-open tools

- Conclusions

- Overlook on CAPE-open tools in SINTEF Industry's projects

Why re-thinking bioprocess modelling?

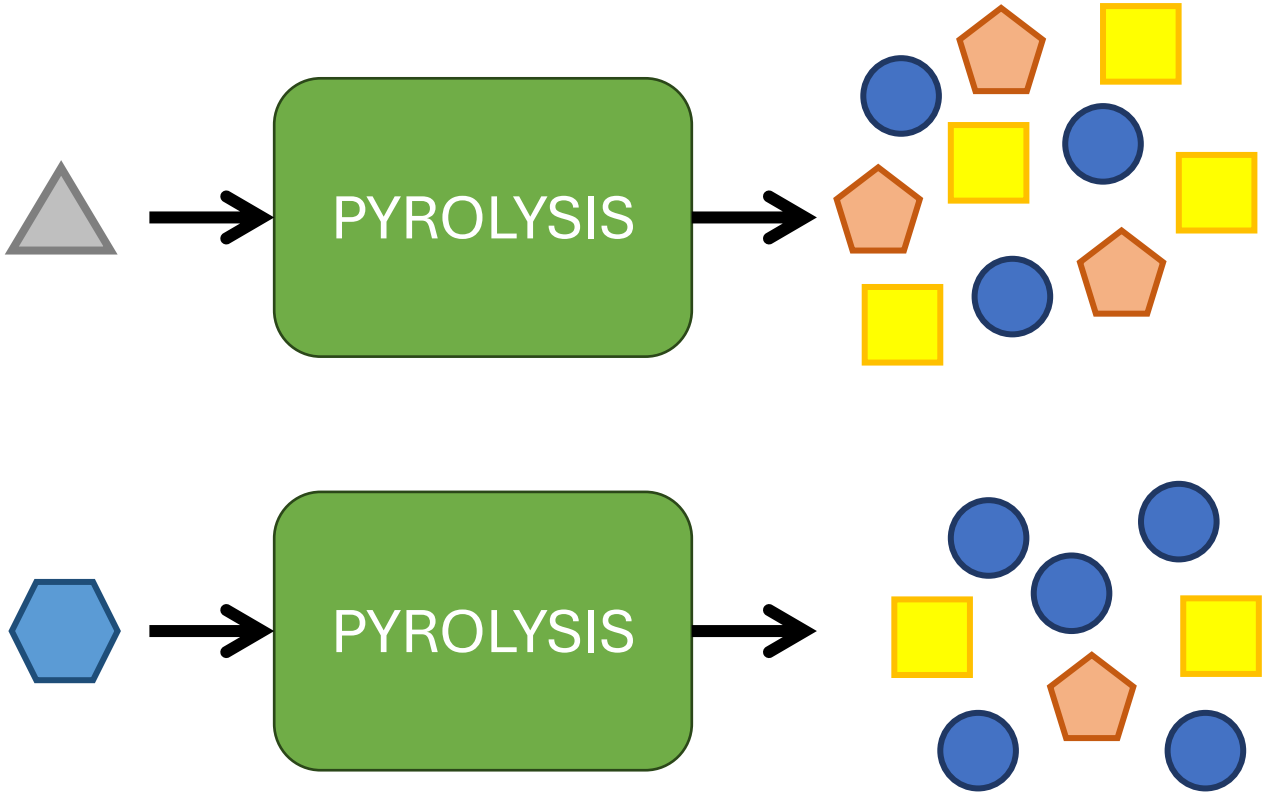
- Current models in **flowsheet simulators** for pyrolysis, gasification, and biomass pre-treatment (steam explosion…) are too simplified
- Often solely based on estimated yields
- **What happens if you change the feed or the operating conditions?**



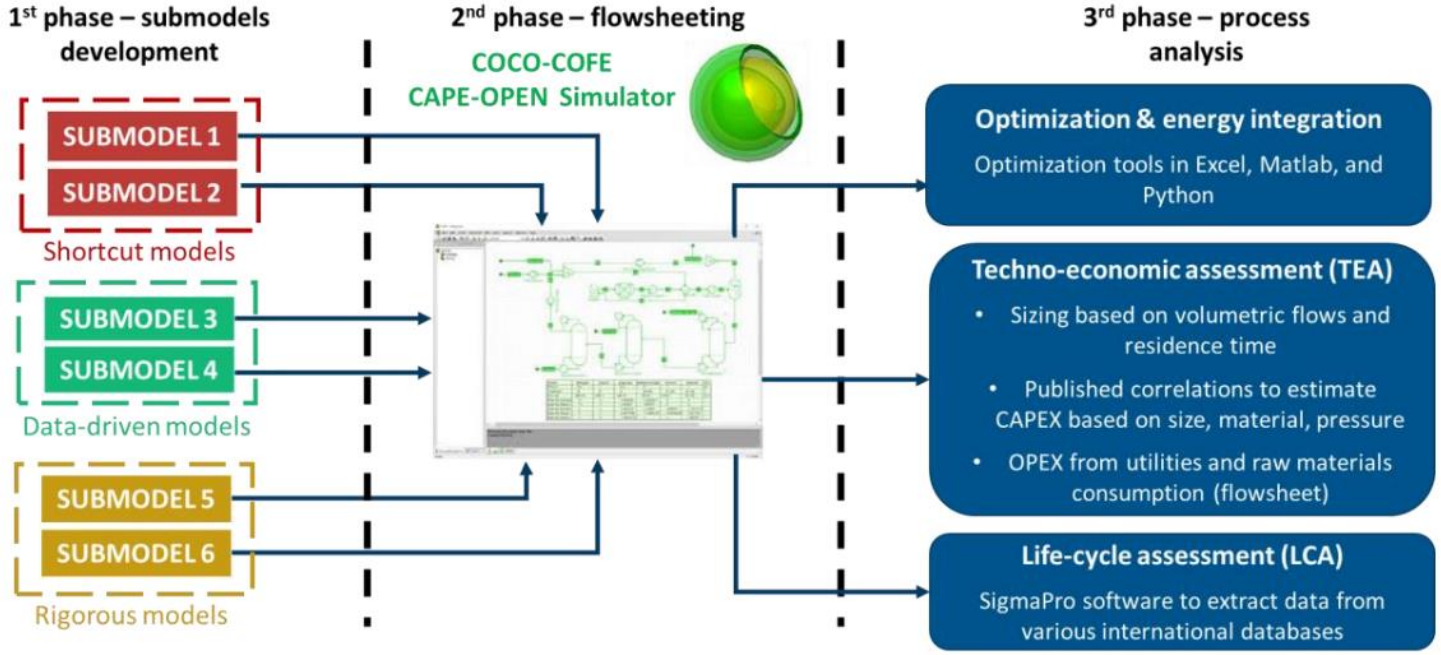
Why re-thinking bioprocess modelling?

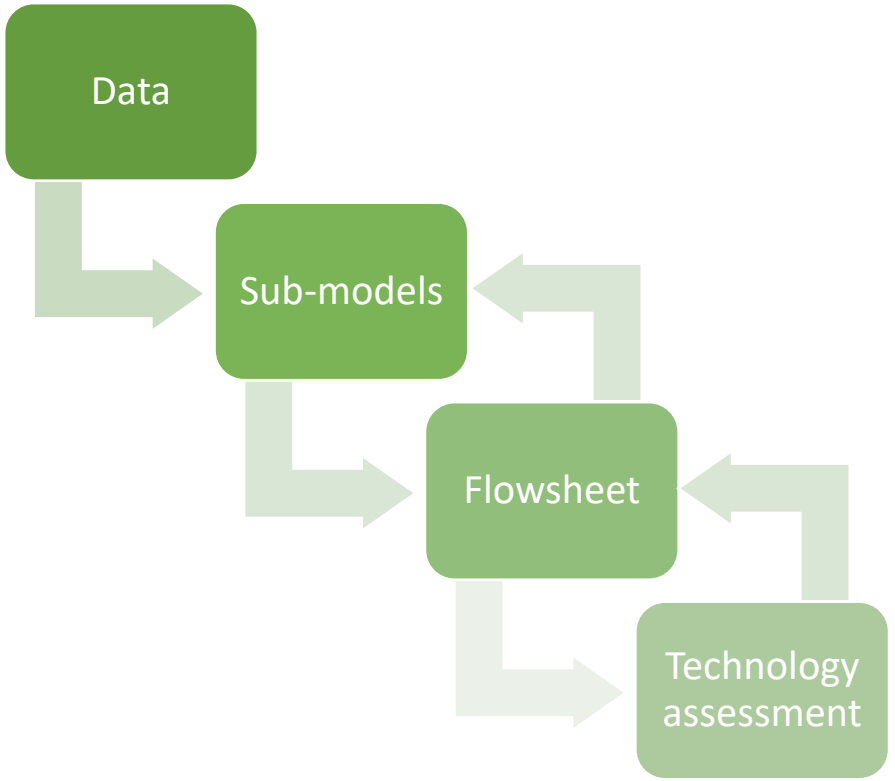
Only rigorous models allow for:

- describing a wide 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"***



Our strategy for Biomass-to-X processes





Select the right model based on data available!

Gilardi, Bisotti et al., Modelling of Biomass-to-X: Challenges and Strategies

The loop of process modelling & design with technology assessment

Need: models for bio-processes

- **Design** purposes
- **Upscaling**
- Environmental assessment
- **Preliminary cost estimates**

Issues

- **Complexity and variability** of the bio-based feedstocks
- **Unconventional processes**
- **Chemistry**
- Complexity of their thermodynamic

Constraints

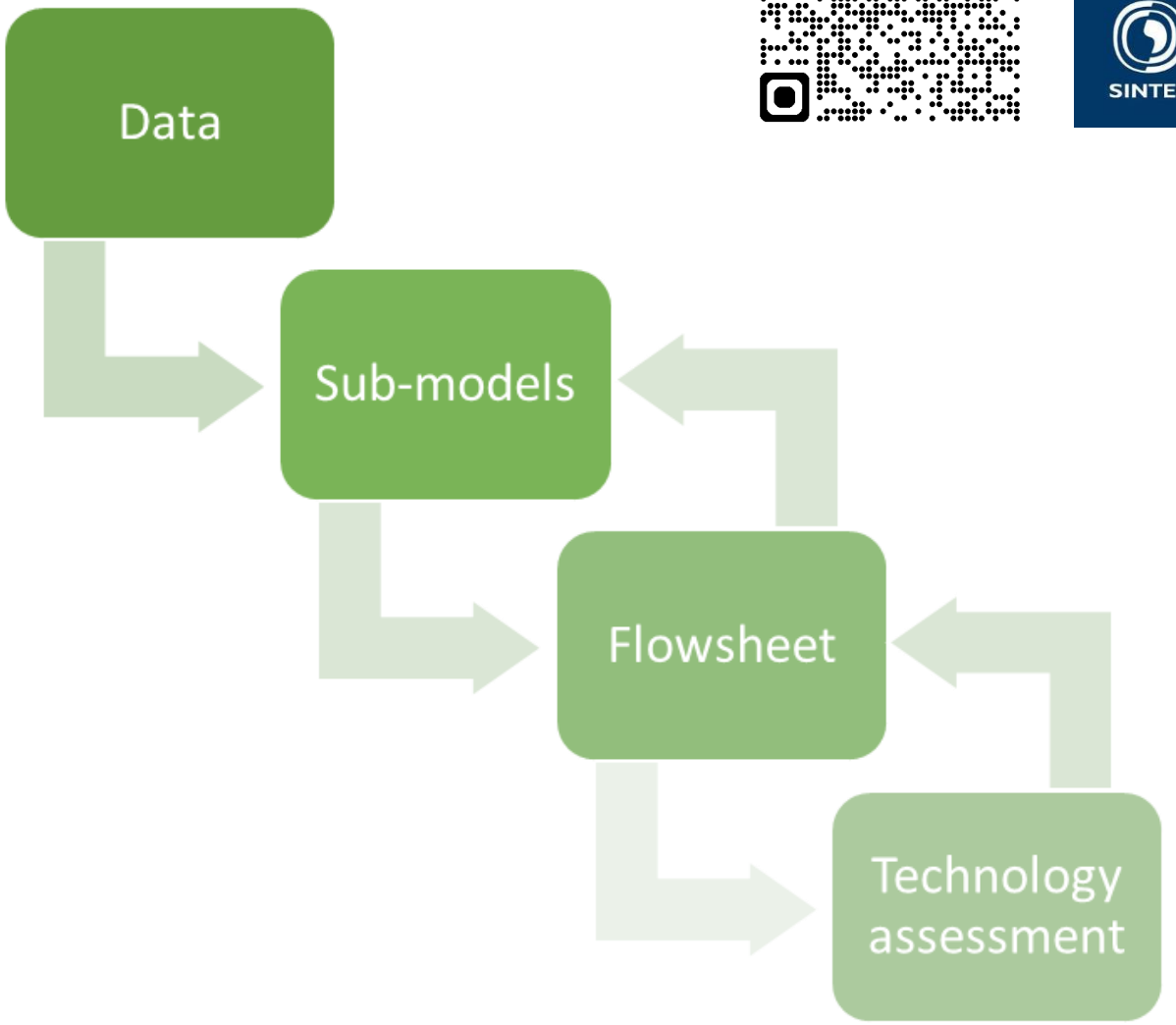
- Simplified but accurate approaches to ensure **good predictability**
- Keep a **reasonable computational effort**

Solution

- Strategies and approaches for the modelling
- Define criteria for flowsheet development of processes from **lab-to-plant**

Transparency

- Data are open
- Models are published and validated or tuned for a specific application
- TEA is transparent (i.e., correlations are retrieved from the literature and estimates documented)
- LCA is trackable (i.e., databases are open-source as the toolbox)

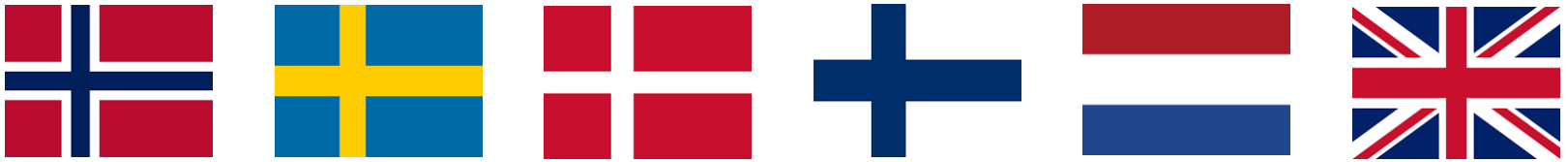


Case study

Bio4Fuels overview

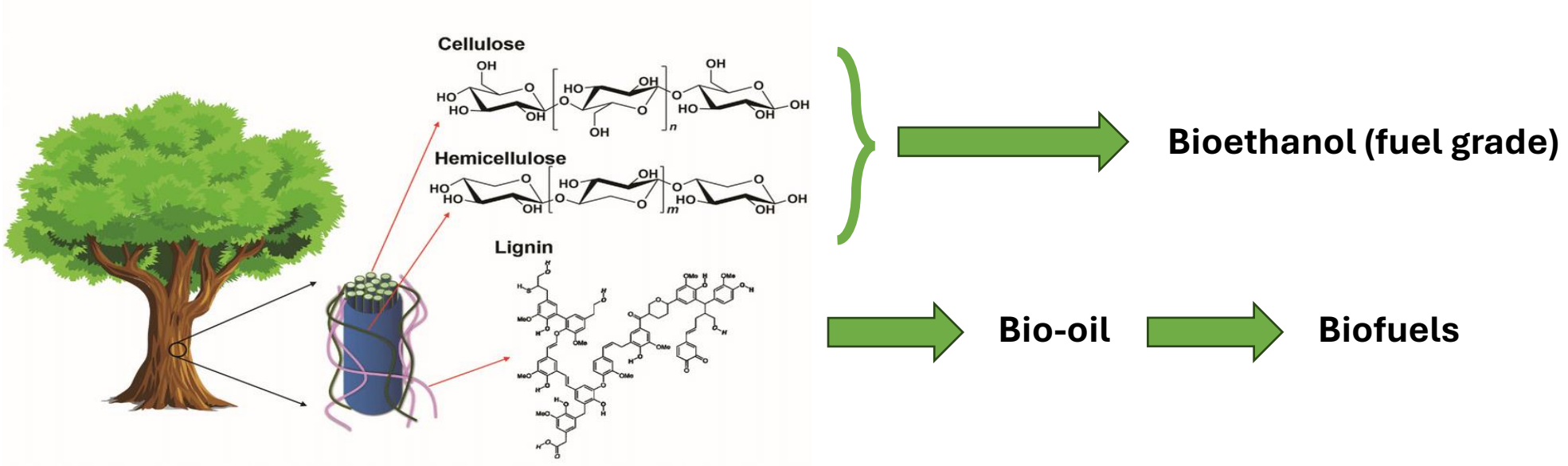
- Funded by the Norwegian Research Institute (Forskningsrådet) for **12.8 M€**
- Bio4Fuels developed **new technologies** to ensure efficient and sustainable use of biomass as a renewable feedstock for integrated **heat, power, and fuel production and transportation**
- International **R&D and industrial partners**

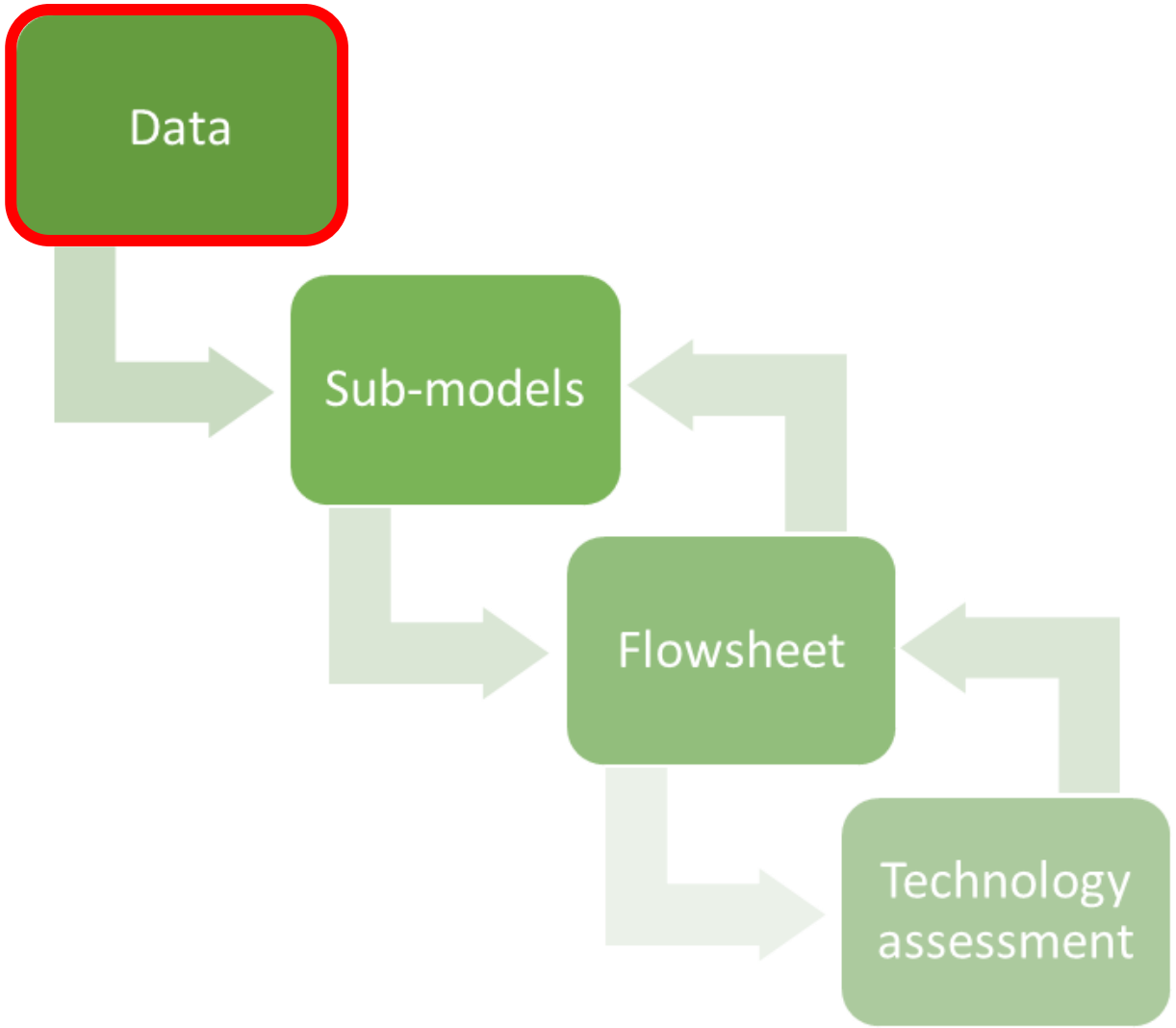
Visit our project website!



Bio4Fuels objectives

- Analysis of an innovative **biorefinery** where **all constituents are converted into fuels**
- Improve cellulose saccharification (i.e., sugar yield) to **increase the overall biorefinery yield**
- Efficiently **valorise each of its building blocks** to optimize the yield and the economics




Data
Sub-models
Flowsheet
Technology assessment

Chemistry and data

INCREASE CARBON EFFICIENCY → Complex chemistry and operations

- **Strategy** → series of operations and reactive steps
  - Separate efficiently cellulose, hemicellulose, lignin
  - Increase sugar yield
  - Valorise wasted carbon in lignin
- **Specific data** (measurements) and **details** on what is happening (molecules and chemistry)

ACS Sustainable Chemistry & Engineering

pubs.acs.org/journal/ascecg

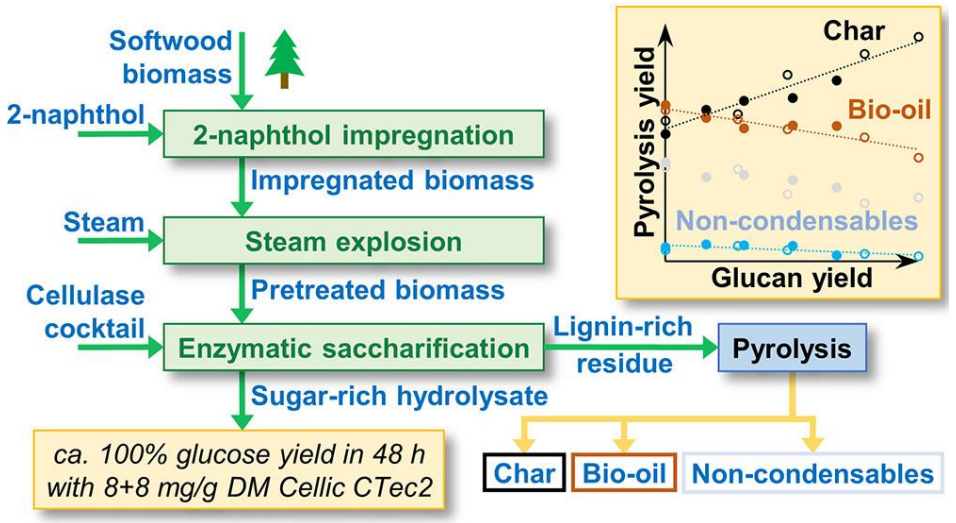
Research Article

2-Naphthol Impregnation Prior to Steam Explosion Promotes LPMO-Assisted Enzymatic Saccharification of Spruce and Yields High-Purity Lignin

Line Degn Hansen, Martin Østensen, Bjørnar Arstad, Roman Tschentscher, Vincent G. H. Eijsink, Svein J. Horn, and Anikó Várnai*

Cite This: *ACS Sustainable Chem. Eng.* 2022, 10, 5233−5242 Read Online

2-Naphthol Impregnation Prior to Steam Explosion Promotes LPMO-Assisted Enzymatic Saccharification of Spruce and Yields High-Purity Lignin | ACS Sustainable Chemistry & Engineering



Species

- Quite “exotic” molecules → potentially missing data
- From hundreds of thousands to a manageable number of species to mimic the system

Identification of the molecule → Definition of structure → Estimate missing thermodynamic properties → Included and stored in the database for the simulation with a fictitious CAS

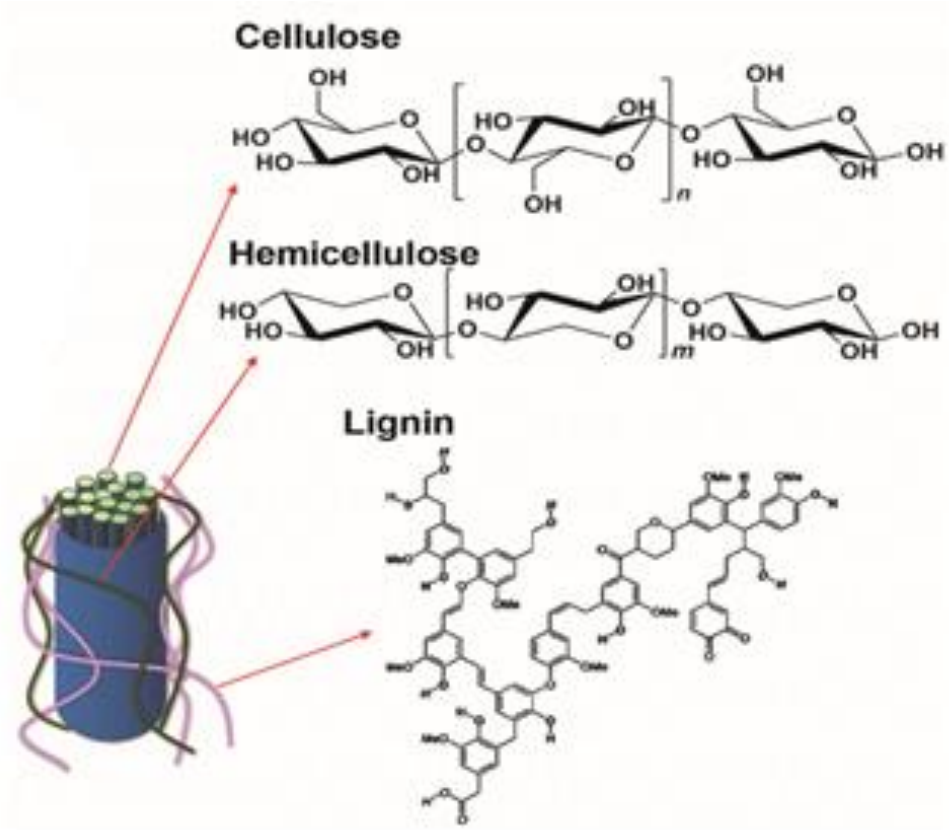
Manageable number of compounds

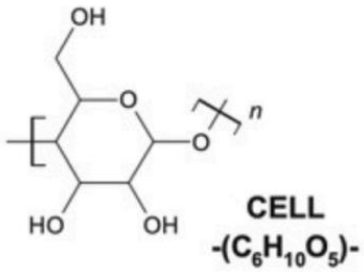
- NIST Webbook (open access)
- Estimated with Gani’s method (group contribution approach)

ChemSep PCDmanager

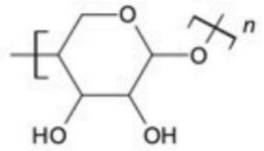
- Enthalpy of formation
- Standard entropy
- Ideal gas heat capacity
- Vapour pressure
- Critical properties
- …

Species: reactants



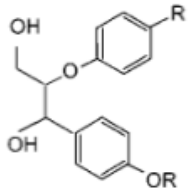


CELL
$-(C_6H_{10}O_5)-$

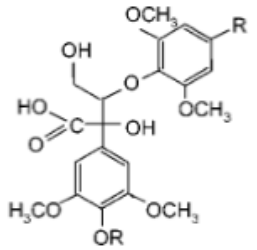


XYHW and GMSW
$-(C_5H_8O_4)-$

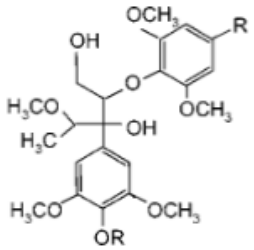
- Mannan
- Arabinan
- Galactan
- Xylan



LIG-C $C_{15}H_{14}O_4$
(69.8%C 5.4%H 24.8%O)



LIG-O $C_{16}H_{10}O_6(OCH_3)_4$
(56.9%C 5.2%H 37.9%O)

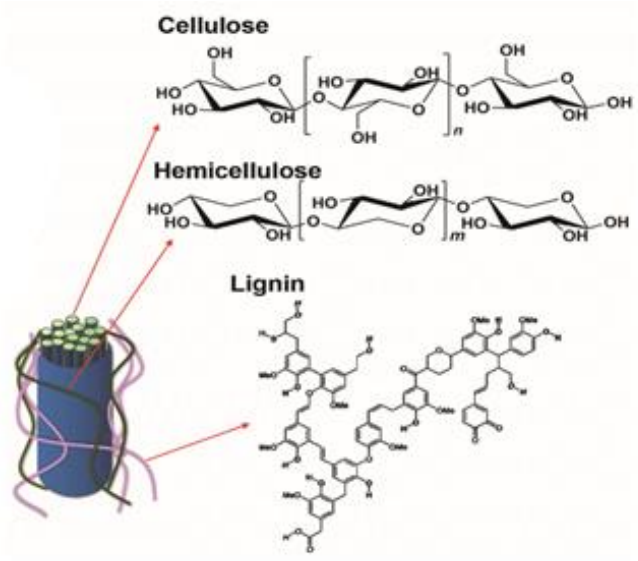


LIG-H $C_{17}H_{13}O_4(OCH_3)_5$
(60.6%C 6.4%H 33.0%O)

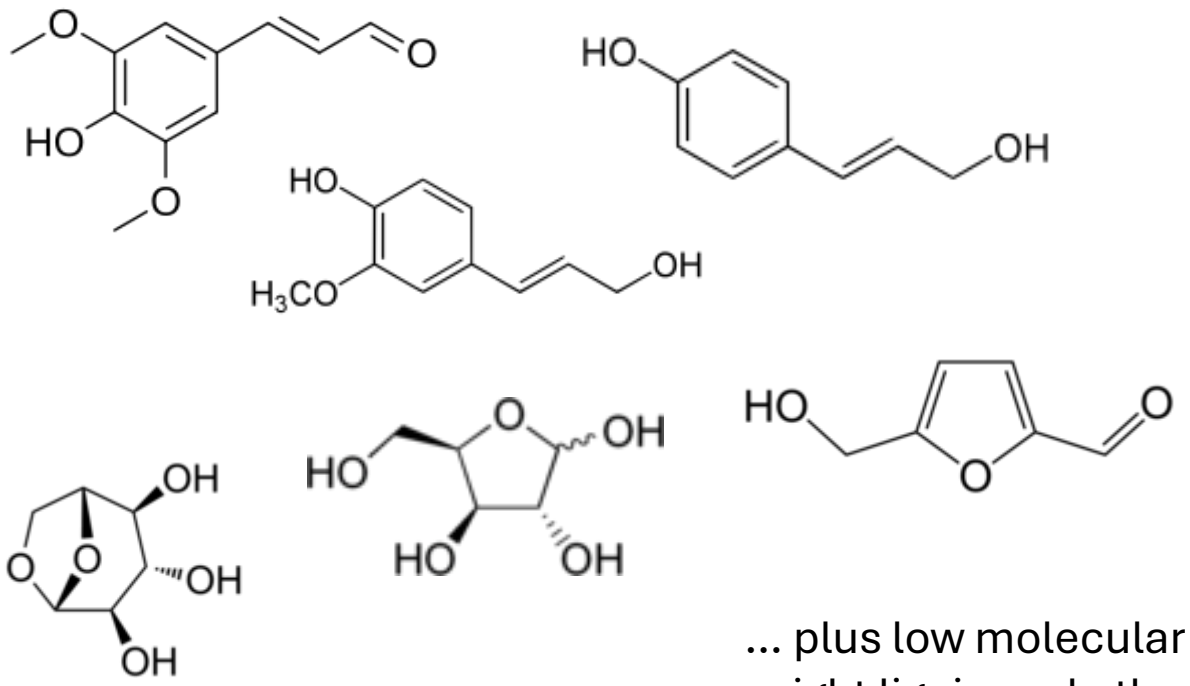
Chemical Kinetics of Biomass Pyrolysis | Energy & Fuels (acs.org)

Development of a multiphase chemical reactor network method as a tool for simulating biomass gasification in fluidized beds - ScienceDirect

Species: bio-”crude” unconventional molecules

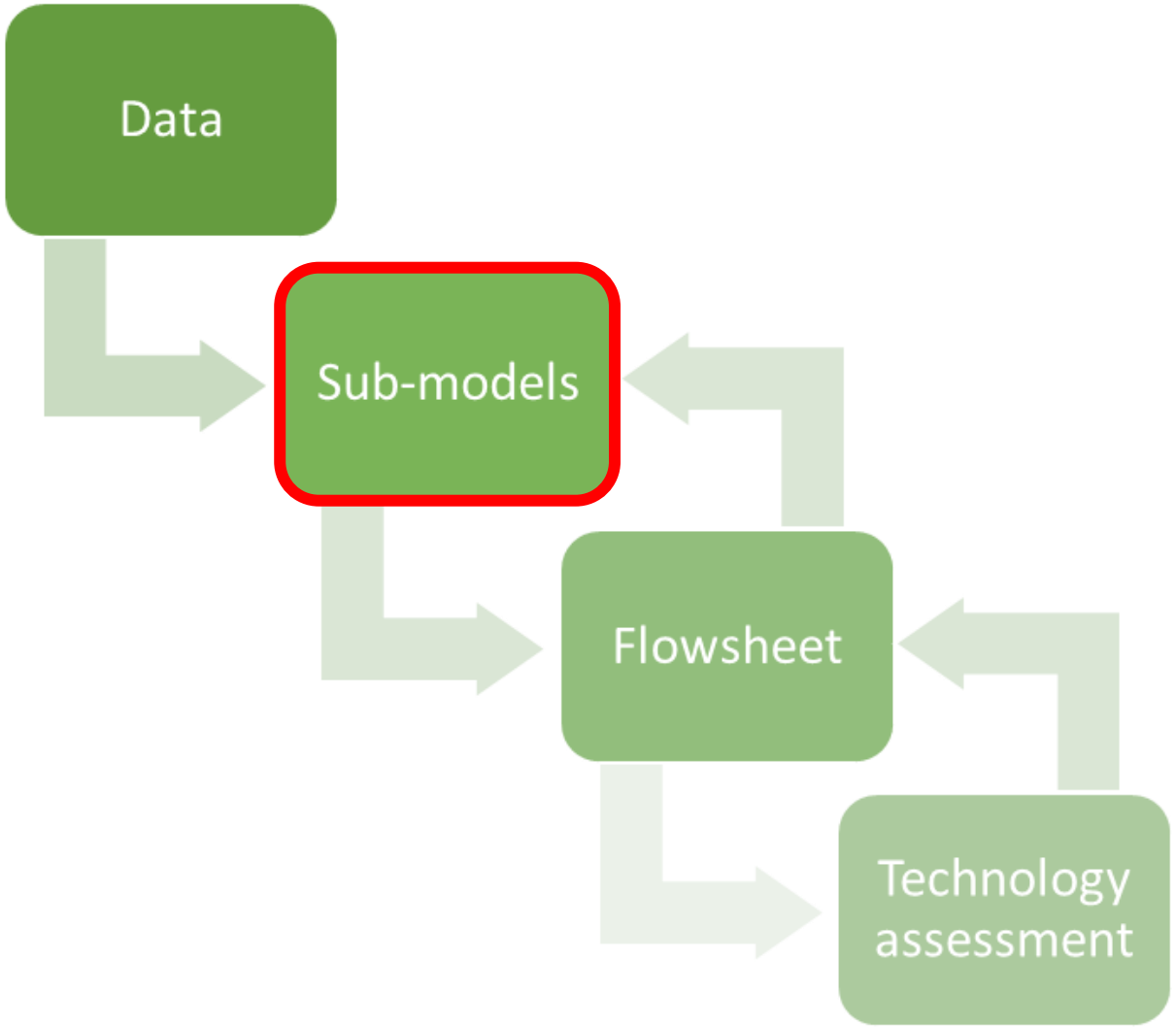


Pyrolysis



… plus low molecular weight lignin and other solid residue

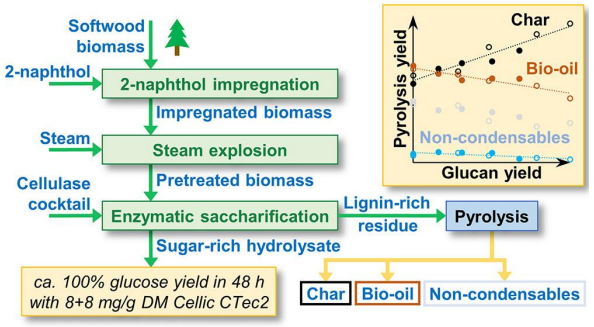
Chemical Kinetics of Biomass Pyrolysis | Energy & Fuels (acs.org)


Data
Sub-models
Flowsheet
Technology assessment

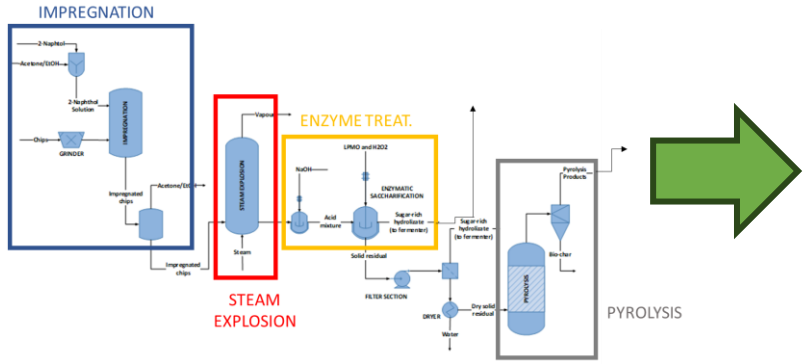
From lab-scale to industrial facility

Sub-block (i.e., sub-models) identification:

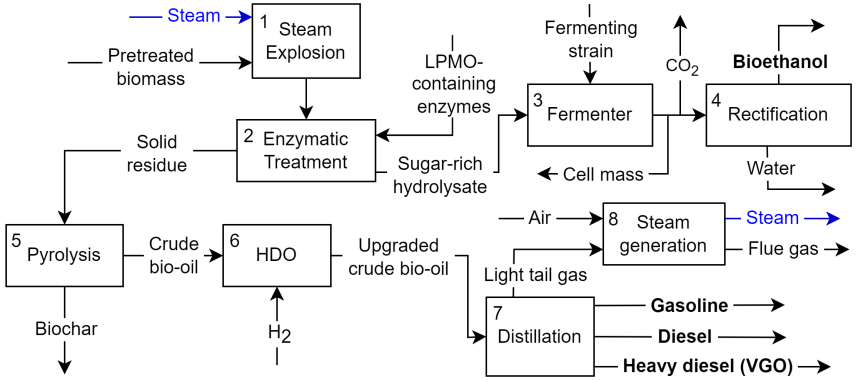
- Remove lab-scale steps that cannot be replicated on an industrial scale
- Identify missing steps and **design a comprehensive process**
- Identify a feasible and **valuable path** to **convert biomass into added-value chemicals**



1. Tested lab-scale concept

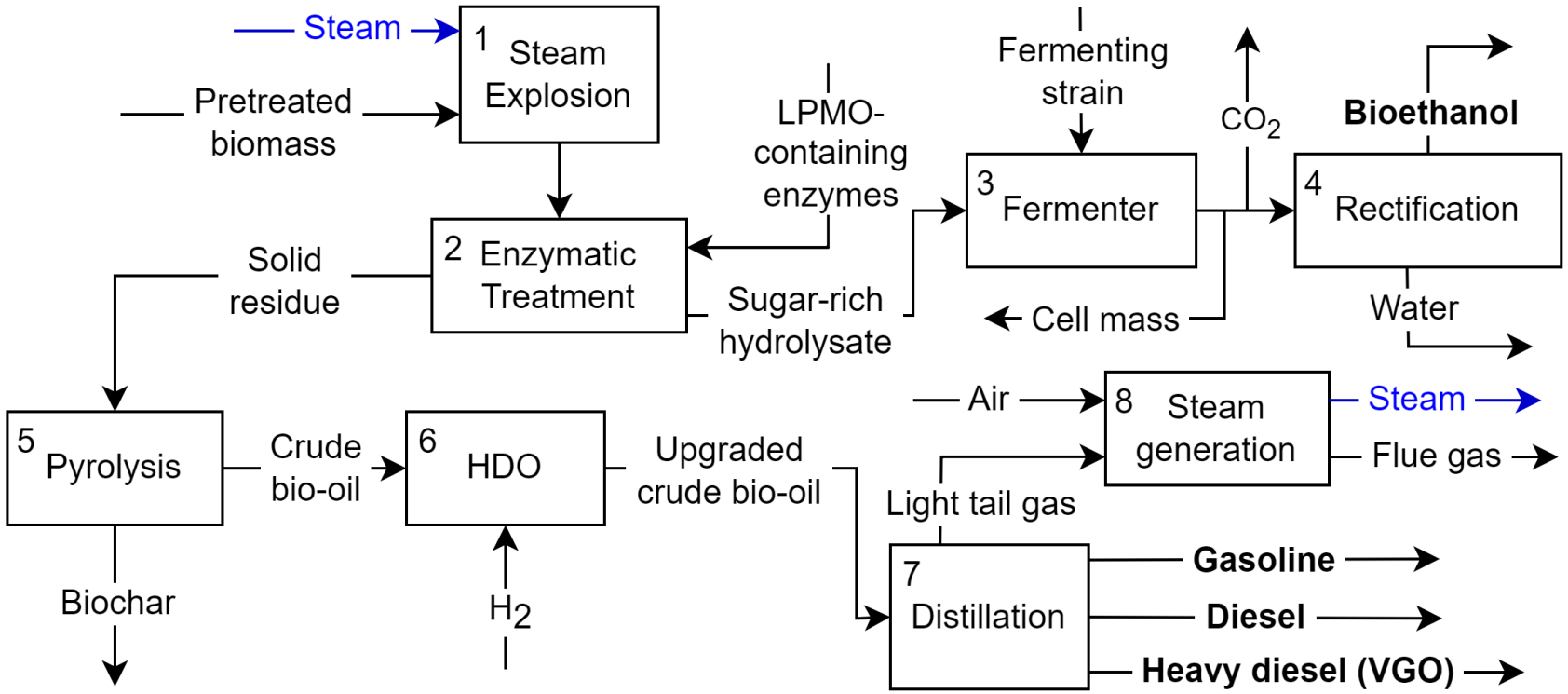


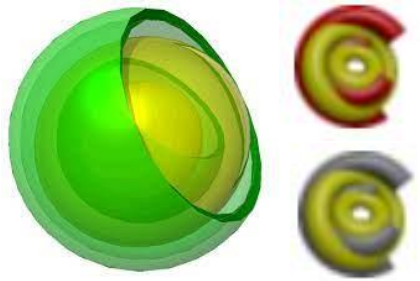
2. Translation into a feasible industrial plant



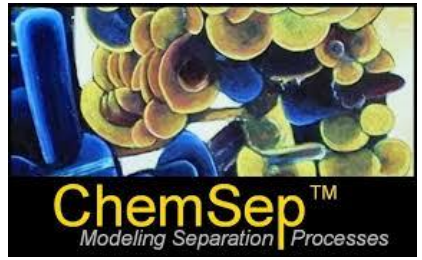
3. BFD completed with missing steps/units

Simulation tools





COCO COFE V3.6
AmsterCHEM



ChemSep 8.40

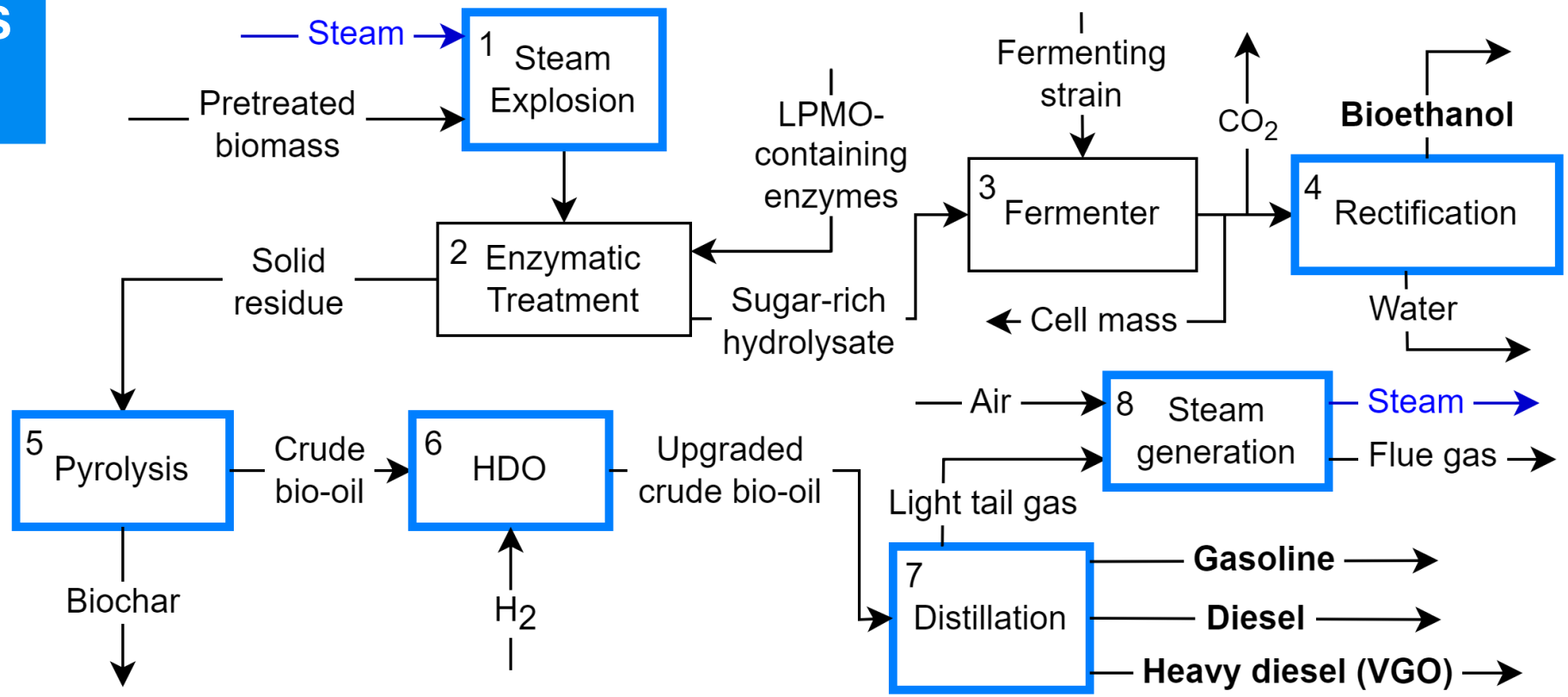
Modelling

Different types of models to characterise each step

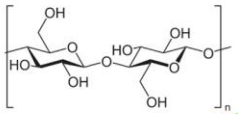
- **Rigorous/detailed**
- **Data-driven**
- **Short-cut**

Sub-models implementation

RIGOROUS MODELS

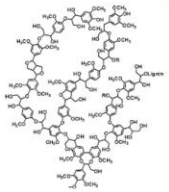


Example: Pyrolisis model



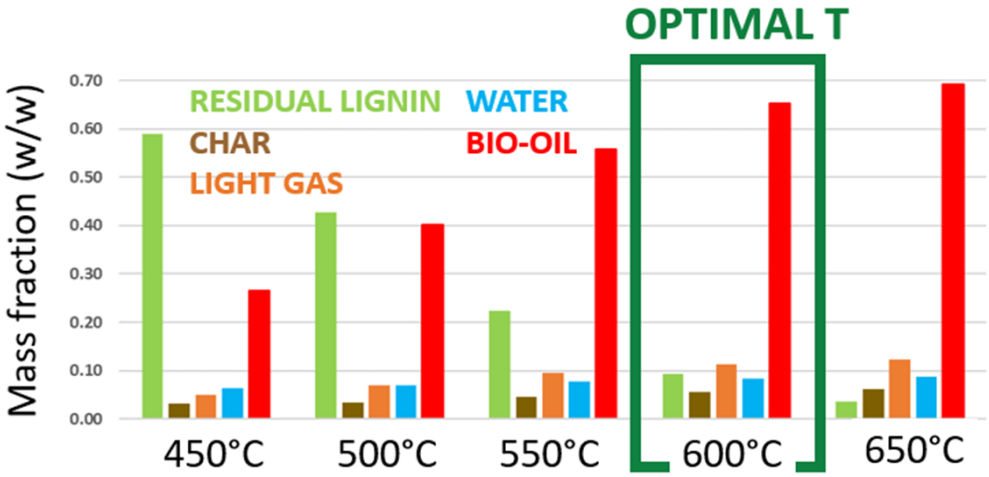
CELLULOSE & HEMICELLULOSE

LIGHT GAS



CELLULOSE & HEMICELLULOSE PYROLYSIS
Ranzi et al., 2008

LIGHT GAS PYROLYSIS
Dussan et al., 2019



Rigorous model from prior literature is used here to optimize the pyrolysis process to maximize bio-oil yield and lignin conversion

Antonis Kokossis, Michael C. Georgiadis, Efstratios N. Pistikopoulos (Eds.)
PROCEEDINGS OF THE 33rd European Symposium on Computer Aided Process Engineering
(ESCAPE33), June 18-21, 2023, Athens, Greece
 http://dx.doi.org/10.1016/B978-0-443-15274-0.50123-2

Soft modelling of spruce conversion into bio-oil through pyrolysis – Note II: pyrolysis

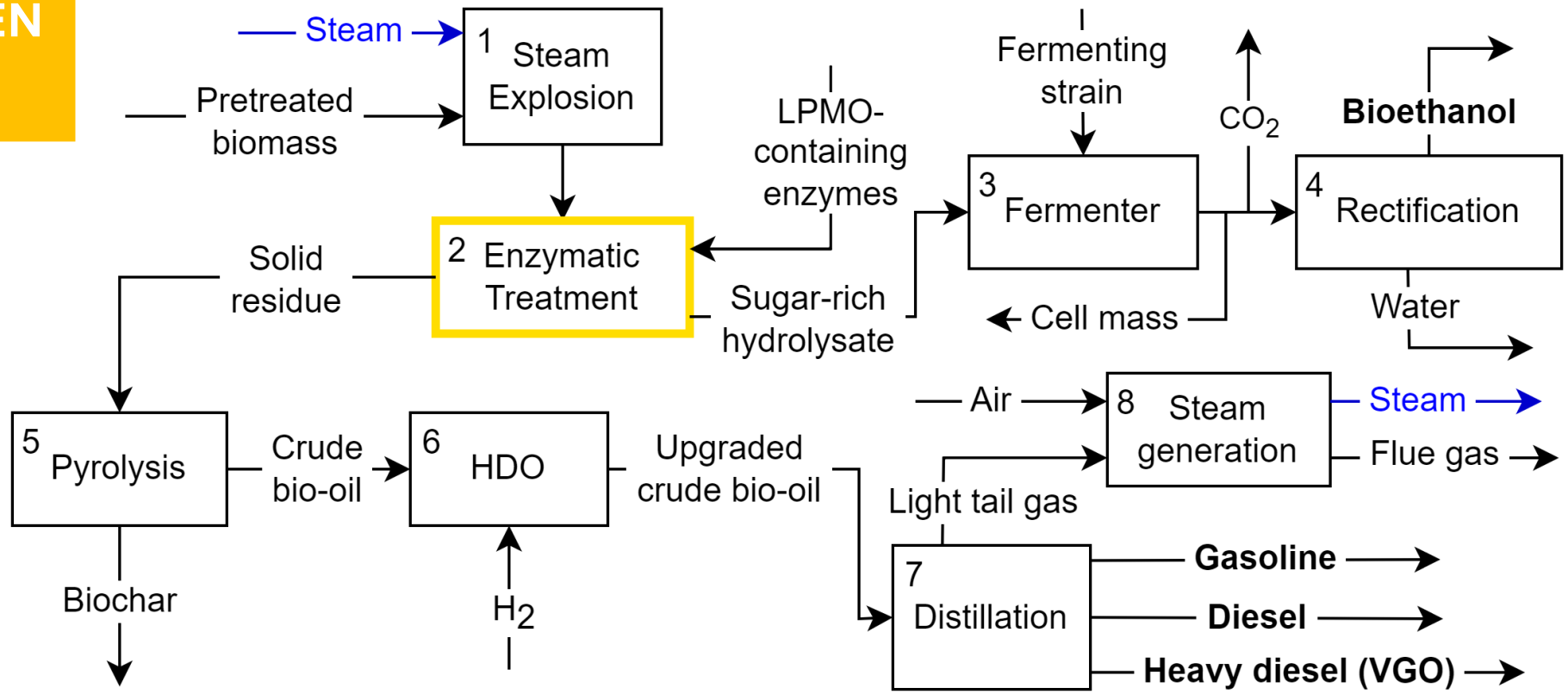
Filippo Bisotti,[a,*] Matteo Gilardi,[a] Olaf T. Berglihn,[a] Roman Tschentscher,[b] Vincent G.H. Eijsink,[c] Anikó Várnai,[c] Bernd Wittgens,[a]

ESCAPE 33 EUROPEAN SYMPOSIUM ON COMPUTER-AIDED PROCESS ENGINEERING
DIGITALIZATION AND GREEN ECONOMY
ATHENS - GREECE
Royal Olympic Hotel

Soft modelling of spruce conversion into bio-oil through pyrolysis – Note II: pyrolysis - ScienceDirect

Sub-models implementation

DATA-DRIVEN MODELS



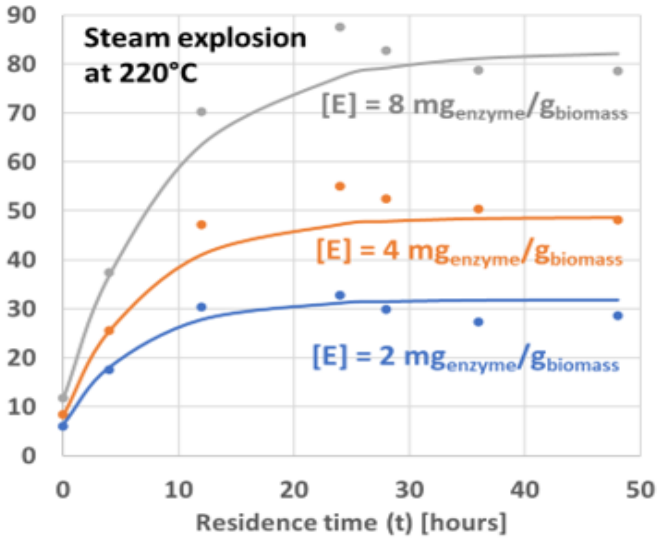
Example: enzymatic saccharification model

$$\gamma(t) = \gamma(0) + h \cdot [1 - \exp(-k_R \cdot t)]$$

$$\gamma(0) = a_1 \cdot [E] + a_2$$

$$h(T_{SE}, [E]) = (a_3 \cdot T_{SE} + a_4) \cdot [E] + (a_5 \cdot T_{SE} + a_6)$$

$$k_R(T_{SE}, [E]) = (a_7 \cdot T_{SE} + a_8) \cdot [E] + (a_9 \cdot T_{SE} + a_{10})$$



- **a_i regressed on experimental data** from lab-scale setup (Hansen et al., 2022, ACS Sustainability)
- Yield depends on DoE parameters
  - residence time (t),
  - enzyme concentration [E],
  - T of steam explosion pre-treatment (T_{SE})

Antonis Kokossis, Michael C. Georgiadis, Efstratios N. Pistikopoulos (Eds.)
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Soft modelling of spruce conversion into bio-oil through pyrolysis – Note I: steam explosion and LPMO-activated enzymatic saccharification

Matteo Gilardi,[a] Filippo Bisotti,[a,*] Olaf T. Berglihn,[a] Roman Tschentscher,[b] Vincent G.H. Eijsink,[c] Anikó Várnai,[c] Bernd Wittgens,[a]

Soft modelling of spruce conversion into bio-oil through pyrolysis – Note I: steam explosion and LPMO-activated enzymatic saccharification - ScienceDirect

Sub-models implementation

BLACK-BOX MODELS


NREL

Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol

Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover

D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, and A. Aden
National Renewable Energy Laboratory
Golden, Colorado

P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton, and D. Dudgeon
Harris Group Inc.
Seattle, Washington and Atlanta, Georgia

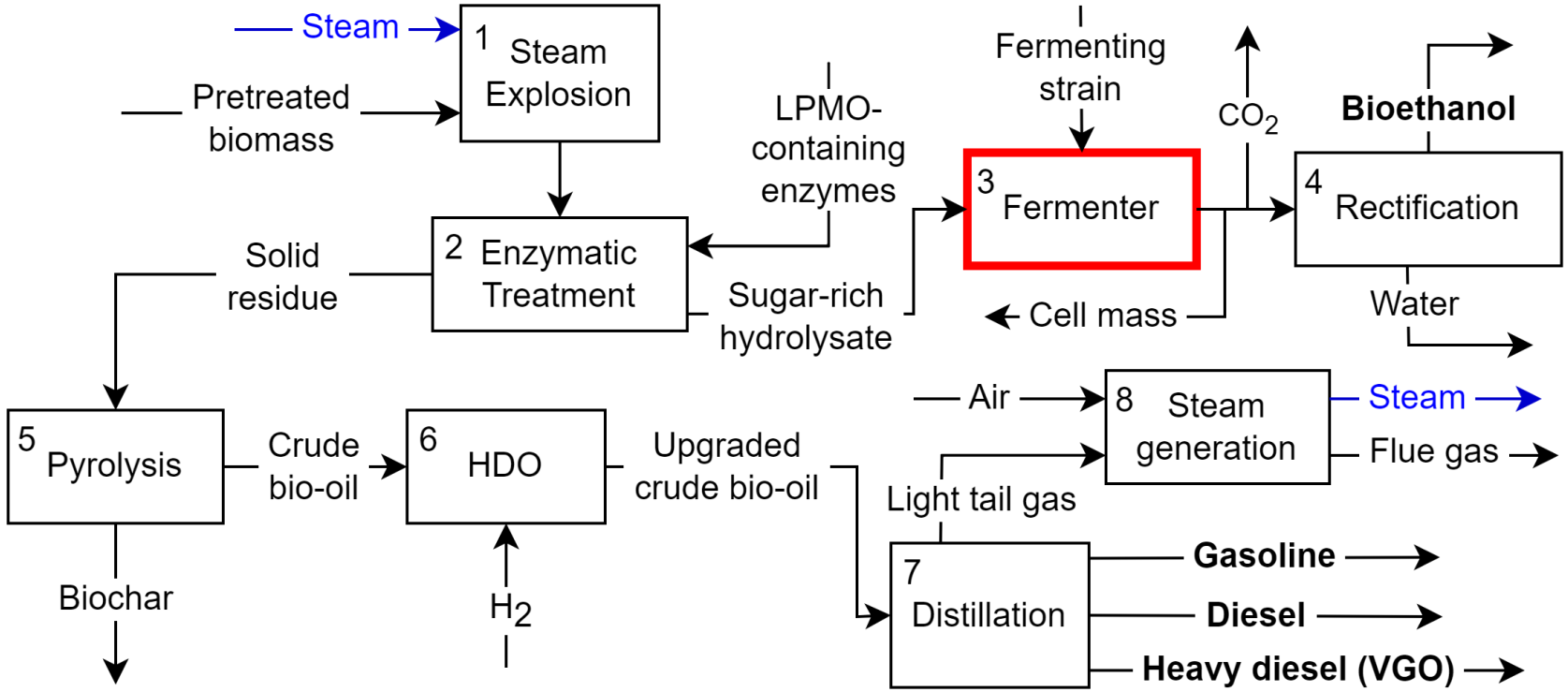
Prepared under Task No. BB07.2410

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

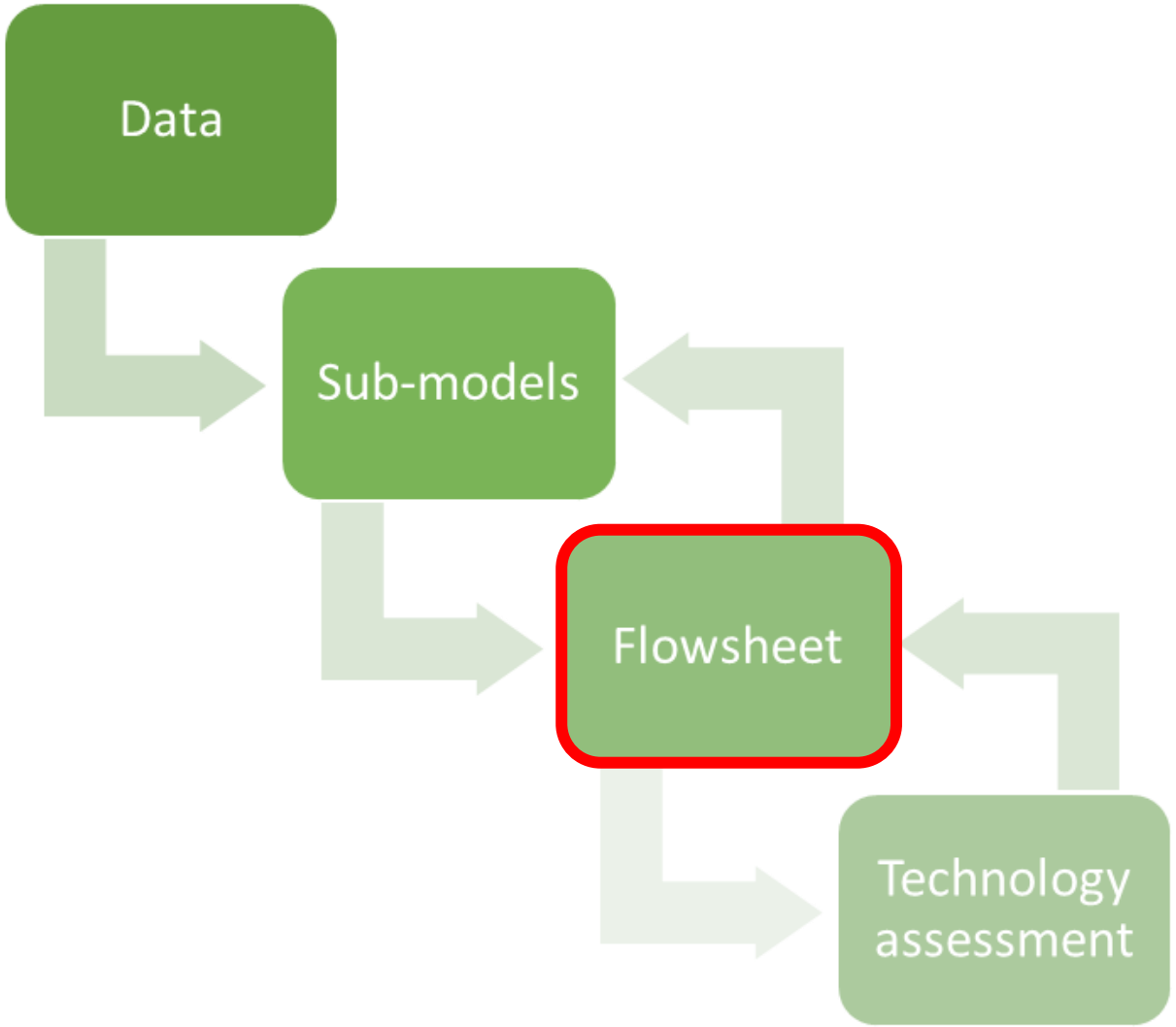
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401
303-275-3000 • www.nrel.gov

Technical Report
NREL/TP-5100-47764
May 2011

Contract No. DE-AC36-08GO28308



Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover (nrel.gov)


Data
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Yields

Norwegian spruce chips

Residue lignin

Lights gas
0.11 ton/ton$_{BM}$

Crude bio-oil
0.24 ton/ton$_{BM}$

Ethanol fuel grade
0.21 ton/ton$_{BM}$

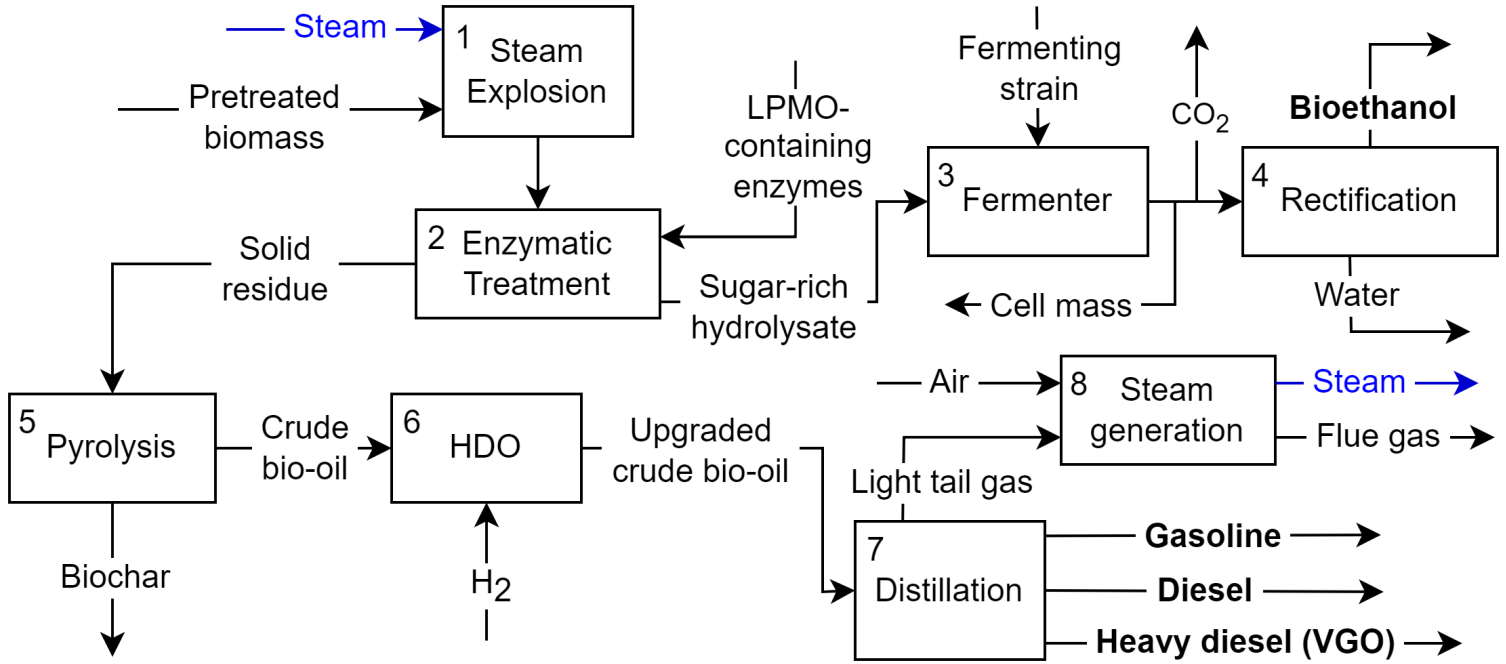
Biochar
0.14 ton/ton$_{BM}$

Flowsheet in COFE

Computer Aided Chemical Engineering
Volume 53, 2024, Pages 2449-2454

From laboratory scale to innovative spruce-based biorefinery. Note I: Conceptual process design and simulation

Filippo Bisotti [a] ✉, Matteo Gilardi [a] ✉, Olaf T. Berglihn [a], Roman Tschentscher [b], Line D. Hansen [c], Svein J. Horn [c], Anikó Várnai [c], Bernd Wittgens [a]



Note I: Conceptual process design and simulation

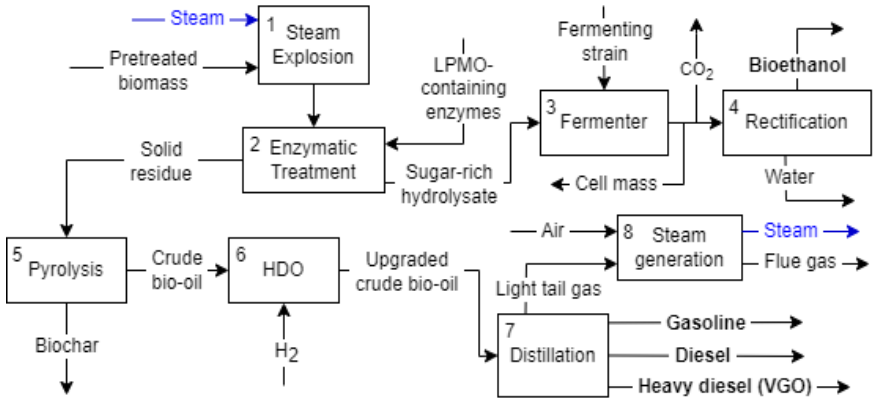
Next step: fully integrated biorefinery

Now we have a flowsheet for standard biorefinery… but we can improve it!

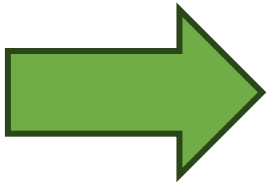
Flowsheet development

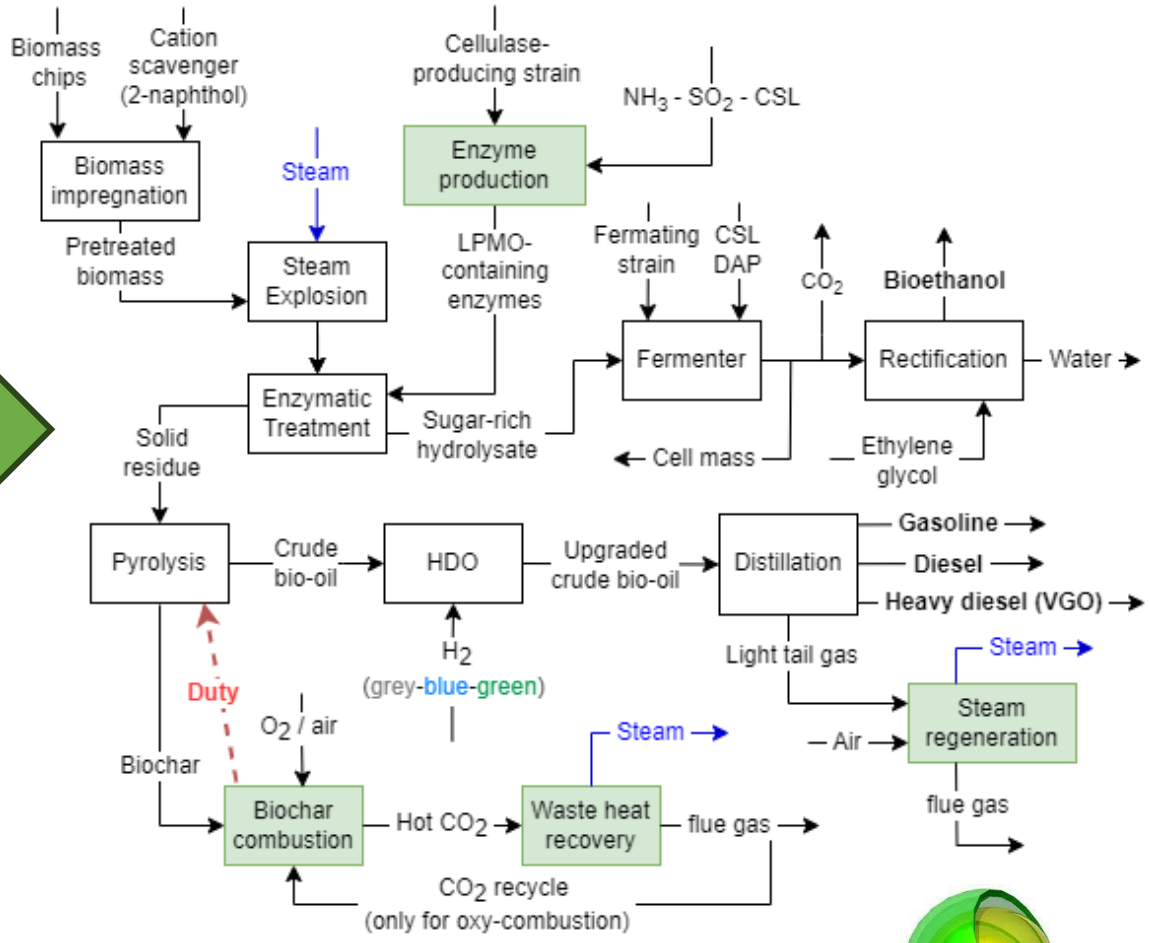
- Process **optimisation**
- Lower consumption: **energy integration**
- Identify process **intensification** loops
- Increase productivity: **valorise wastes** and **low-value streams**

Optimization: to a fully integrated biorefinery

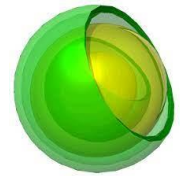


Simple flowsheet





Fully-integrated flowsheet



From laboratory scale to innovative spruce-based biorefinery. Note II: Preliminary techno-economic assessment

Matteo Gilardi [a] ✉, Filippo Bisotti [a] ✉, Olaf T. Berglihn [a], Roman Tschentscher [b], Line D. Hansen [c], Svein J. Horn [c], Anikó Várnai [c], Bernd Wittgens [a]

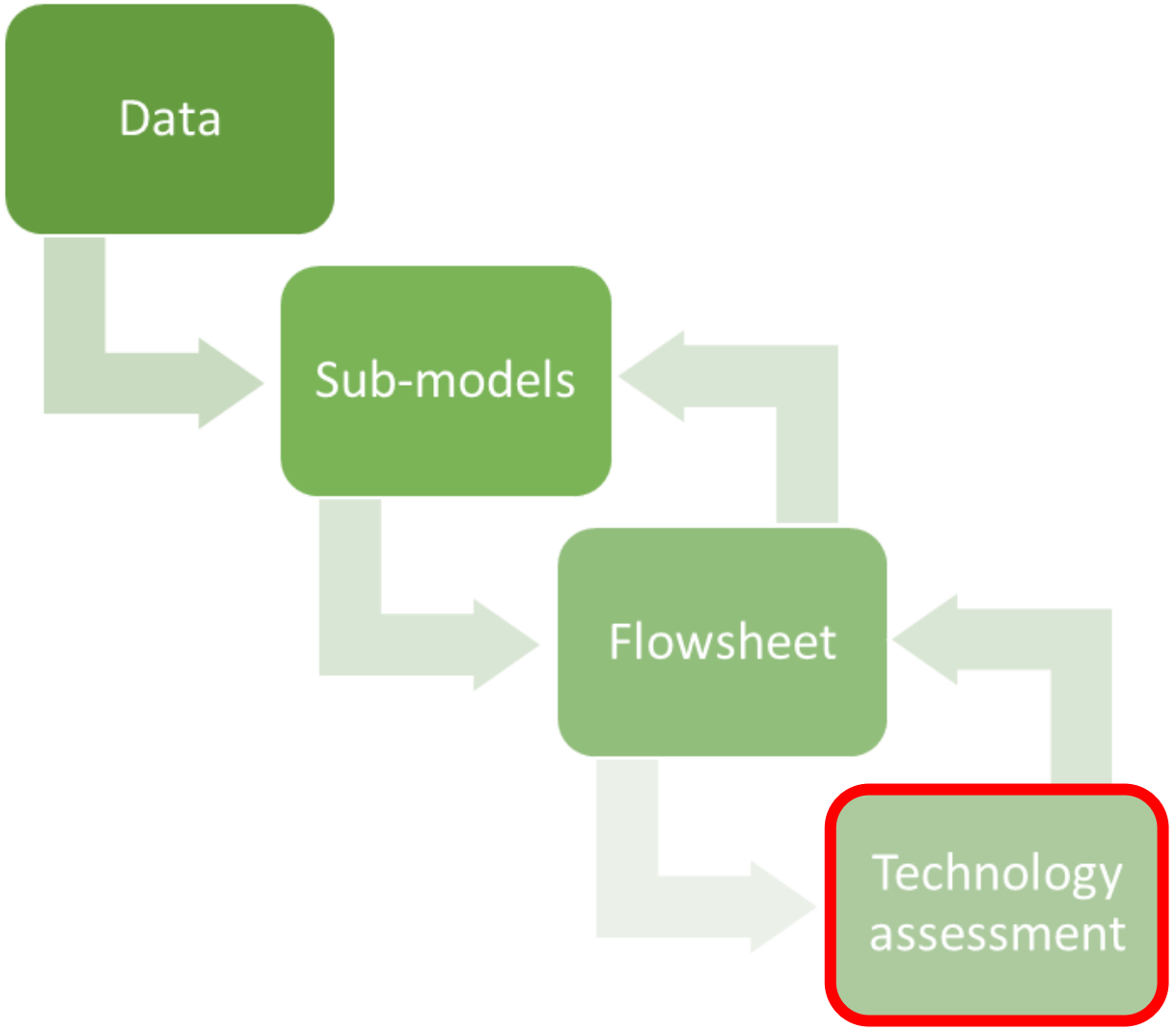
Note II: Preliminary techno-economic assessment

Next step: assessment

Now you have anything in place…

Technology investigation

- Technoeconomic assessment (**TEA**) → **PROFITABLE?**
- Life cycle analysis (**LCA**) → **CARBON MITIGATION?**


Data
Sub-models
Flowsheet
Technology assessment

An iterative process

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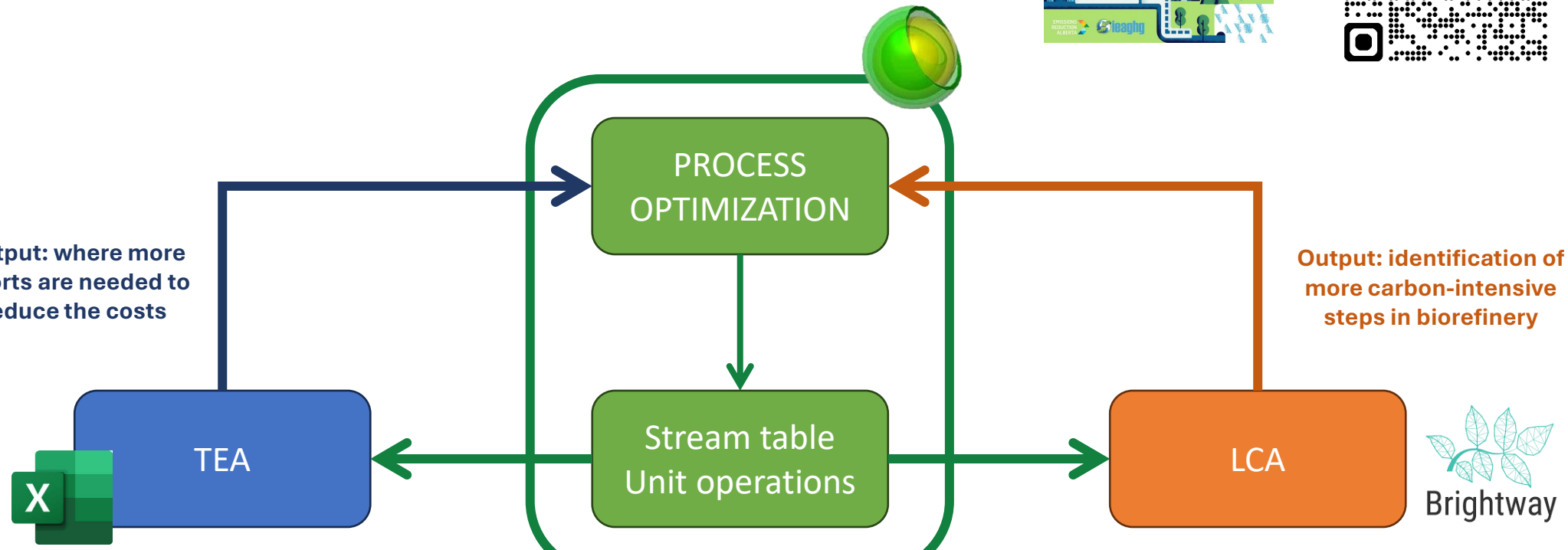
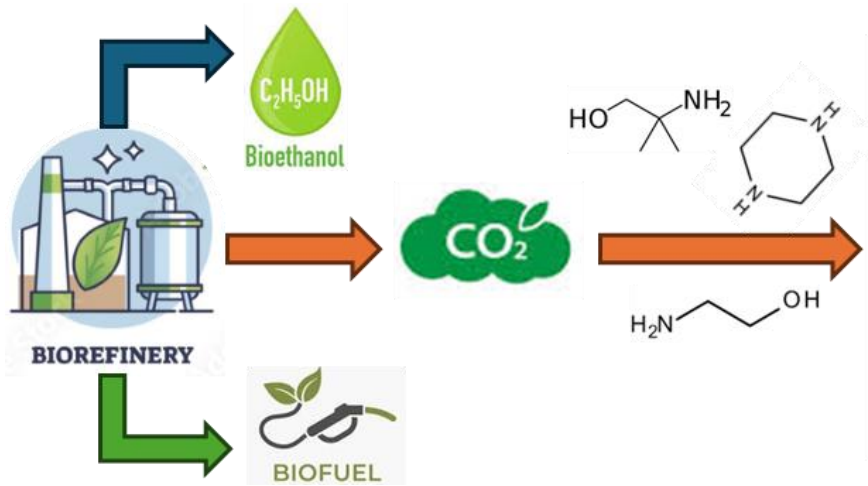


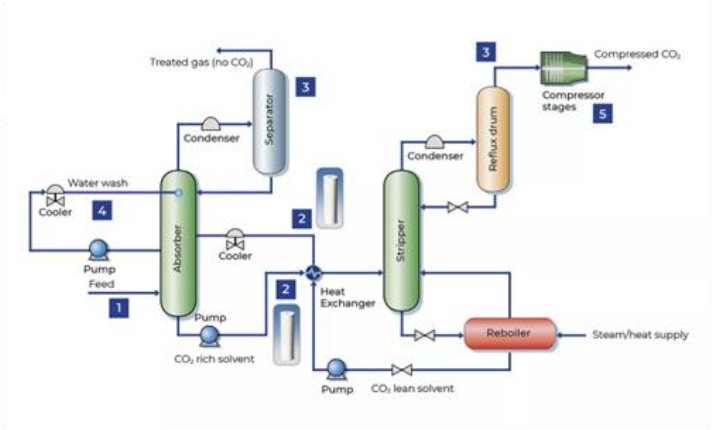
- CapEx & OpEx
- **Costs for all the supply chain**
- Economic **impact of H_2 quality**
- **Selling price** to be competitive

Is carbon reduction feasible?

- **Environmental impact** of H_2 quality
- **Carbon neutrality**
- Full **supply chain** assessment

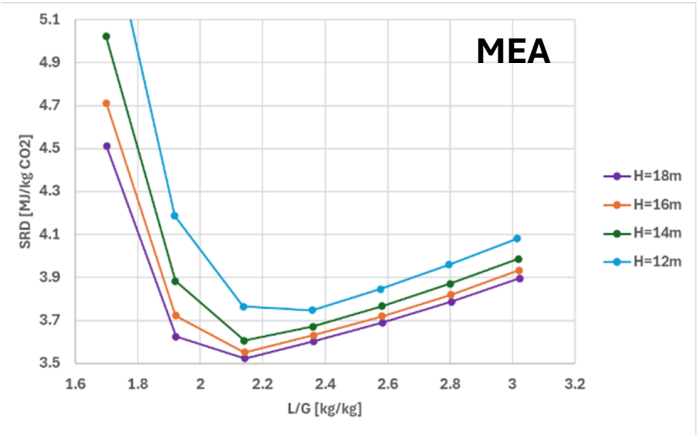
Can it be carbon negative? Yes

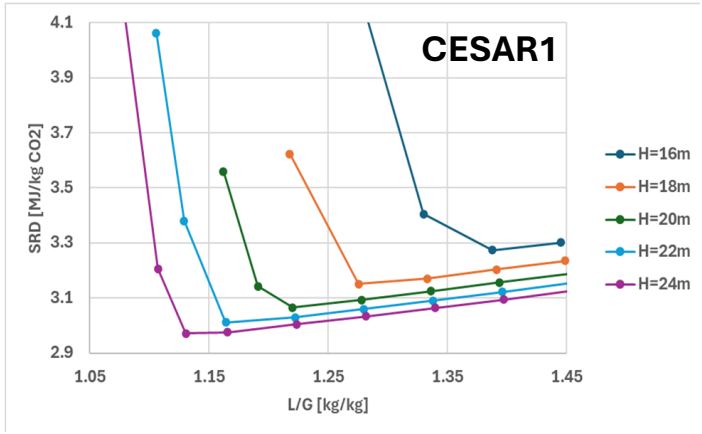




CO_2 SIM

SINTEF Industry's in-house tool for CO2 capture simulation and optimization





Project portfolio with CAPE-open tools…

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In SINTEF Industry – Process Technology we are CAPE-open and COFE friendly!

hyield

REFOLUTION
Unlocking the potential of biofuels

VALUABLE

SEMPRE-BIO

FuelUp

ELOXYCHEM

HYDROGENi

… and dissemination on CAPE-open potential!

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Thank you for your kind attention

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