OCTOBER 24 2023

Empowering Reaction Engineering for a Net Zero Chemical Industry

Kevin M. Van Geem[1]

[1]Laboratory for Chemical Technology, Ghent University, Belgium
CTO CAPTURE

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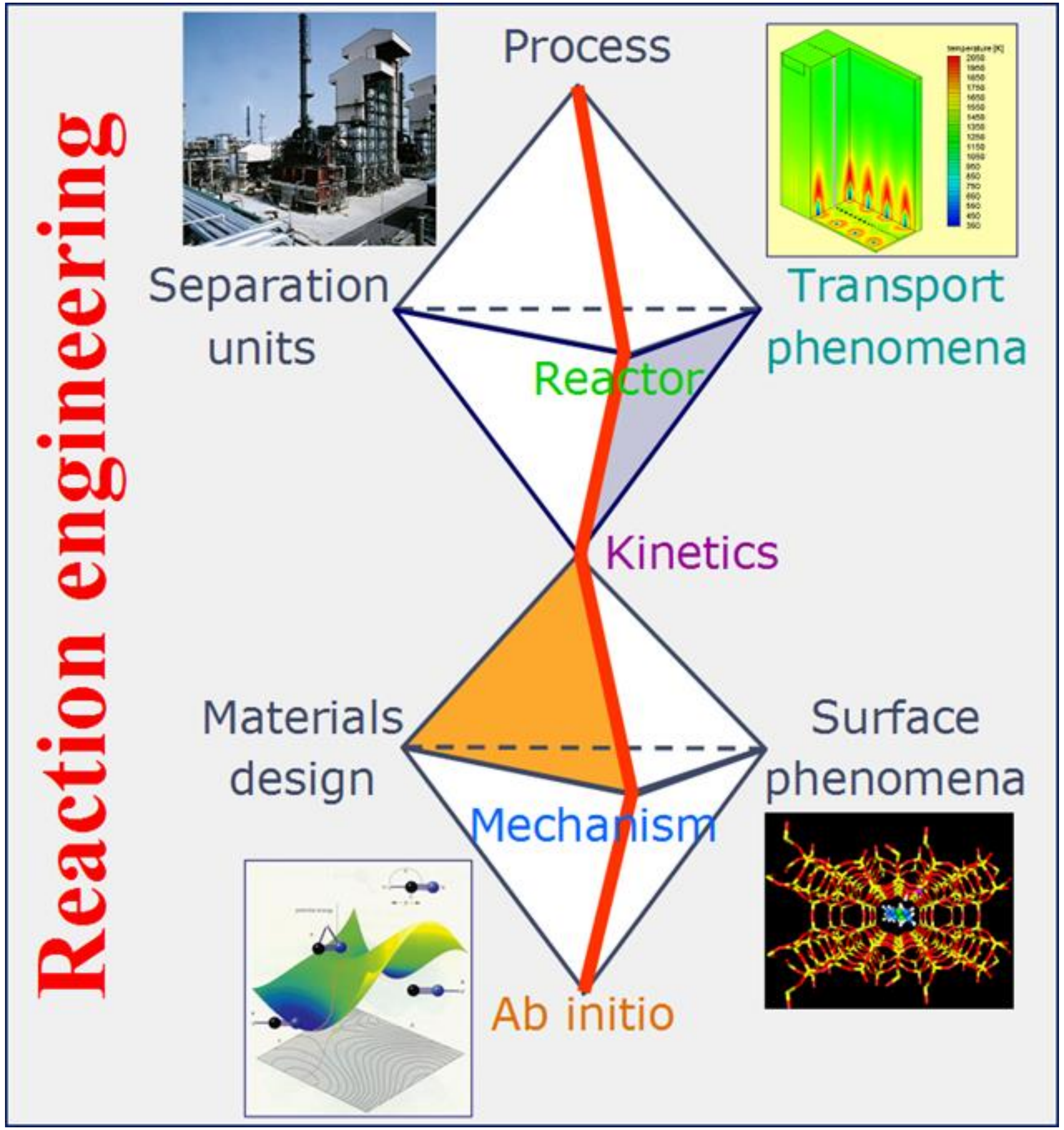
DRIVING CHEMICAL TECHNOLOGY

From molecule to process



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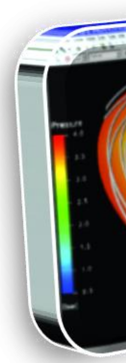
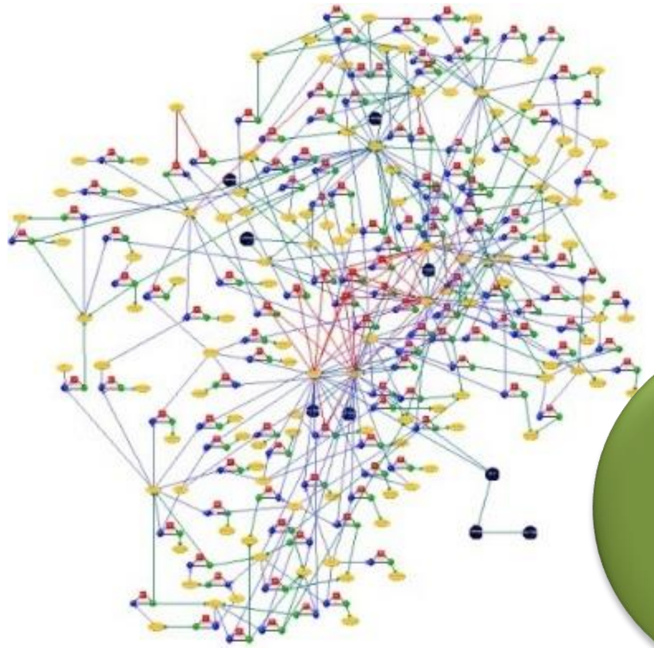
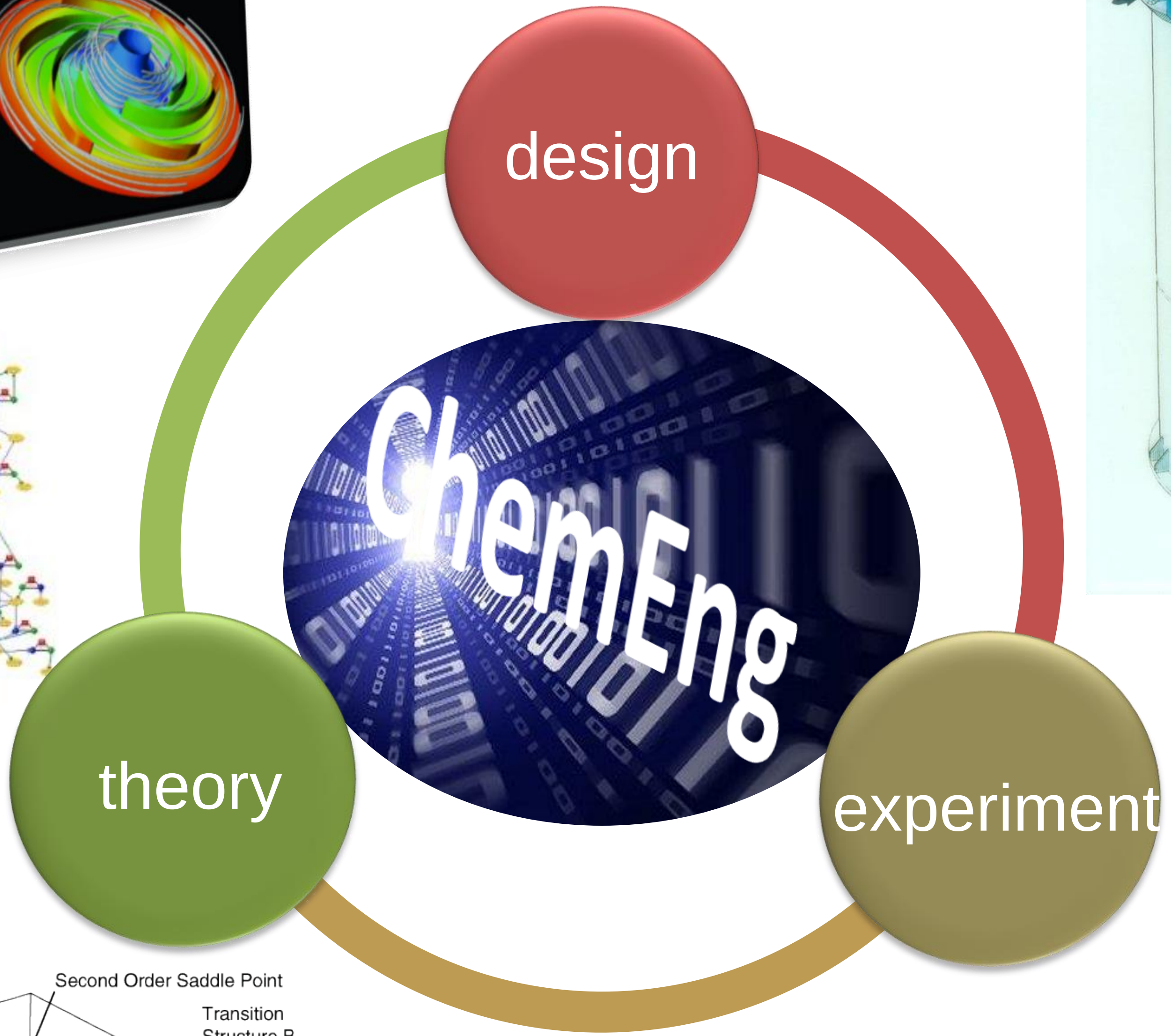
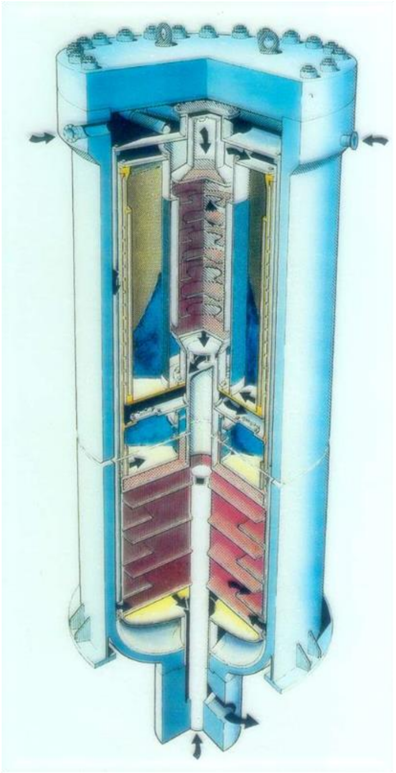
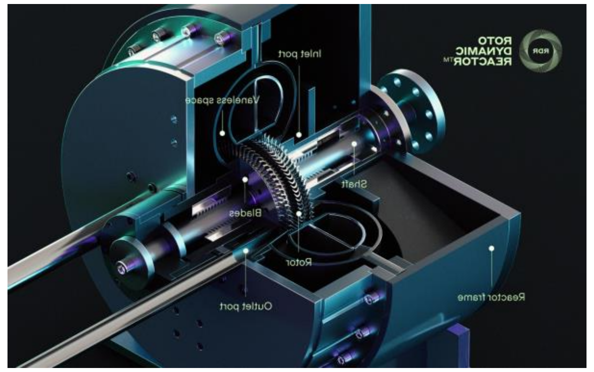
Chemical reaction and reactor engineering: a big driver

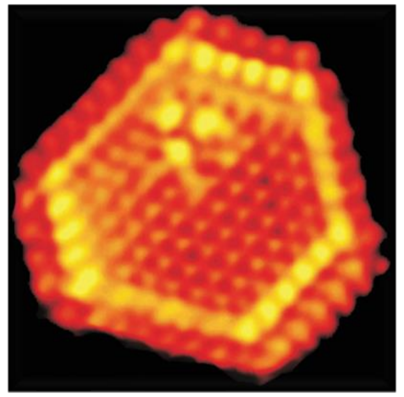


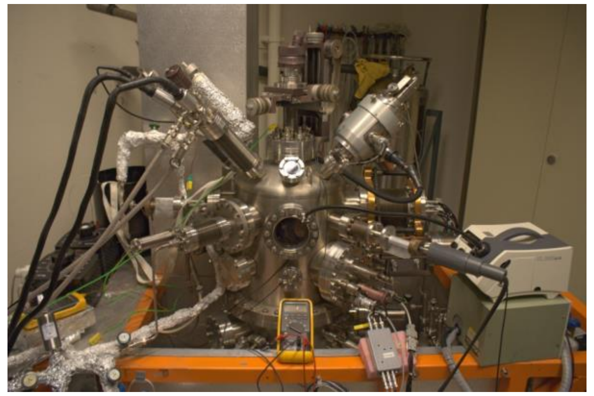


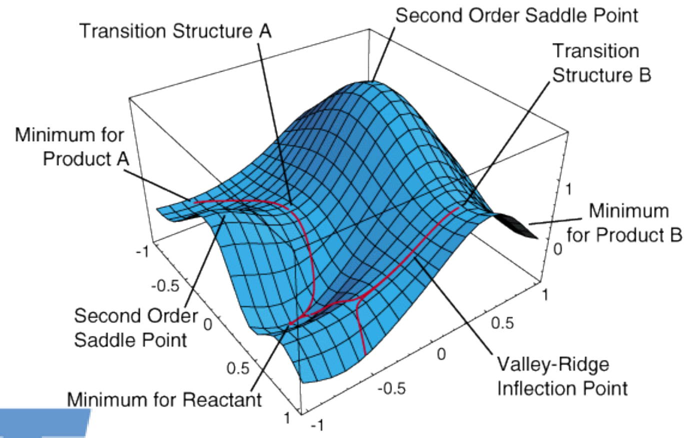


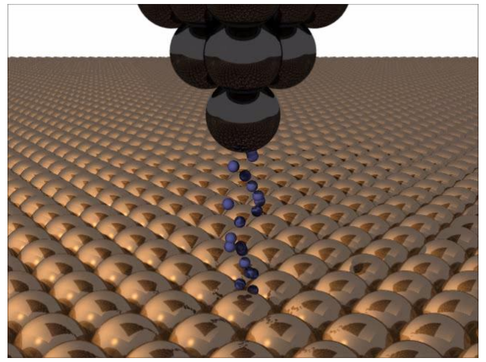












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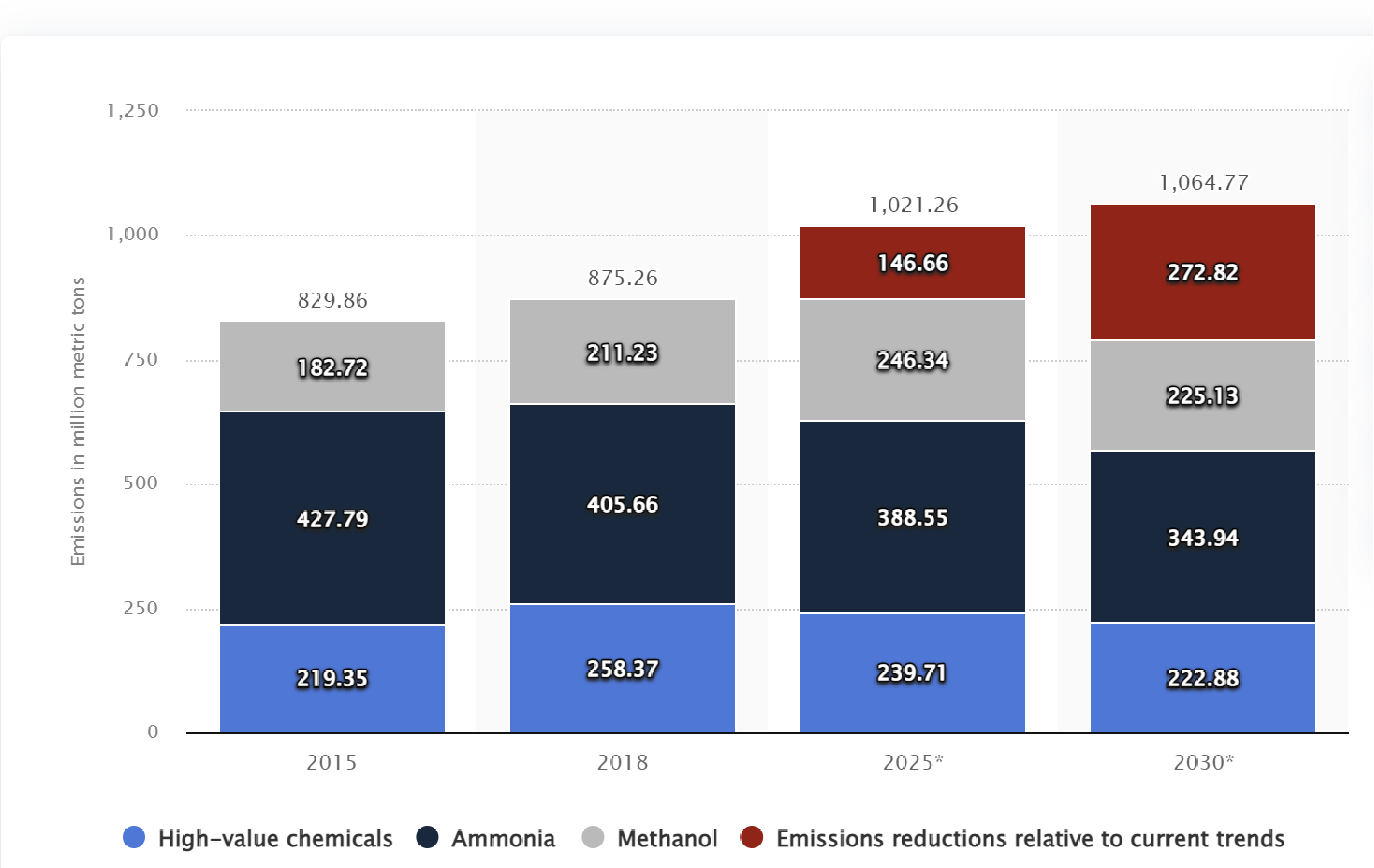
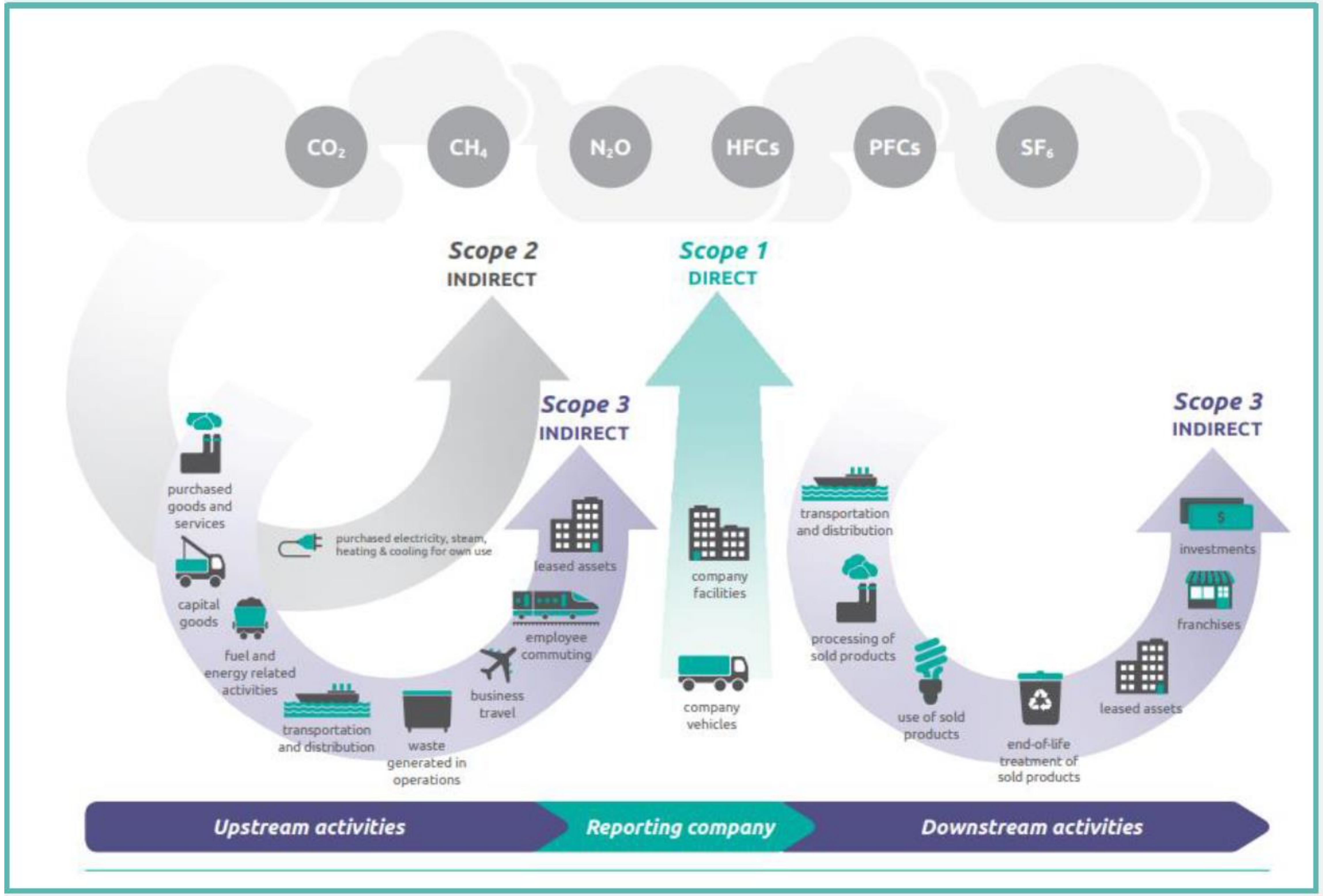
CO2 emissions of chemical production worldwide from 2015 to 2030, by chemical source

(in million metric tons)



https://www.statista.com/statistics/272474/emissions-of-the-chemical-industry-since-2000/

SCOPE definition according GHG protocol



- Scope 1 – All Direct Emissions from the activities of an organization or under their control. Including fuel combustion on site such as gas boilers, fleet vehicles and air-conditioning leaks.
- Scope 2 – Indirect Emissions from electricity purchased and used by the organization. Emissions are created during the production of the energy and eventually used by the organization.
- Scope 3 – All Other Indirect Emissions from activities of the organization, occurring from sources that they do not own or control. These are usually the greatest share of the carbon footprint, covering emissions associated with business travel, procurement, waste and water.

Unlike LCA, GHG protocol standards estimate the GHG footprint and are based on ISO 14064

GHG protocol for the chemical industry

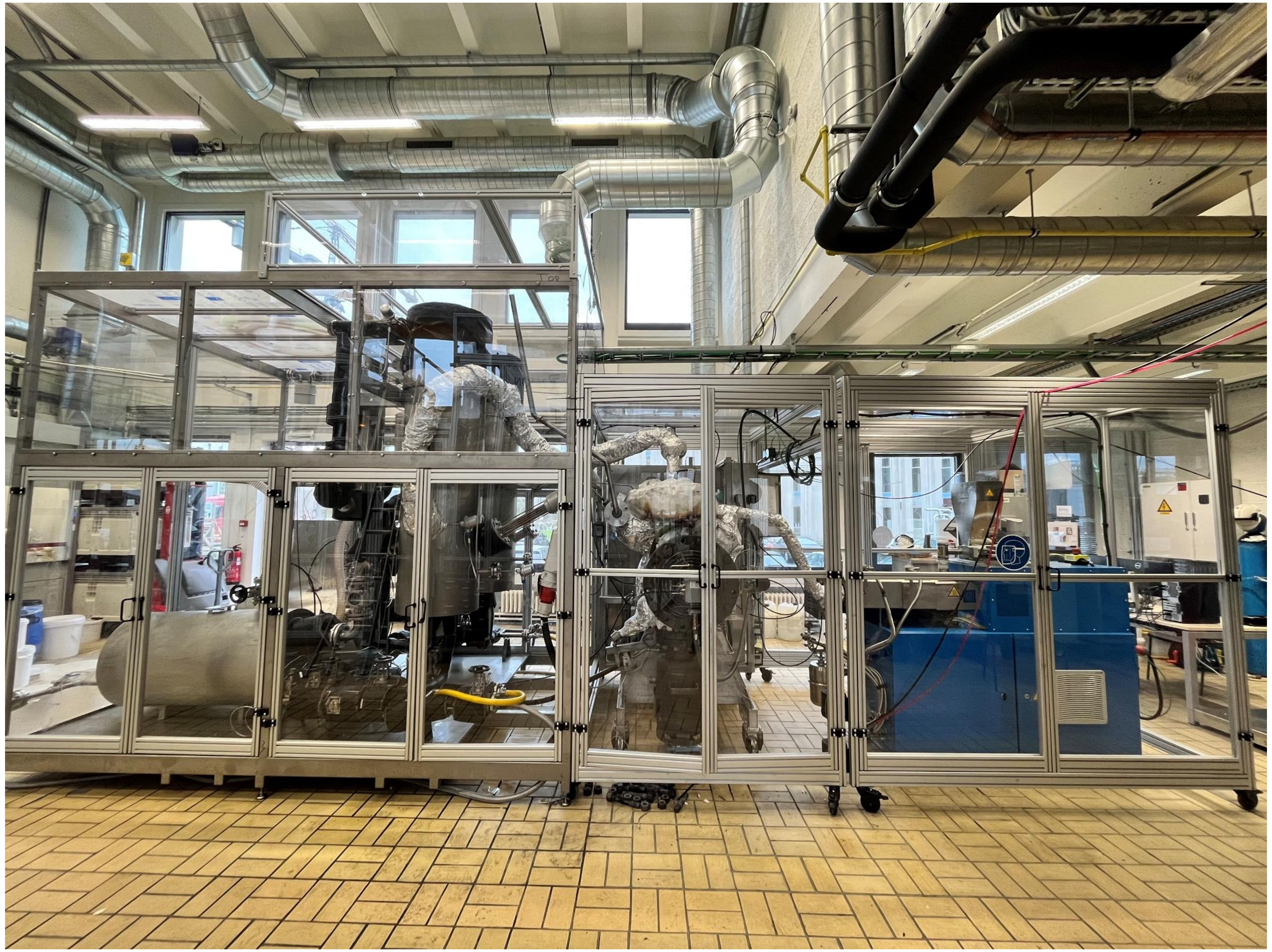
- '….I applaud the breadth and depth of this unprecedented report that quantitatively analyzed pathways for **the chemical industry to reach net zero not only in scope 1 & 2, but also scope 3 upstream and downstream**….'
- '…..The production of basic chemical intermediates in-scope for this report has a Scope 1, 2 & 3 emissions of 2.3 Gt CO_{2eq}, representing just under 4% of the 59 Gt global annual emissions and an estimated 72% of all chemical system emissions. Within the 2.3 Gt, Scope 3 represents the majority at 64% (1.5 Gt CO_{2eq}), while Scope 1&2 only represent 36% (0.8 Gt CO_{2eq}). **The magnitude of Scope 3 in the chemical system is driven by its dependence on fossil, leading to high upstream scope 3 emissions from oil and gas extraction (0.5 Gt CO_{2eq}), as well as carbon-dense products such as plastics and urea resulting in high associated downstream Scope 3 emissions (1.0 Gt CO_{2eq}). It is for this reason that focusing on Scope 3 in the chemical system transition to net zero is so essential**…..'
- '….There is growing recognition that the chemical industry needs to address its Scope 1&2 and, **increasingly, end-of-life Scope 3 emissions**….'
- '….**The vast bulk of total in-scope system emissions stem from Scope 3 (~64% today).** Therefore, abating Scope 3 is the biggest driver for system emissions reduction and the driver of the bulk of the technology shifts needed to abate the system…'

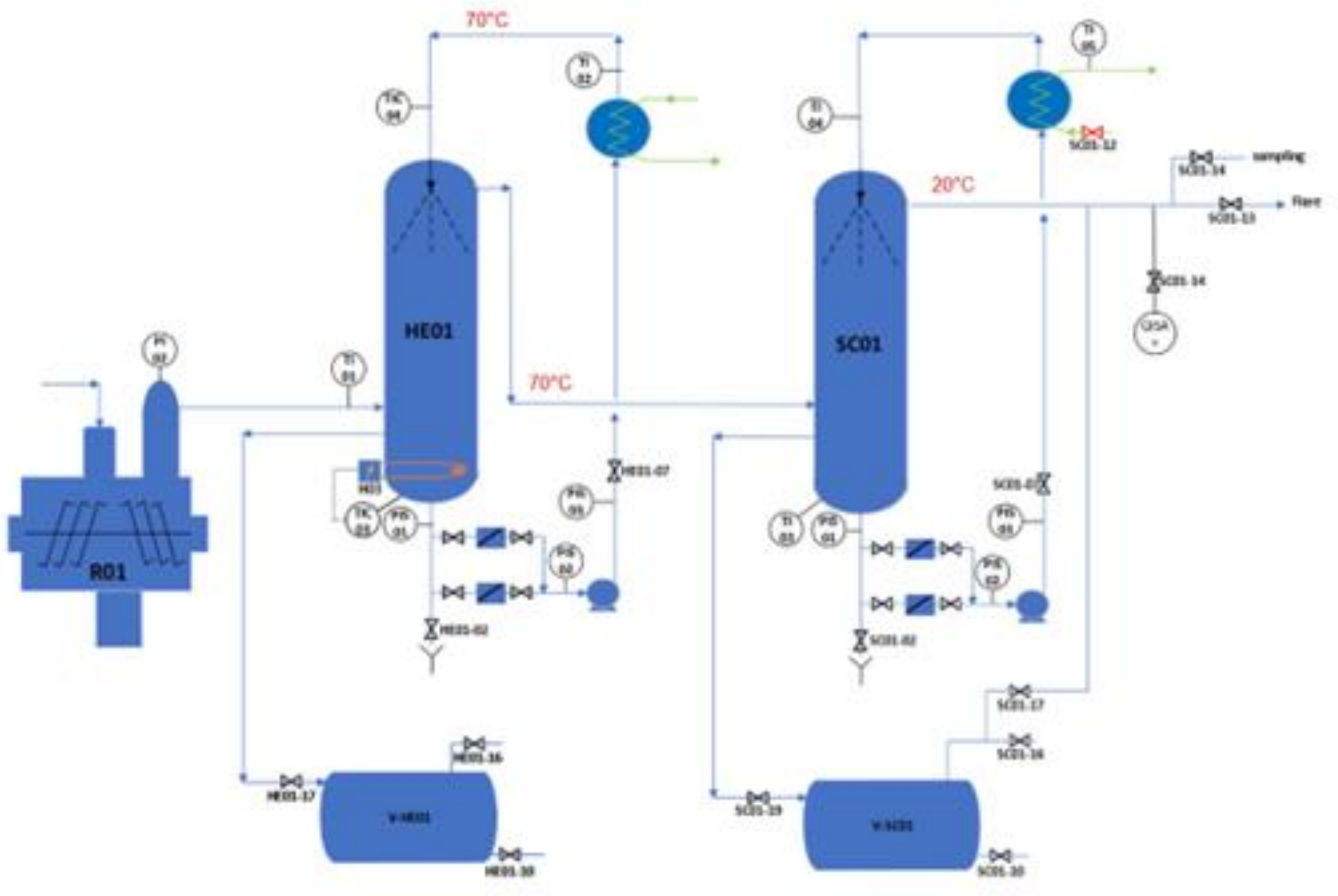
From a report commissioned by The Center for Global Commons, The University of Tokyo, Japan. Published September 2022. (Refer https://www.systemiq.earth/planet-positive-chemicals/)

Accurate experimental data for plastic waste conversion

We need experimental data!

New large scale chemical recycling pilot





Impurity removal/reduction in extruder

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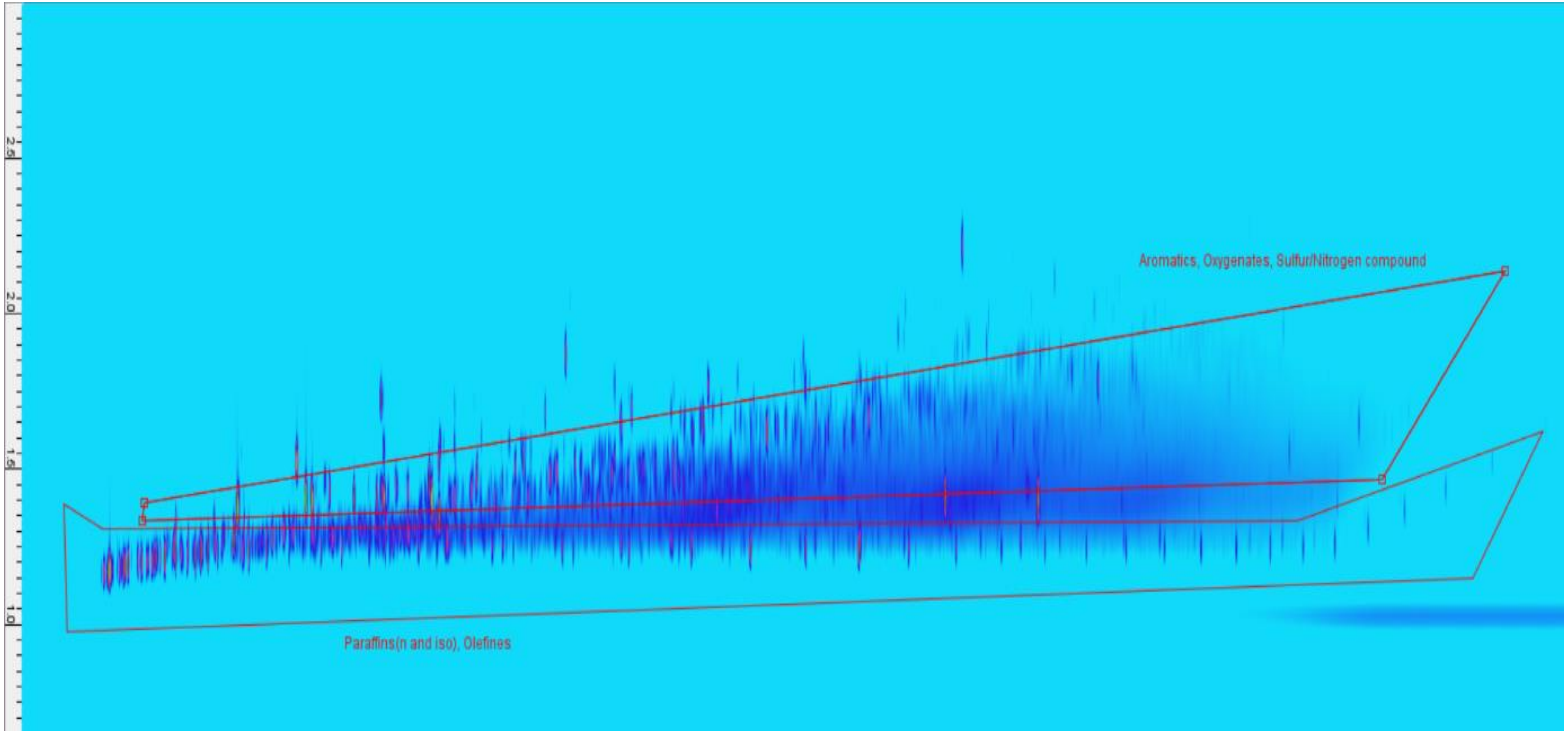
Typical more complex than what managers want!



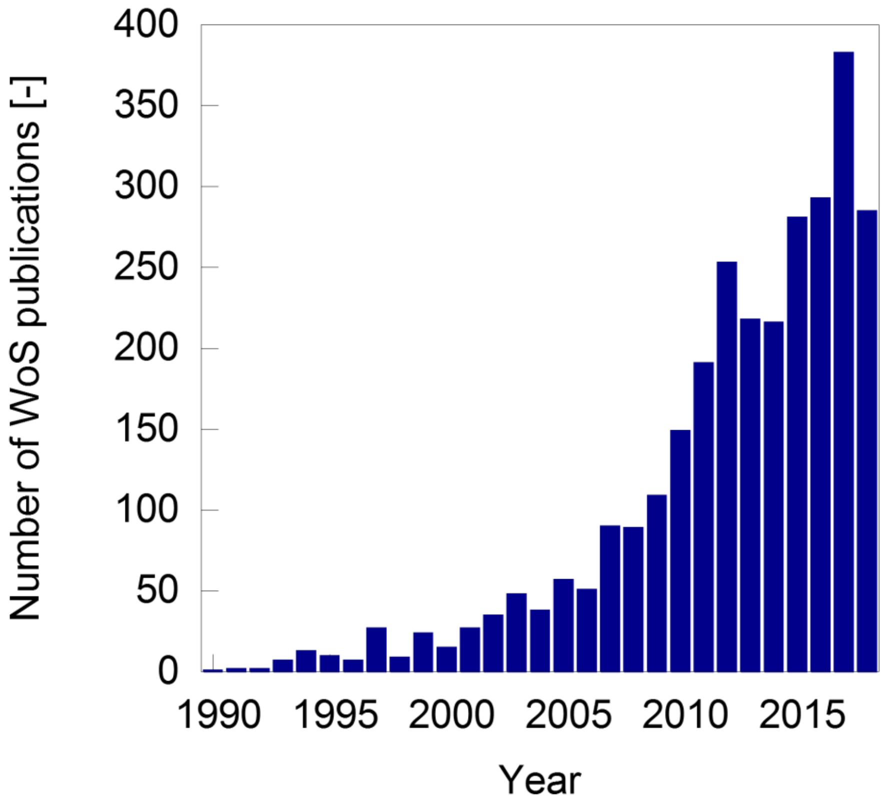
Process intensification:

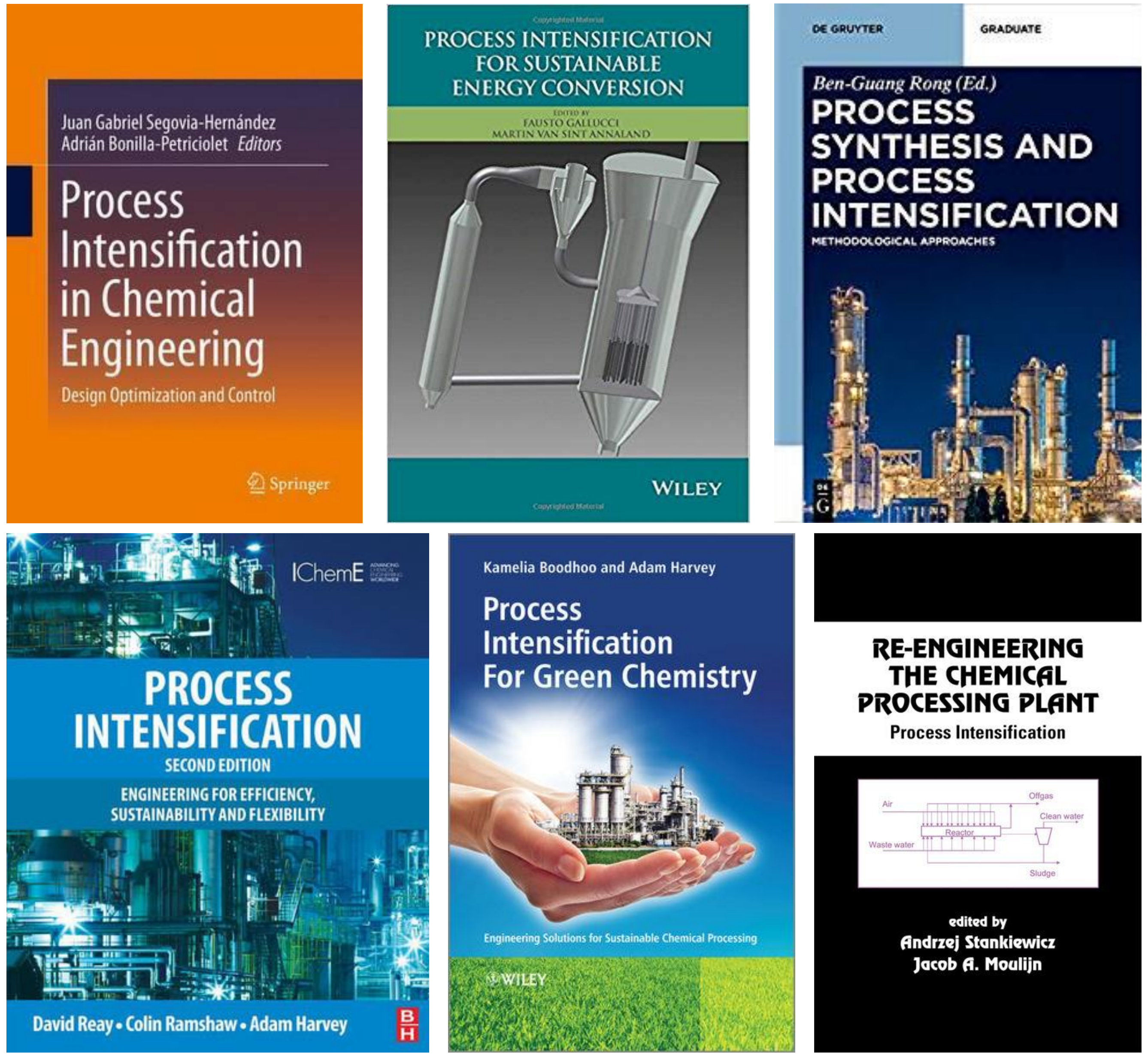
develop new technology

Process intensification – what?

"any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology"

A. Stankiewicz, J. Moulijn





Juan Gabriel Segovia-Hernández
Adrián Bonilla-Petriciolet *Editors*
Process Intensification in Chemical Engineering
Design Optimization and Control
Springer

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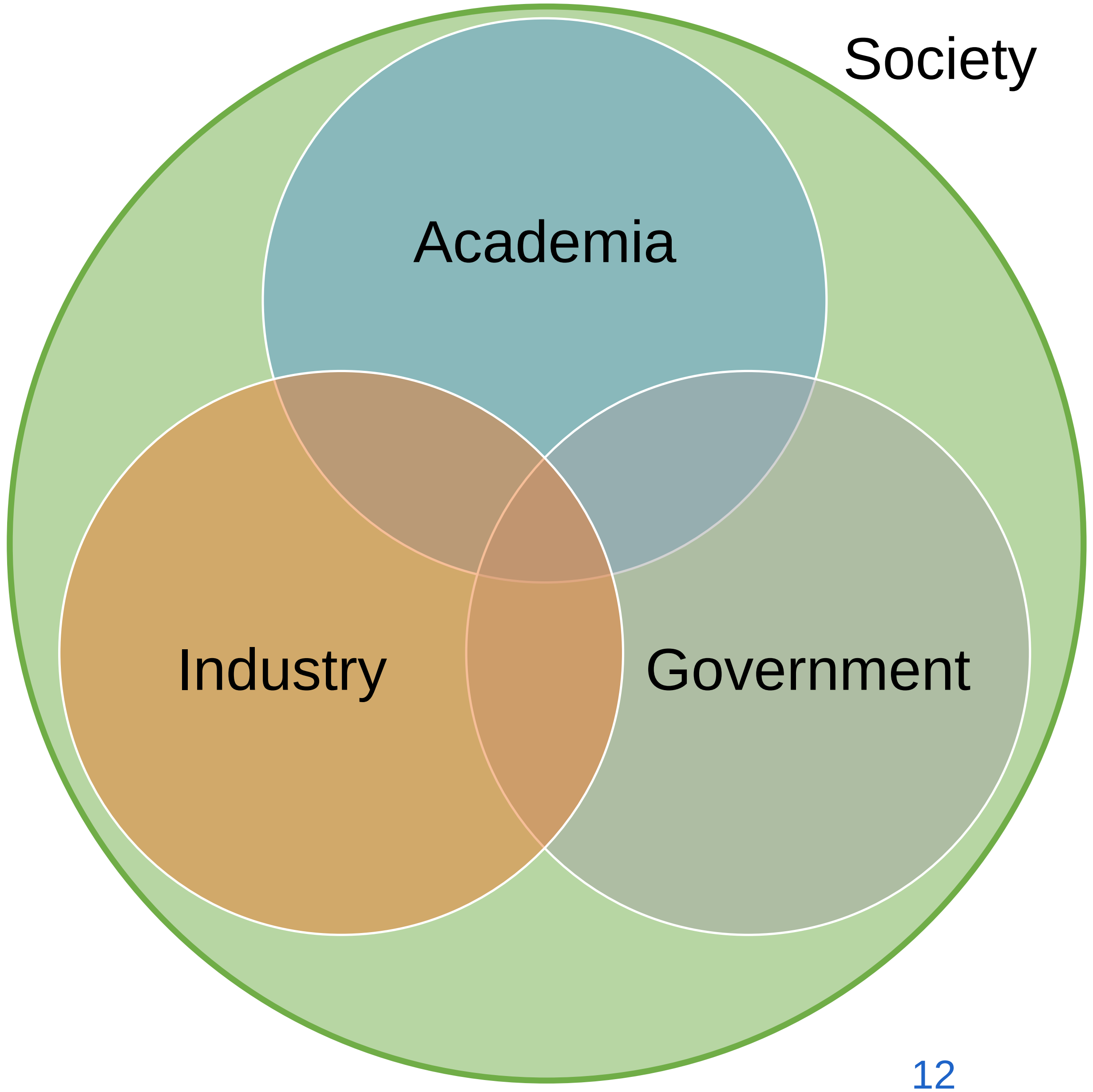
Process Intensification
edited by
Andrzej Stankiewicz
Jacob A. Moulijn



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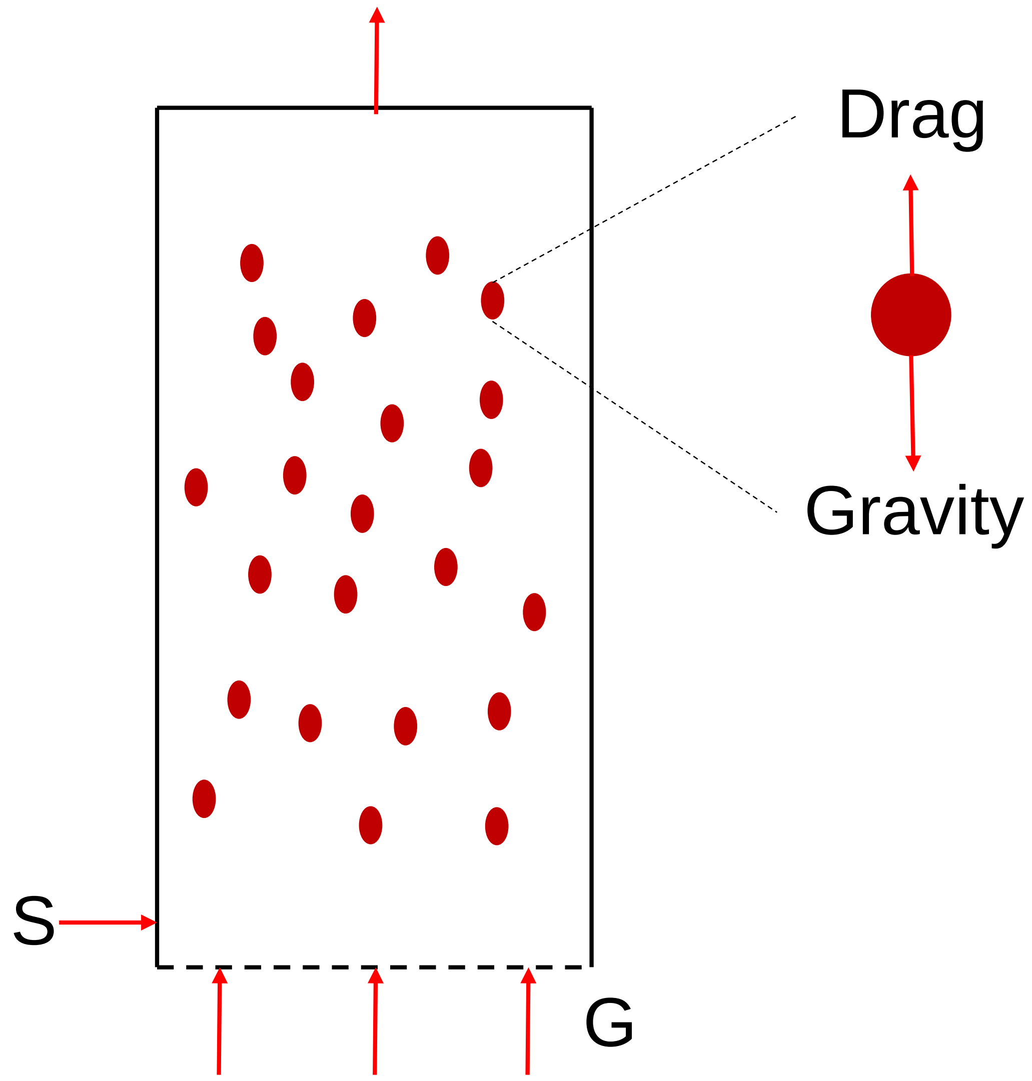
Stankiewicz, A. I.; Moulijn, J. A., Process Intensification: Transforming Chemical Engineering. Chemical Engineering Progress 2000, 22.
https://www.ugent.be/csc/en

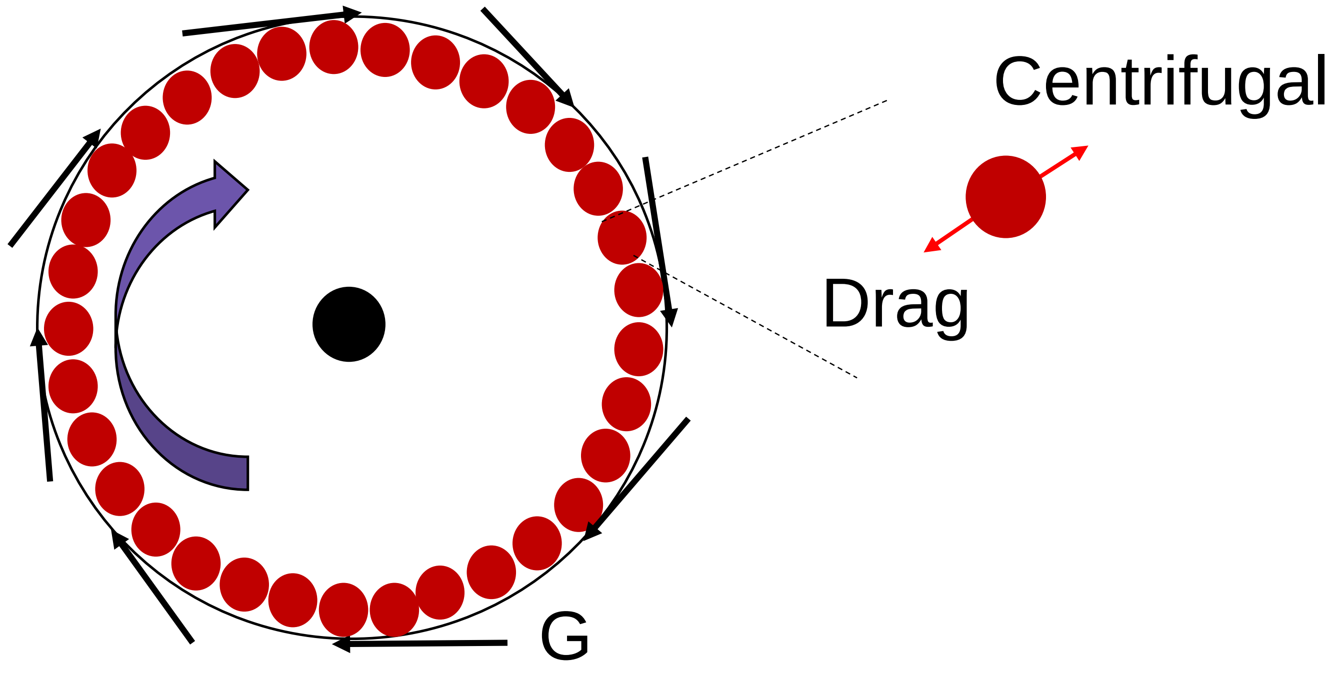
Multiphase Chemical Reactors



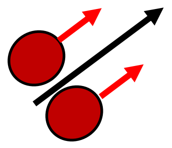
- Gas flow restrictions
- Dilute beds

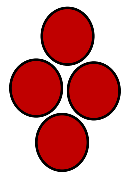
Fluidized Bed Reactor

Gas-Solid Vortex Reactors



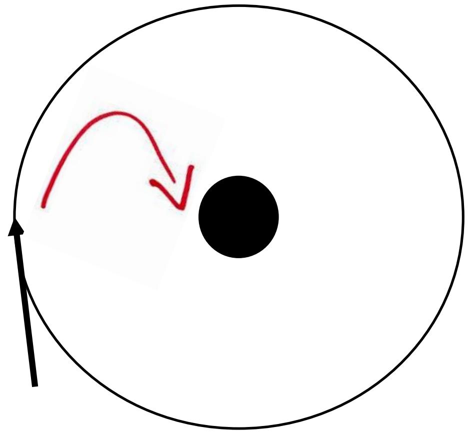
Gas-Solid slip velocities





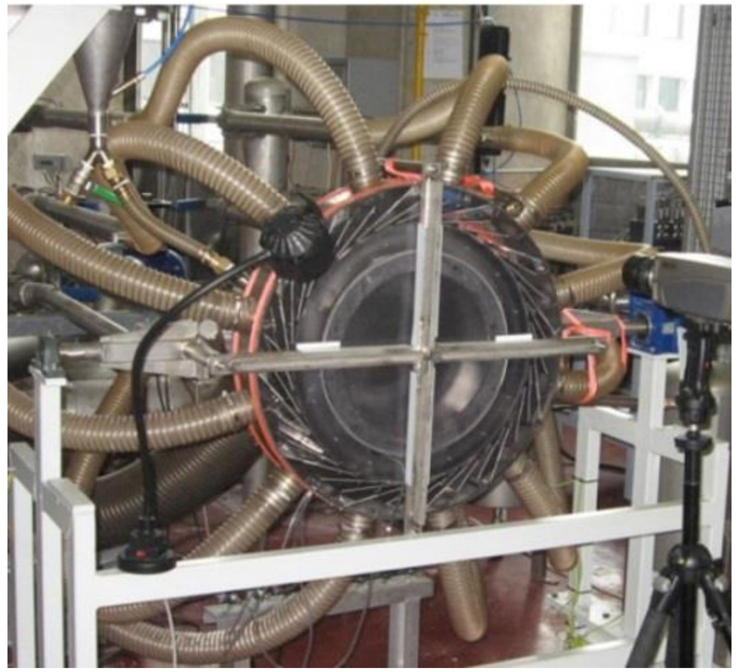
Packed beds

Short Gas Residence time



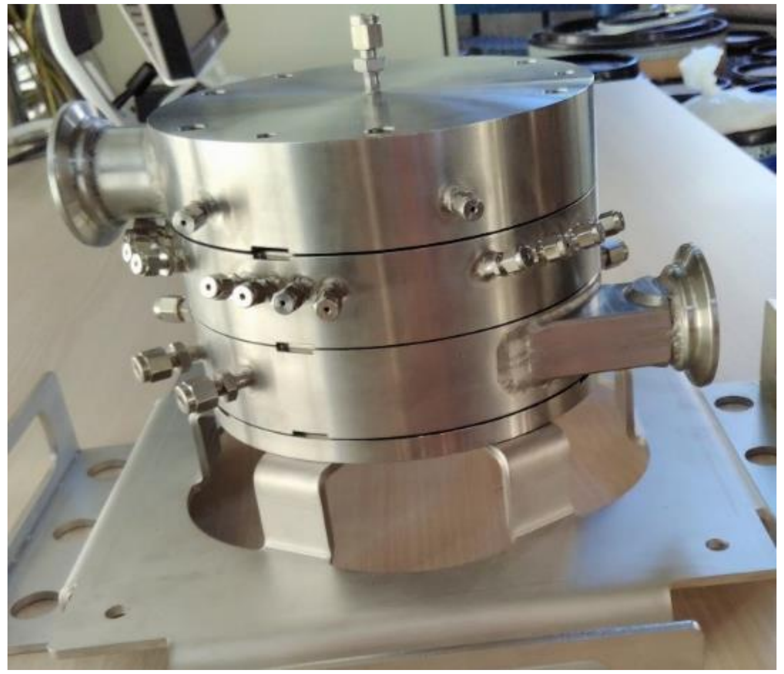
Process intensification in terms of heat & mass transfer

GSVR

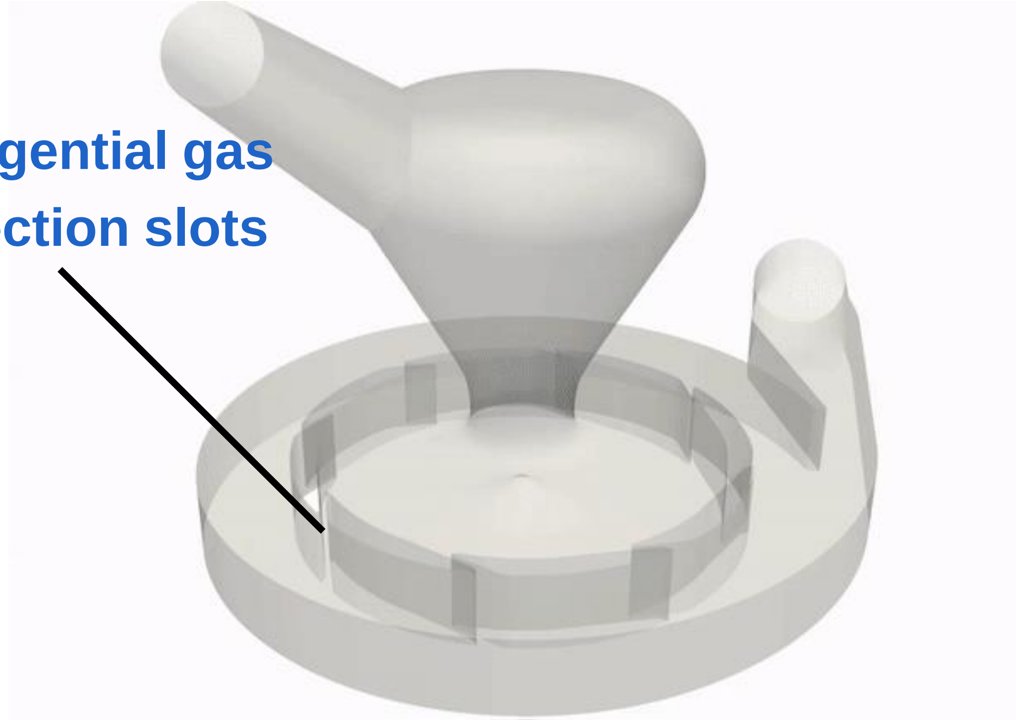


Cold flow

Hot flow



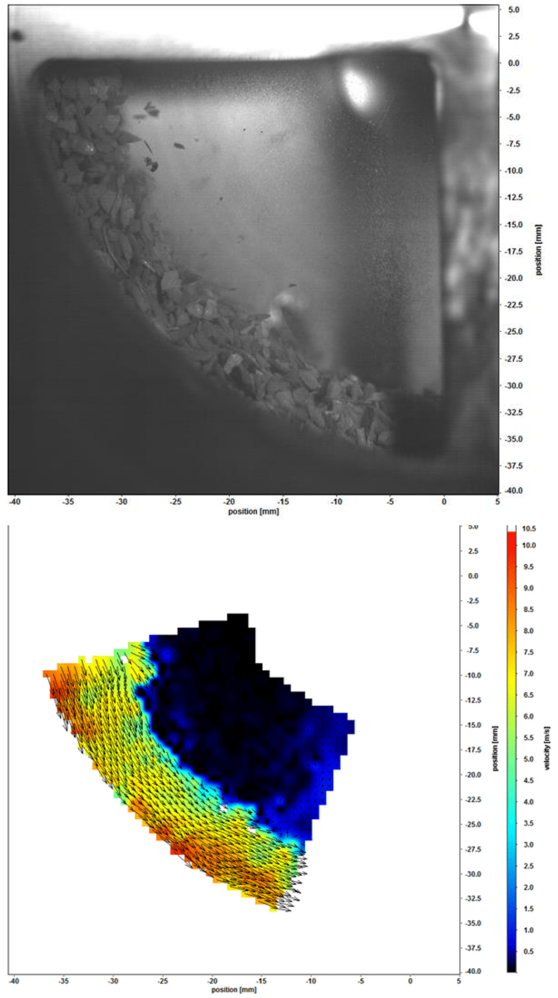
Reactive flow



Tangential gas injection slots

Rotating bed in vortex reactor

Gas-Solid

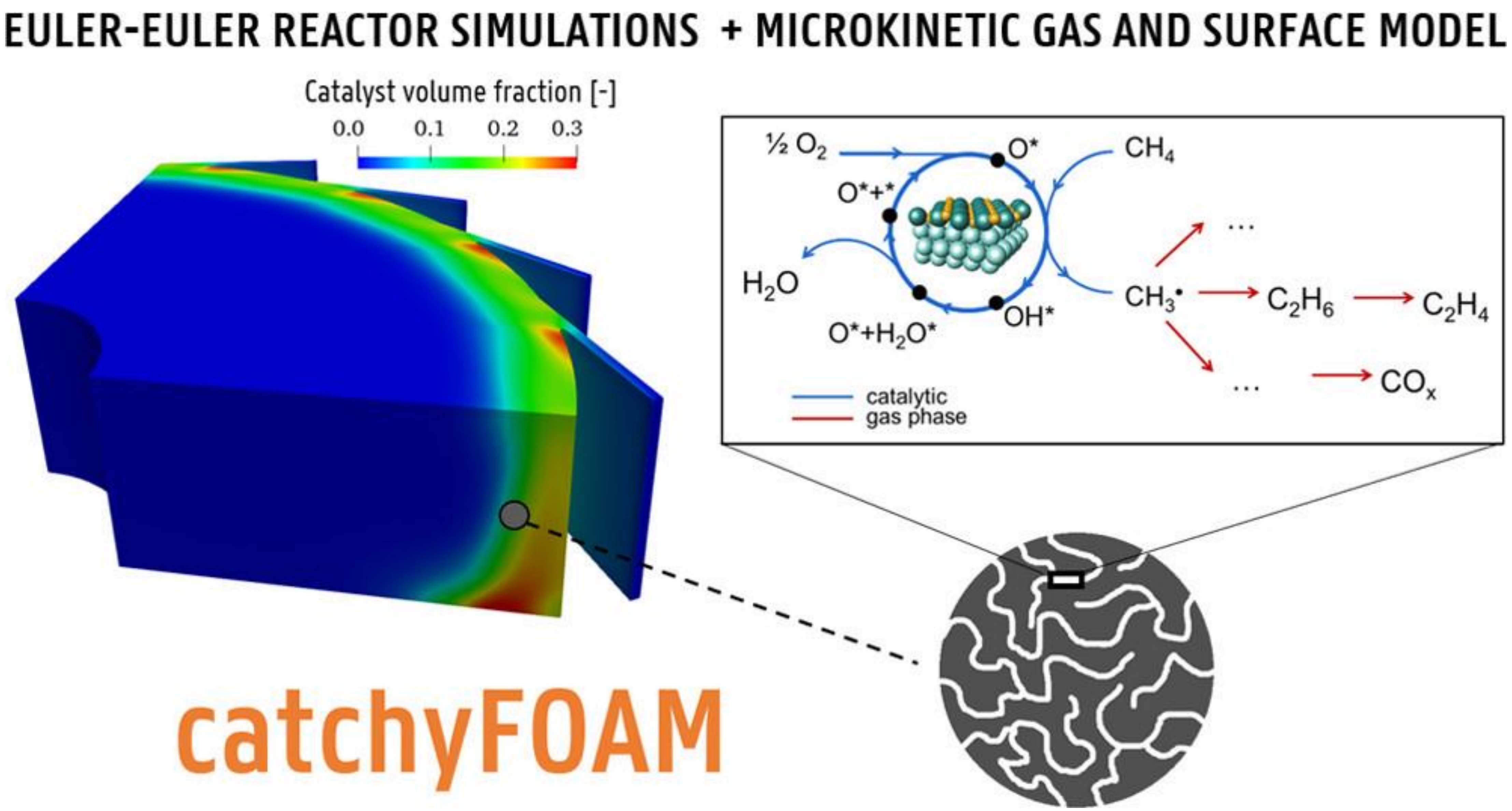


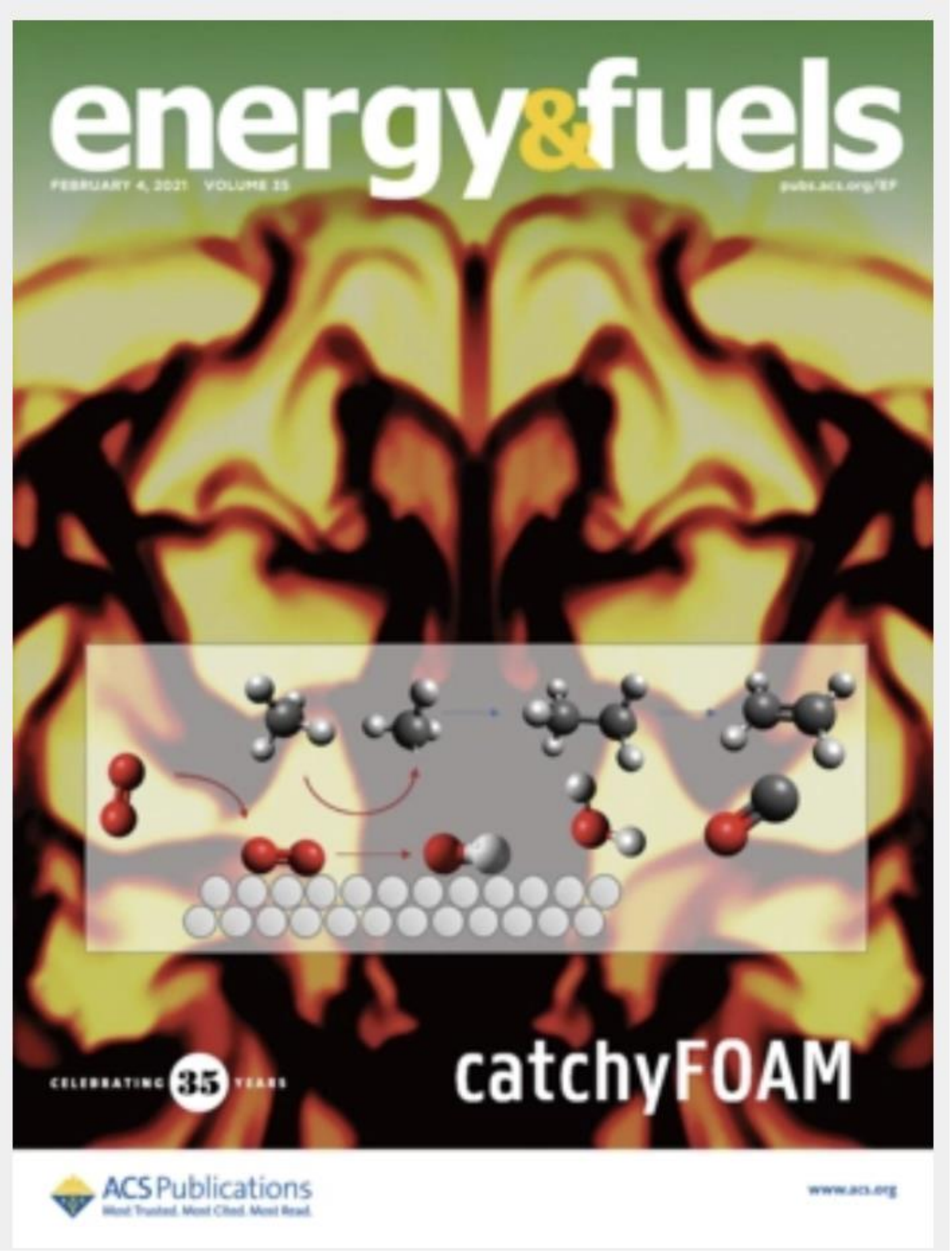
- High interphase slip velocity
- Strong vortex flow and centrifugal force field
- No mechanical rotation
- Small equipment size

- Low solids loading
- High gas flow rate
  - low residence time of gas
  - Loss of gas energy

Gonzalez-Quiroga, Arturo, et al. "Azimuthal and radial flow patterns of 1g-Geldart B-type particles in a gas-solid vortex reactor." Powder Technology 354 (2019): 410-422.

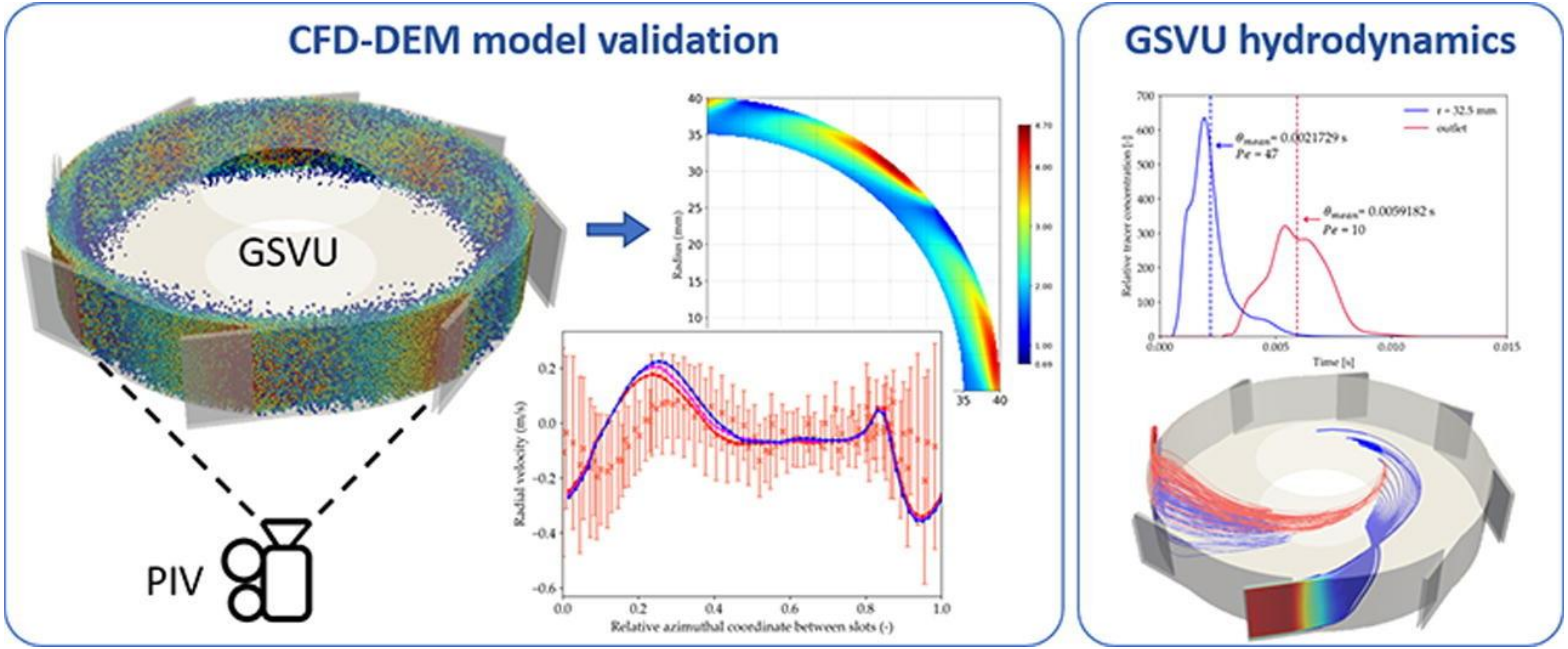
catchyFOAM

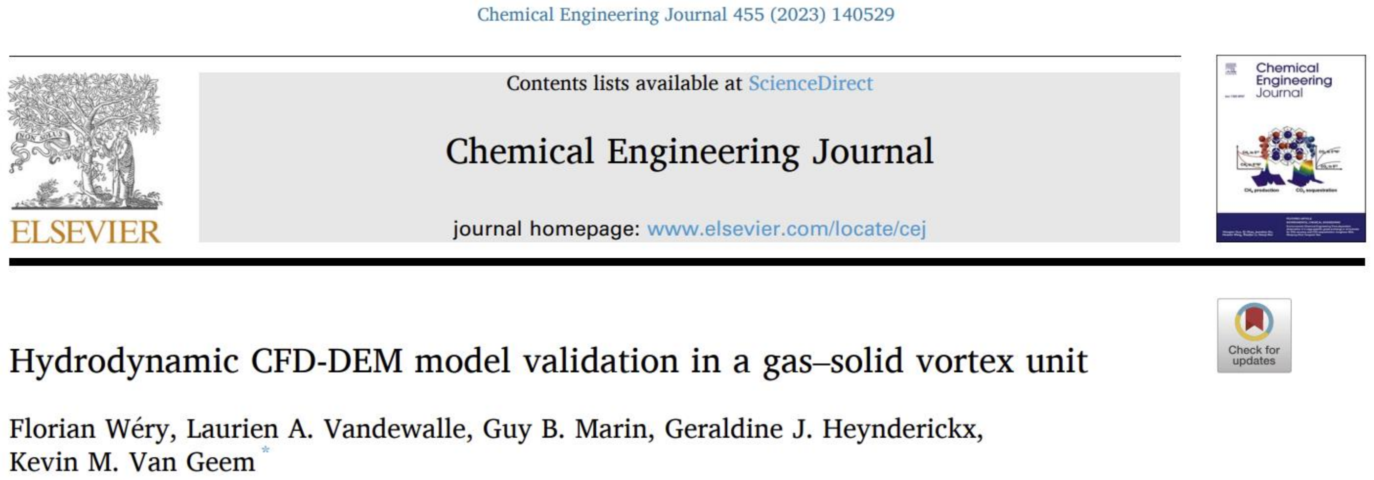




https://github.com/lavdwall/catchyFOAM

Vortex dryer: design by CFD DEM




Chemical Engineering Journal 455 (2023) 140529

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journal homepage: www.elsevier.com/locate/cej

Hydrodynamic CFD-DEM model validation in a gas–solid vortex unit

Florian Wéry, Laurien A. Vandewalle, Guy B. Marin, Geraldine J. Heynderickx, Kevin M. Van Geem

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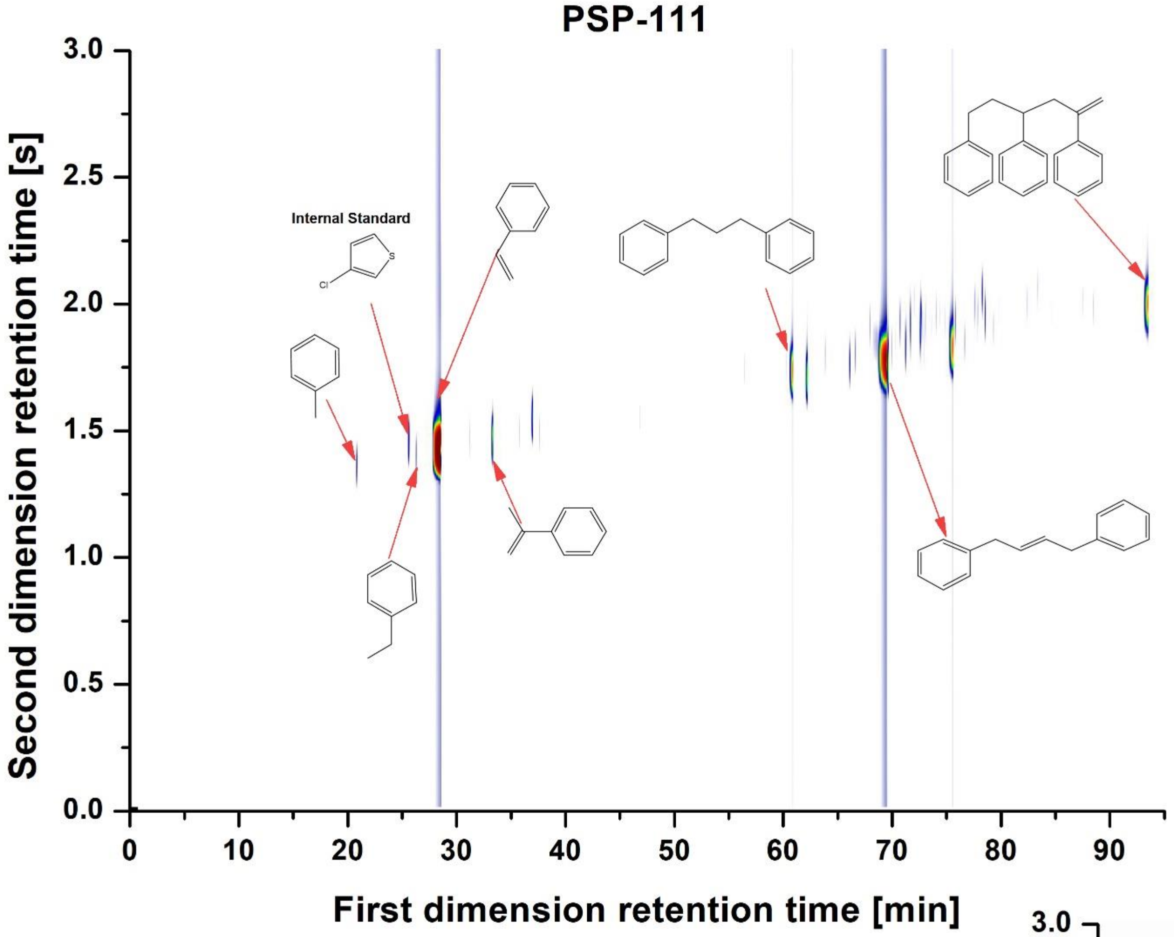
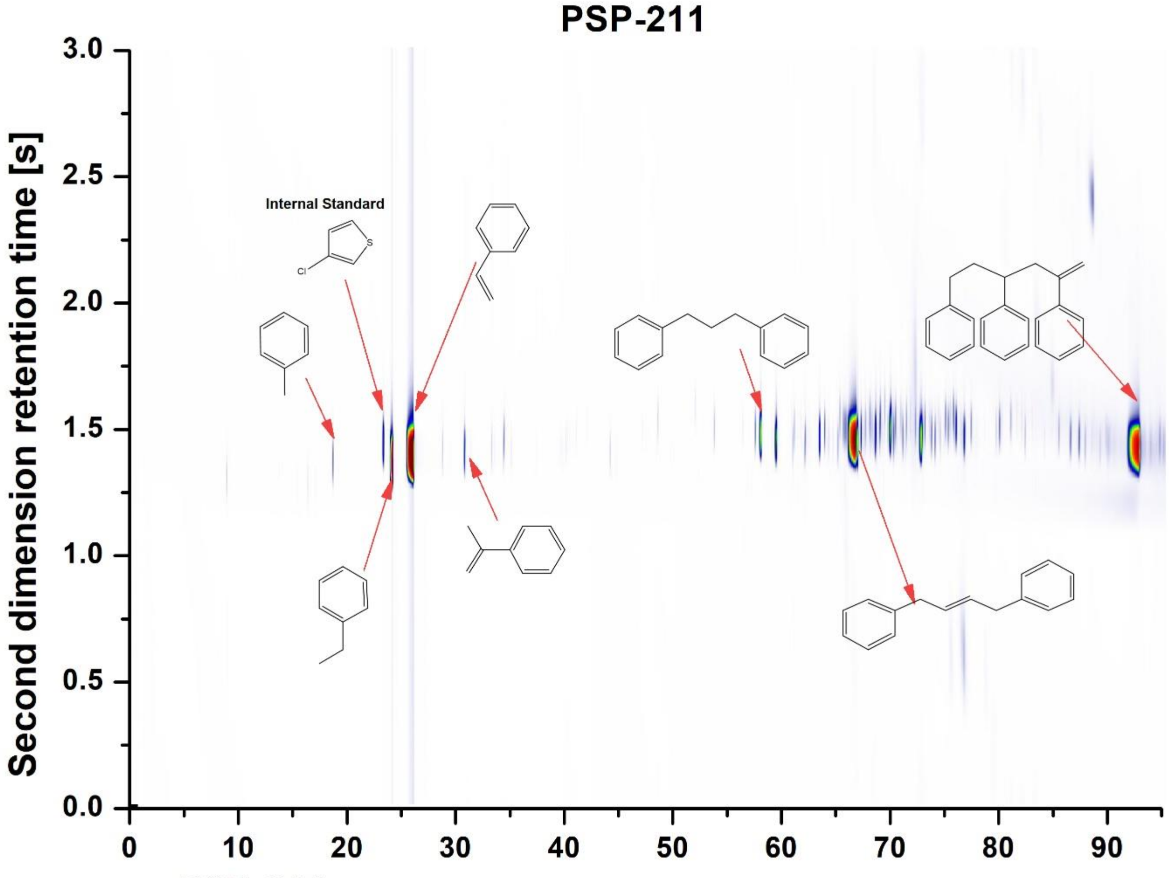
PS Pyrolysis Experiment in the VR

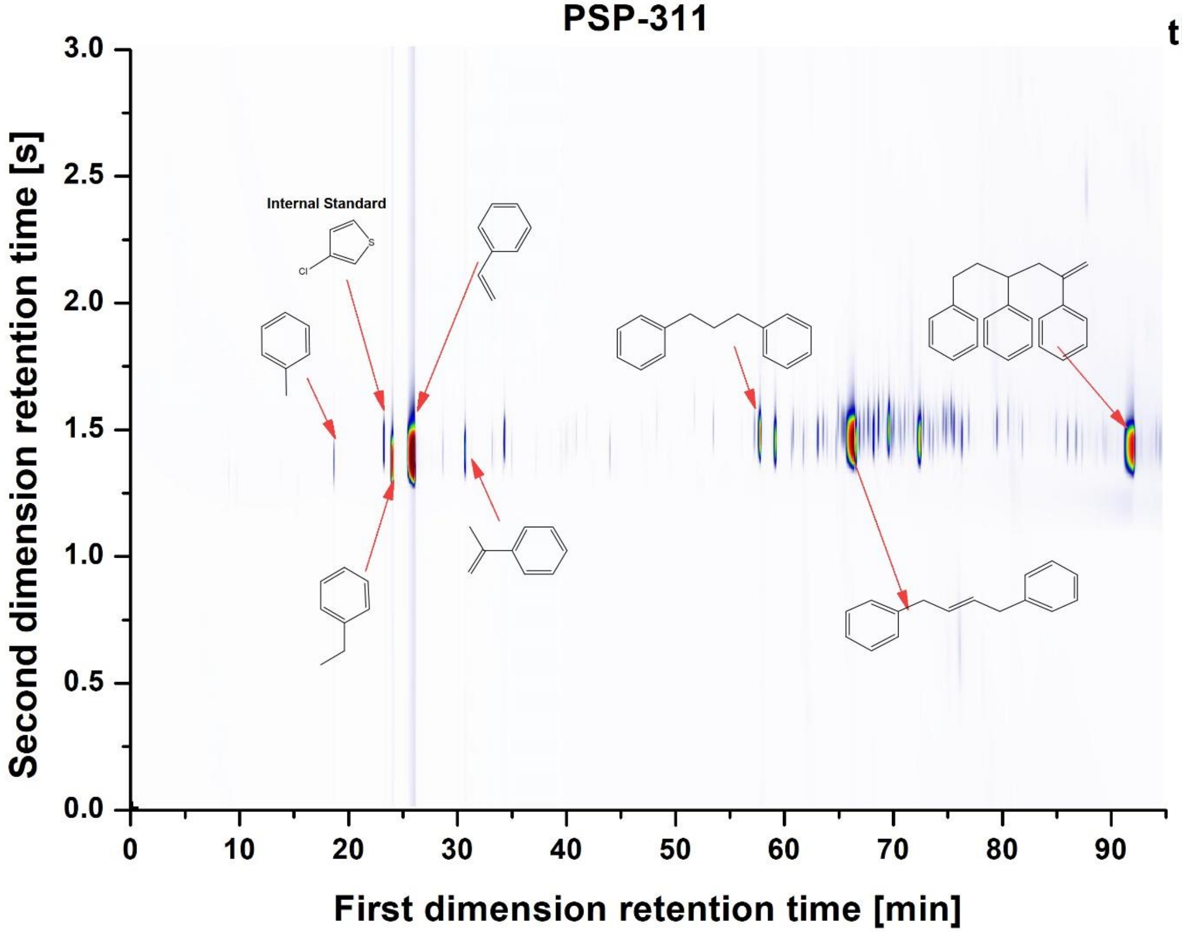
- Expected liquid production in PS pyrolysis ~ 70-90%
- High flow of gas → short residence time

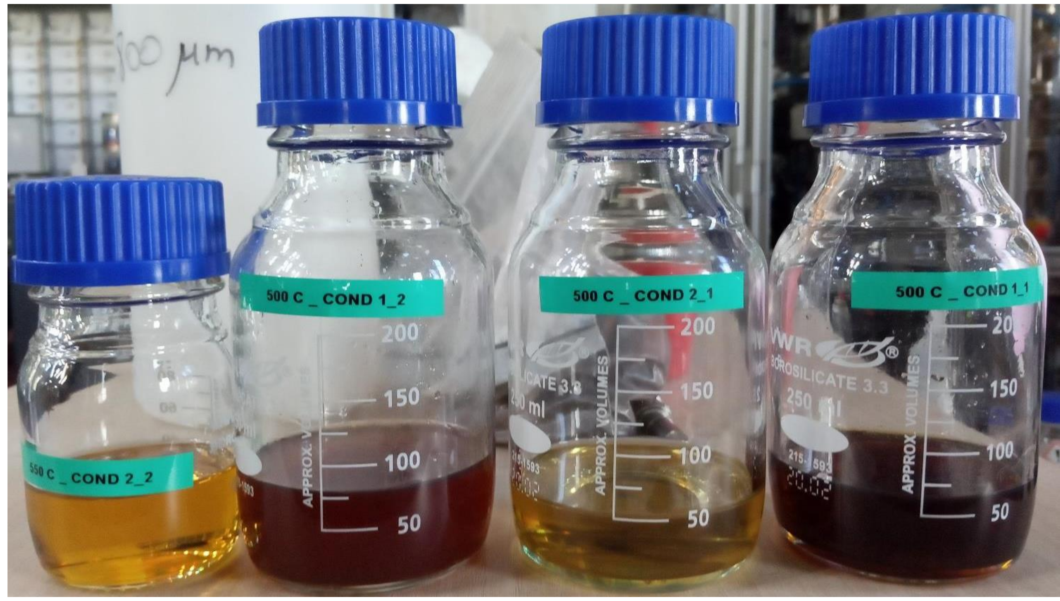
Challenges		**Possible Solutions**
Quantifying the liquid production rate	→	• Online sampling and analysis with injecting the IS
Collecting all the produced liquid	→	Modifying the condensers (Packing or S&T condenser)

Liquid Products Analysis





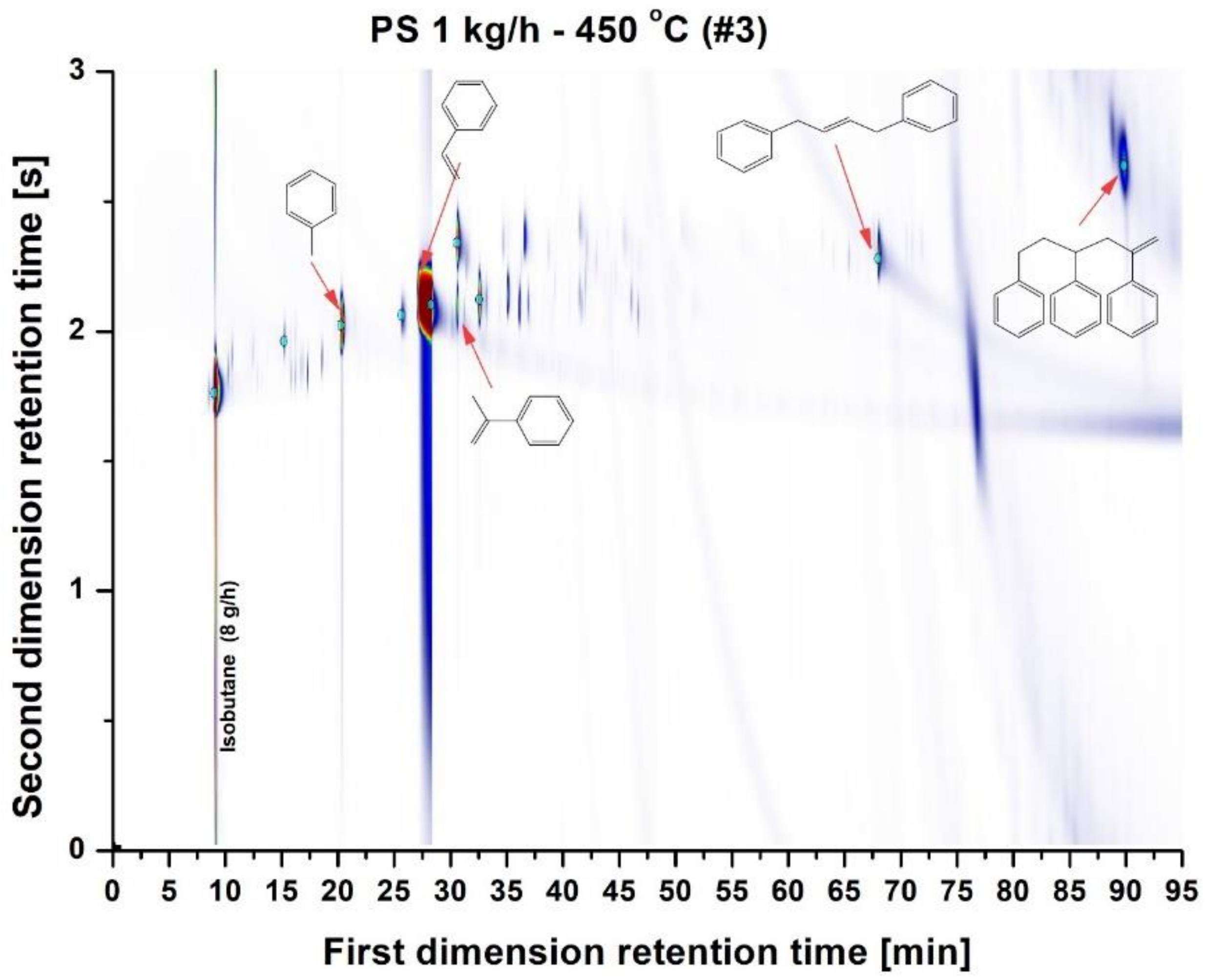


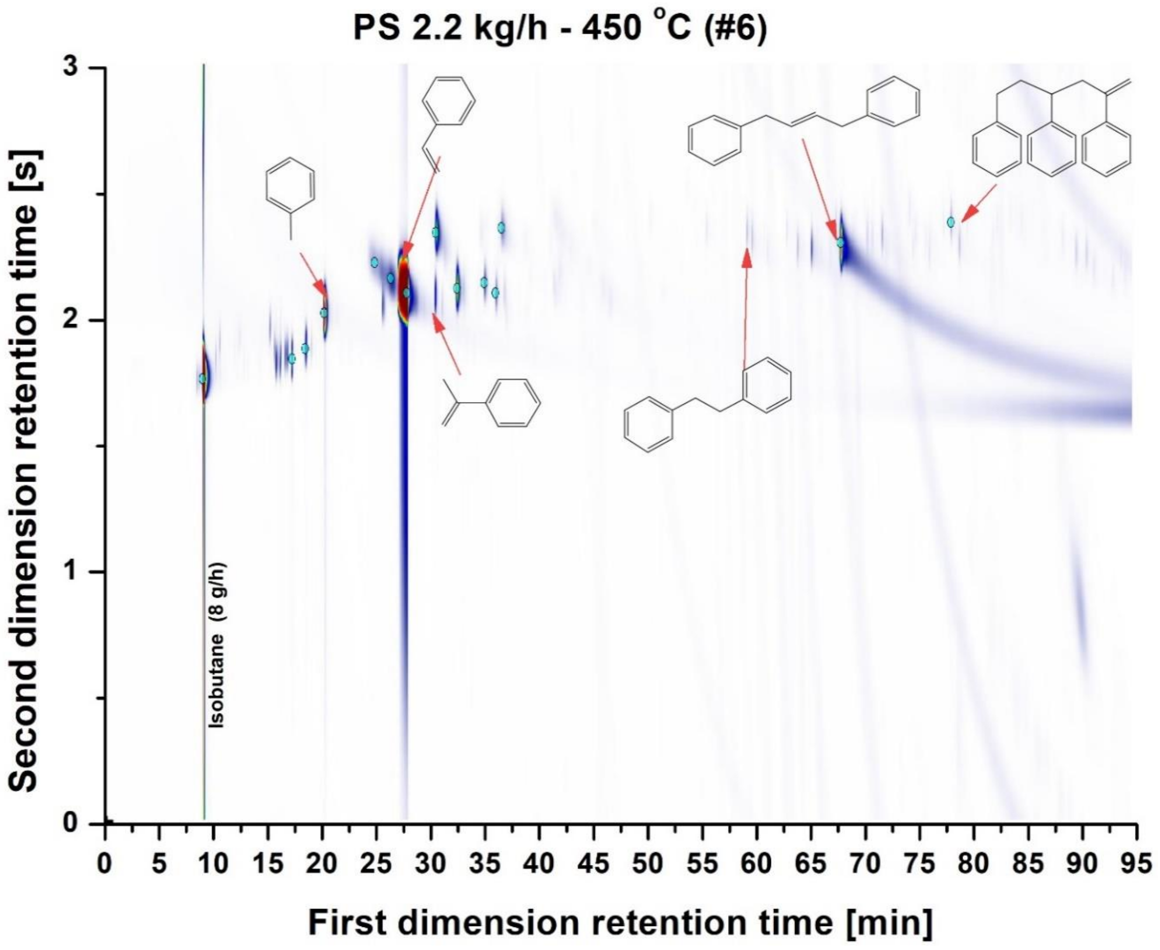


Results

Parameter	Values
PS flow rate [kg/h]	1.0, 2.2
Primary N_2 flow rate [Nm^3/h]	15
Average Bed Temperature (Bed and Throat) [ºC]	450

Species	Yield (%)		
	75th min	85th min	95th min
Benzene	0.6	0.4	0.3
Toluene	0.8	1.0	1.1
Ethylbenzene	0.3	0.1	0.2
Styrene	**91.0**	**95.4**	**95.8**
other monoaromatics	1.0	1.0	0.9
bis-phenyls	5.8	1.7	1.0
tris+-phenyls	0.0	0.0	0.0
Dimer	0.3	0.1	0.1
Trimer	0.0	0.0	0.0


PS 1 kg/h - 450 °C (#3)

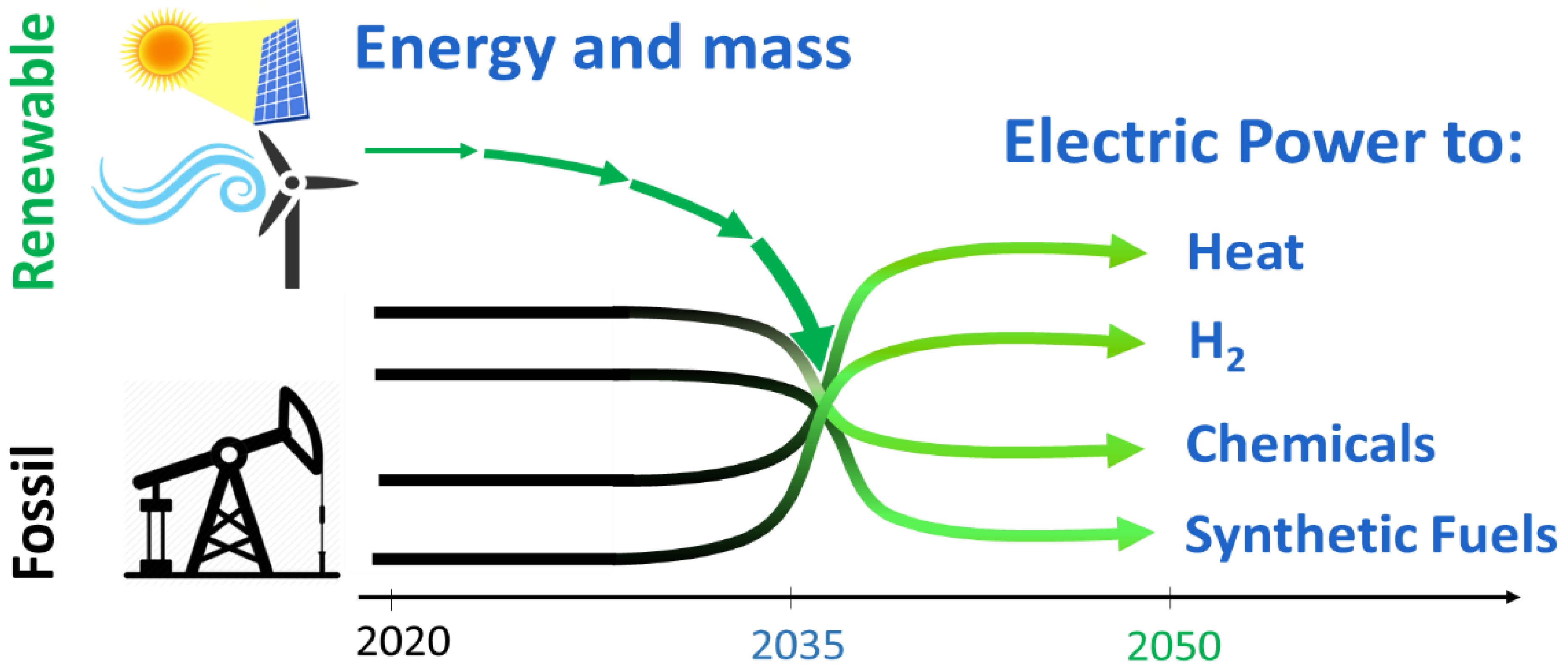

PS 2.2 kg/h - 450 °C (#6)

Electrification:

develop new technology

Electrification: defenition

– Electrification of the chemical industry is the use of electricity to drive a chemical process including conversion, separation, purification and providing the utilities to assist in operating and controlling the process



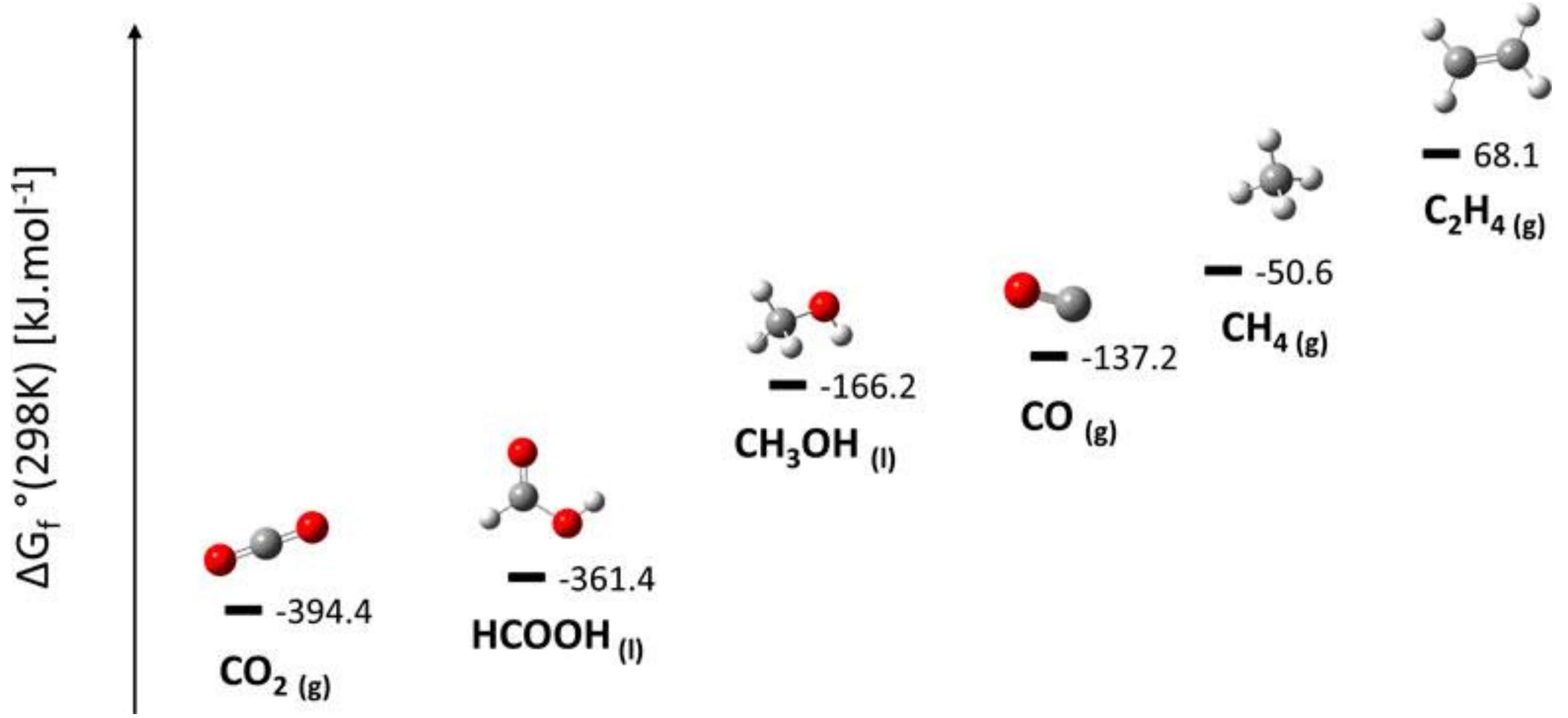
Making chemicals with electricity, **Kevin M. Van Geem, Vladimir V. Galvita, Guy B. Marin** *Science* 24 May 2019

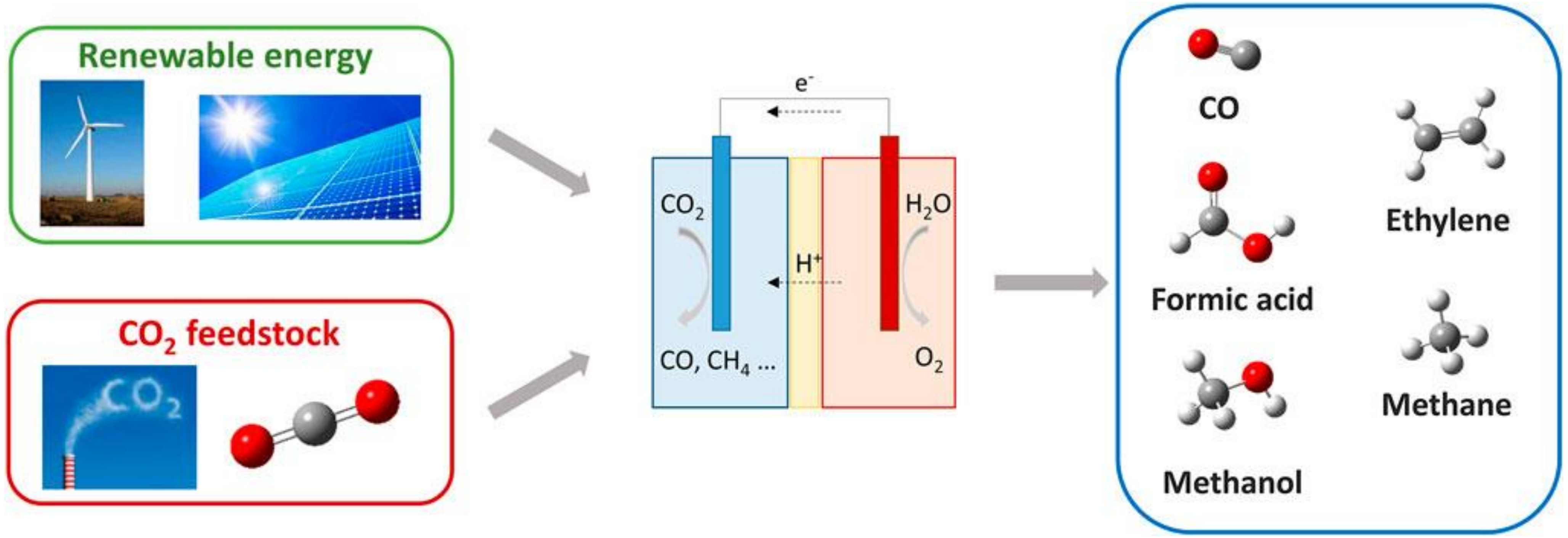
It is all about priority

Challenges and Opportunities of Carbon Capture and Utilization: Electrochemical Conversion of CO_2 to Ethylene

Cato A. R. Pappijn[1], Matthijs Ruitenbeek[2], Marie-Françoise Reyniers[1] and Kevin M. Van Geem[1]*

[1] Laboratory for Chemical Technology, Department of Materials, Textiles and Chemical Engineering, Ghent University, Ghent, Belgium
[2] Dow Benelux BV, PSPH R&D, Terneuzen, Netherlands





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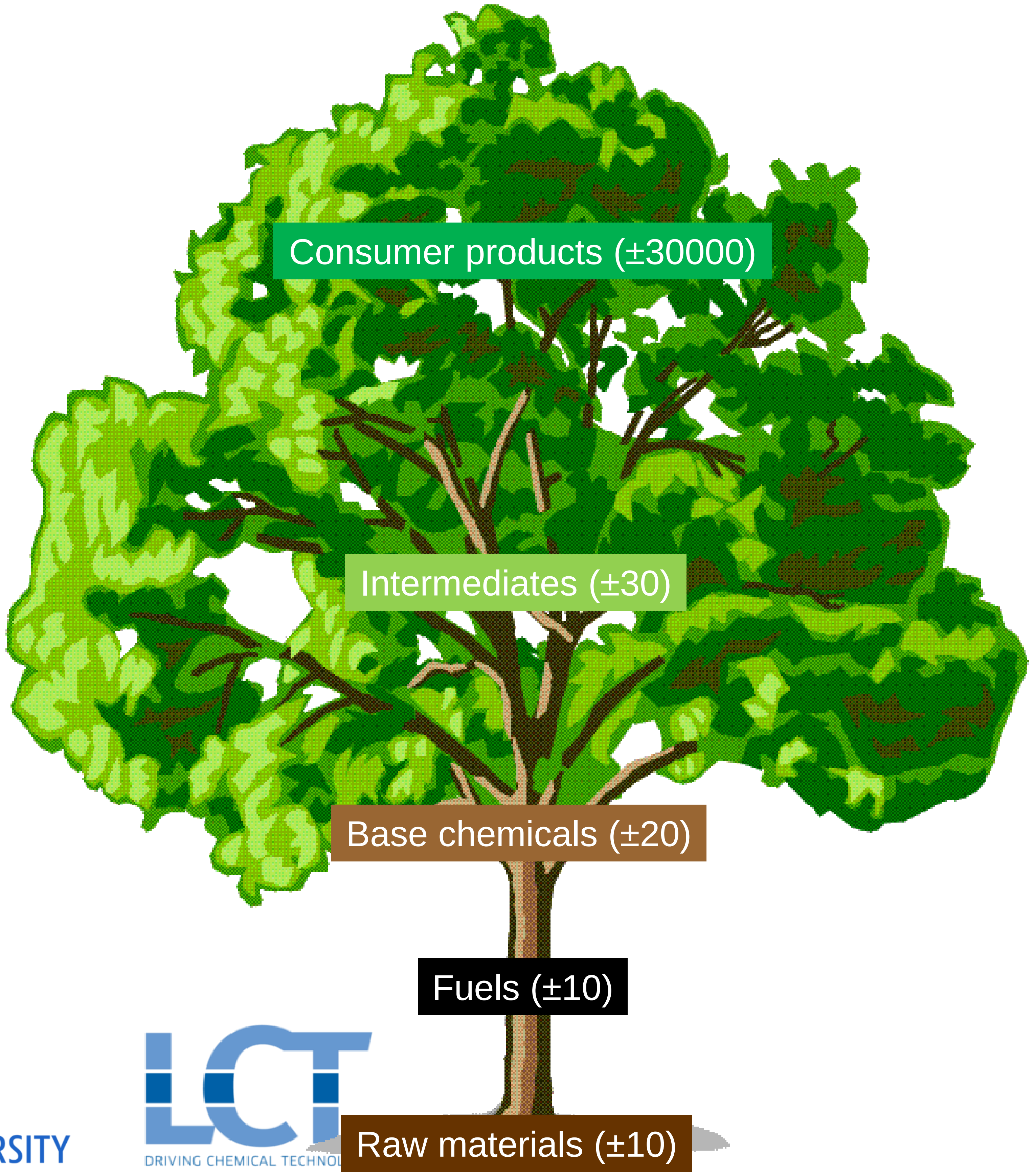
Current Opinion in Chemical Engineering

Carbon dioxide mitigation using renewable power

James R Lattner

Structure of the chemical industry: chemistree



Plastics, electronic materials,
Fibers, solvents, detergents,
insecticides, pharmaceuticals

Specialty chemicals

Acetic acid, formaldehyde,
Urea, ethene oxide,
Acrylonitrile, acetaldehyde,
Terephtalic acid

Ethene, propene, 1,3-butadiene,
Benzene, synthesis gas, ammonia
Methanol sulfuric acid, chlorine

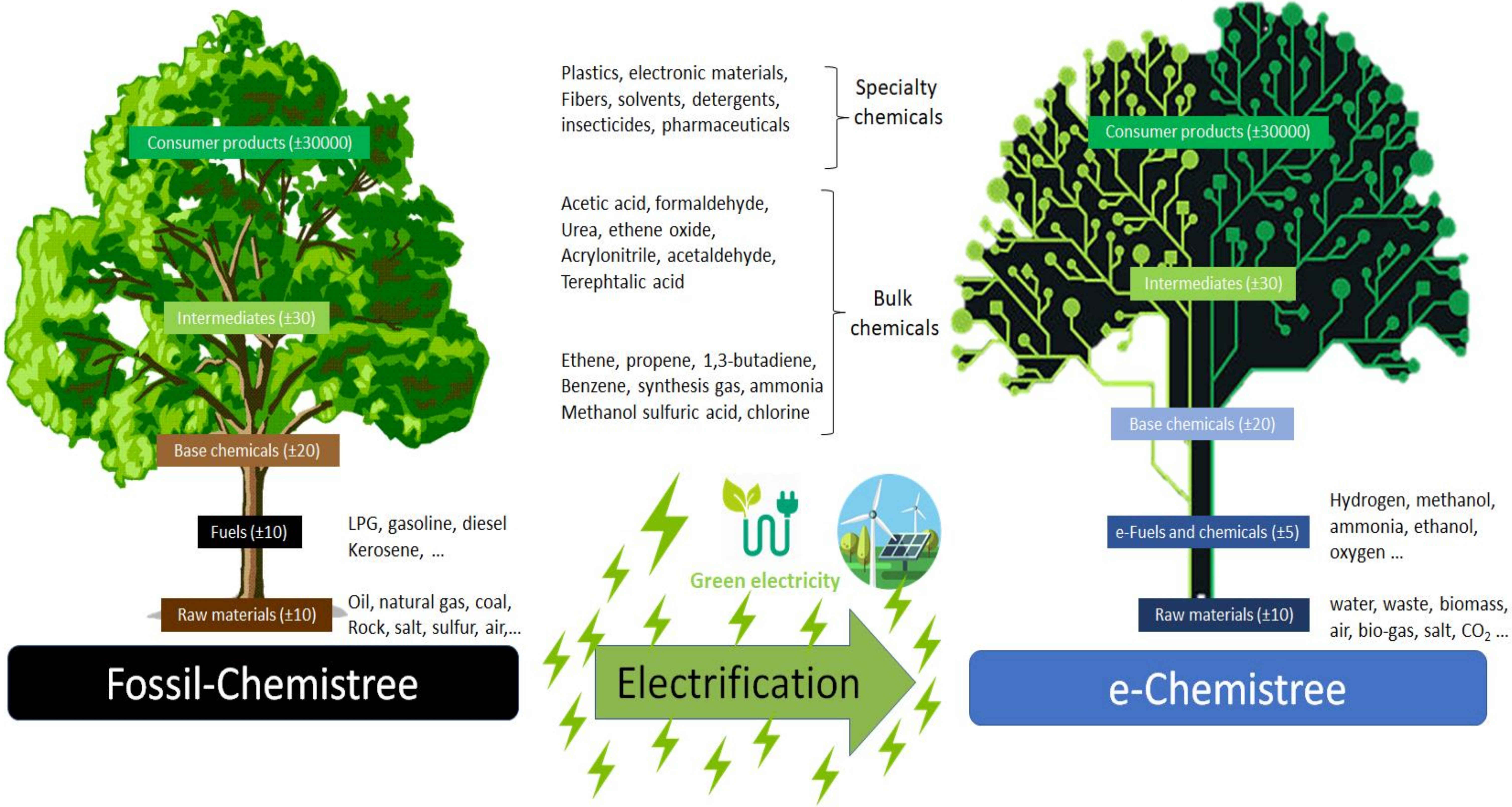
Bulk chemicals

LPG, gasoline, diesel
Kerosene

Oil, natural gas, coal, biomass,
Rock, salt, sulfur, air, water

e-Chemstree

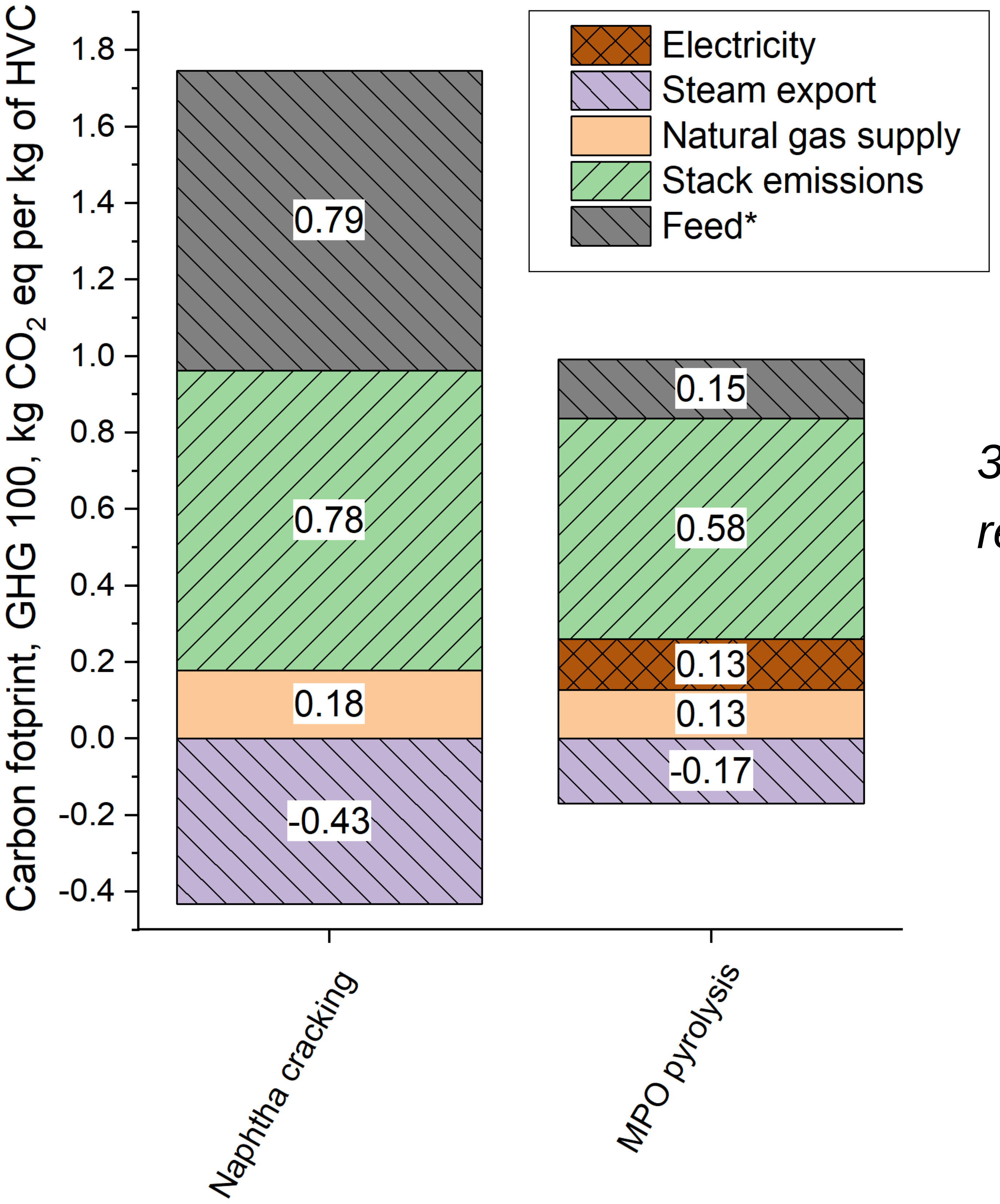
Toward an e-chemistree : materials for electrification of the chemical industry
Kevin Van Geem (UGent) and Bert M. Weckhuysen
(2021) MRS BULLETIN. 46(12). p.1187-1196



Carbon footprint: olefin production from Py-oil

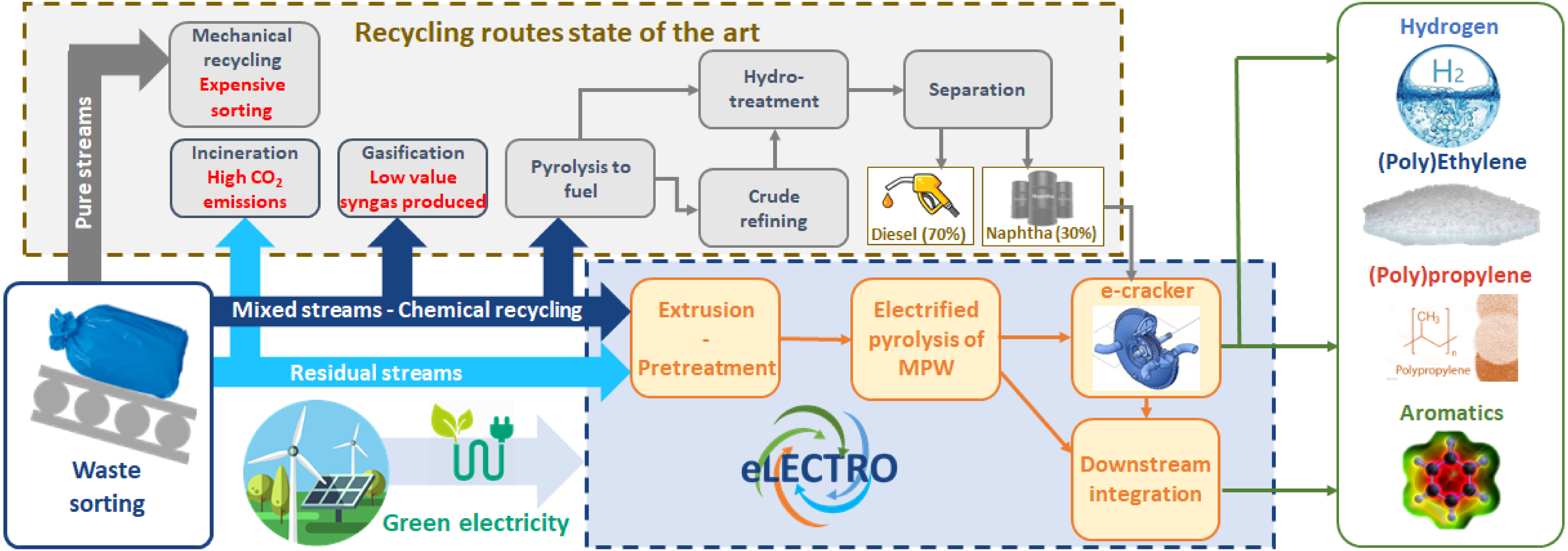
Cradle – to - gate LCA
(at this scope effectively equal to
SCOPE 1+2+3 emissions)

* - Fossil naphtha for baseline scenario (steam cracking of naphtha), toluene upkeep stream for MPO pyrolysis process



37% reduction

ELECTRO: Electrified olefin production



Recycling routes state of the art

Pure streams

Mechanical recycling
Expensive sorting

Incineration
High CO_2 emissions

Gasification
Low value syngas produced

Pyrolysis to fuel

Hydro-treatment

Crude refining

Separation

Diesel (70%)

Naphtha (30%)

Waste sorting

Mixed streams - Chemical recycling

Residual streams

Green electricity

Extrusion - Pretreatment

Electrified pyrolysis of MPW

e-cracker

Downstream integration

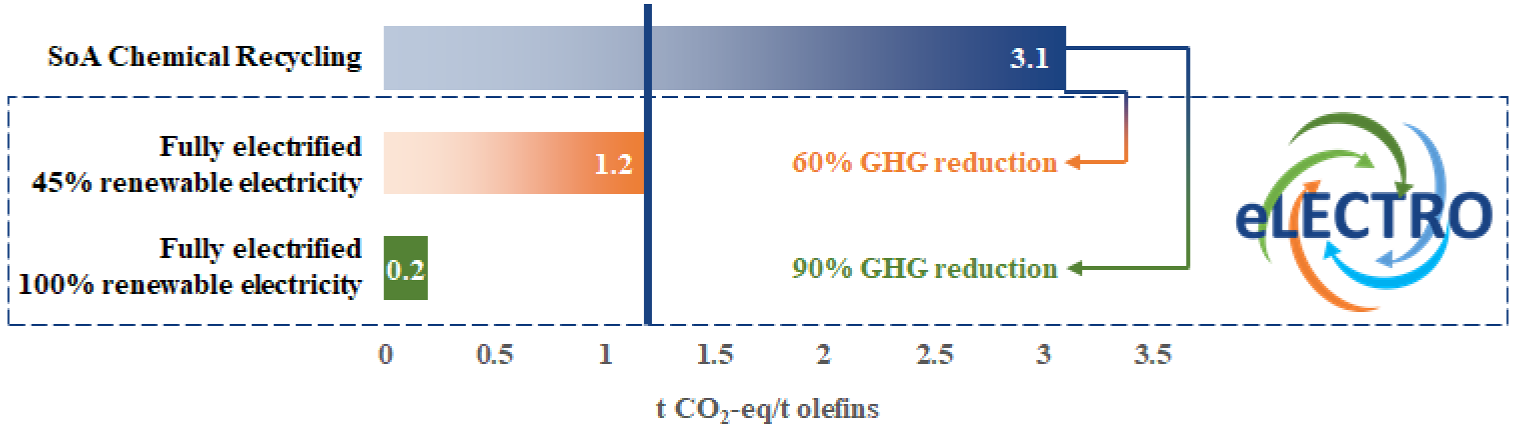
eLECTRO

Hydrogen

(Poly)Ethylene

(Poly)propylene

Aromatics



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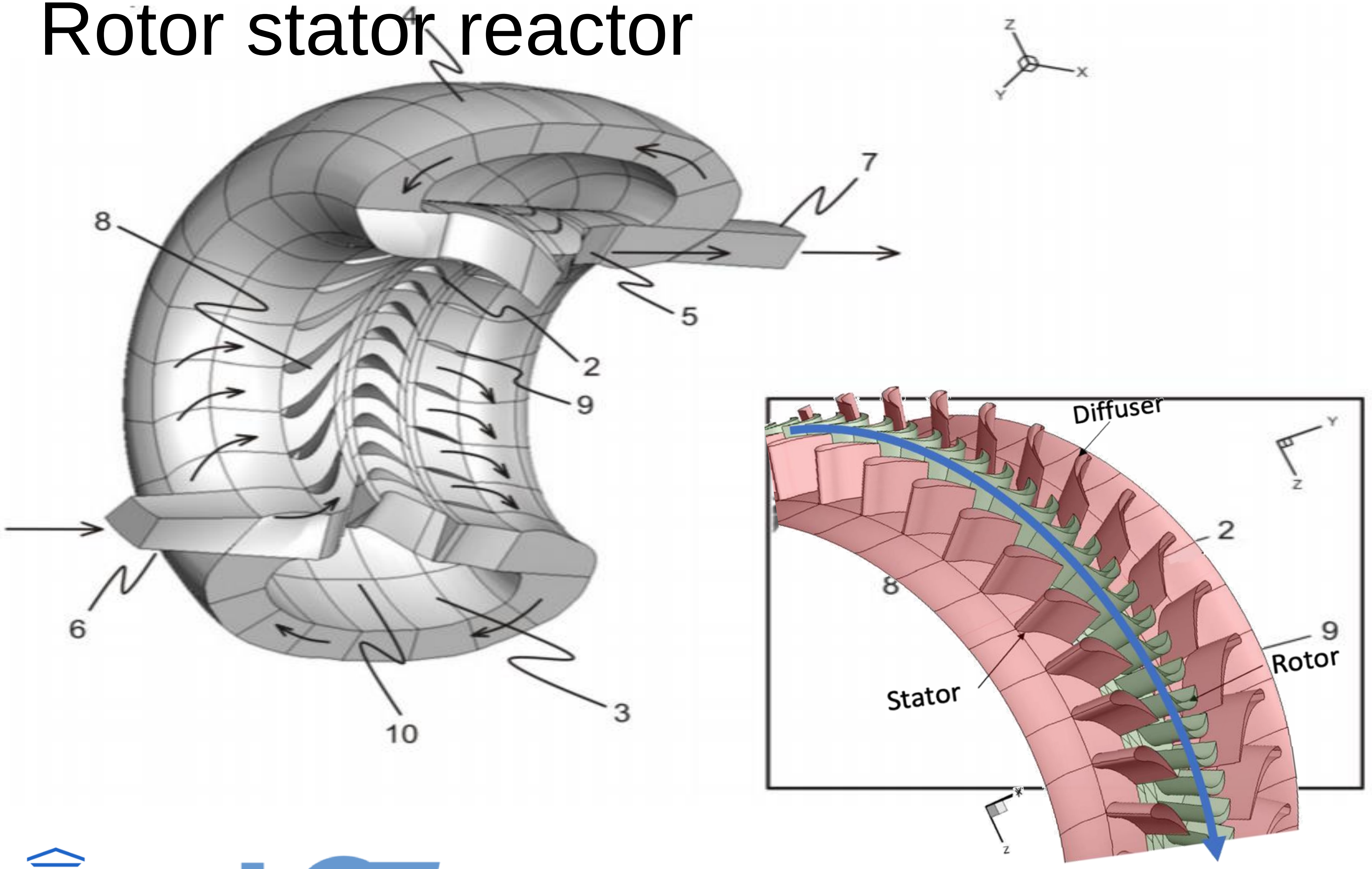
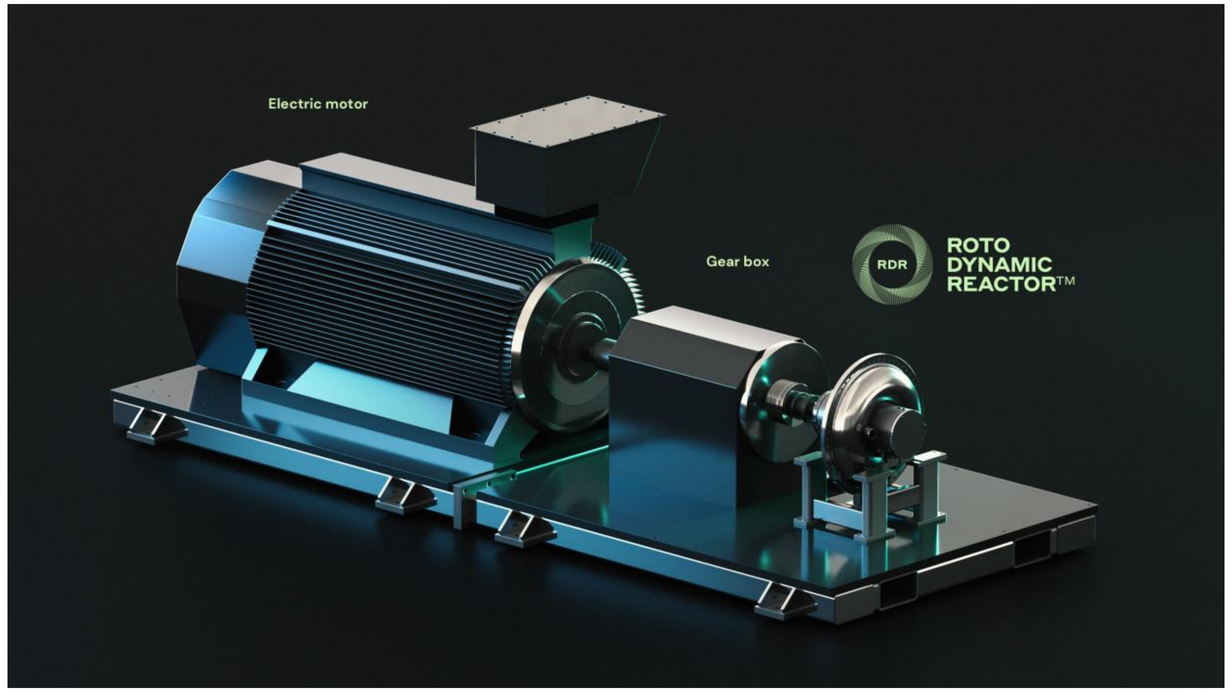
More disruptive changes for CO2 neutrale olefins

Rotor stator reactor



Electrification of plastic waste to olefins

“RDR (Roto Dynamic Reactor) is a revolutionary technology that uses rocket engineering, mechanical engineering and chemistry to solve the biggest challenges in olefins production today.”



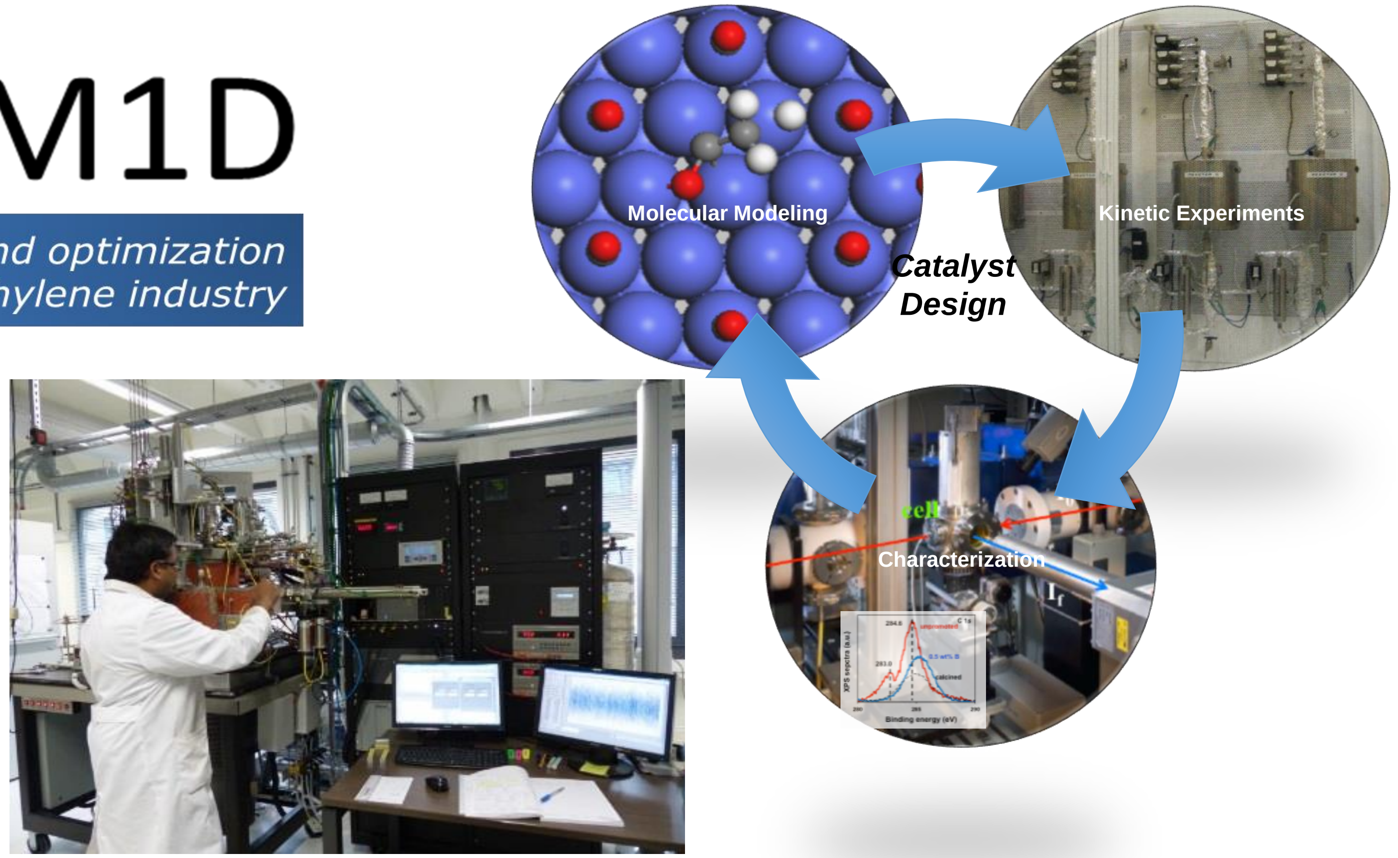
- Convert kinetic energy into heat
- Lower residence times then conventional steam cracking and thus higher selectivity
- Offers the possibility to use (green) electric power in the cracking process
- Lower capex cost

Laboratory for chemical Technology

Design and **optimization** of sustainable products and processes

COILSIM1D

The advanced simulation and optimization software for the ethylene industry



Application Domains:

Transportation fuels and Energy carriers
Large scale Chemicals
Functional materials (catalysts, polymers)

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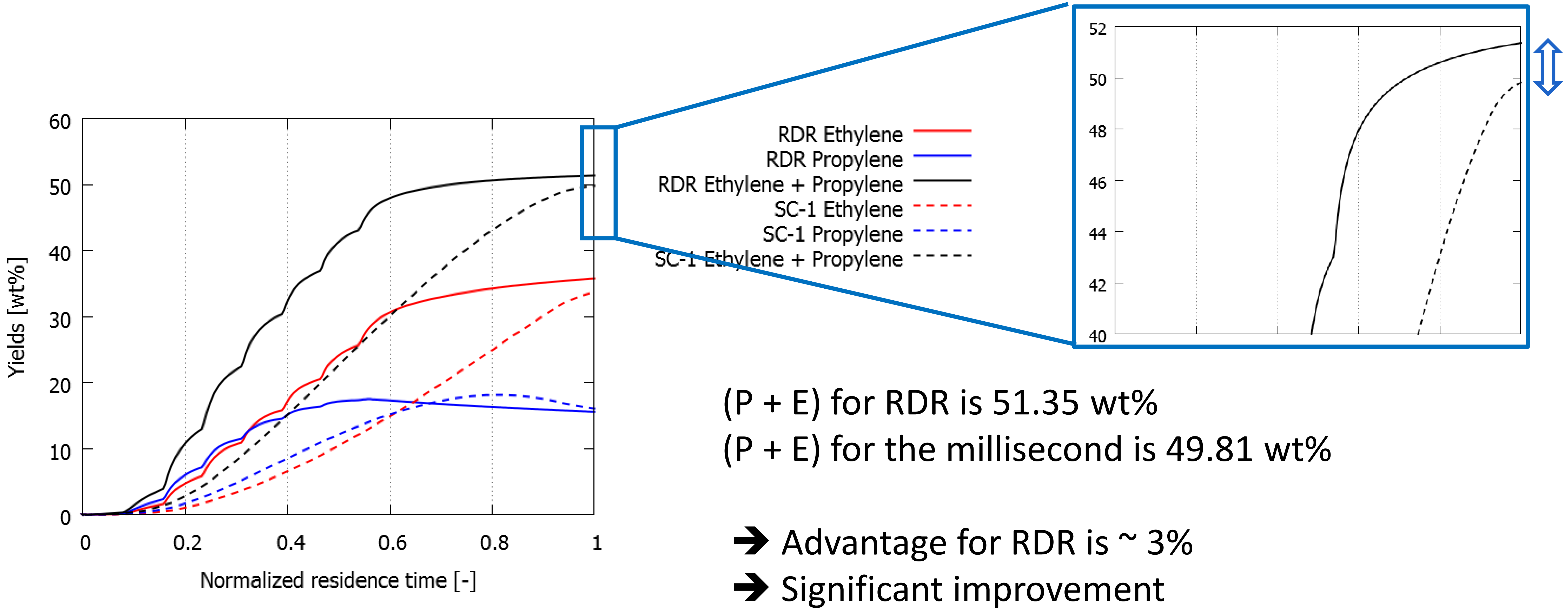
RDR vs conventional steam cracking

Yield comparison (normalized residence time)

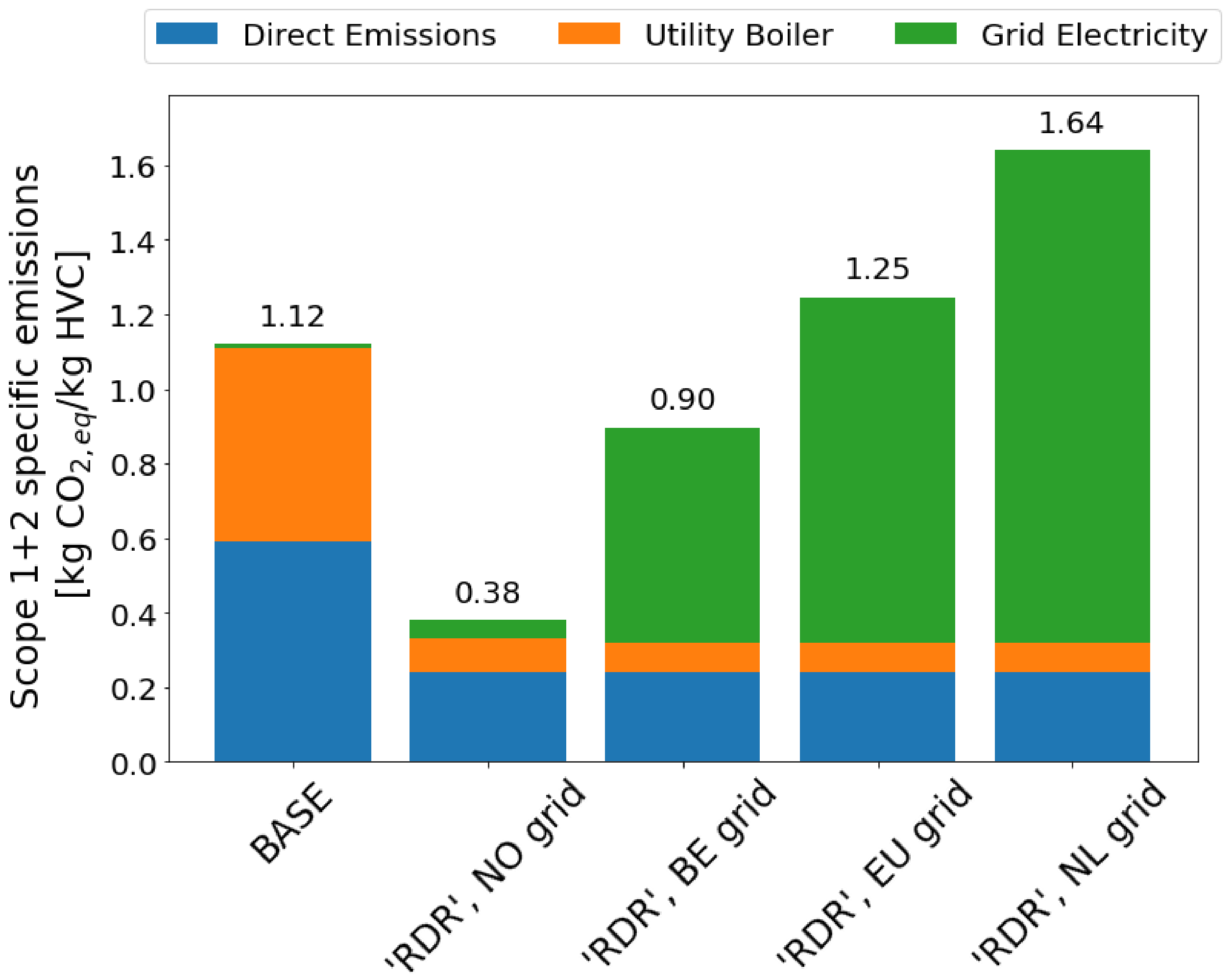


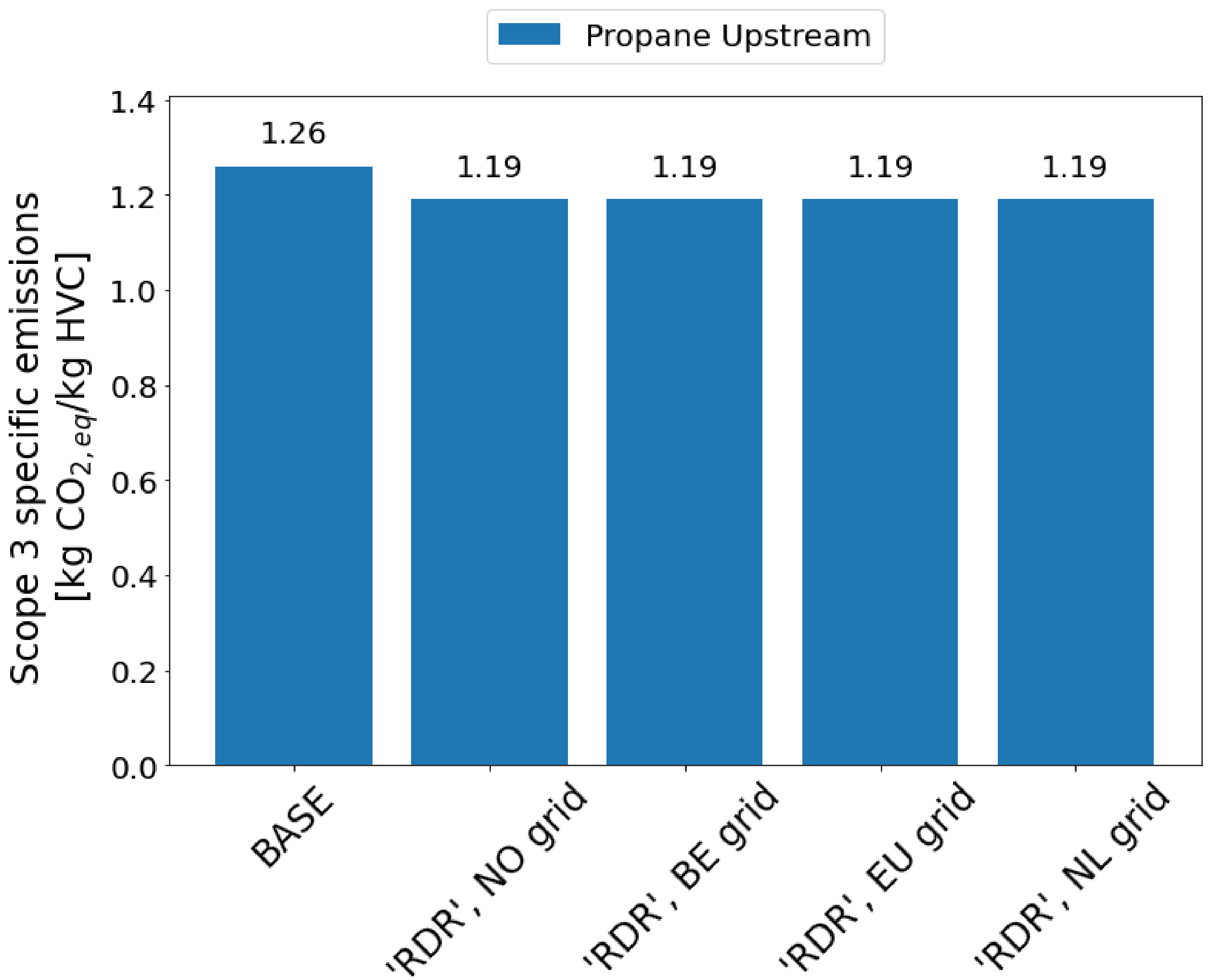
(P + E) for RDR is 51.35 wt%

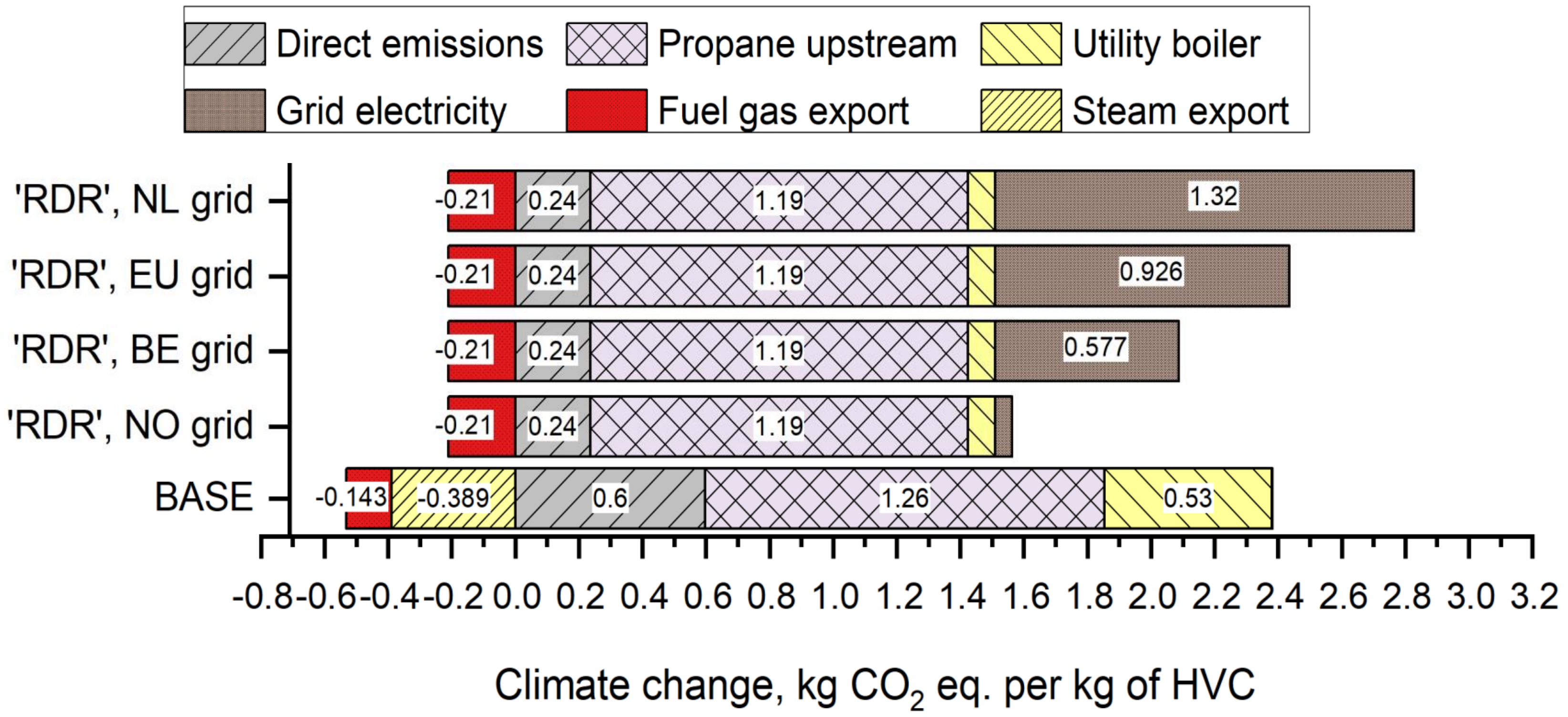
(P + E) for the millisecond is 49.81 wt%

- ➔ Advantage for RDR is ~ 3%
- ➔ Significant improvement

GHG Protocol: e-Cracking







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Conclusions

- Reaction engineering will be a key driver to move to a net-zero World
- Collaboration is key: local but also on global scale (industry & Academia)
- Waste can become an important feed for the CPI
- Process intensification is a necessity
- **It is more than Technology**

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fwo

Chemical or advanced recycling: definition

Feedstock recycling, also known as chemical recycling, **aims to convert plastic waste into chemicals**. It is a process where the chemical structure of the polymer is changed and converted into chemical building blocks including monomers that are then used again as a raw material in chemical processes.

There is no silver bullet

Multiple technologies…feedstock dependent

Each chemical recycling technology can treat specific feedstock and therefore offer a complementary model to support a circular economy for all plastics.

- Deploymerisation mostly focuses on monostreams independently sorted by plastic types: PET (including fibers), PA, PU, PMMA and PLA.
- Pyrolysis and hydrothermal upgrading mostly focus on mixed polymers (including multilayers, multi-materials within controlled limits): LDPE, HDPE, PP, PS.
- Gasification mostly focuses on mixed polymers.

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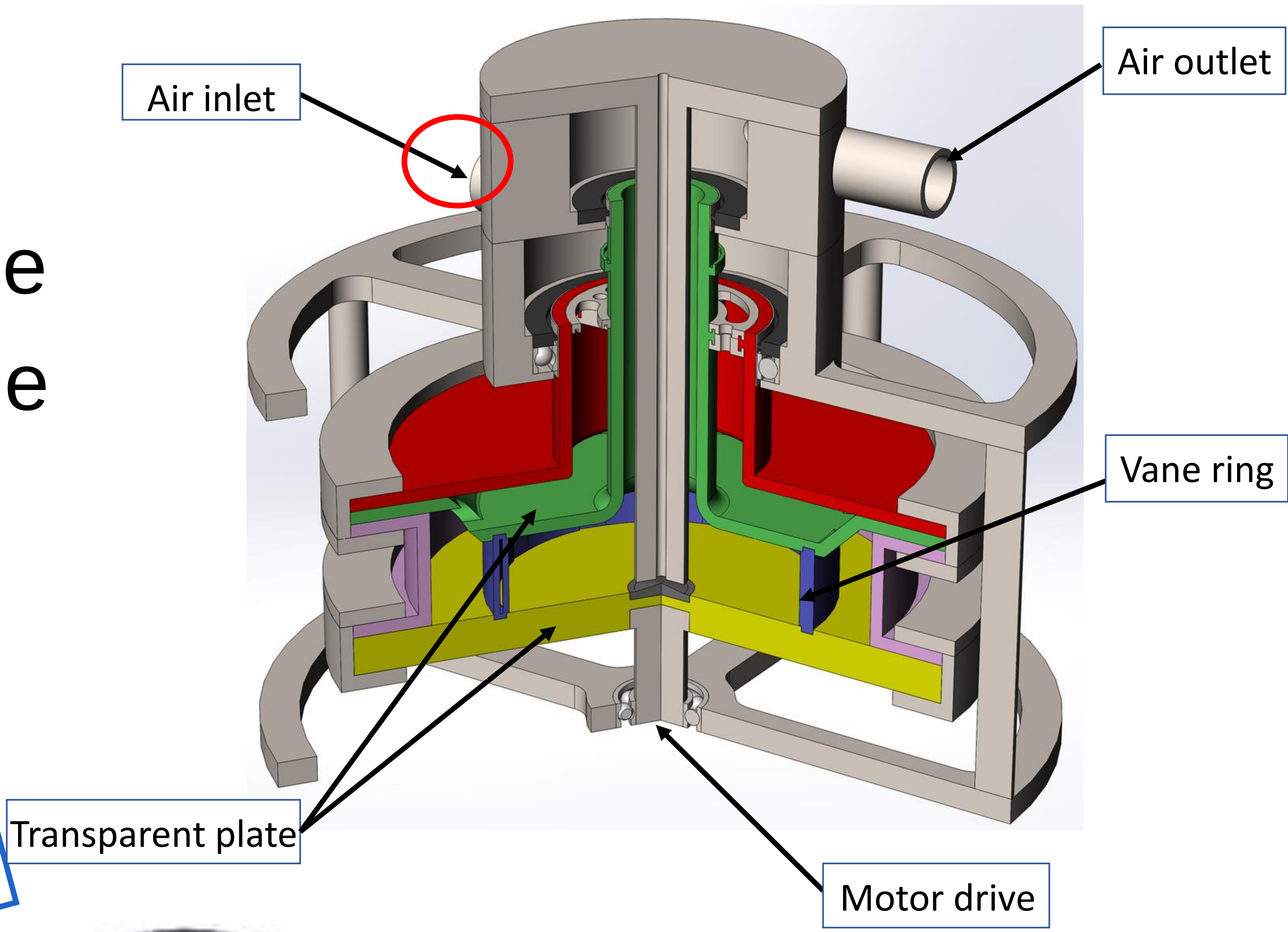
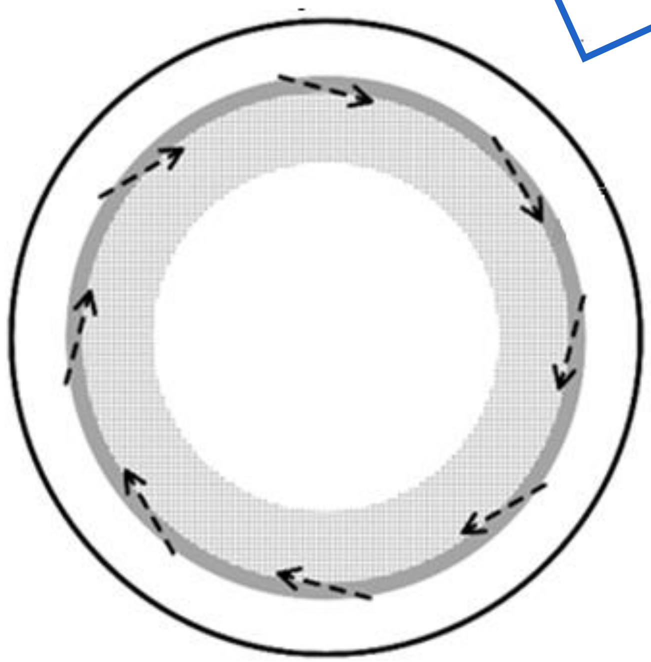
FOCUS

Vortex Technology

- Decouple F_c and F_d by introducing external force
- Offer guidance for design the blade-driven mode



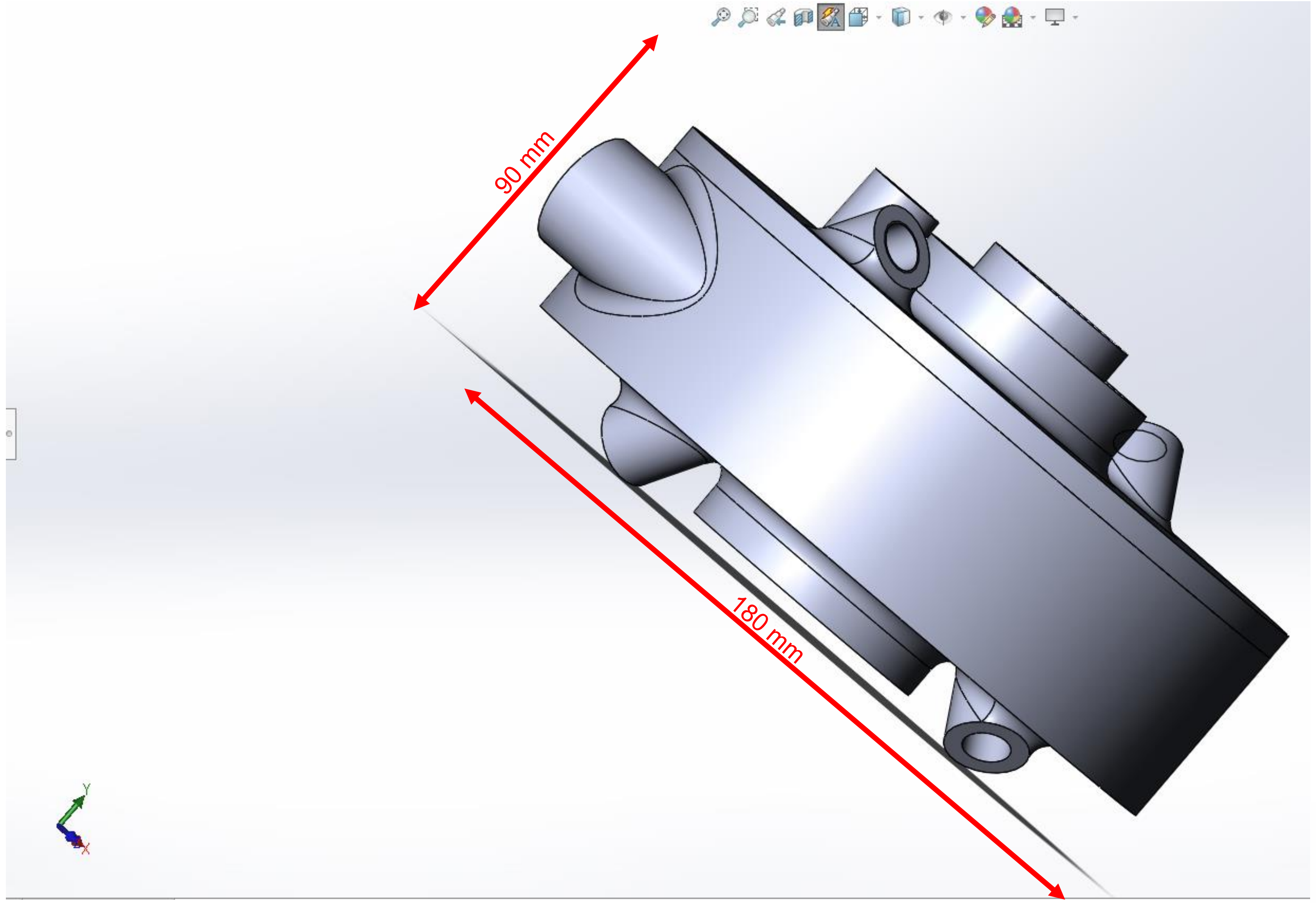
Static



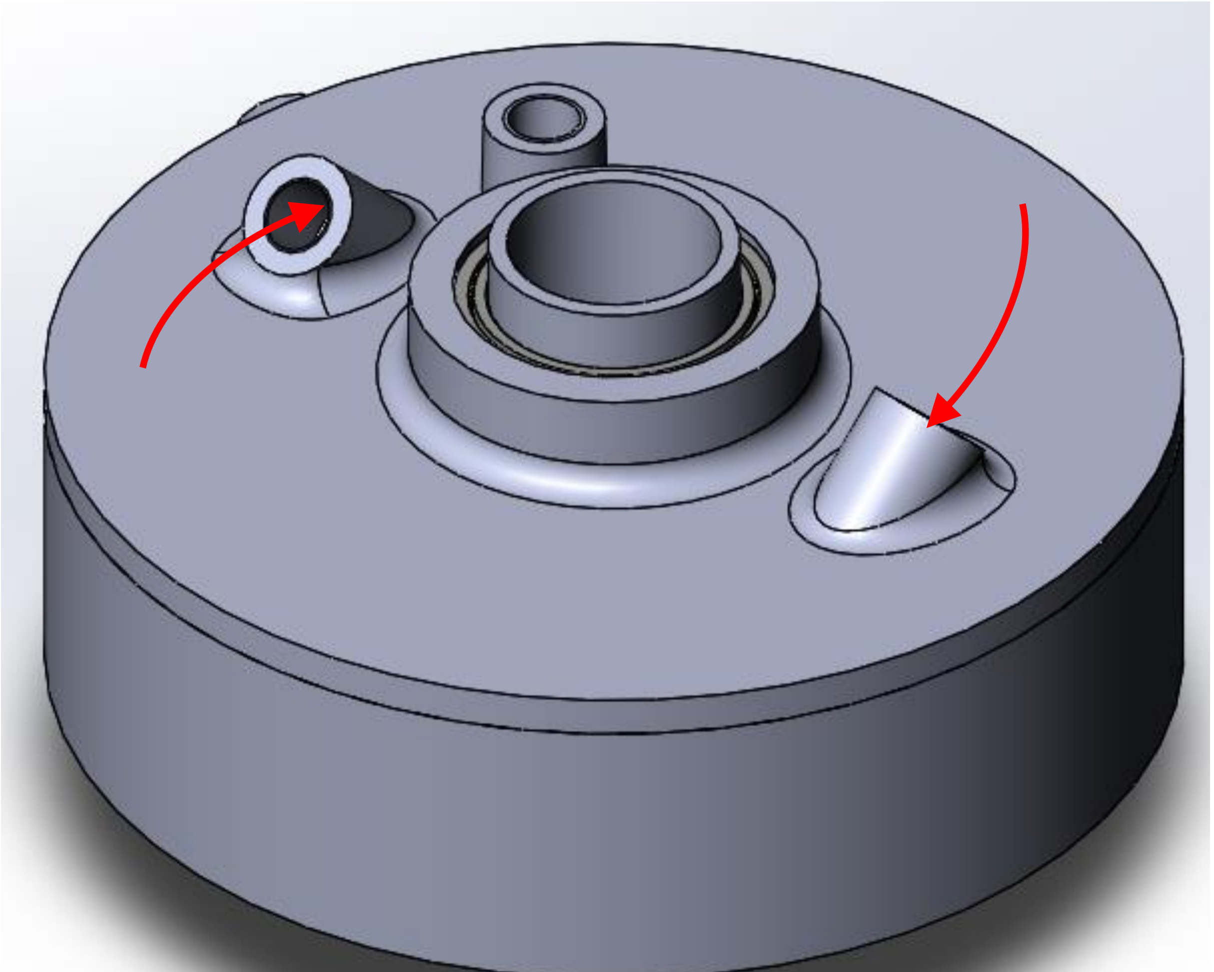
Starvoc2
Decoupled
F_c and F_d

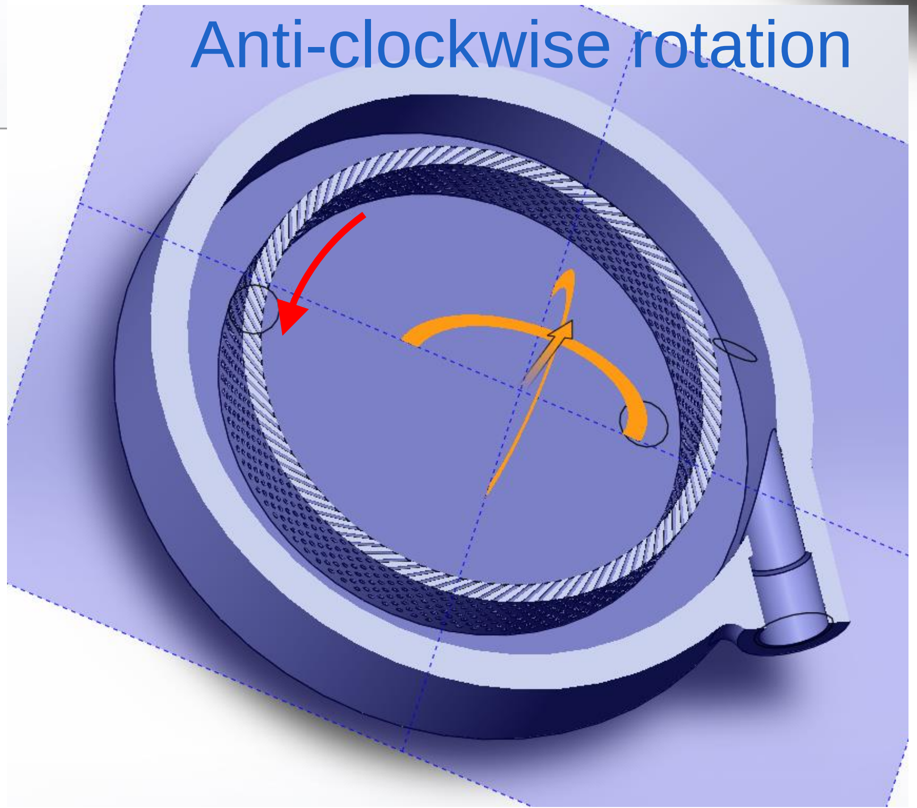
Rotating

STARVOC-3 (patented design)



Clockwise rotation (when viewed from top)





Anti-clockwise rotation

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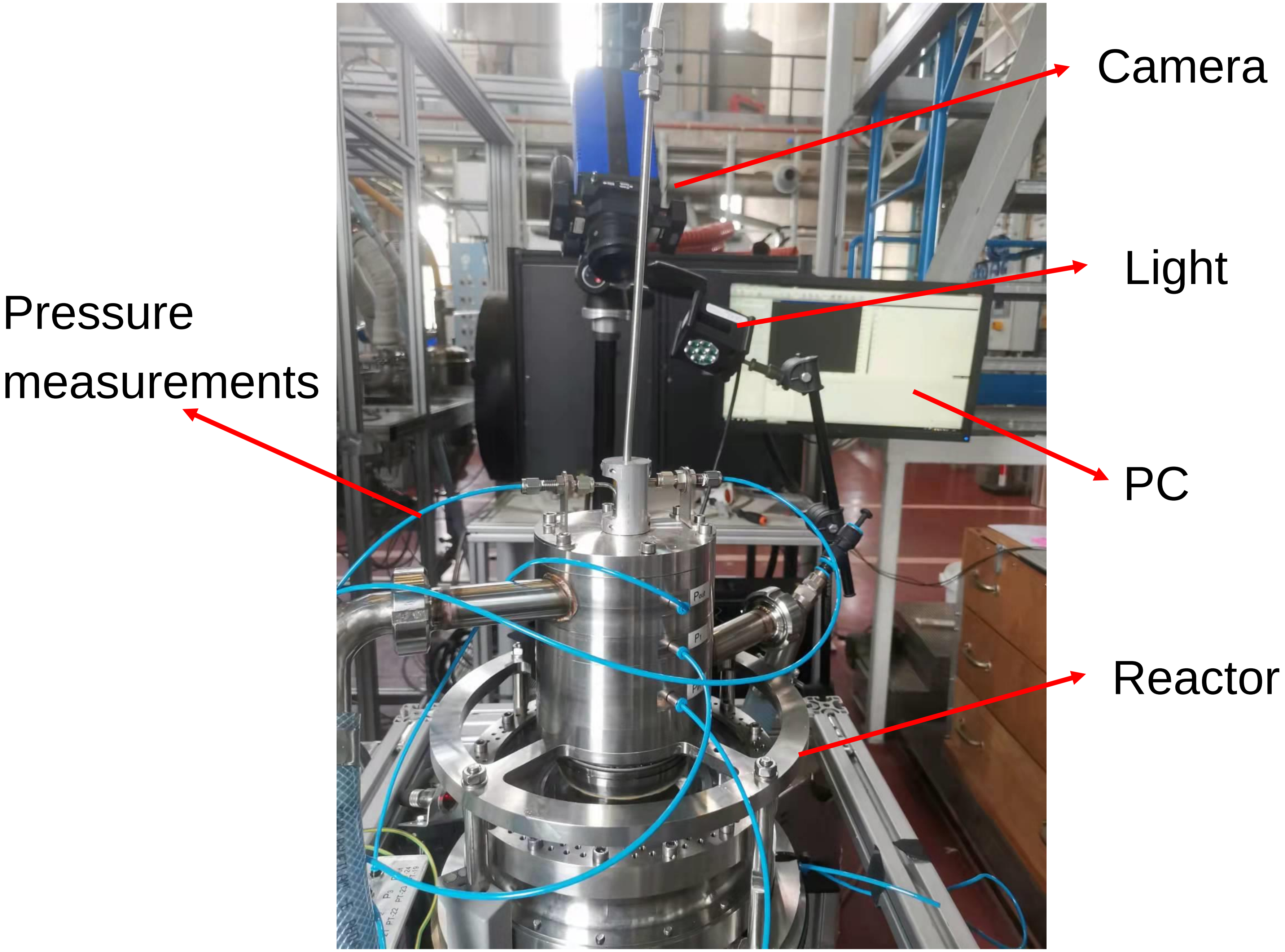
Methodology

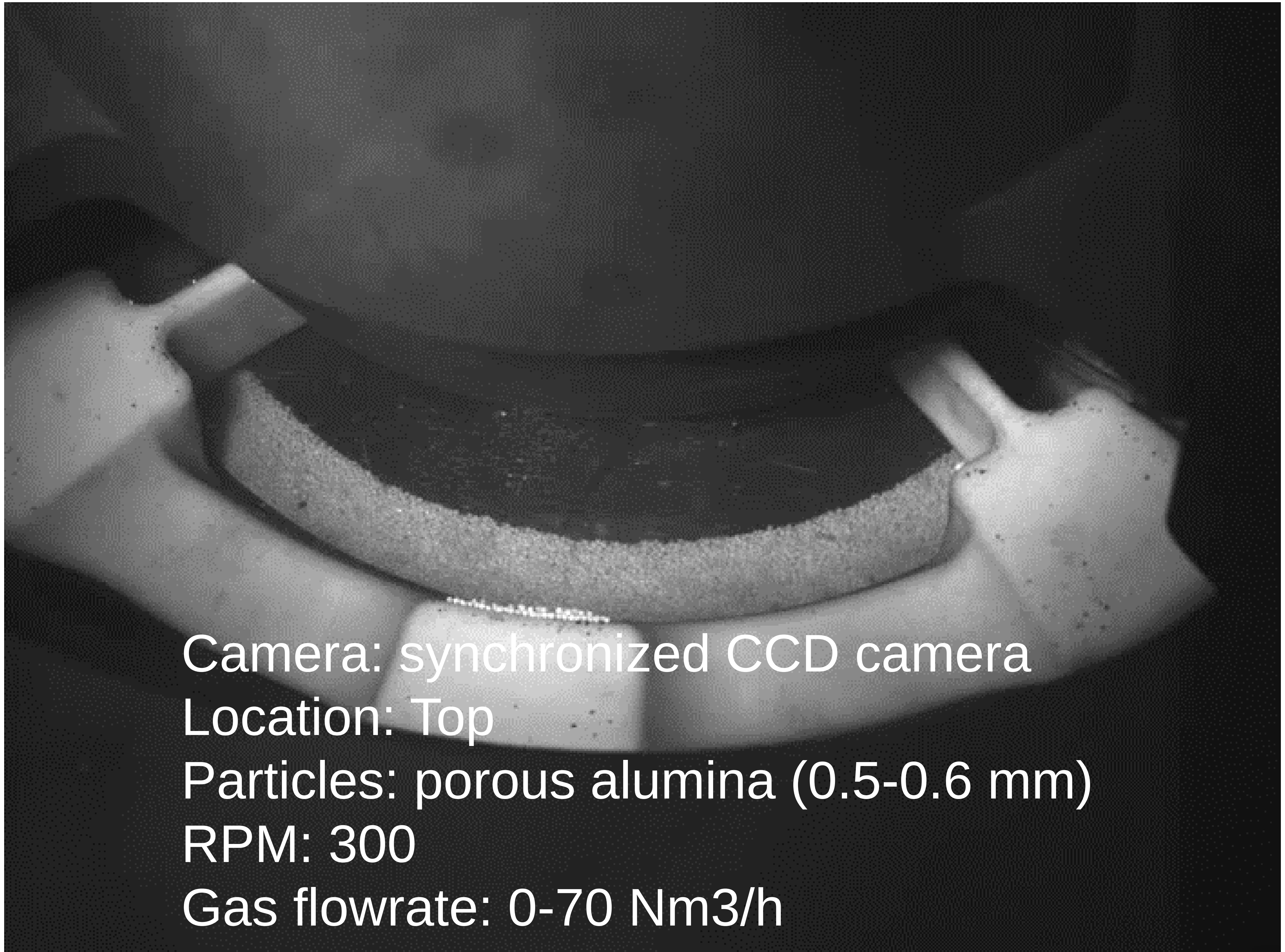
- Setup

  Reactor with transparent endplates

  PIV camera above or below the reactor
- Data acquisition
  - PIV camera is synchronized
    - Images/videos
  - Pressure drop over the solids bed is measured



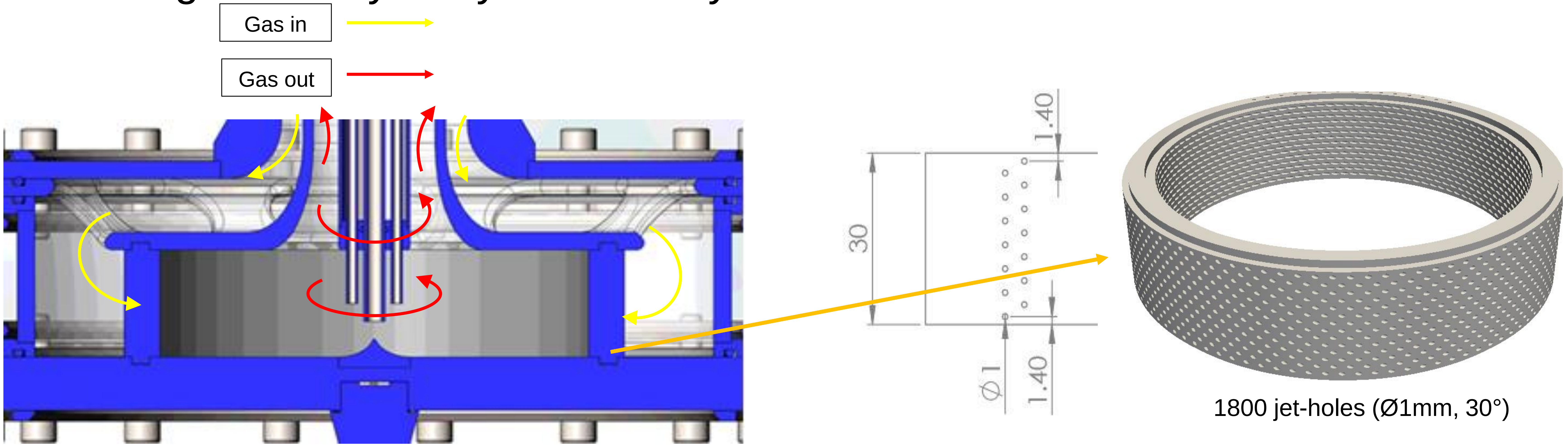
Incipient entrainment



Camera: synchronized CCD camera
Location: Top
Particles: porous alumina (0.5-0.6 mm)
RPM: 300
Gas flowrate: 0-70 Nm3/h

Experimental setup

- Motor-driven chamber as an approach to:
  - Independently control of flowrate and rotating speed
  - Investigate the hydrodynamic study of these variables



1800 jet-holes (Ø1mm, 30°)

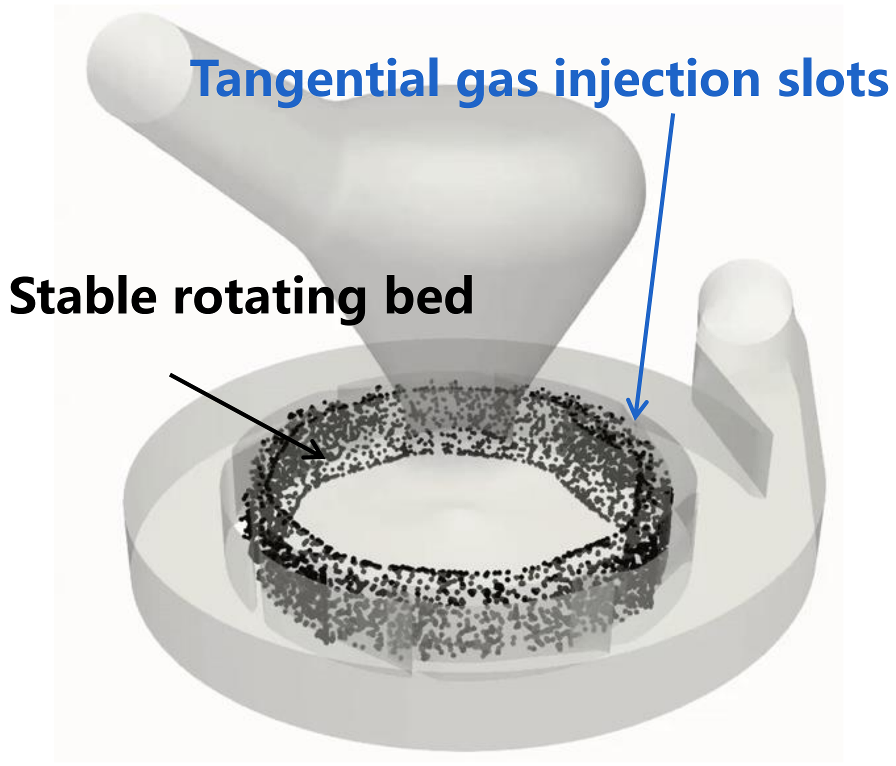
Gas distributor

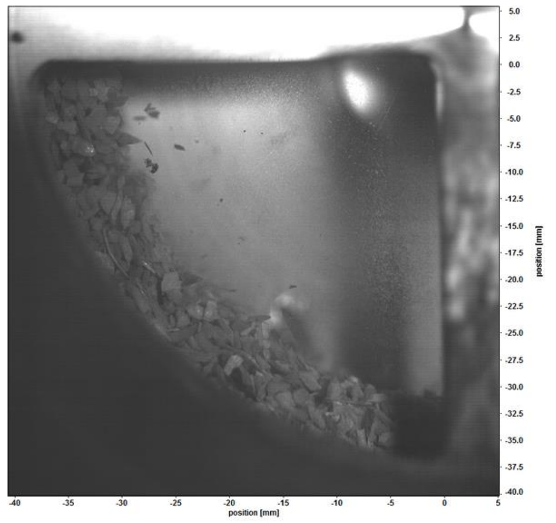
Van Geem et al. U.S. Patent Application No. 16/680,430.

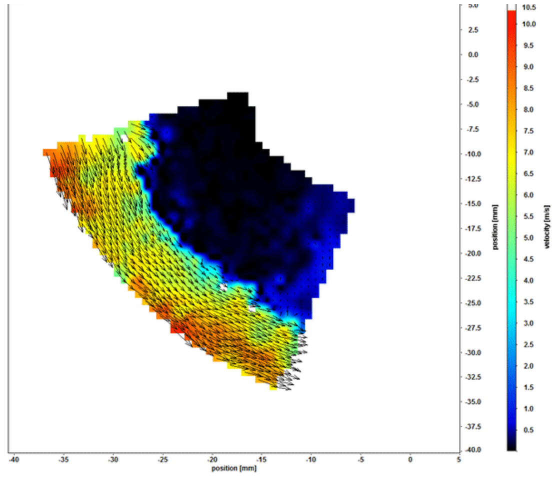
Static vortex technology

- Gas-solid vortex reactor (GSVR)[2-4]
  - Tangential gas injection
  - Vortex flow
  - Centrifugal force field
  - High interphase slip velocity
  - No mechanical rotation

- Gas-liquid vortex reactor (GLVR)[5-7]
  - Tangential gas injection
  - Centrifugal force field by gas energy input
  - Momentum transfer from gas to liquid
  - Large interfacial area
  - High energy dissipation rate







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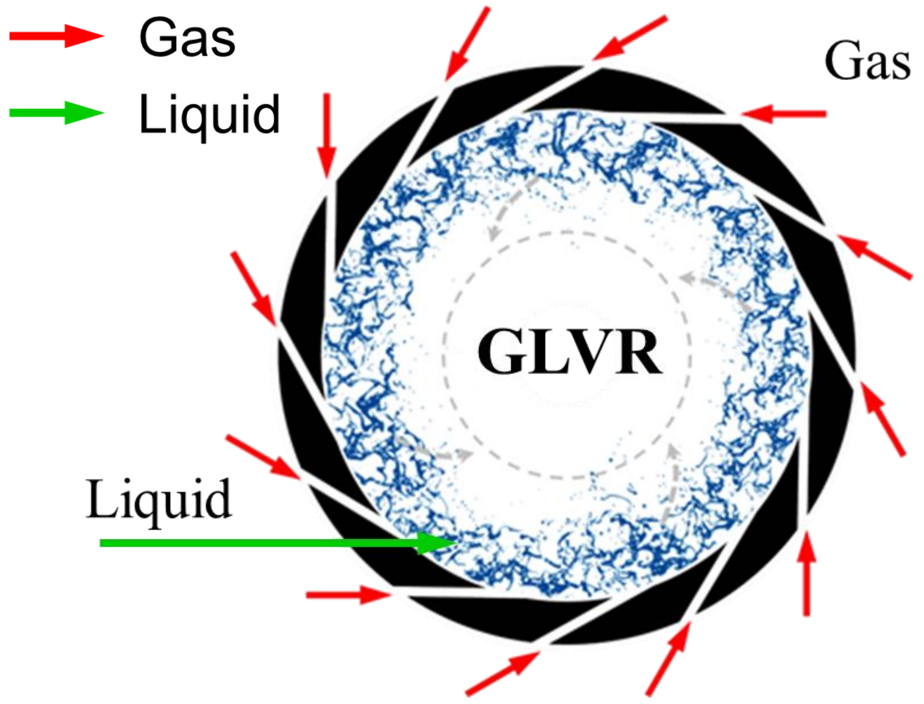
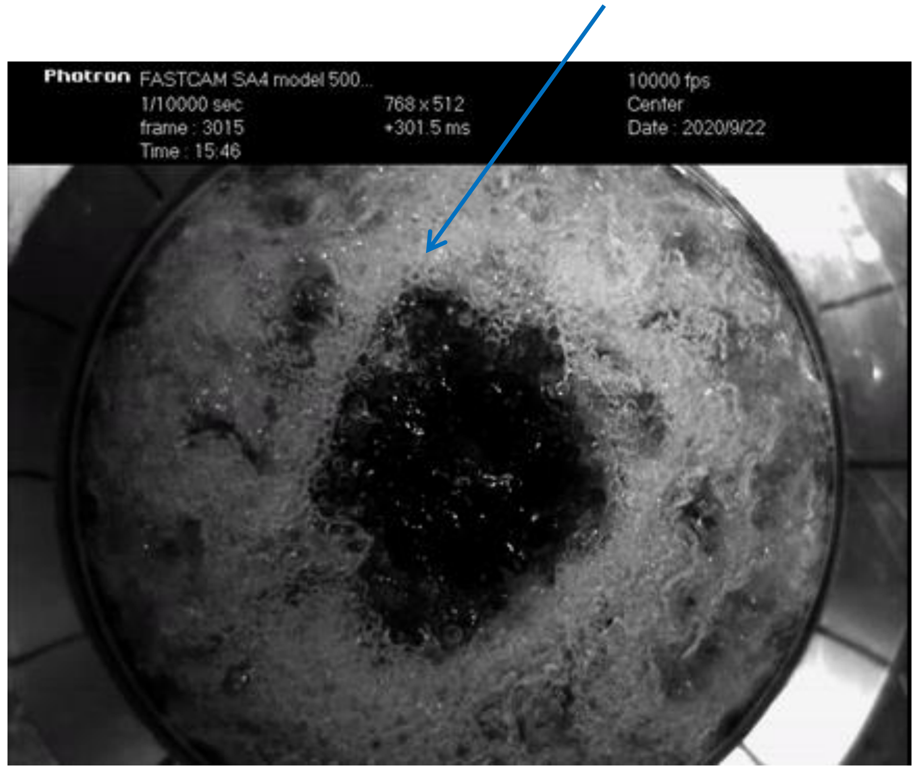


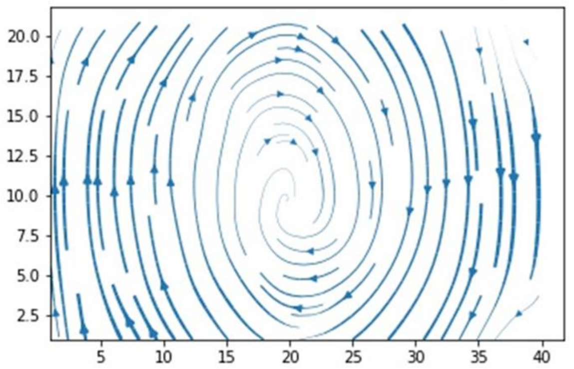
Stable rotating liquid layer



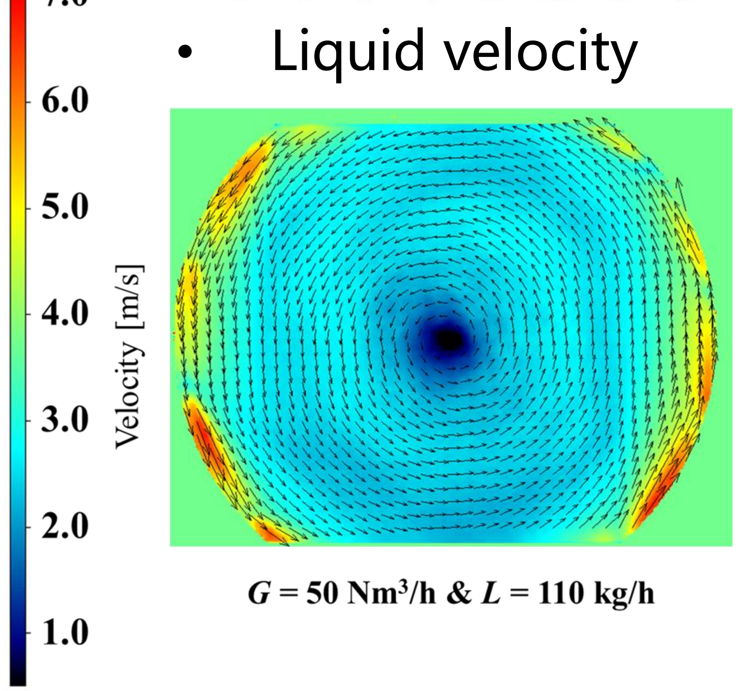
GLVR research at the LCT

- Hydrodynamics[5]
  - Streamline

G = 30 m³/h – *L* = 20 kg/h



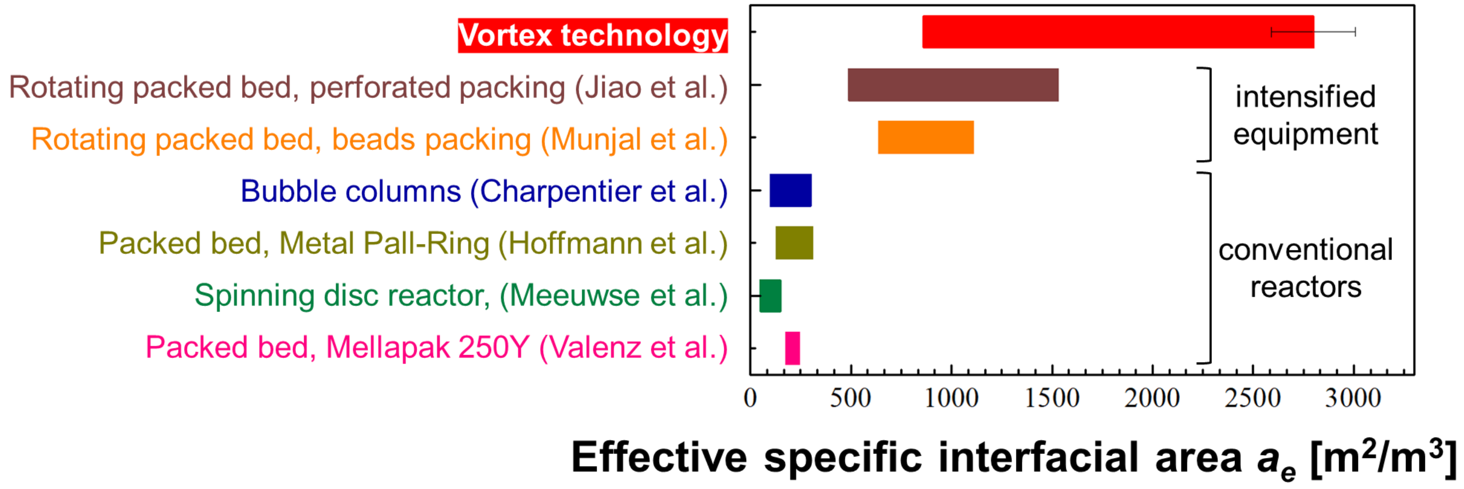
  - Liquid velocity

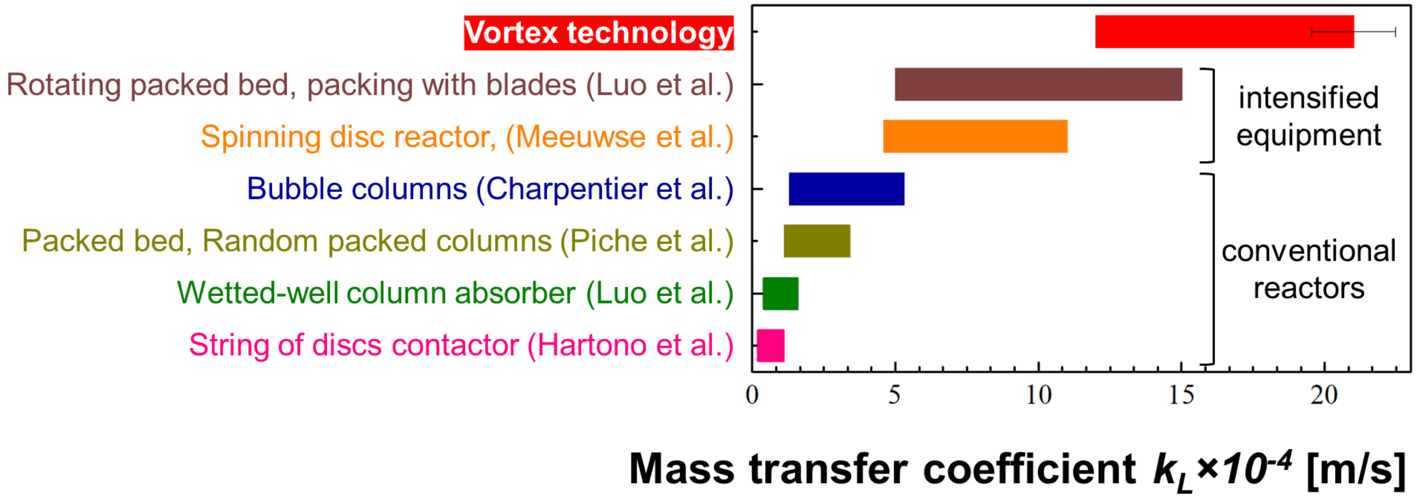


G = 50 Nm³/h & *L* = 110 kg/h

  - Flow pattern, liquid layer thickness,…

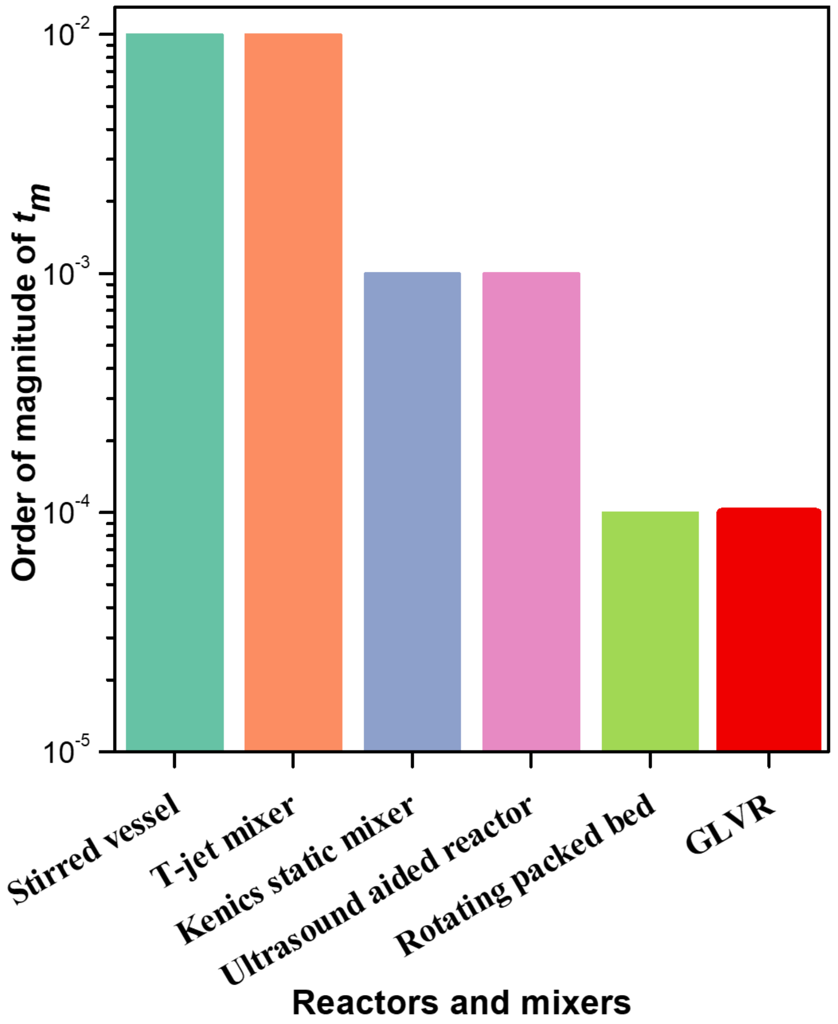
- Interface mass transfer





- a_e & k_L:
- Enhancement factor of 10 compared to conventional reactors
- Enhancement factor of 2 compared to intensified equipment

- Micromixing time[6]

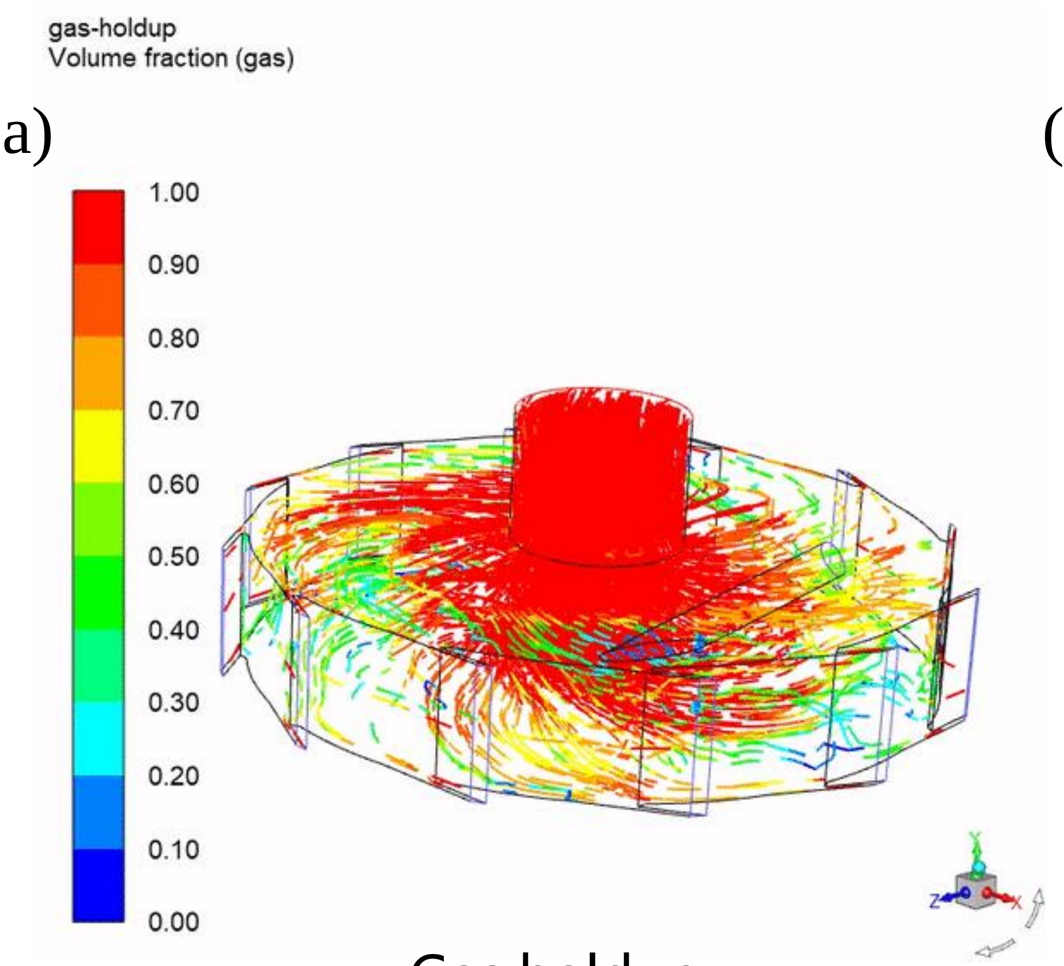


- t_m :
- Micromixing time is reduced by 2 magnitudes compared to conventional reactors

Liquid and gas flow patterns for CO2 capture

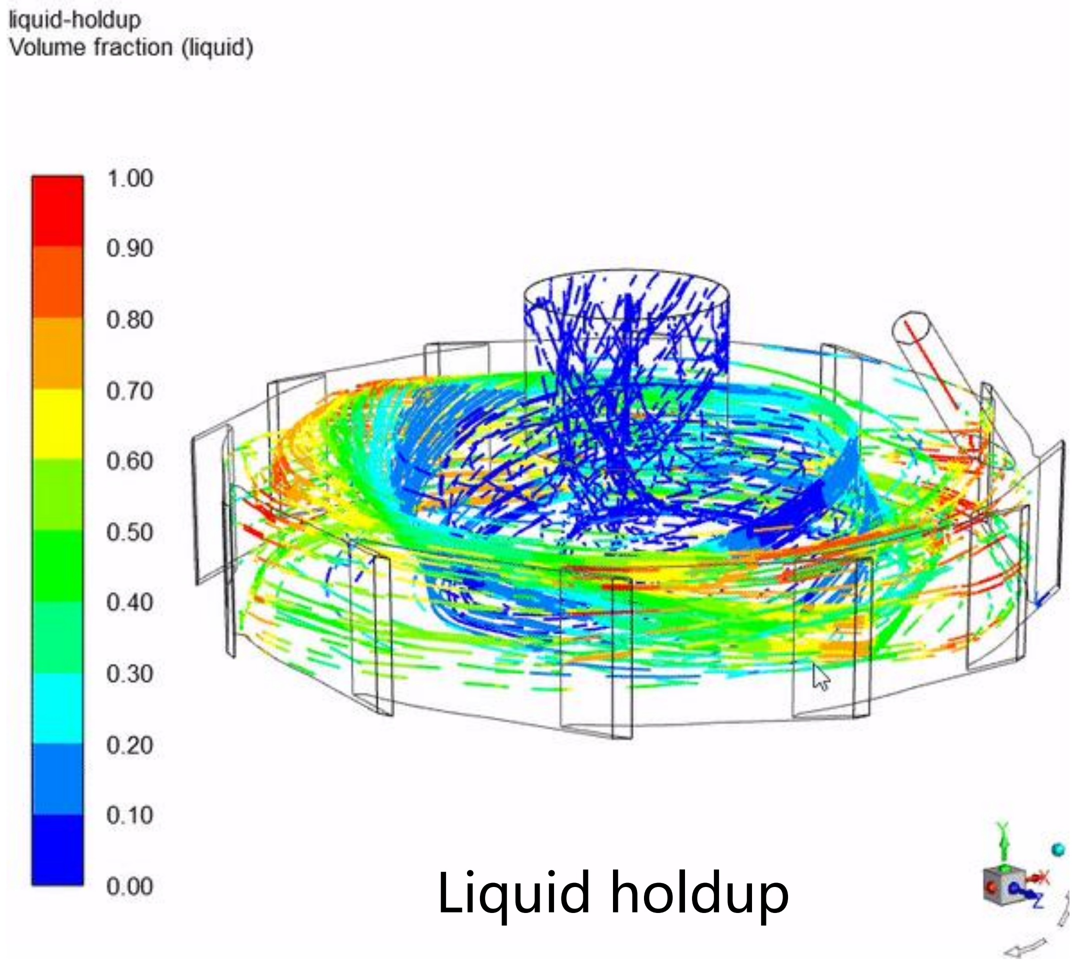
3D streamlines for gas and liquid phases

(a)



Gas holdup

(b)



Liquid holdup

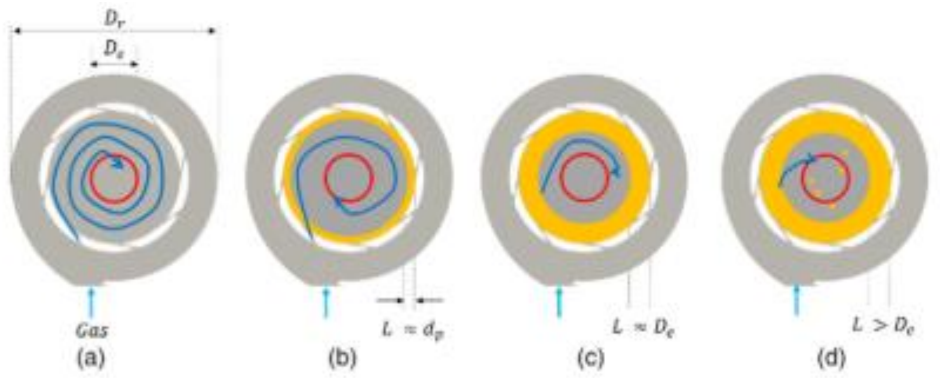


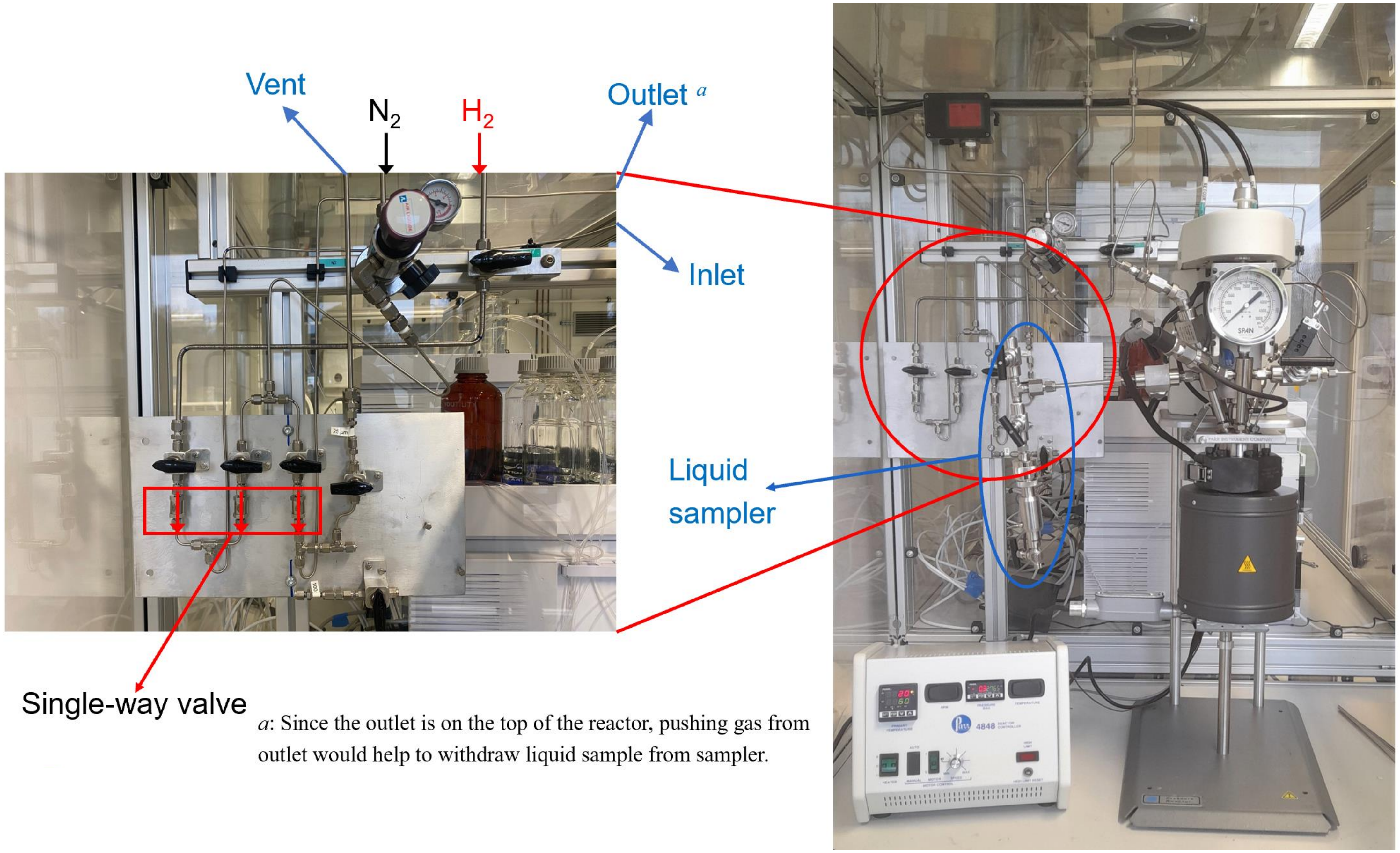
FIGURE 6 Top view of various flow patterns in a vortex unit (with vertical axis) covering (a) gas-only flow showing swirling gas motion, (b) bed at vortex suppression condition, (c) bed operating at maximum solids loading capacity, and (d) bed operating at solids entrainment limit with excess particles deposited on the unit bottom plate. Red circle depicts the exhaust diameter and the yellow region corresponds to solids bed [Color figure can be viewed at wileyonlinelibrary.com]

Gas streamline in GSVR with solid[7]

$G = 50 m^3/h$ $L = 110 kg/h$

- The gas vortex flow is broken due to the liquid injection/solid loading
- The liquid is rotating in the chamber

We need both large scale and small scale



a: Since the outlet is on the top of the reactor, pushing gas from outlet would help to withdraw liquid sample from sampler.

Supercritical water treatment and hydrogenolysis