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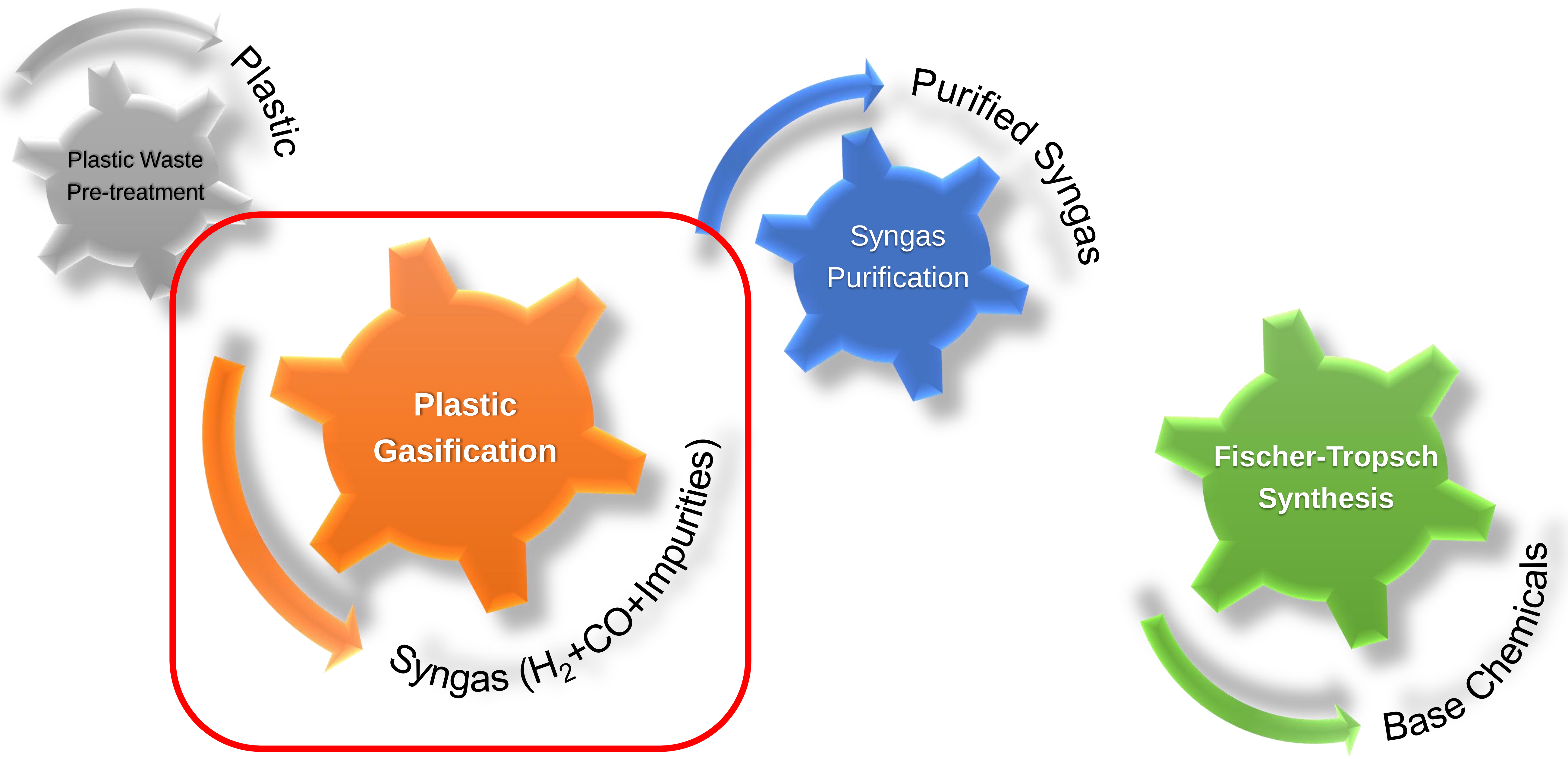
Avec le soutien du Fonds européen de développement régional
Met steun van het Europees Fonds voor Regionale Ontwikkeling

PSYCHE Consortium Meeting

10/12/2020

PSYCHE Project



LCT (UGent) + IMAP (UCL)

State of the art of plastic waste gasification

materials

MDPI

Review

Multi-scale Modeling of Plastic Waste Gasification: Opportunities and Challenges

Sepehr Madanikashani [1,3], Laurien Vandewalle [1], Steven De Meester [2], Juray De Wilde[3] and Kevin M. Van Geem[1,*]

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[2] Laboratory for Circular Process Engineering (LCPE), Faculty of Bioscience Engineering, Ghent University – Campus Kortrijk, Graaf Karel de Goedelaan 5, 8500 Kortrijk, Belgium

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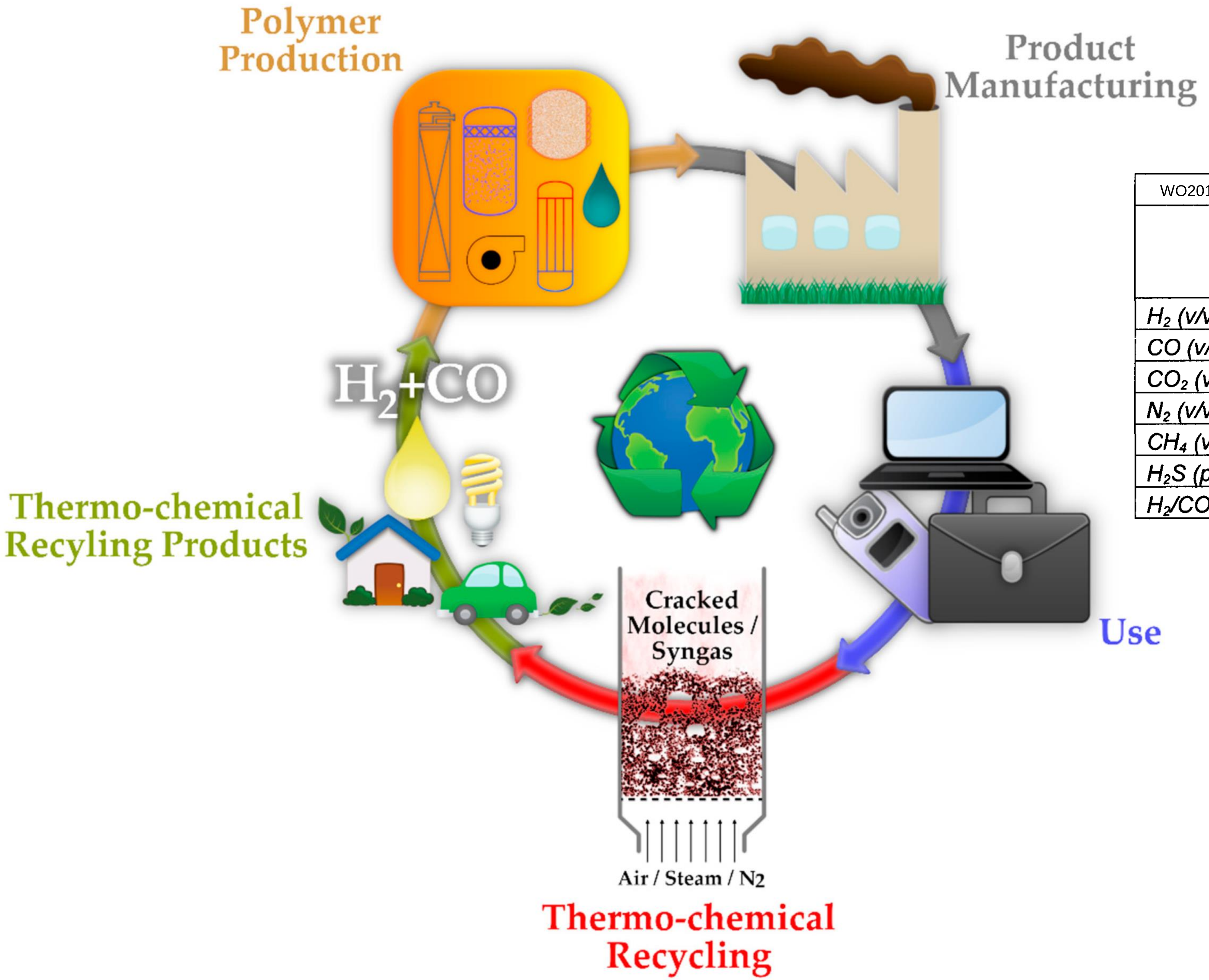
* Correspondence: Kevin.VanGeem@UGent.be

https://www.mdpi.com/1996-1944/15/12/4215

Essential is the syngas quality: feed dependent



WO2012064936A1	Natural Gas	Asphaltene	Coal	Pet Coke
	vol% dry gas, O_2 fired	*vol% dry gas, O_2 fired*	*vol% dry gas, O_2 fired*	*vol% dry gas, O_2 fired*
H_2 (v/v %)	63.0	44.7	38.0	33.0
CO (v/v%)	33.5	45.0	45.0	53.2
CO_2 (v/v%)	3.0	10.0	15.0	12.0
N_2 (v/v%)	0.2	0.3	2.0	0.6
CH_4 (v/v%)	0.3	500 ppm	250 ppm	0.2
H_2S (ppm)	0	1.3	0.9	1.5
H_2/CO	1.8	1.0	0.9	0.6

Syngas quality: air versus oxygen

- Air-blown gasifiers avoid the large capital cost of an ASU but produce a much lower calorific value syngas than oxygenblown gasifiers. The nitrogen in the air typically dilutes the syngas by a factor of 3 compared to oxygen-blown gasification.

- In the future O_2 could come from electrolysis…

- This has a significant impact on the design of the combustion system. Because the nitrogen in air must be heated to the gasifier exit temperature by burning some of the syngas, air-blown gasification is more favourable for gasifiers which operate at lower temperatures (i.e. non-slagging).

- Air-blown gasifiers also have a negative impact on CO_2 capture. Because of the dilution effect of the nitrogen, the partial pressure of CO_2 in air-blown gasifier syngas will be one-third of that from an oxygen-blown gasifier. This increases the cost and decreases the effectiveness of the CO_2 removal equipment

	Gasifier A	Gasifier B	Gasifier A	Gasifier B
WO2012064936A1	*vol% dry gas, Air fired*	*vol% dry gas, Air fired*	*vol% dry gas, Oxygen-fired*	*vol% dry gas, Oxygen-fired*
H2 (v/v %)	5-39	10-30	5-39	10-35
CO (v/v%)	5-39	10-39	5-39	15-39
CO2 (v/v%)	15-50	15-35	15-50	15-40
N2 (v/v%)	10-60	10-30	8-30	8-15
CH4 (v/v%)	0-10	0-10	0-10	0-10
CxHy(v/v%)	0-4	0-4	0-4	0-4
H2S (ppm)	400-2000	400-2000	400-2000	400-2000
COS (ppm)	5-400	5-400	5-400	5-400
HCl (ppm)	1000-5000	1000-5000	1000-5000	1000-5000
NH3 (ppm)	1000-5000	1000-5000	1000-5000	1000-5000
Ar (v/v%)	0-2	0-2	0-2	0-2
H2/CO	0.3-2	0.6-1.5	0.3-2	0.6-1.5
H2O (v/v%) in wet gas	15-50	15-30	15-50	15-30
Particulate matter (mg/Nm3)	Up to 50,000	From 5,000 to 29,500 or from 30,500 to 50,000	Up to 50,000	From 5,000 to 29,500 or from 30,500 to 50,000

Crude Syngas Compositions from the Gasification of Waste

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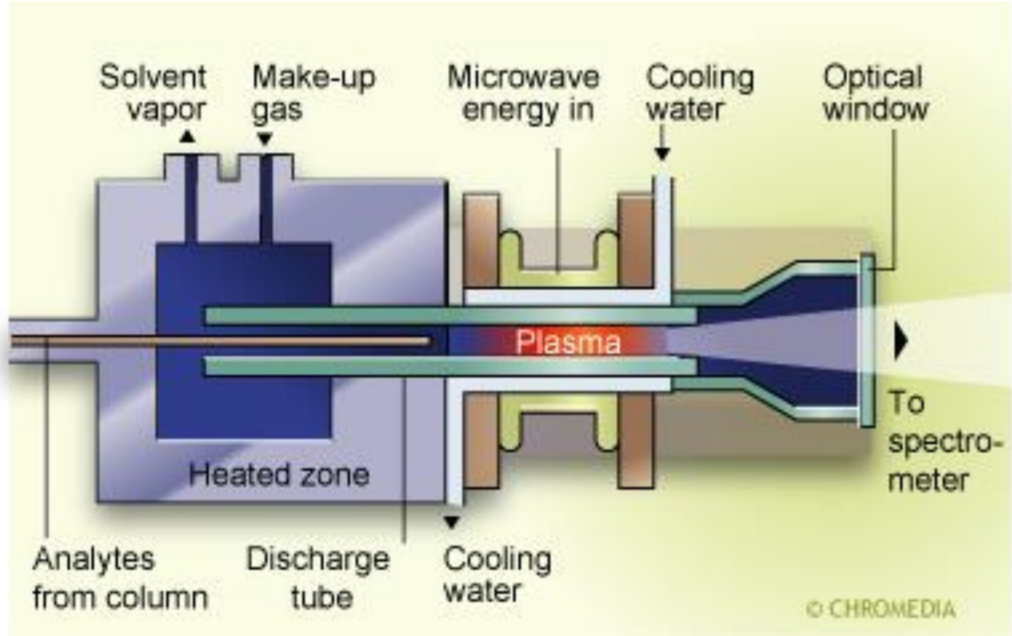
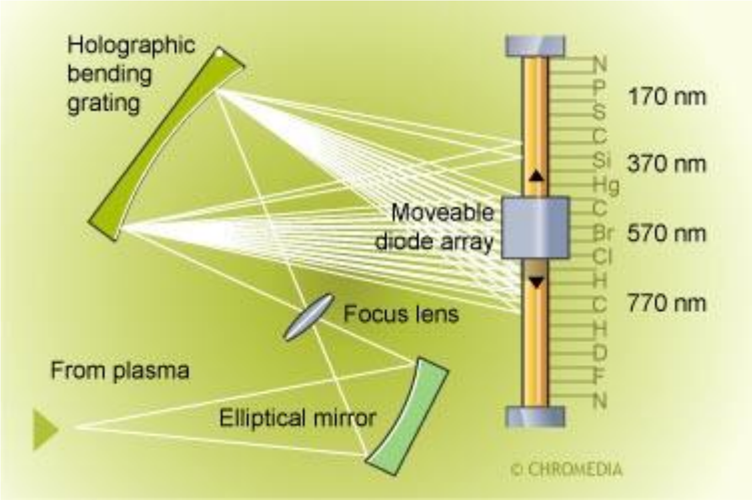
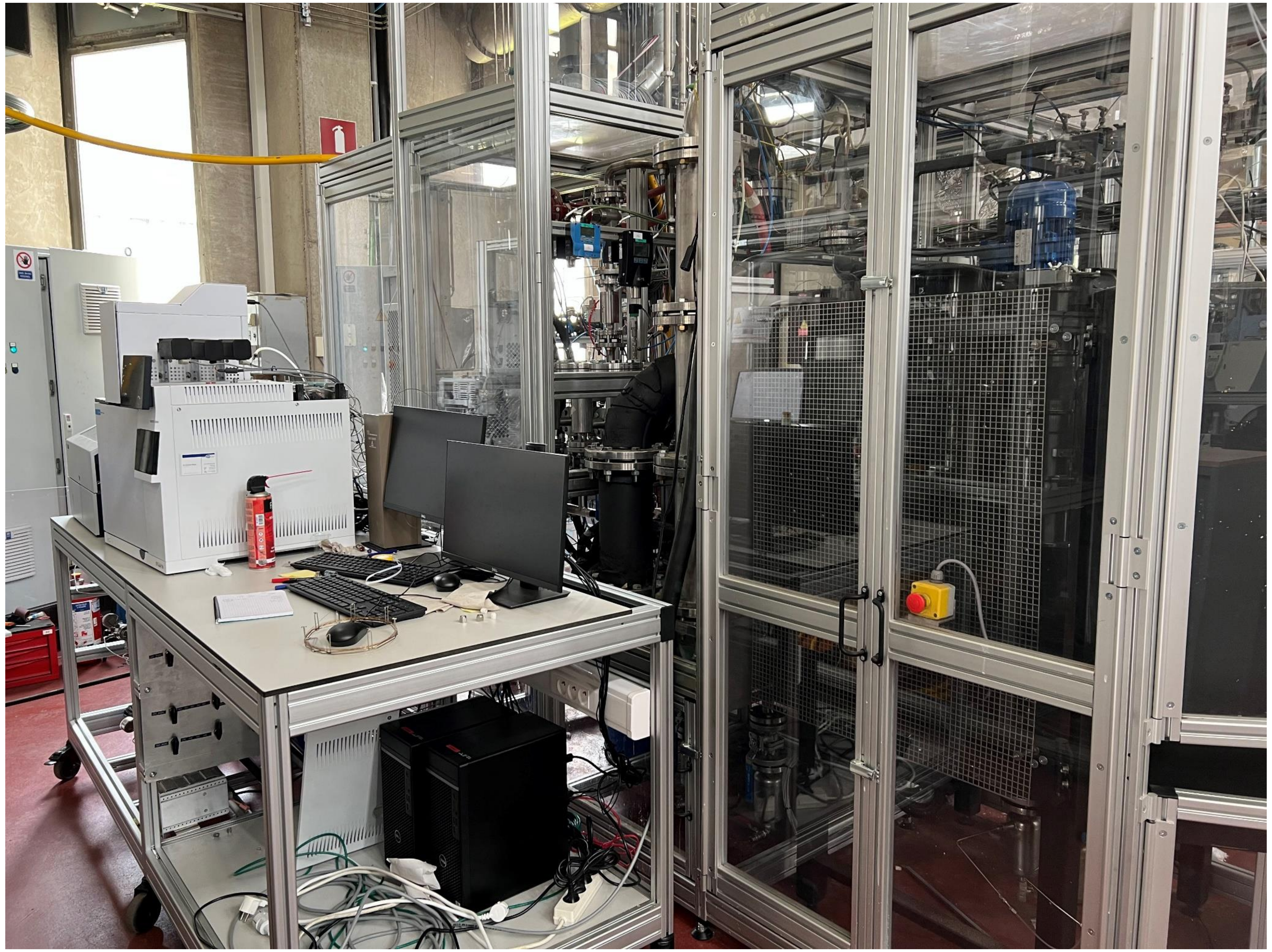
Measuring syngas composition/impuirties: AED

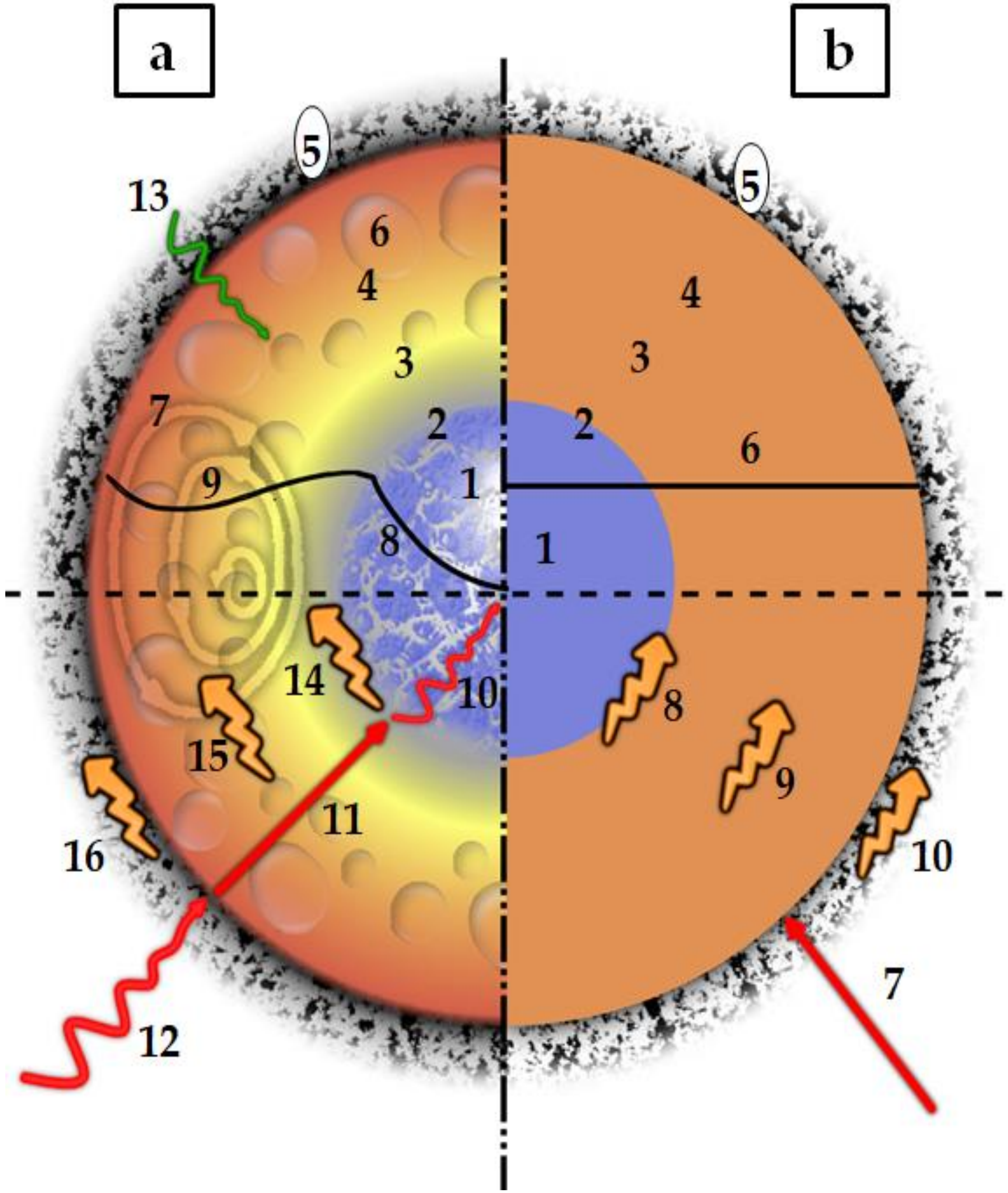


The atomic emission detector (AED) is based on the intense emission properties of elements, particularly halogens, phosphorus, nitrogen, and sulphur, following excitation in a helium plasma.





Modeling approach: Comprehensive vs. Simplified



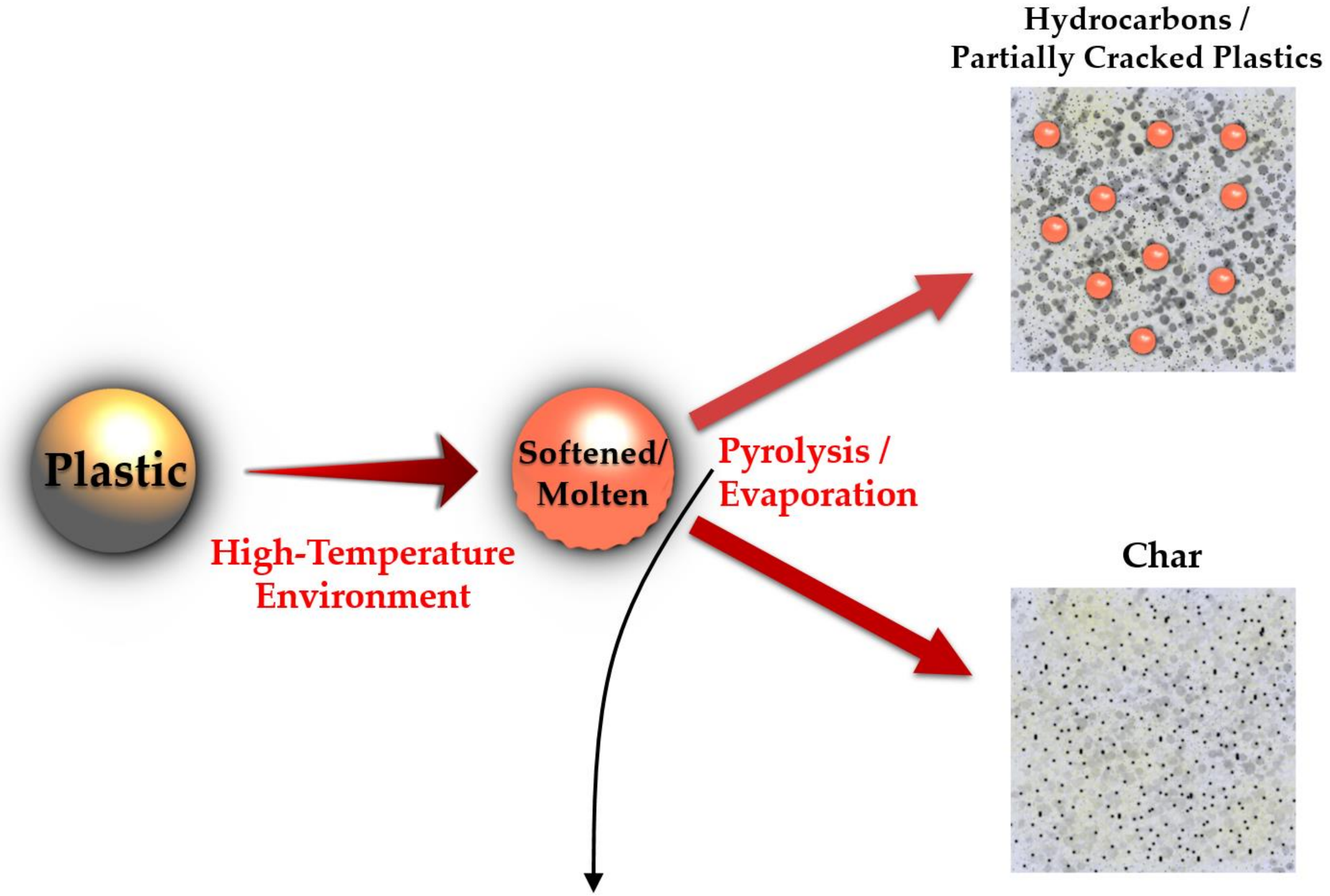
COMPREHENSIVE

1) Porous solid plastic core; 2) Melt front; 3) Liquid layer; 4) Pyrolysis and evaporation (devolatilization) layer; 5) Gasification layer (including char); 6) Bubbles present in the liquid layer as the result of pyrolysis and evaporation; 7) Vortex-pattern flows as the result of Marangoni and convection effects; 8) Diffusive transport phenomena; 9) Possible temperature (or concentration) profile as the result of internal circulations in the liquid phase; 10) Internal radiative and conductive heat transfer; 11) Conductive and convective heat and mass transfer; 12) Radiation and convective heat and mass transfer; 13) Mass diffusion; 14) Heat of melting; 15) Heat of decomposition and evaporation; 16) Heat of gasification

SIMPLIFIED

1) Solid plastic core; 2) Sharp melt front; 3) Liquid layer; 4) Pyrolysis and evaporation (devolatilization) layer; 5) Gasification layer (including char); 6) Infinite internal heat and mass transfer; 7) Convective heat and mass transfer; 8) Heat of melting; 9) Heat of decomposition and evaporation; 10) Heat of gasification

The chemistry is complex even without impurities



Gasification Reactions

$$C_nH_m + O_2 \rightarrow CO_2 + H_2$$
$$C_nH_m + H_2O \rightarrow CO + H_2$$
$$C_nH_m + CO_2 \rightarrow CO + H_2$$
$$CO + O_2 \rightarrow CO_2$$
$$CO + H_2O \leftrightarrow CO_2 + H_2$$
$$CO + 3H_2 \leftrightarrow CH_4 + H_2O$$
$$2CO + 2H_2 \rightarrow CH_4 + CO_2$$
$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

$$C + O_2 \rightarrow CO_2$$
$$C + {}^1/_2\, O_2 \rightarrow CO$$
$$C + H_2O \rightarrow CO + H_2$$
$$C + 2H_2O \rightarrow CO_2 + 2H_2$$
$$C + CO_2 \leftrightarrow 2CO$$
$$C + 2H_2 \rightarrow CH_4$$

Simplified Single-Step Pyrolysis Reaction and Evaporation

$$C_nH_mO_pN_q \rightarrow aH_2 + bCO + cCO_2 + dCH_4 + eC_2H_4 + fC_2H_6 + gC_xH_y + hN_2 + iC$$

Contaminants in post-consumer plastic waste

Halogen content (in ppmw) of representative products analysed via **Ion Chromatography** [1]

	Cl	Br	F	I
Cap Tr.	**320**	<50	<40	<50
Cap Red	200	<50	<40	<50
Bottle	**710**	<50	<40	<50
Label	**2300**	<50	<40	<50
Cap	200	<50	<40	<50
Bottle	<150	<50	<40	<50
Label	**320**	<50	<40	<50
Tray	<150	<50	<40	<50
Lid	<150	<50	<40	<50
Cap	**900**	<50	<40	<50
Bottle	180	<50	<40	<50
Cap	200	<50	<40	<50
Bottle	<150	<50	<40	<50
Label	<150	<50	<40	<50

Metal content of post-consumer mixed polyolefin (MPO) waste analysed via **ICP-OES** [2]

Element	ppmw
Li	4
Na	**578**
Mg	220
Ca	**3435**
Sr	6
Ti	170
Cr	24
Mn	2
Fe	124
Cu	20
Zn	63
Al	**258**
Tl	3
Pb	3
Sb	17
As	3

Elemental analysis of post-consumer MPO [2]

Element	wt.%
N	0.9
C	82.0
H	13.3
S	<LOD
O	3.8

Post-consumer plastic waste is a diverse feedstock with a huge range of elements

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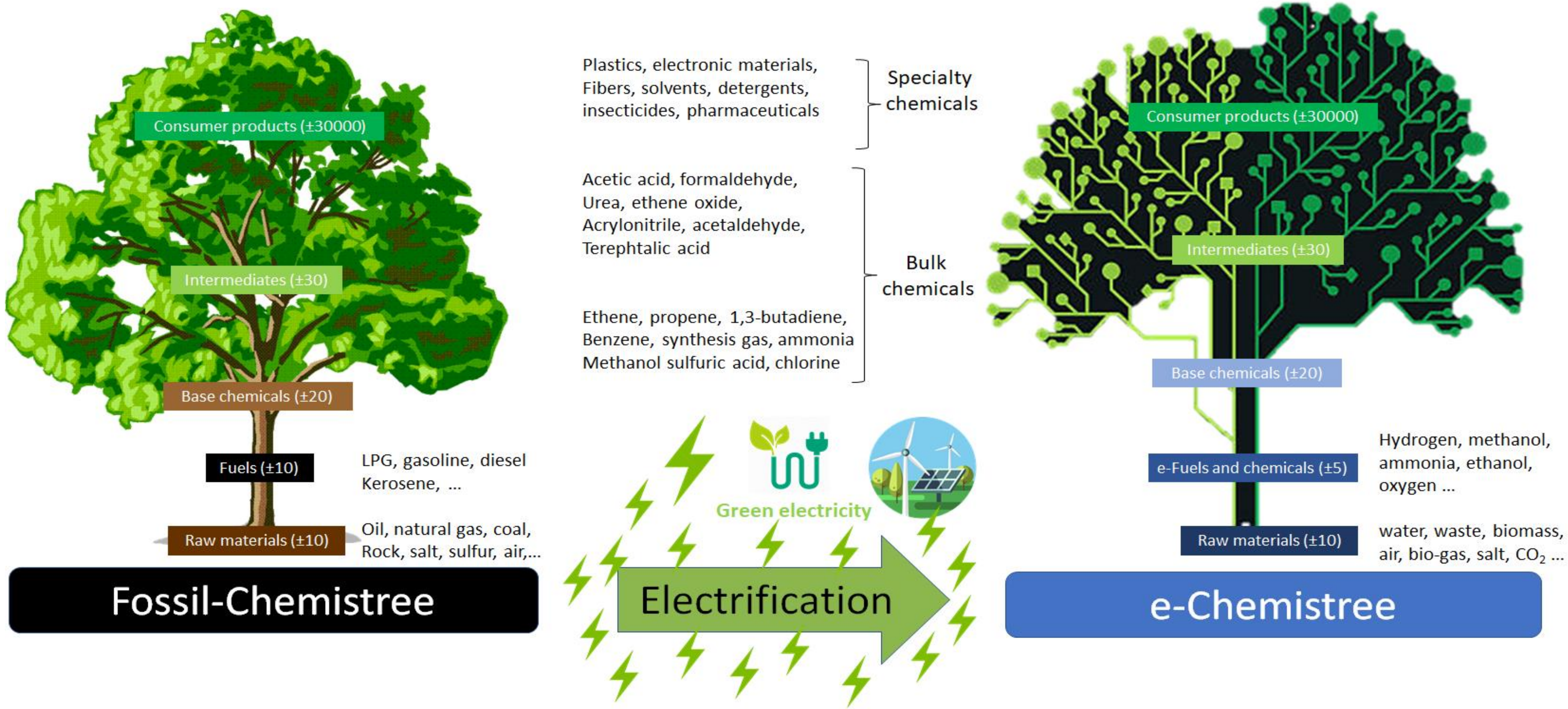
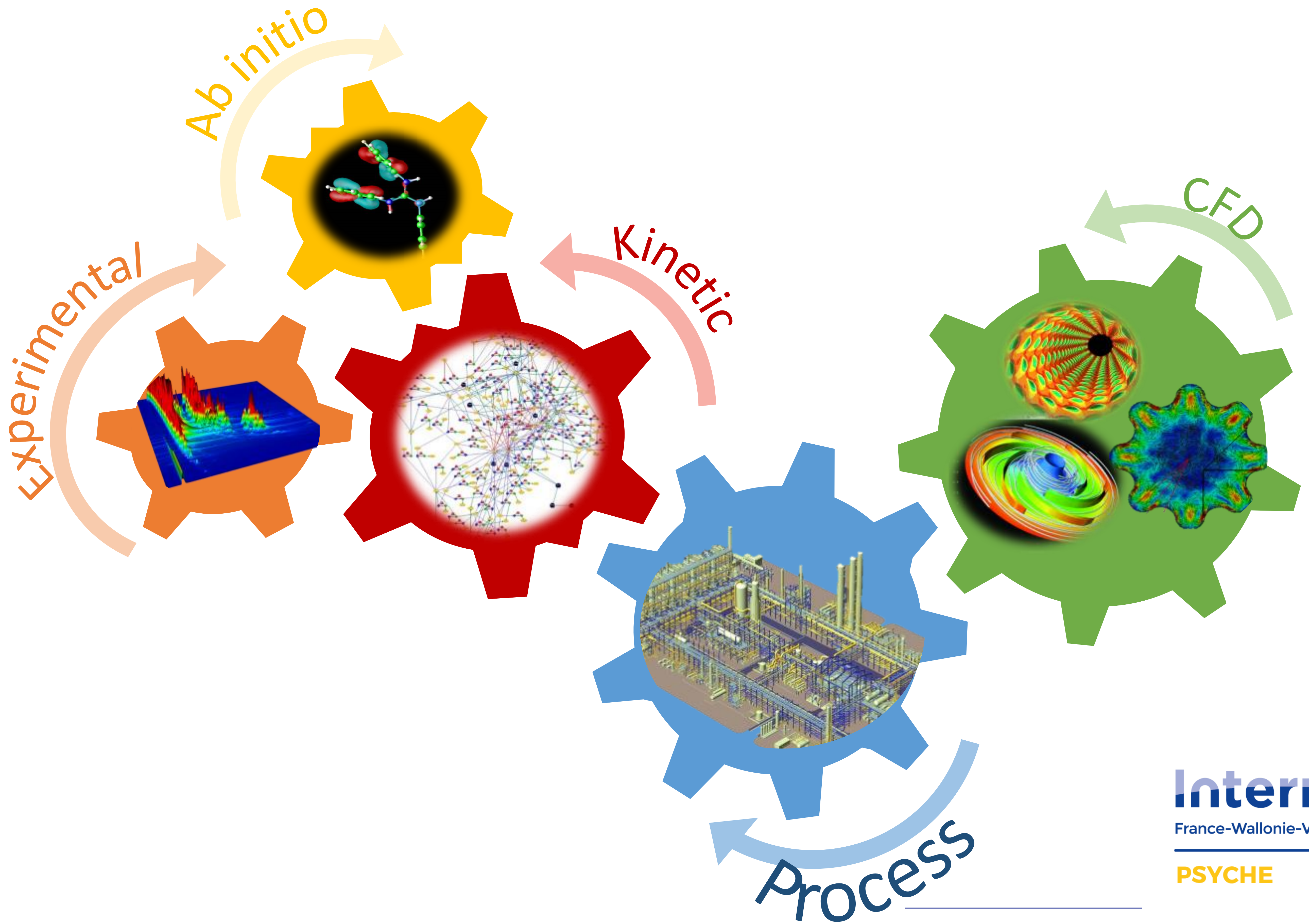
[1] Roosen et al. (2020). Environ Sci Technol 54(20): 13282-13293. [2] Kusenberg et al. (2022). Fuel Process Technol 227: 107090.

Electrification: can we use green electricity?

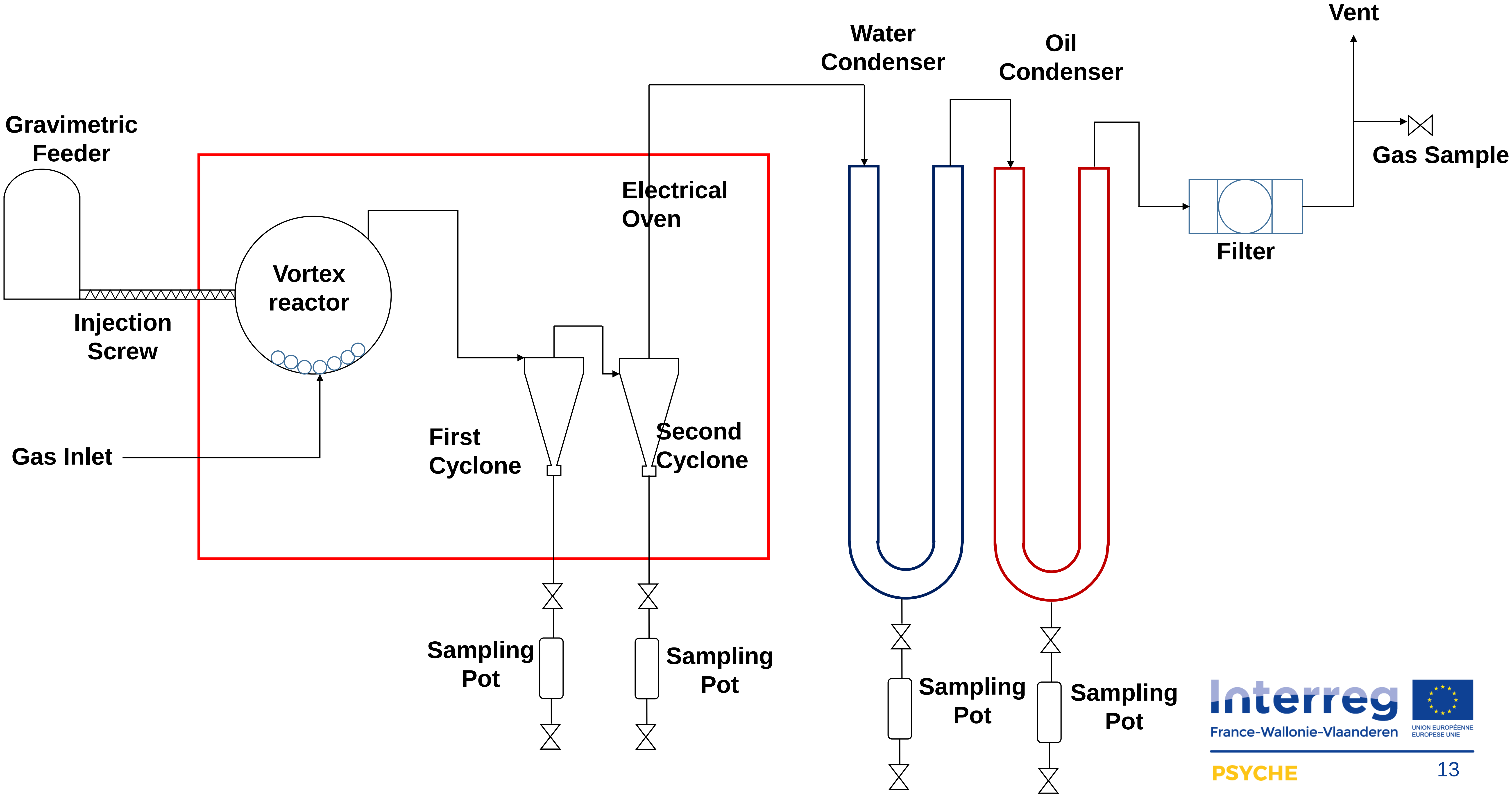
Van Geem and Weckhuysen (2022): Toward an e-chemistree : materials for electrification of the chemical industry



Multiscale modeling approach for gasifier design



Highlight 1: vortex gasification unit constructed!



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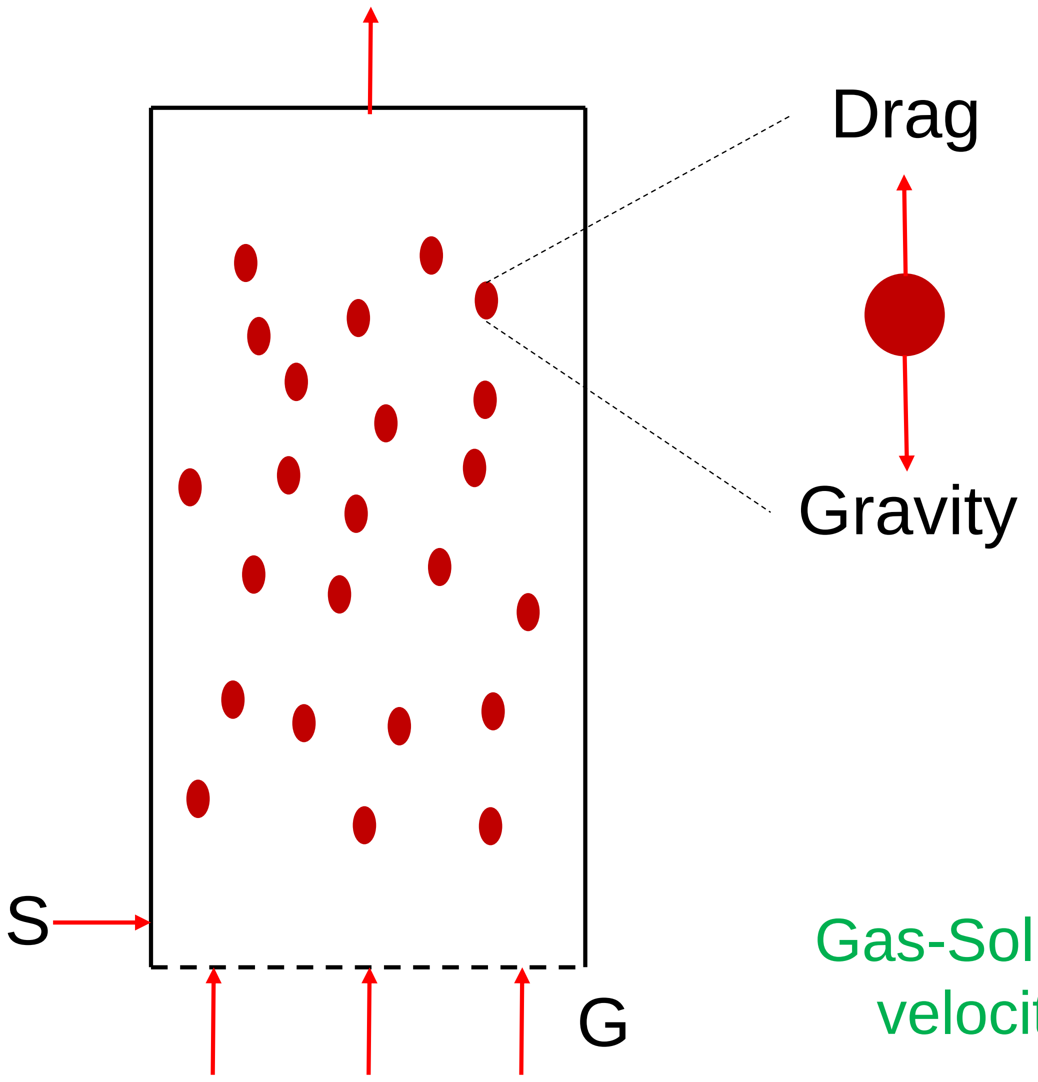
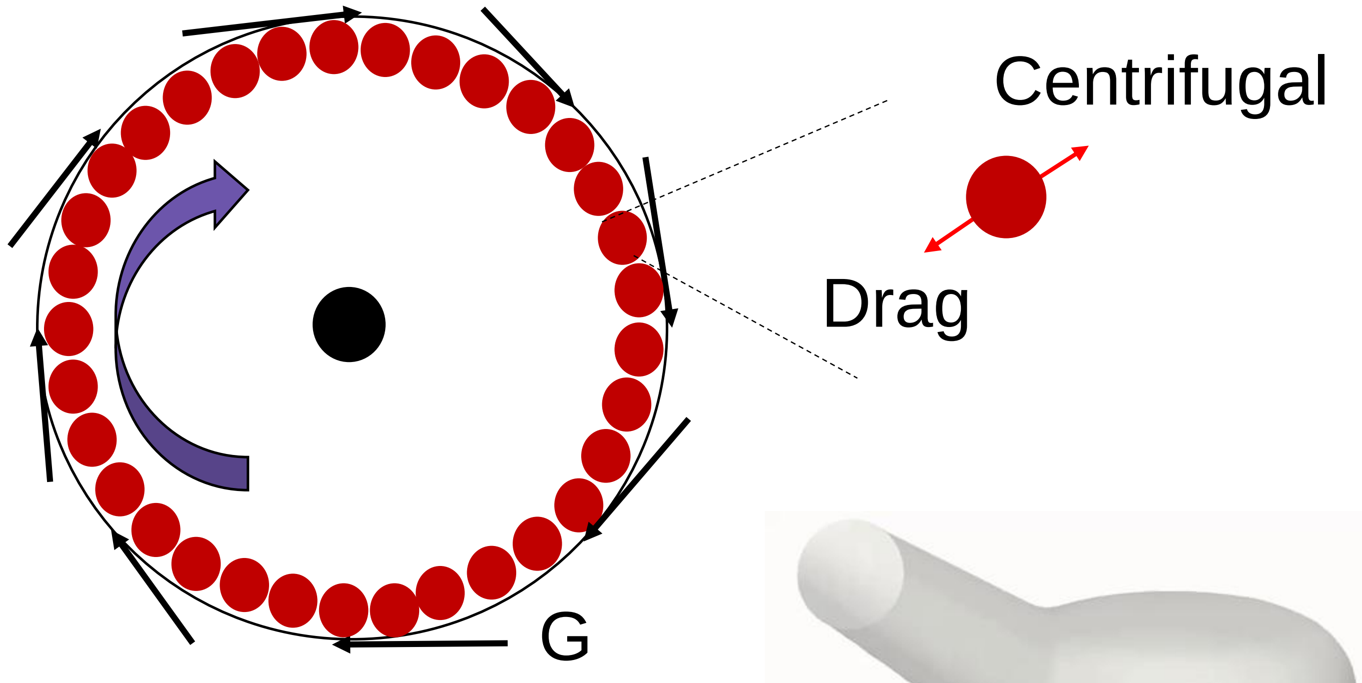
Multiphase Chemical Reactors



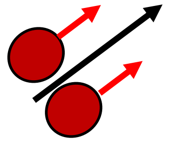
- Gas flow restrictions
- Dilute beds

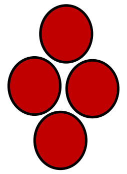
Fluidized Bed Reactor

Gas-Solid Vortex Reactors



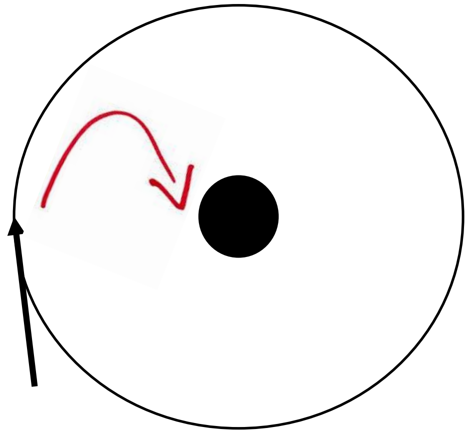
Gas-Solid slip velocities





Packed beds

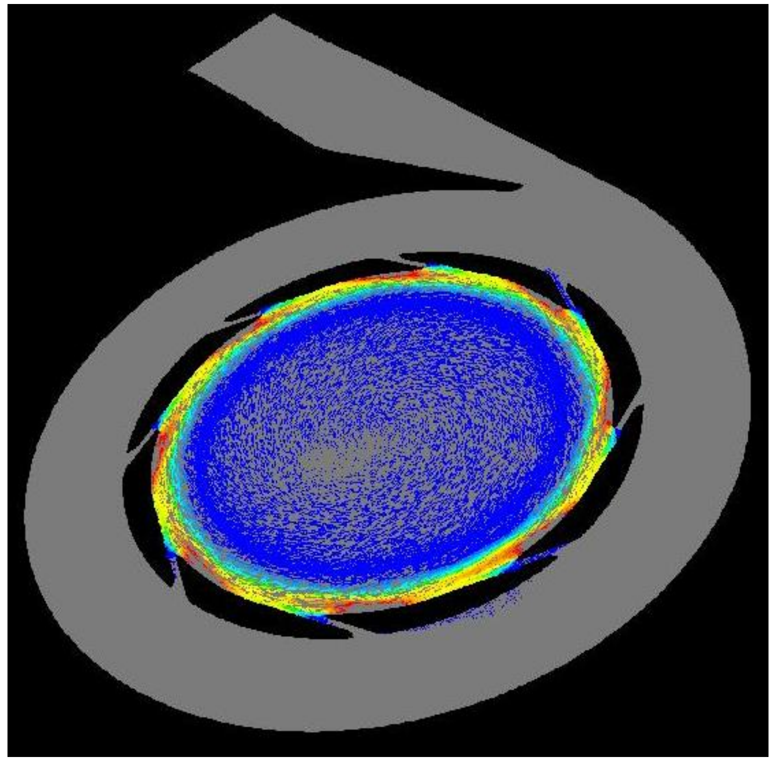
Short Gas Residence time



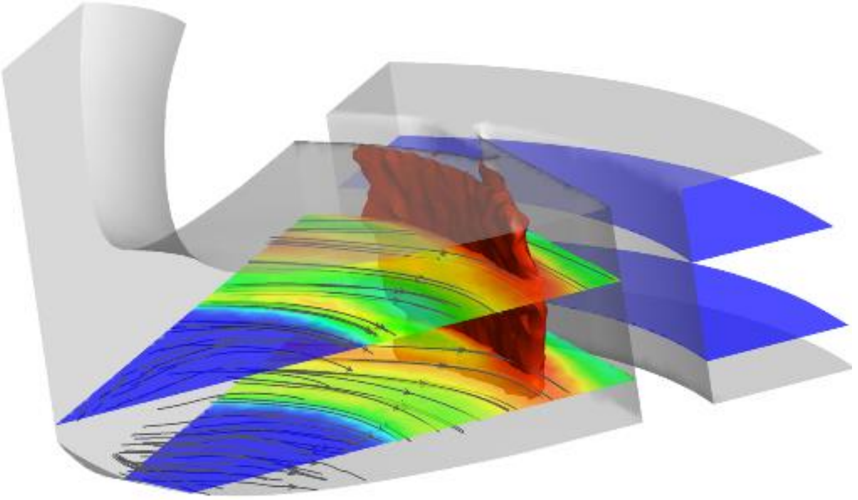
Gas-Solid

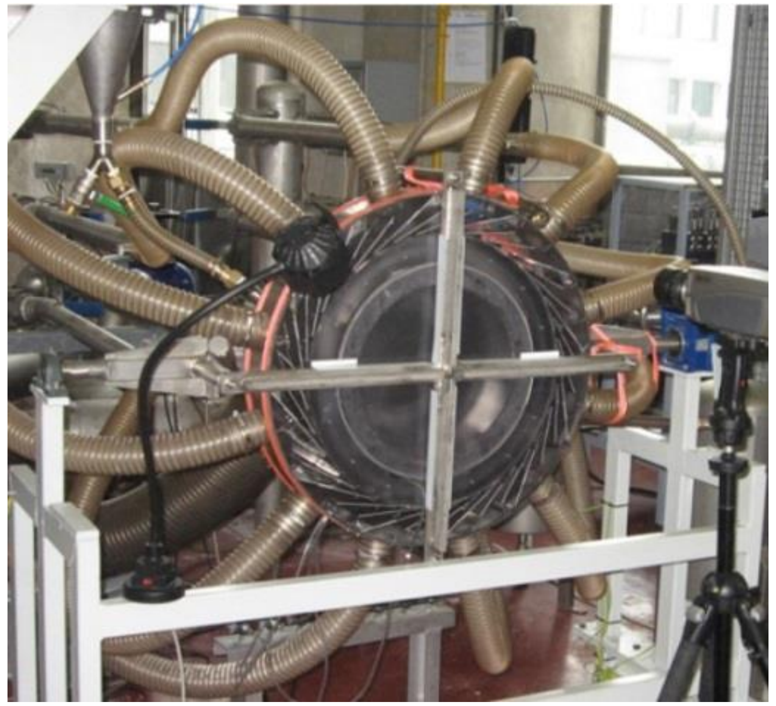
Process intensification in terms of heat & mass transfer

GSVR Research @ LCT

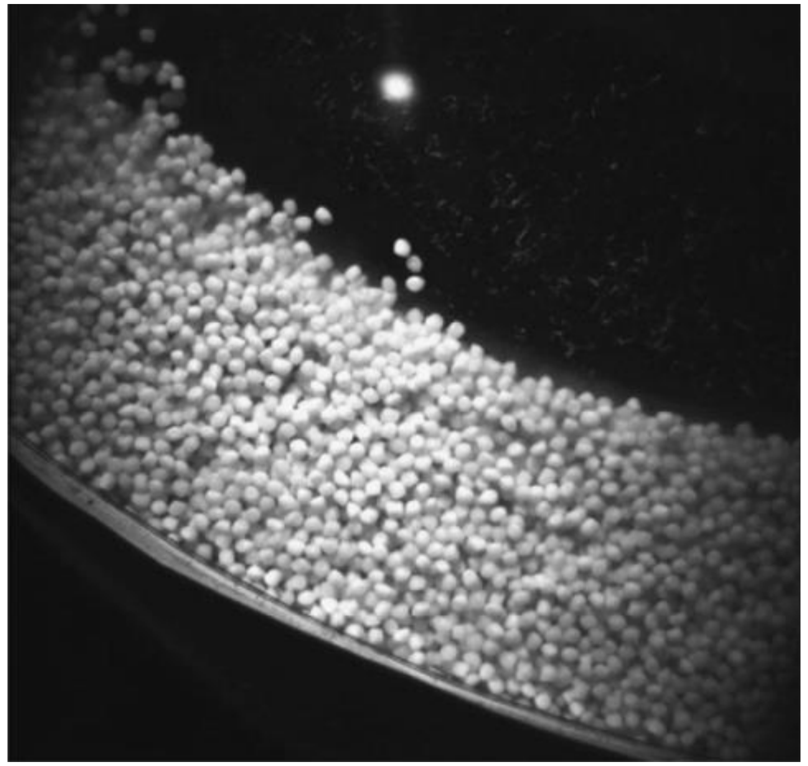


CFD

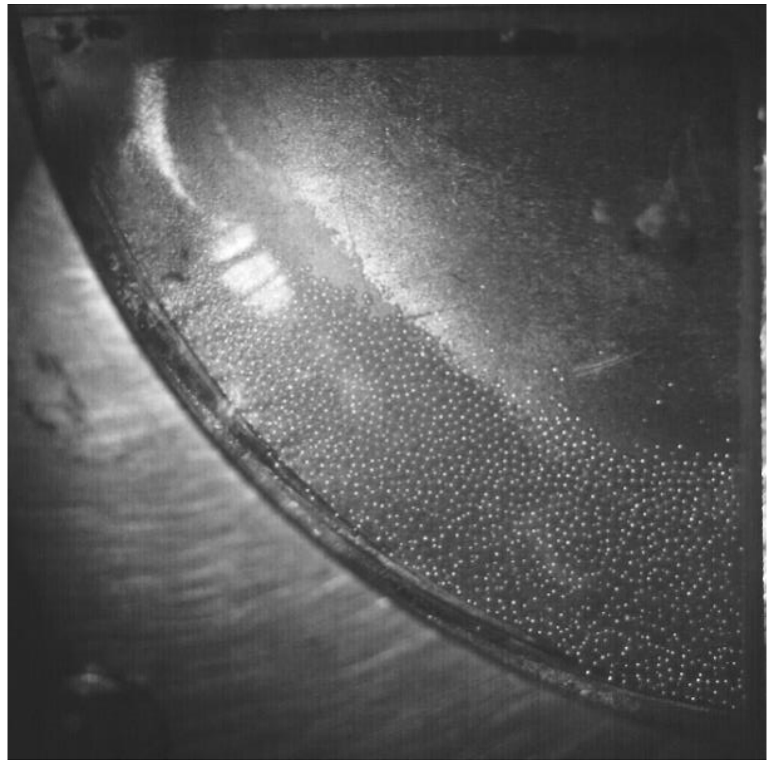


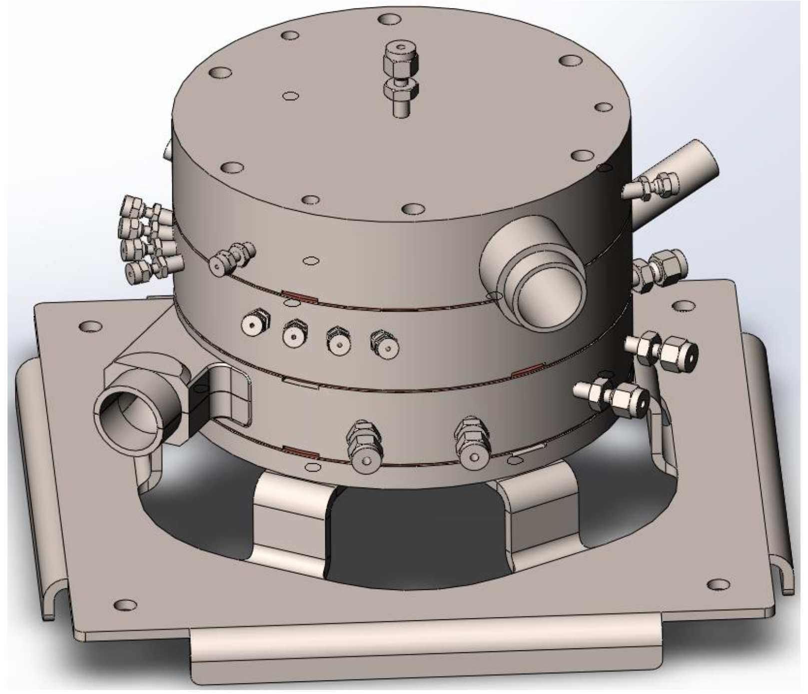


Cold-Flow GSVR

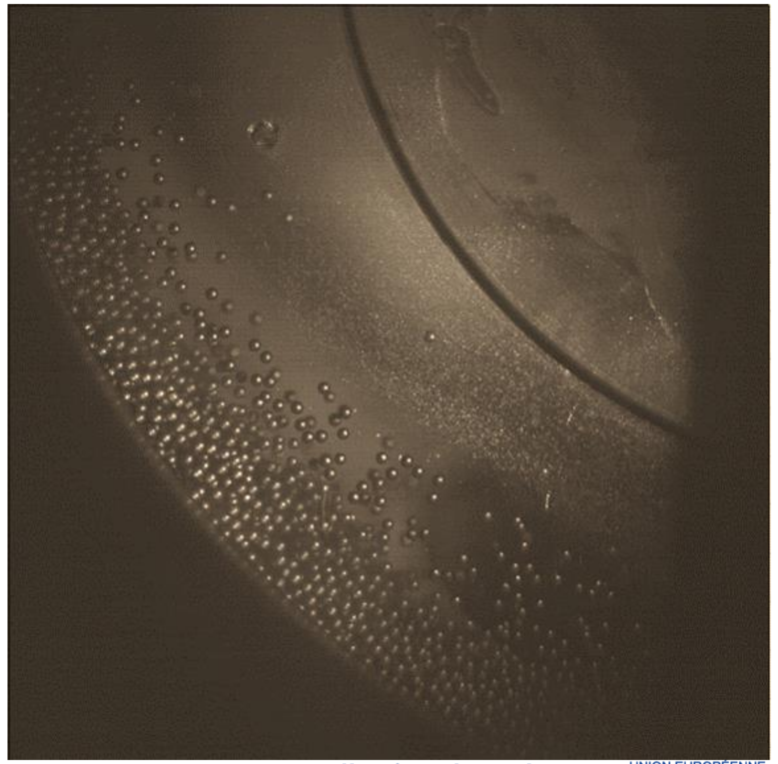


Hot-Flow GSVR





Reactive GSVR



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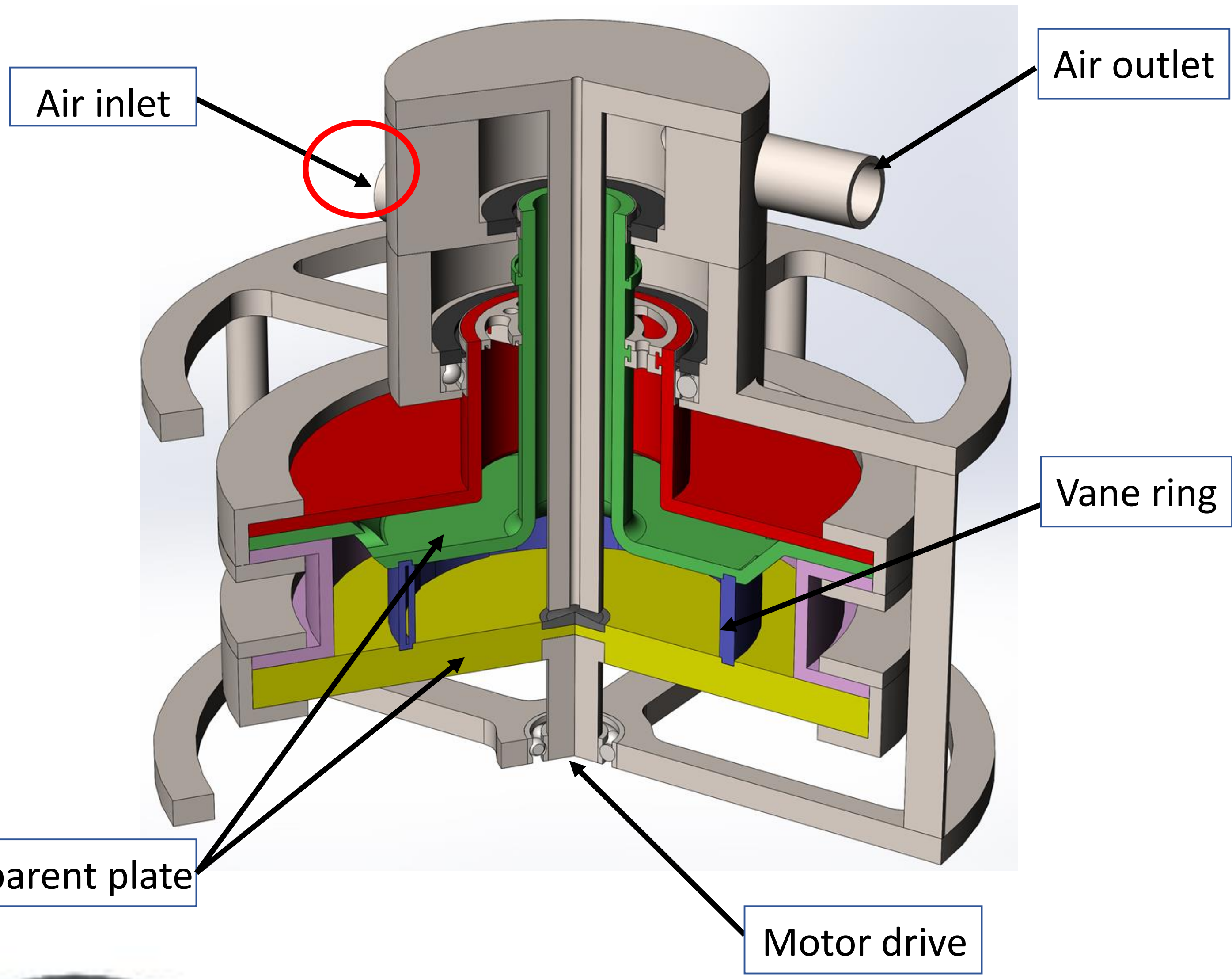
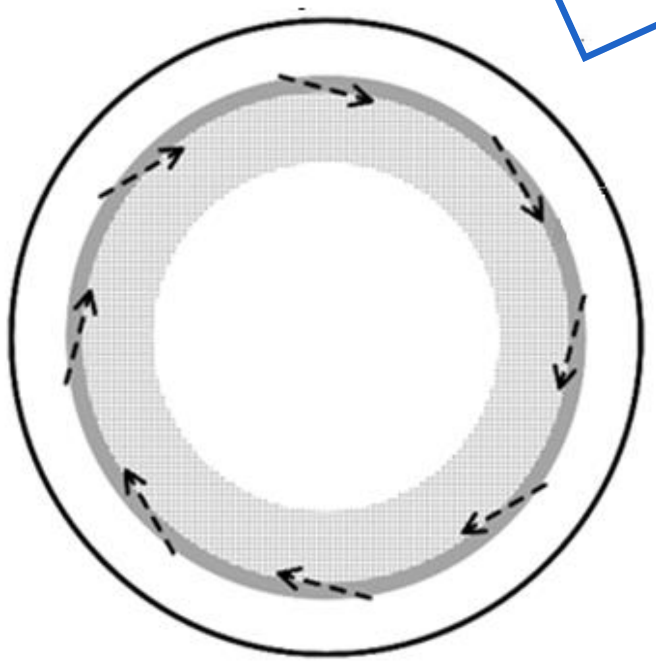
Vortex Technology

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



Starvoc2
Decoupled
F_c and F_d

Static



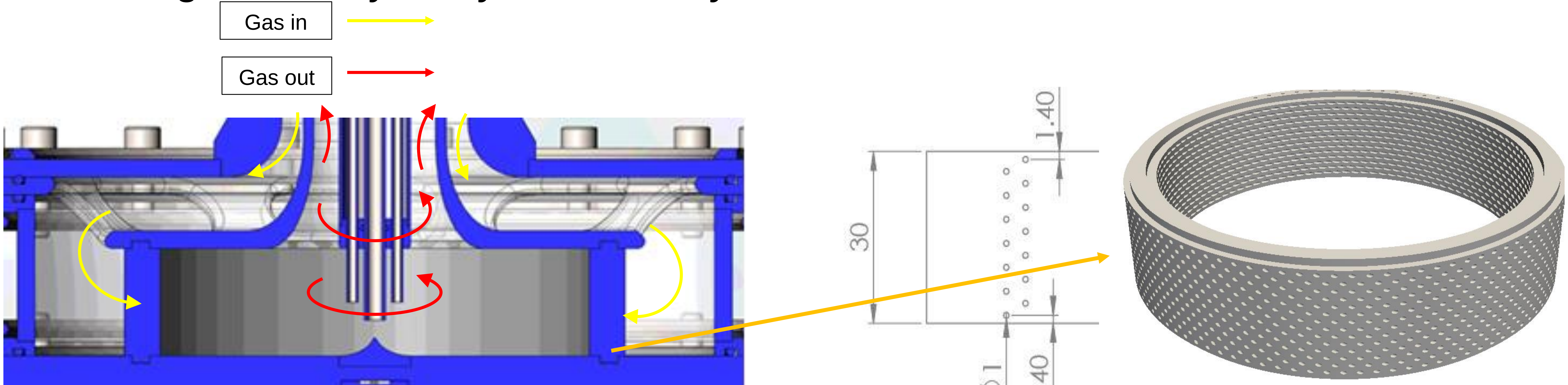
Rotating

Van Geem et al.., et al. U.S. Patent Application No. 16/627,430.

Experimental setup

Controlled chamber rotation as an approach to:

- Independently control of flowrate and rotating speed
- Investigate the hydrodynamic study of these variables

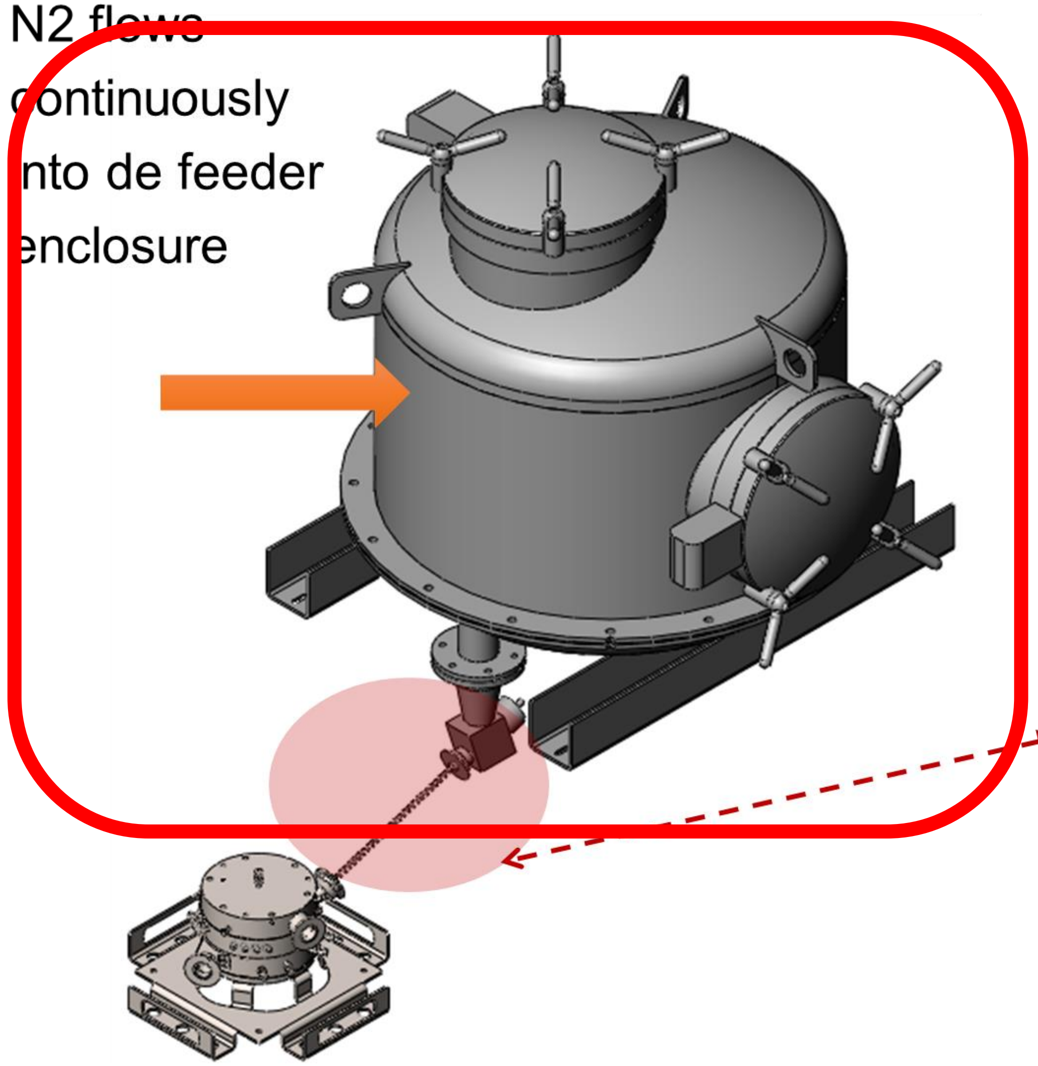


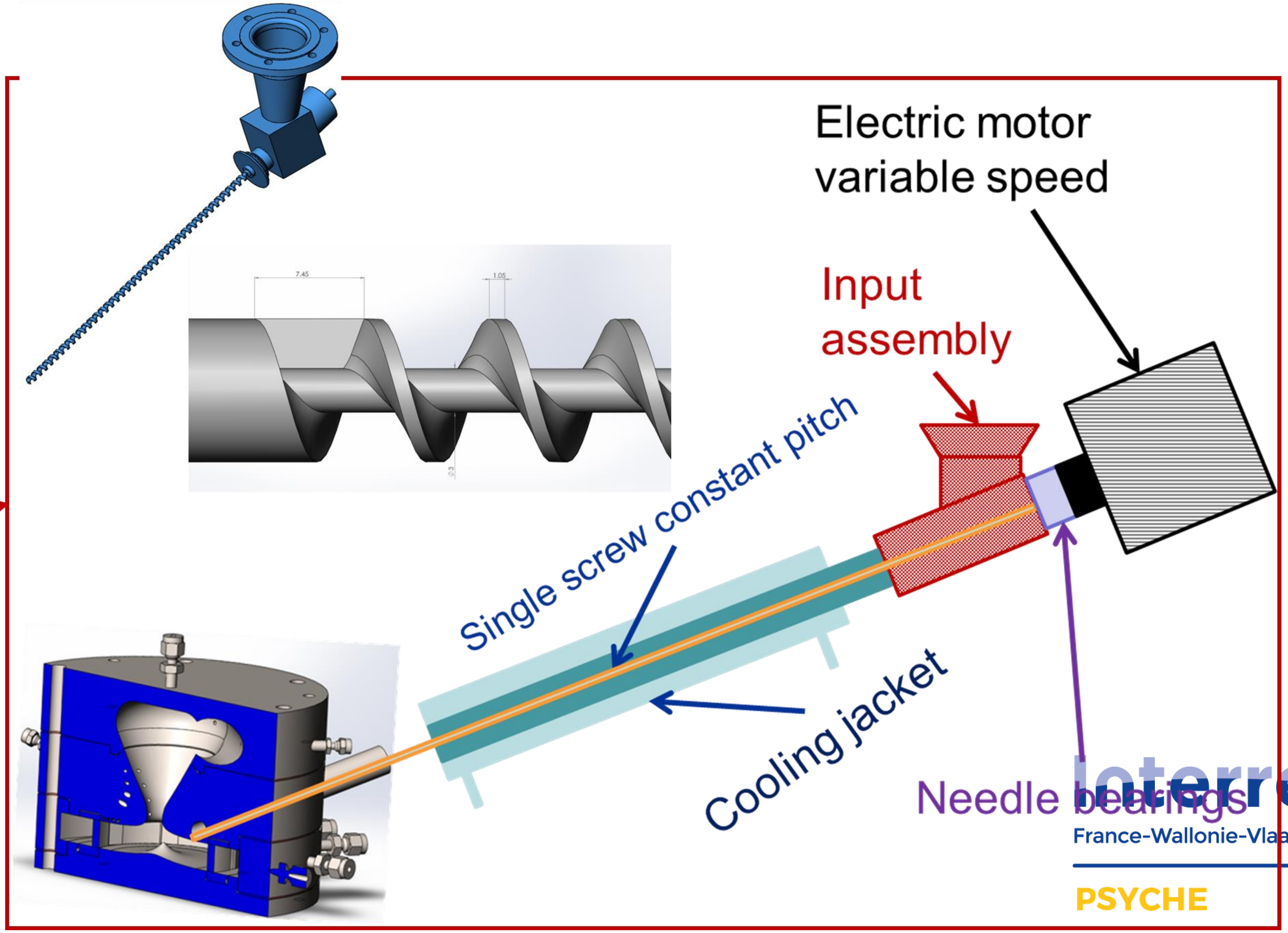
1400 jet-holes (Ø1mm, 30°)

Gas distributor

Feeding is more challenging then expected

– First using the previous gravimetric feeder: Comparable to the biomass pyrolysis experiments





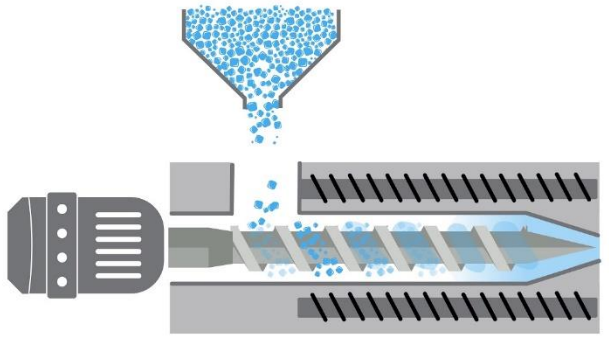
Large → Relocate the analytical section → Test the performance first

UCL work

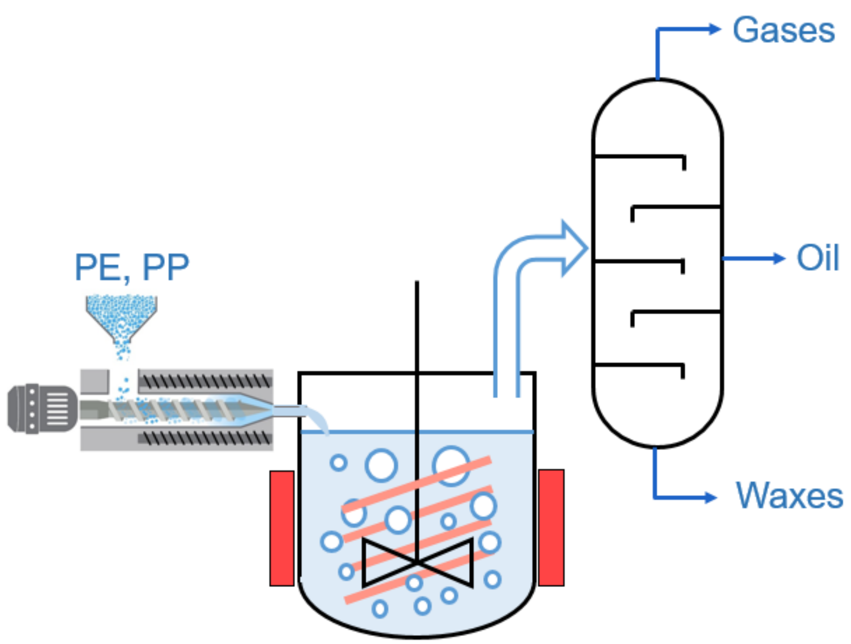
- Pyrolysis of plastic: Vortex and/or conventional technology based on plastic as **continuous** or **dispersed** phase?

Plastic as **continuous** phase

- Feeding system: extrusion screw

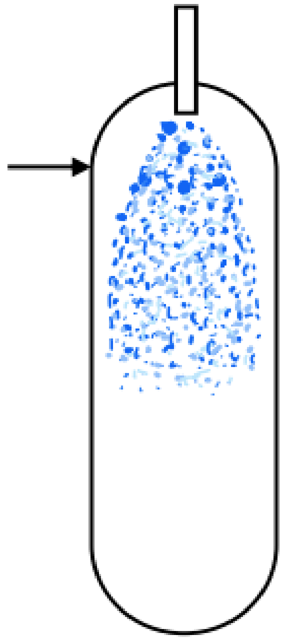


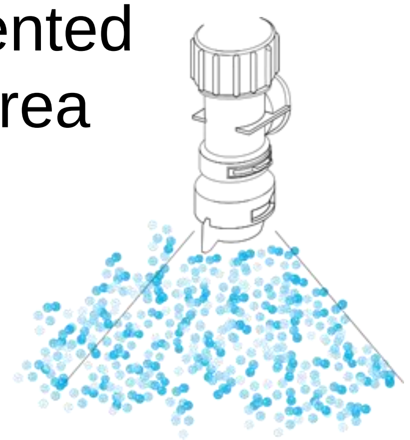
  - Simplicity of design



Plastic as **dispersed** phase

- Feeding system: spray nozzle
  - Reduced wall friction
  - Wall fouling can be prevented
  - High interfacial surface area liquid phase





Added value of Vortex chamber technology?

Pros

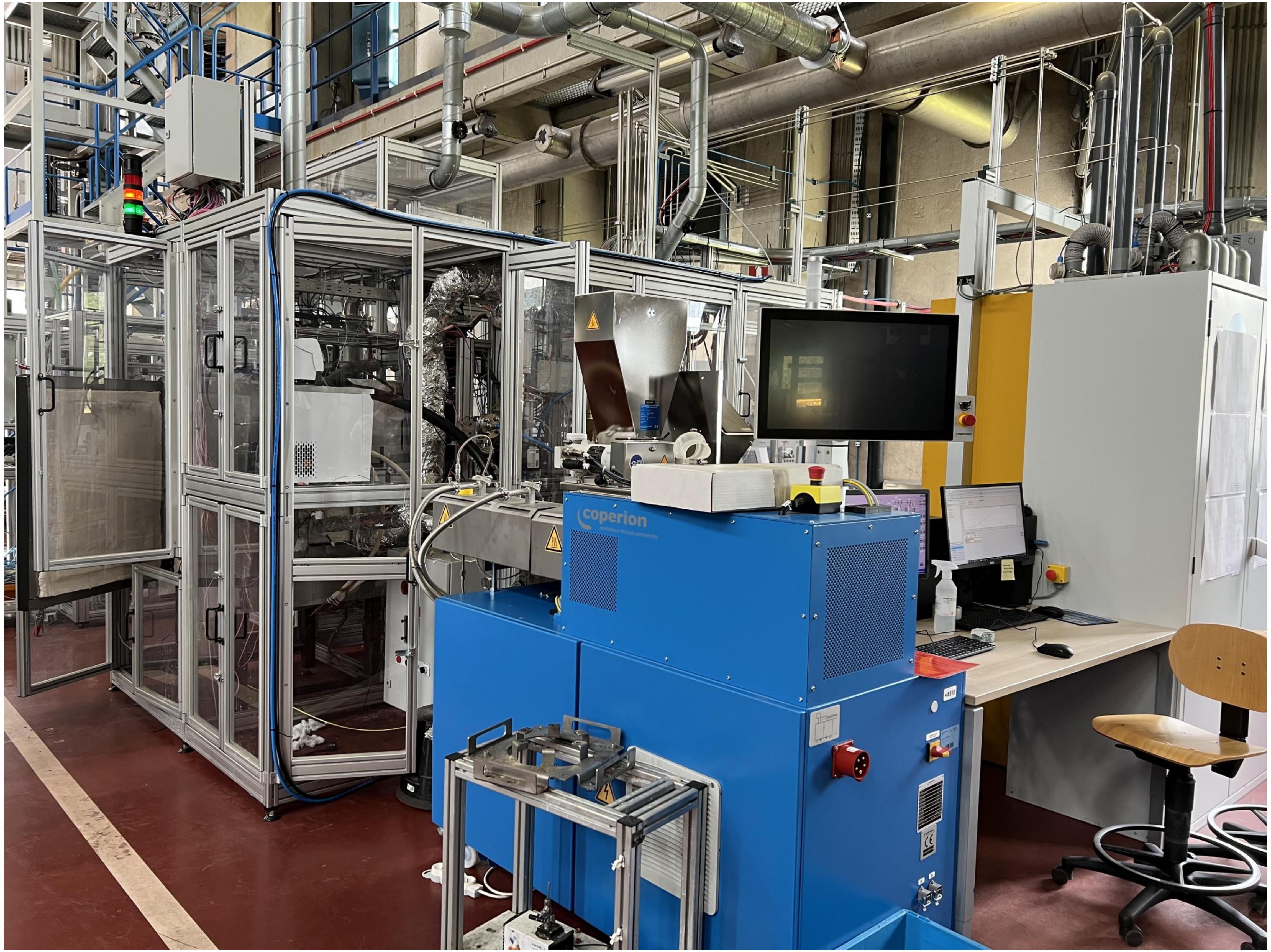
- Intensification of interfacial mass and heat transfer
- Different types of multi-zone operations possible

Cons

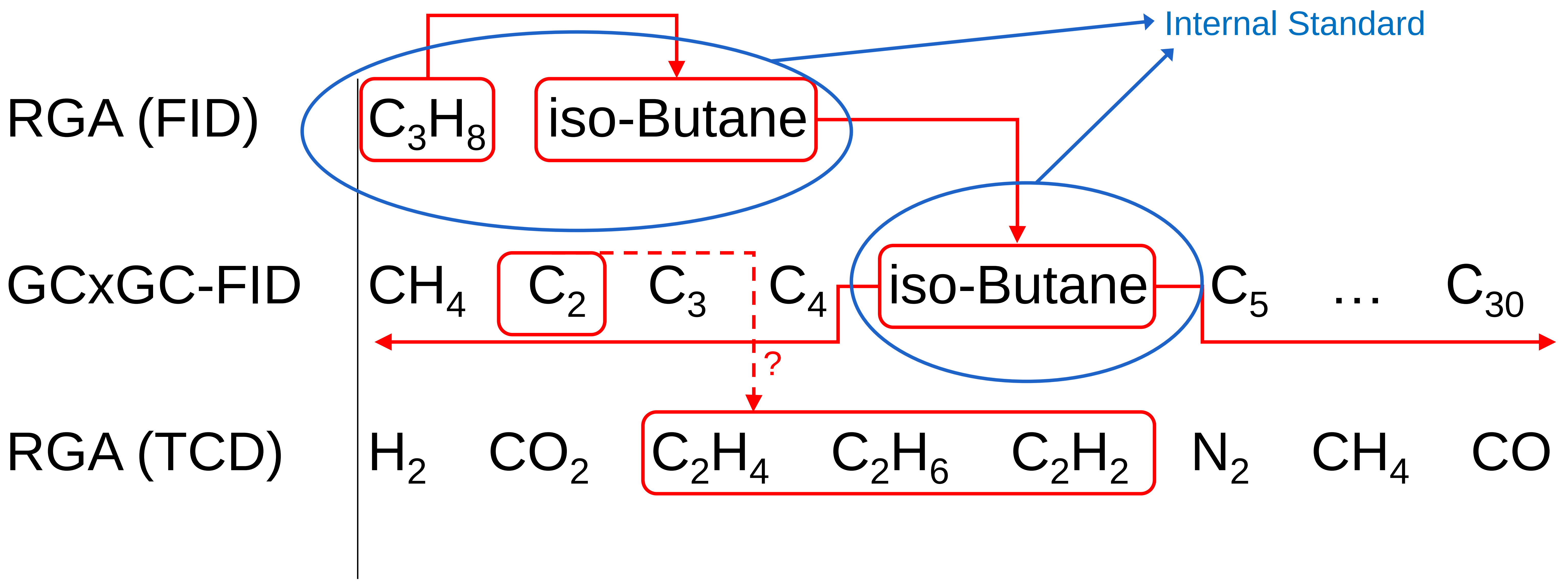
- Flow complexity & control
- Minimum flow rate requirement in order to ensure vortex regime
- Energy consumption related to bed rotation to be analyzed
- Lower length-to-diameter ratio (lower heat exchanging surface area per unit reactor volume)

spray tower could be interesting technology but blockages of spray nozzle are the main concern

Extruder works better for vortex reactor



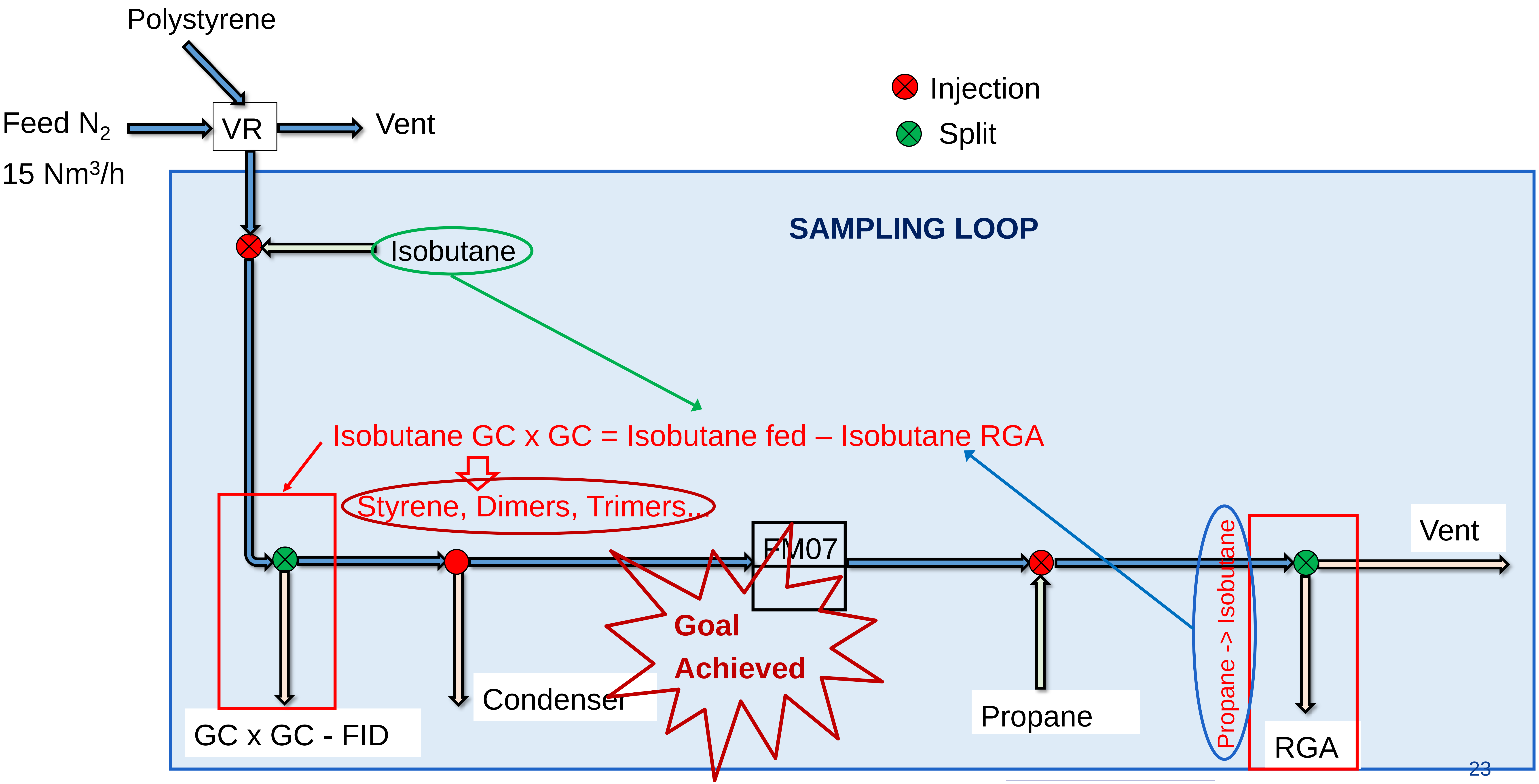
Development of Online Sampling System



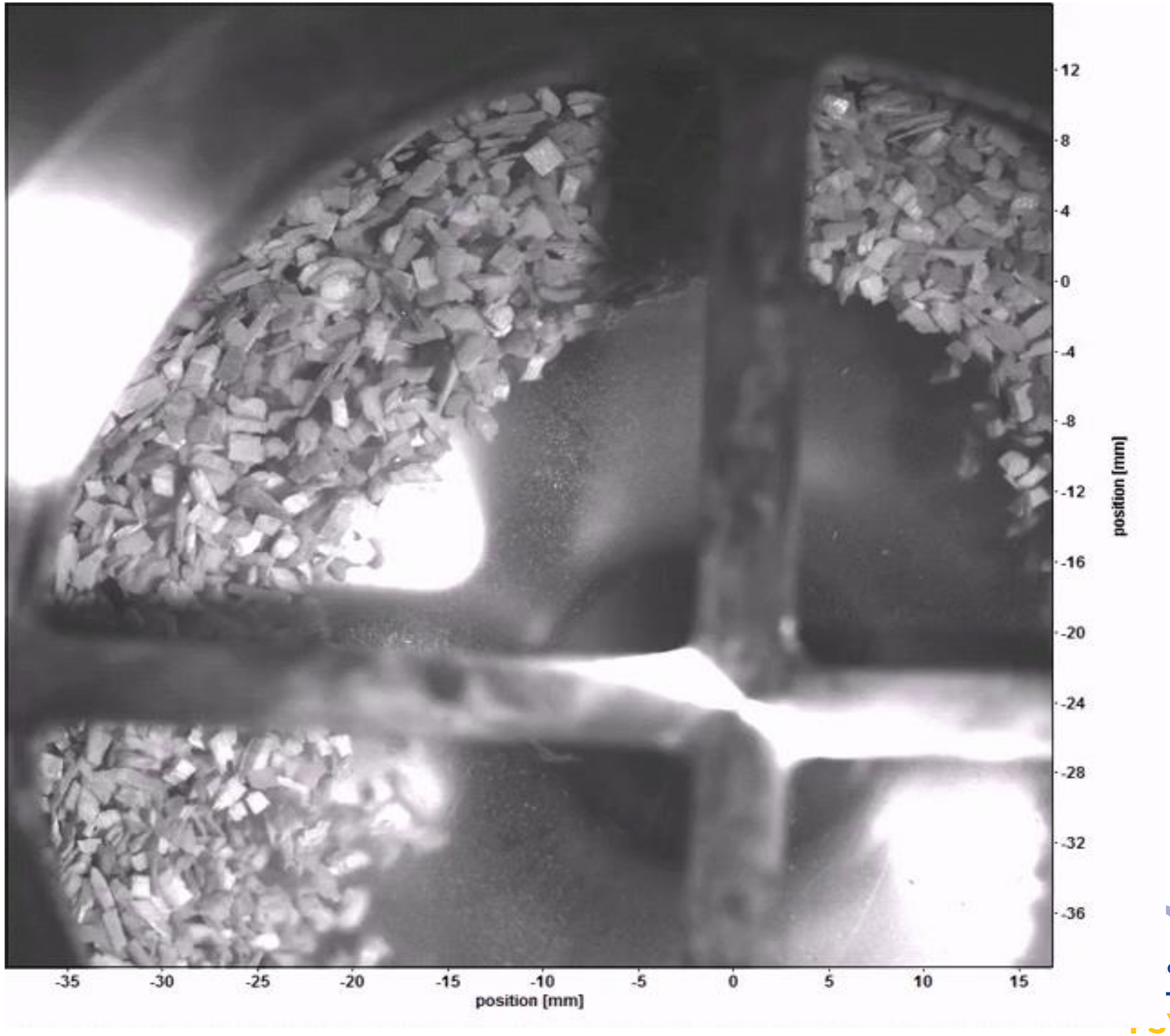
C_3H_8 - To quantify isobutane and non-condensable gases in RGA

iso-Butane – To characterize liquid products and gases in GC x GC

Schematic of the Sampling System



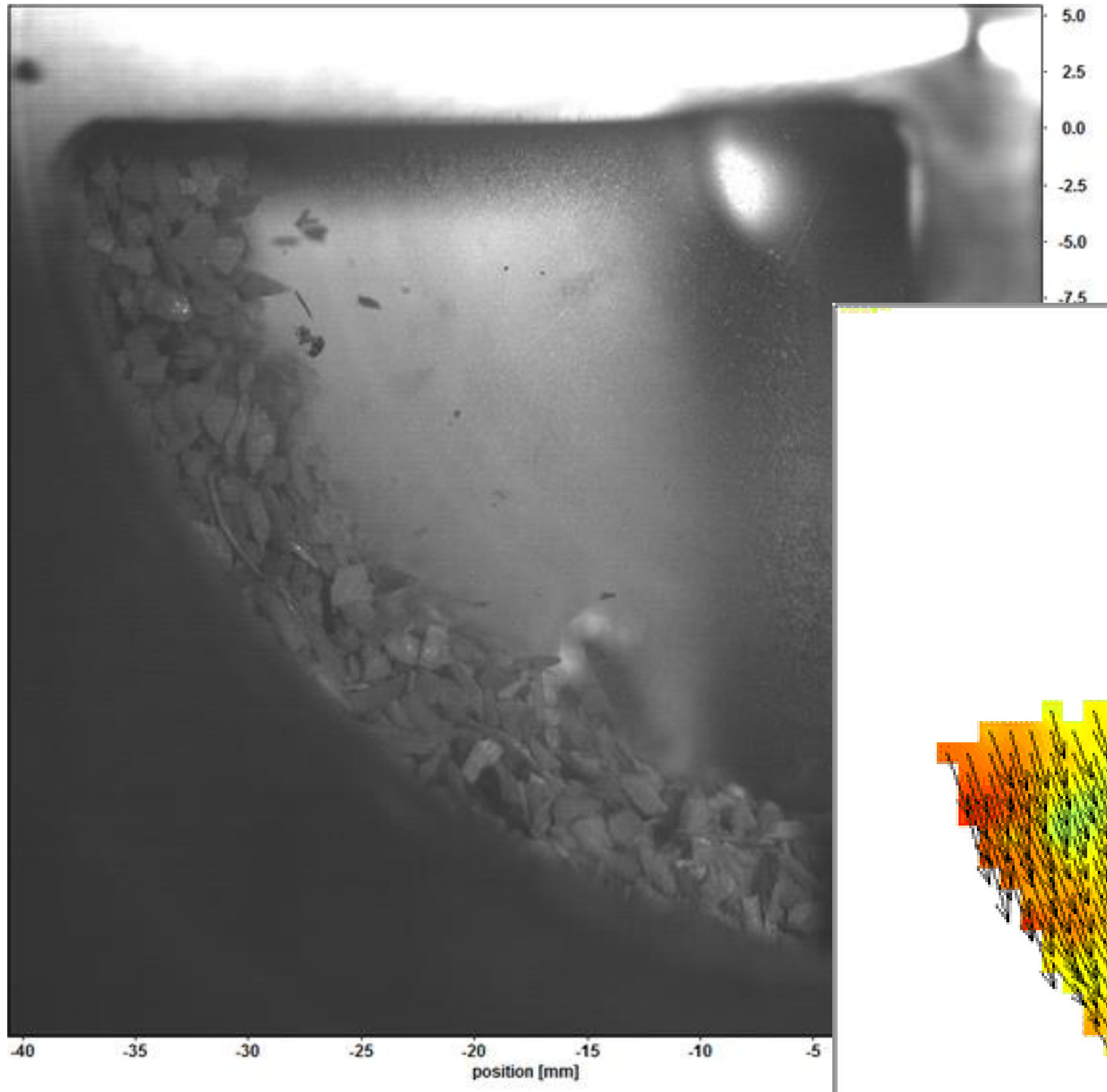
How does it work?

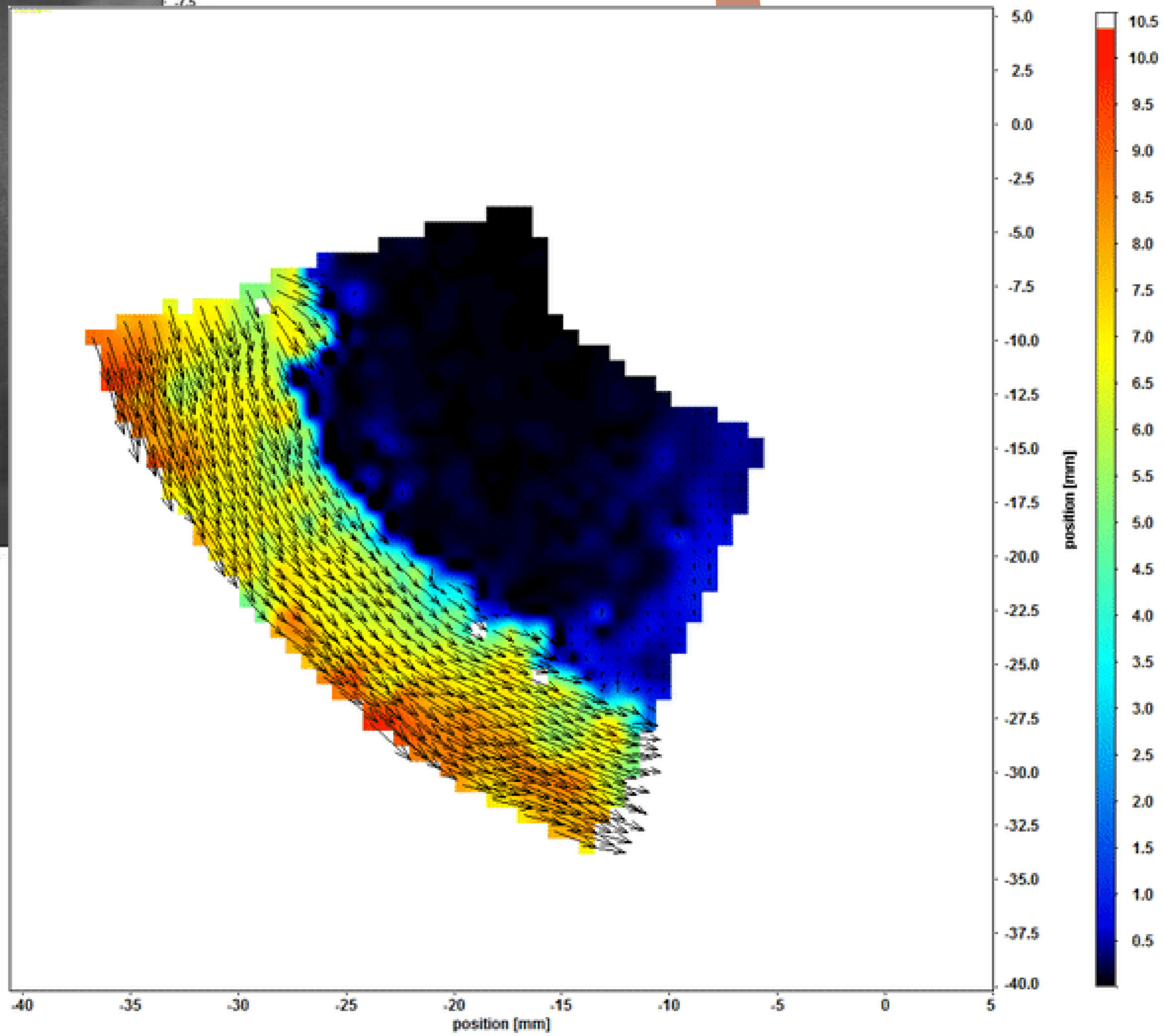


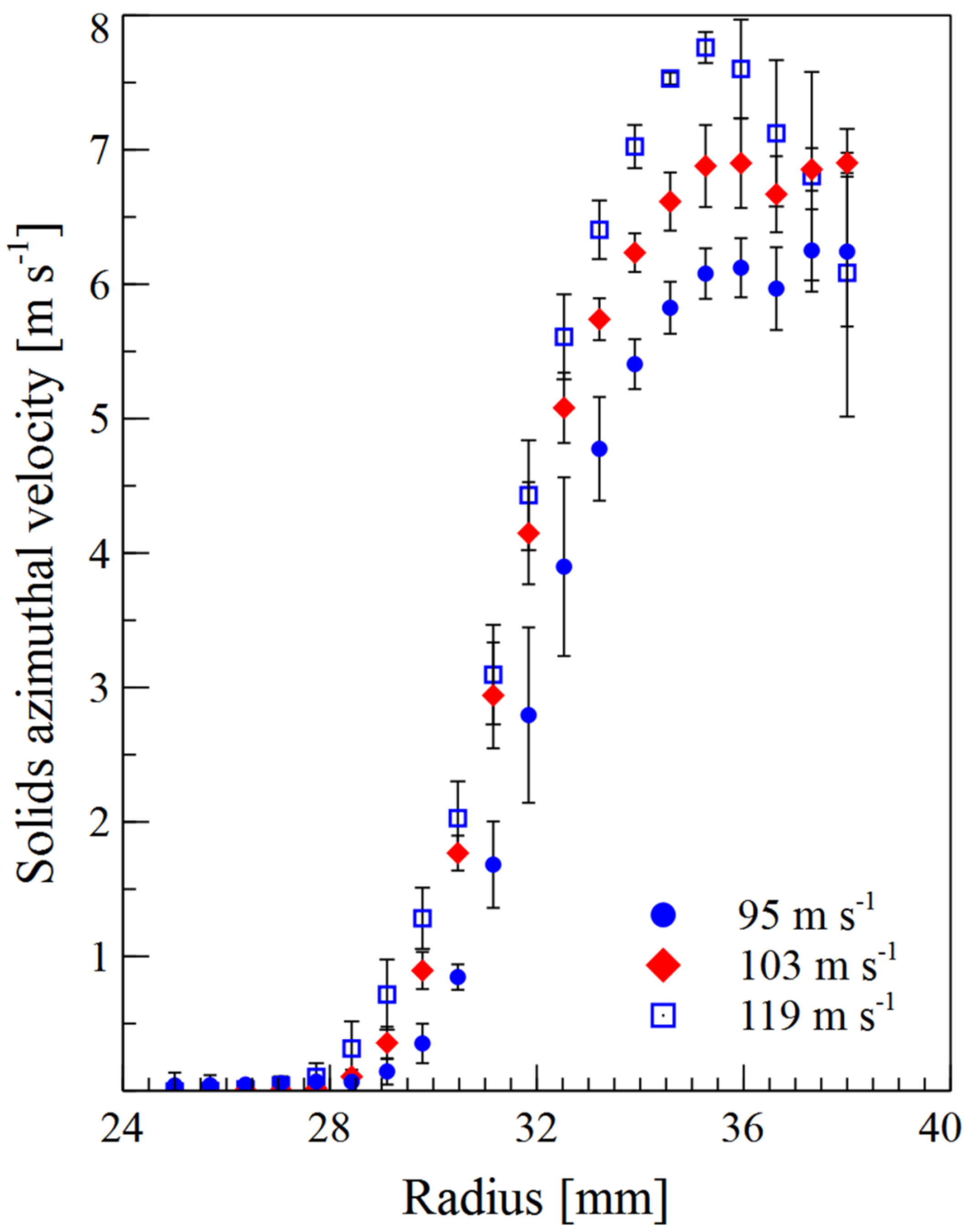
Pine biomass particles rotating in the GSVR

Cold flow testing and data acquisition

Particle image velocimetry







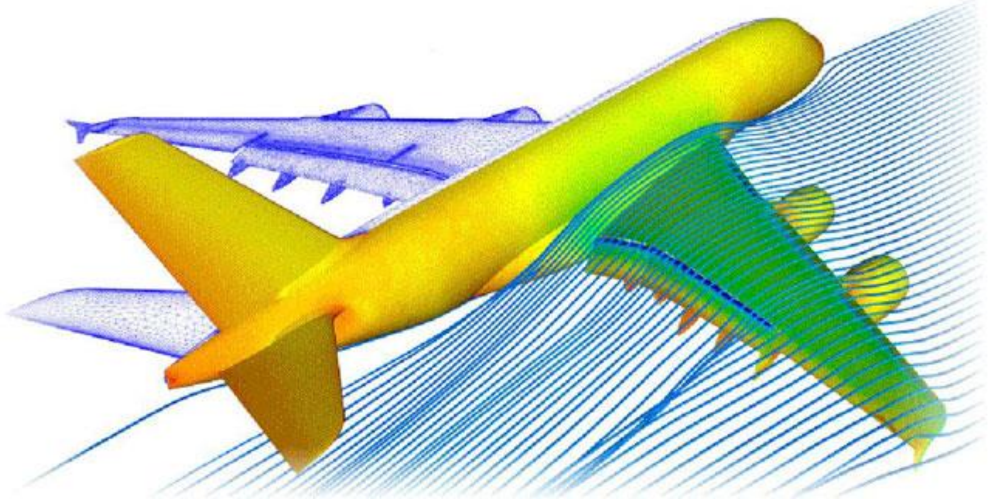
Gonzalez-Quiroga A. et al., *Chem. Eng. J.* **329** 198, 2016; *Powder Technology* **354** 410, 2019

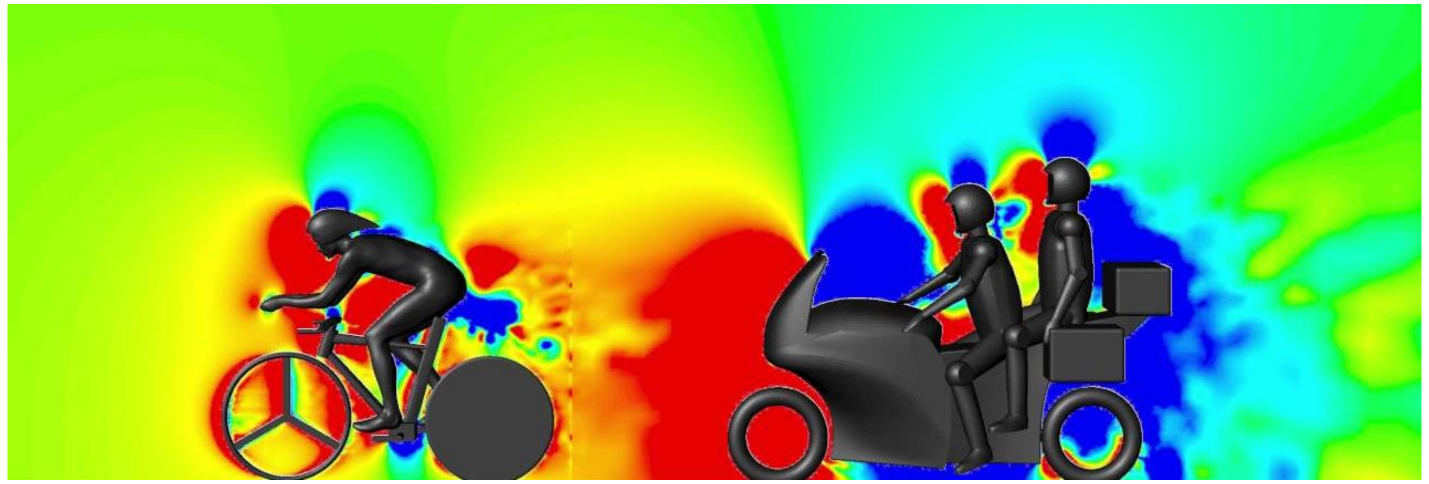
Computational fluid dynamics (CFD)

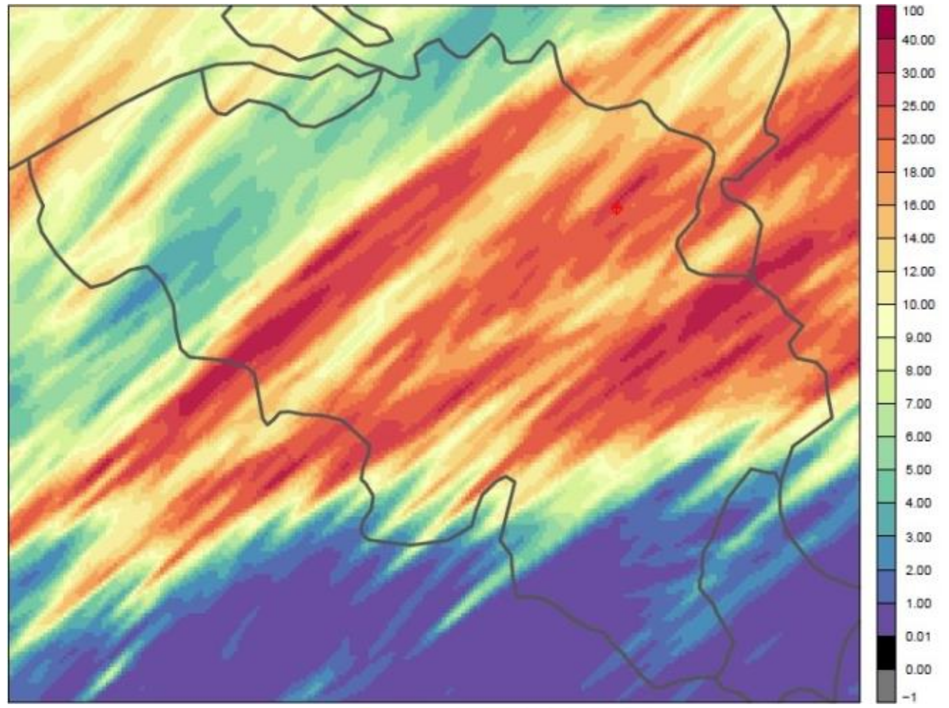
“cleverly forged data” *“contract for difference”*

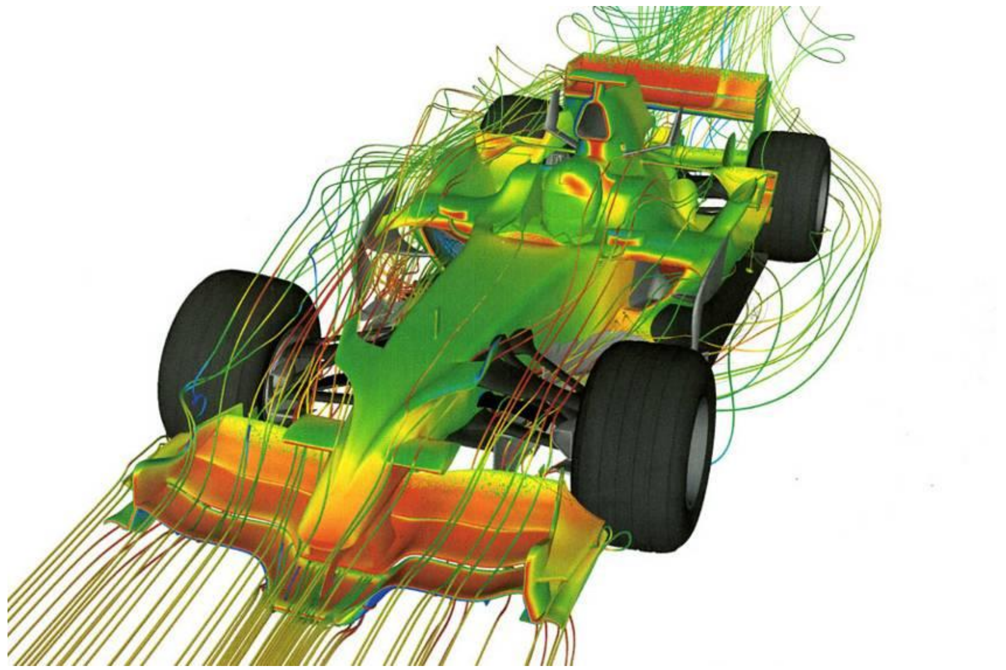
“colors for directors”

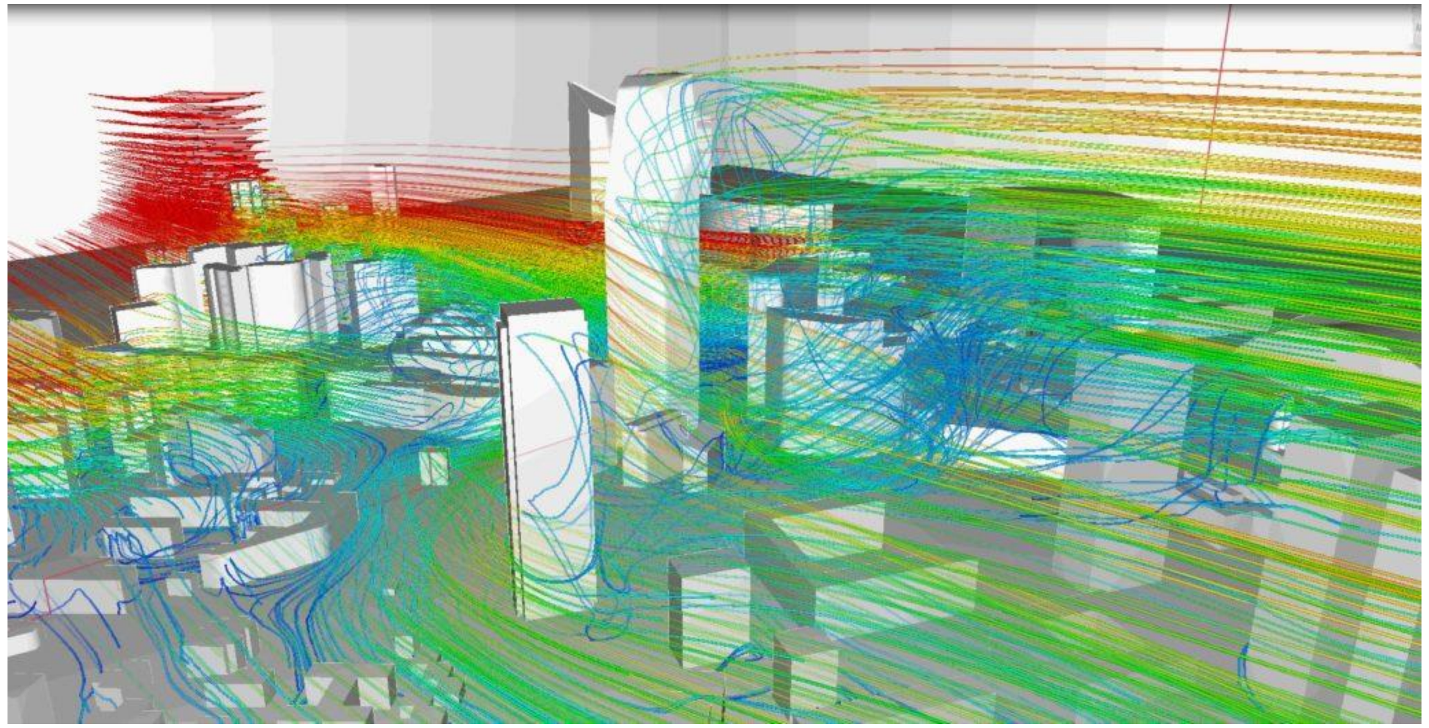
Simulate **fluid flow** based on conservation equations

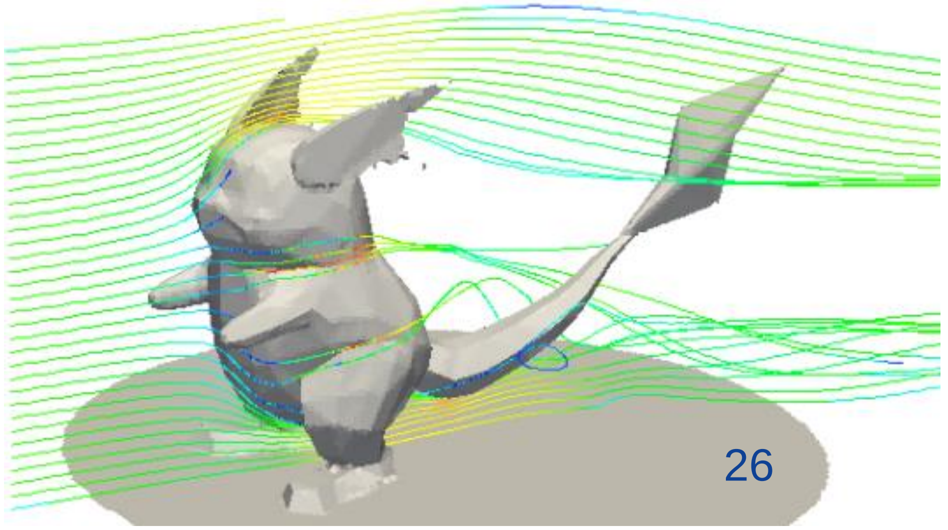








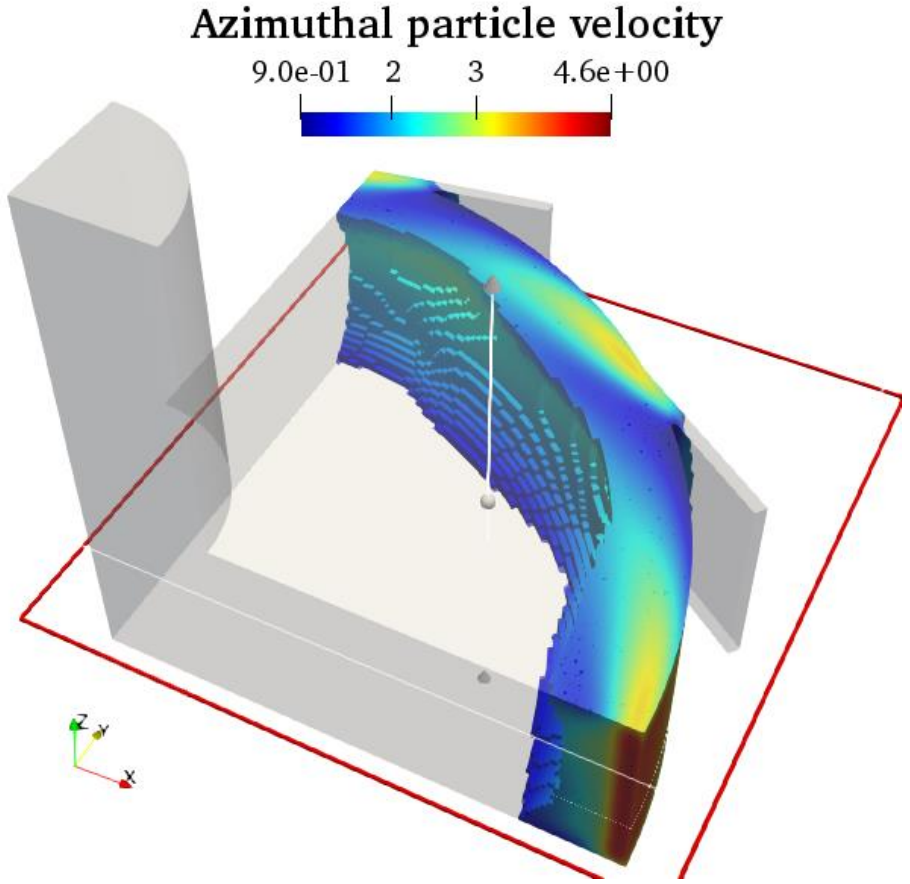


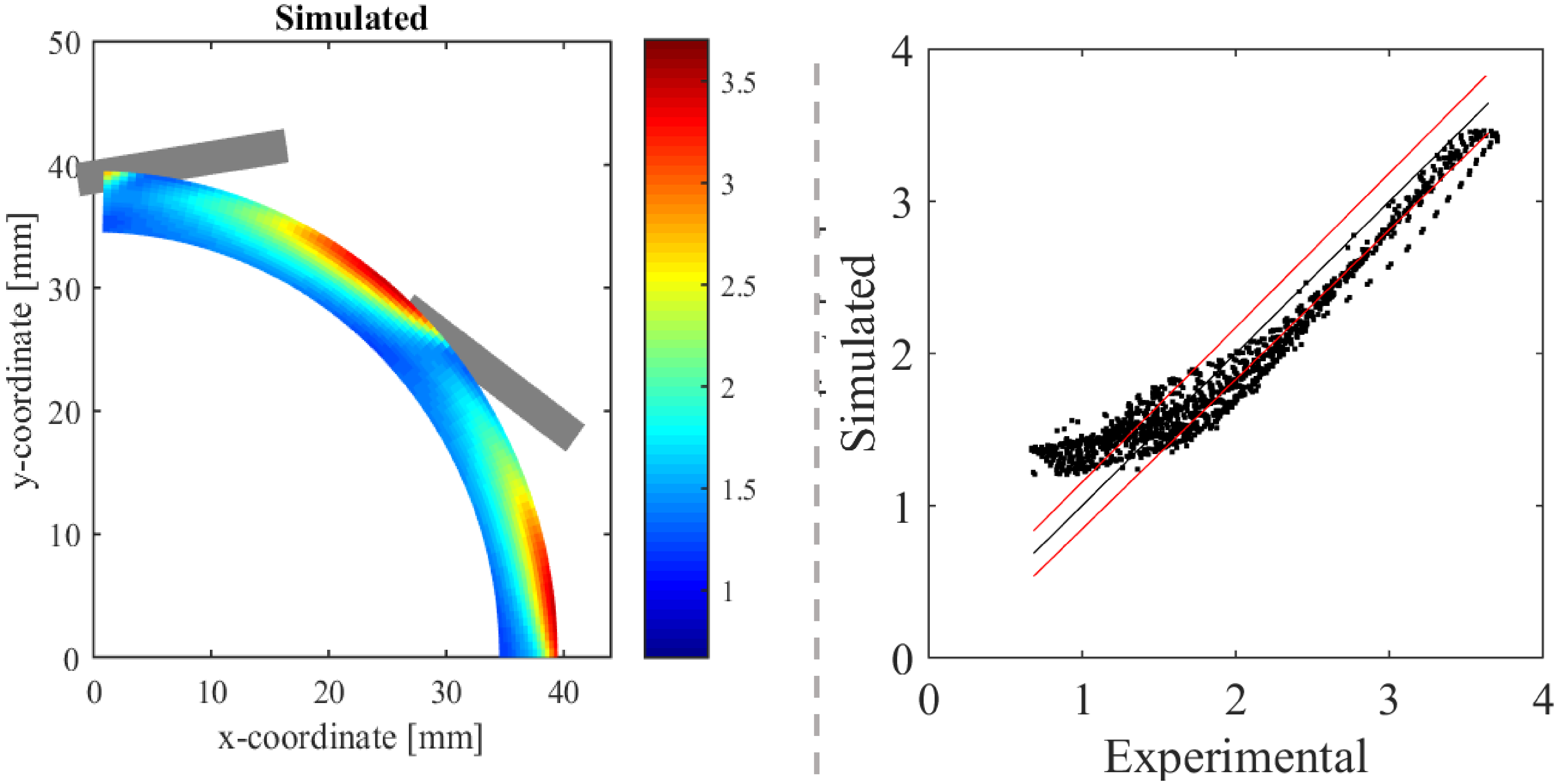


CFD validation

Probing or interpolating the PIV data and CFD results at the exact same positions, allows a one-on-one comparison of the experiments and simulations

Operating conditions: 40 Nm^3/hr air @ 291 K, 10.7 g Al (500 µm, 2700 kg/m^3)
Specularity coefficients: Φ_w = 0.075, Φ_b = 0.05

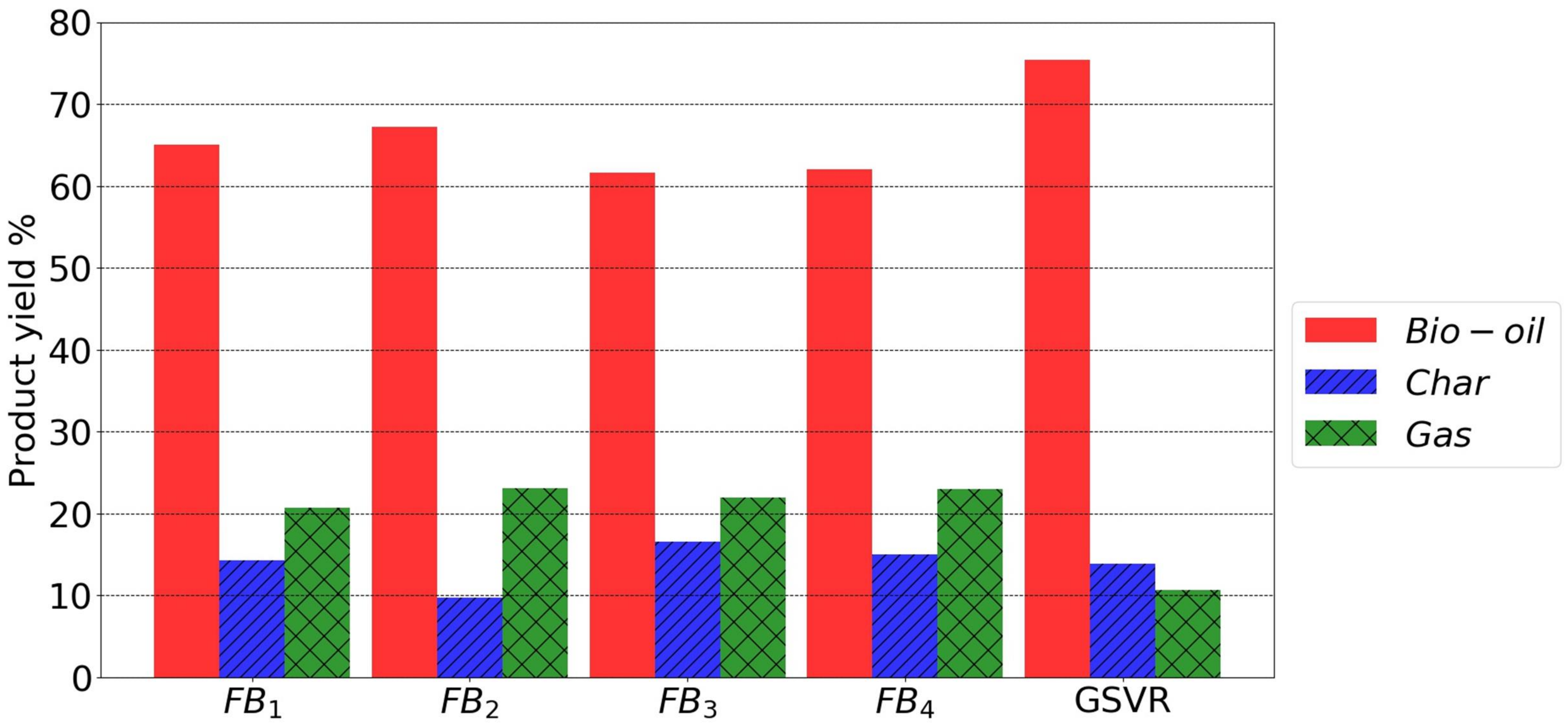




Vandewalle, L., González Quiroga, A., Perreault, P., Van Geem, K.M., & Marin, G.B. (2019). Process intensification in a gas–solid vortex unit : computational fluid dynamics model based analysis and design. *INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH*, *58*(28), 12751–12765

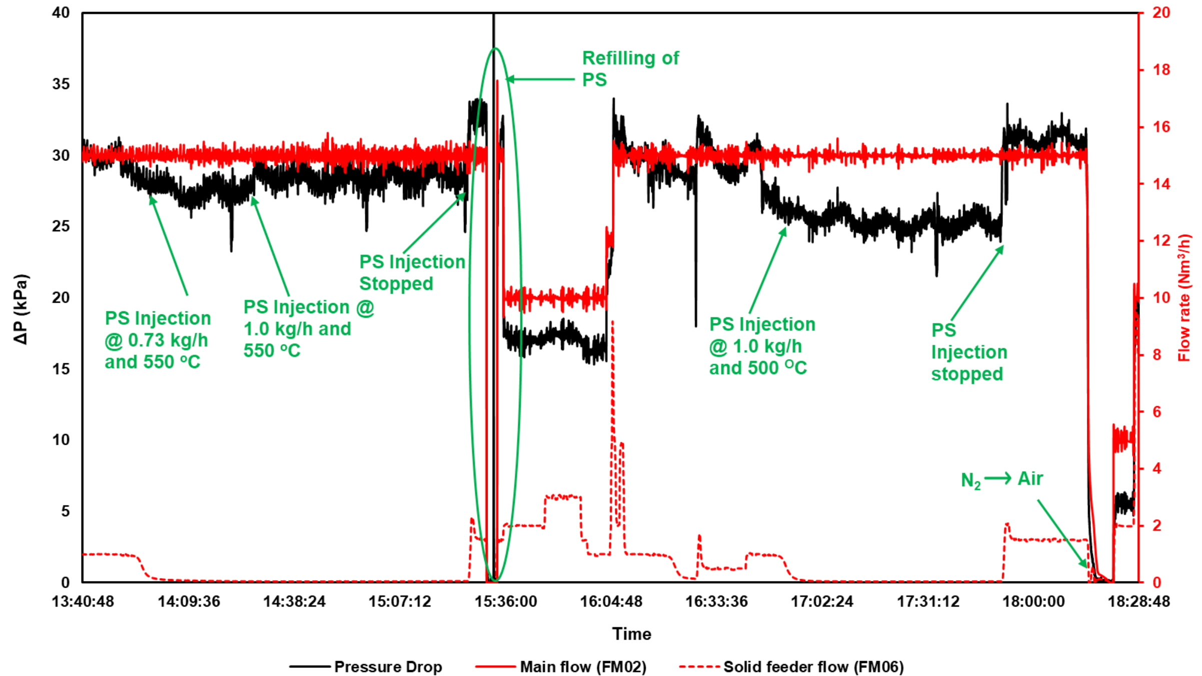
Tested feedstocks

- Biomass
- Natural gas
- Polystyrene
- Polyethylene



FB1 - DeSisto et al. Energy Fuels (2010) 24:2646−2651
FB2 - Men et al. Bioresource Technol (2012) 111:439-446
FB3 - Kim et al. Renewable Energy (2013) 50:188-195
FB4 - Westerhof et al. Ind. Eng. Chem. Res. (2010) 49:1160-1168

Stable operation:

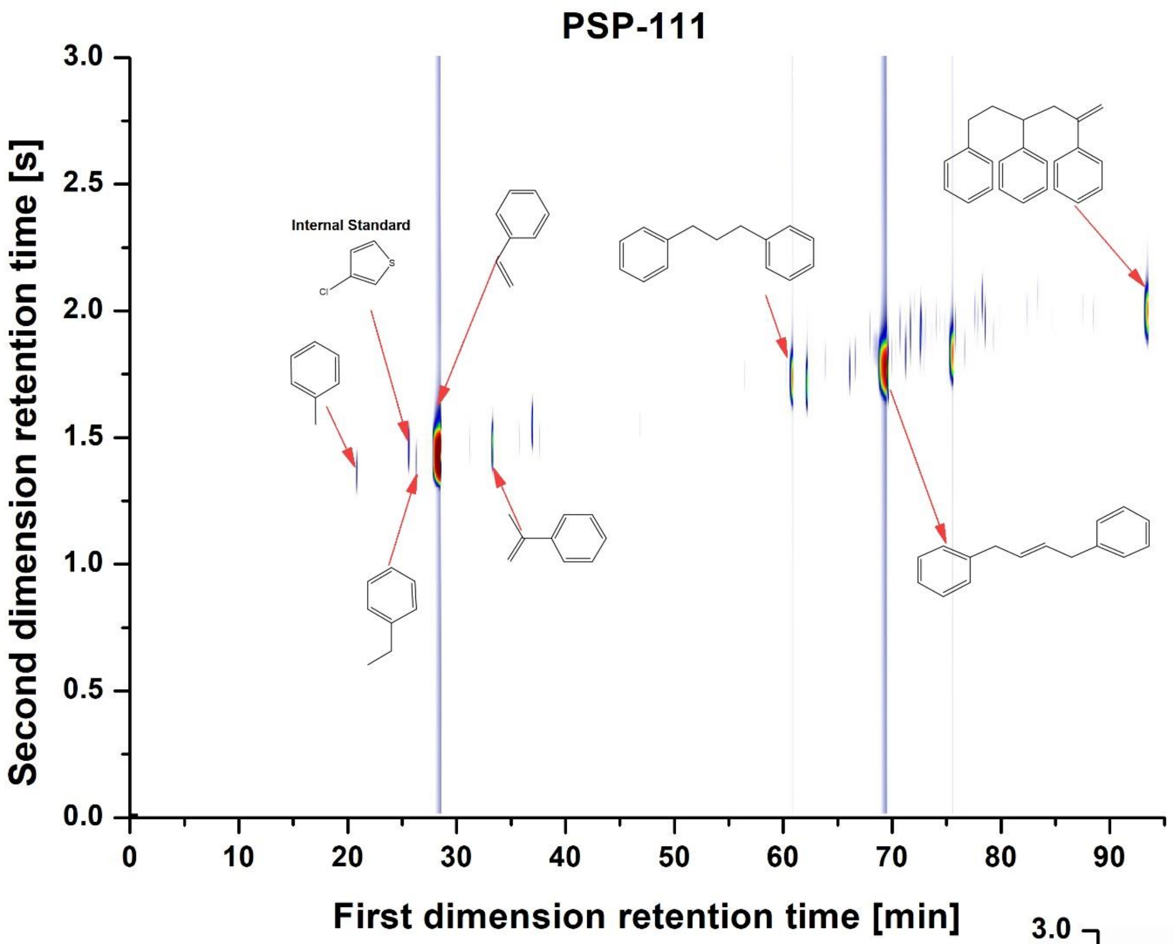


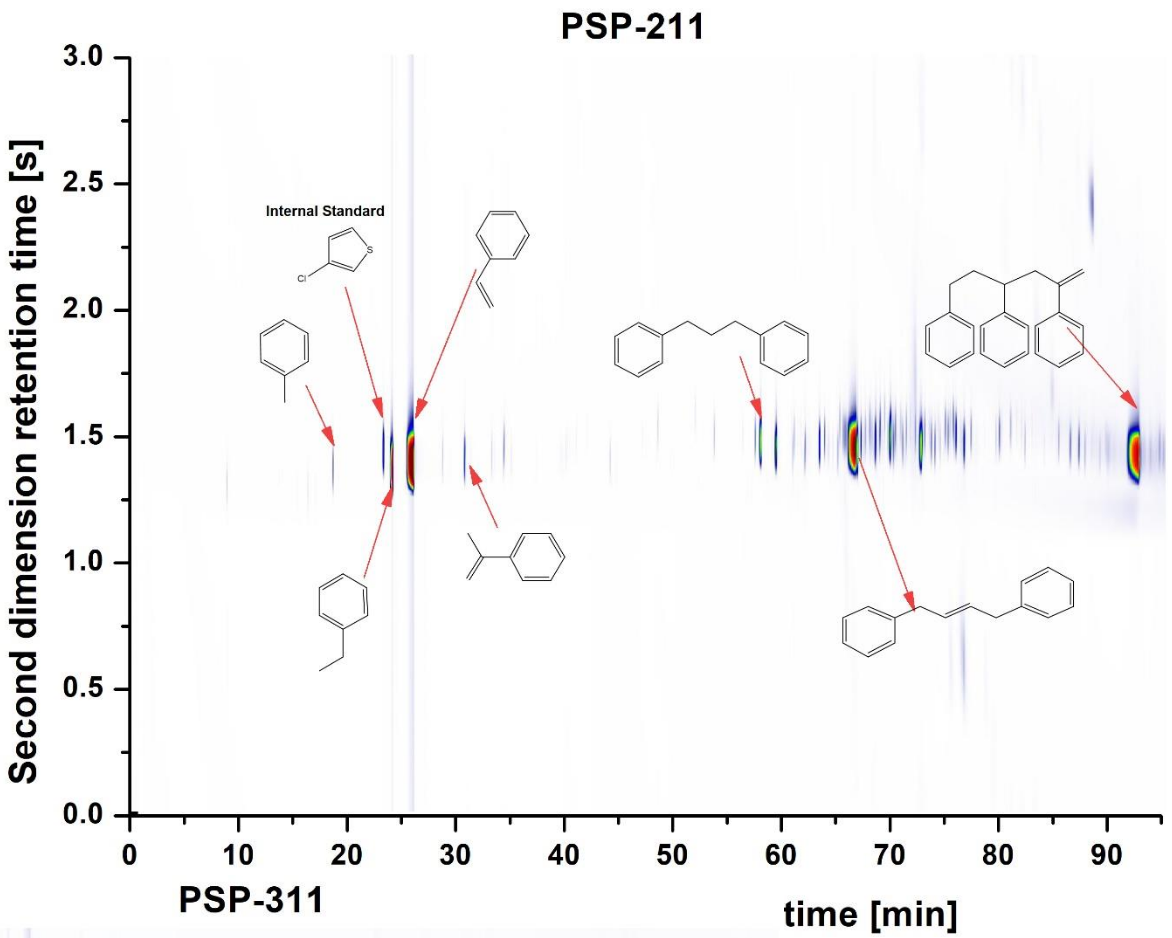
PS Pyrolysis Experiment in the VR

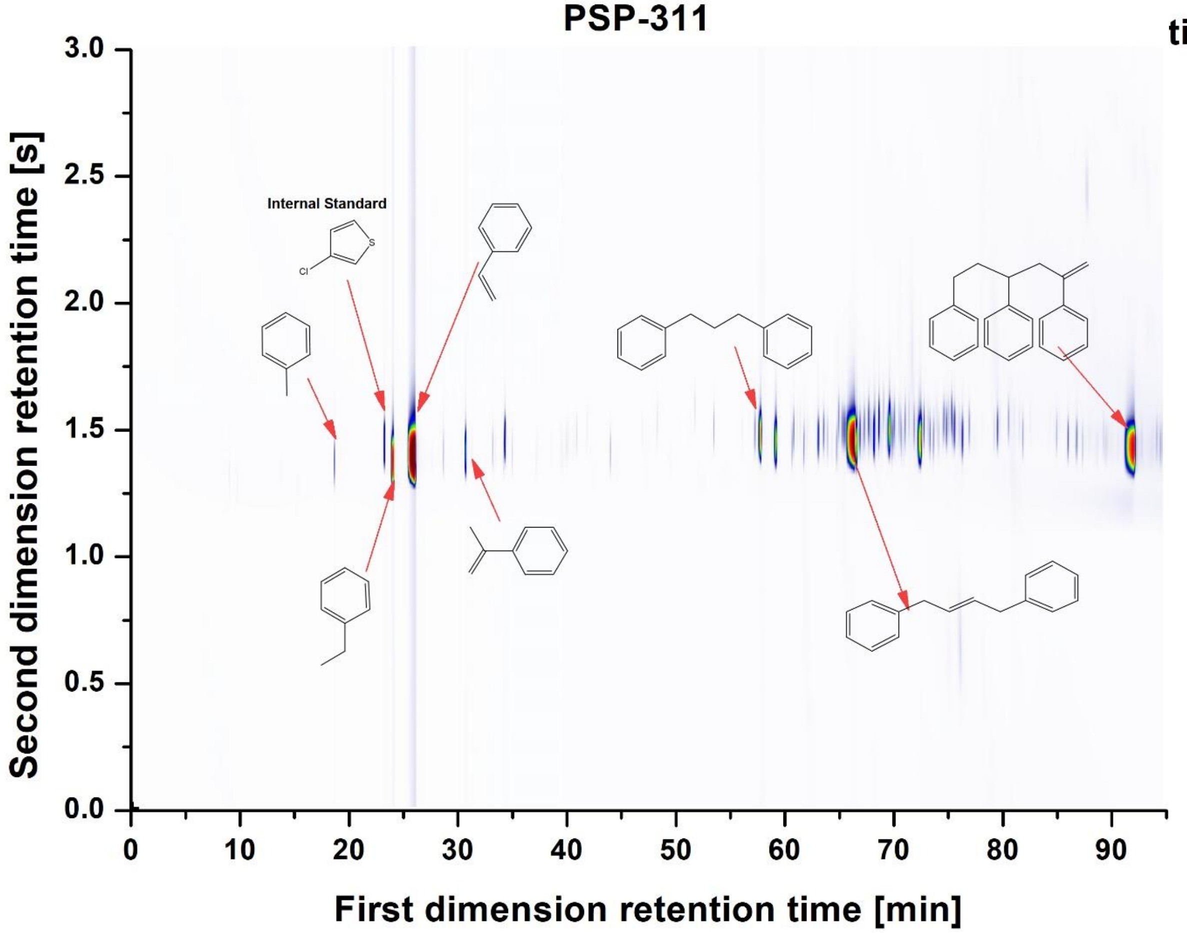
- Expected liquid production in PS pyrolysis ~ 70-90%
- Obtained liquid product ~ 14%
- High flow of gas → short residence time
- low surface area → Incapability of condensers

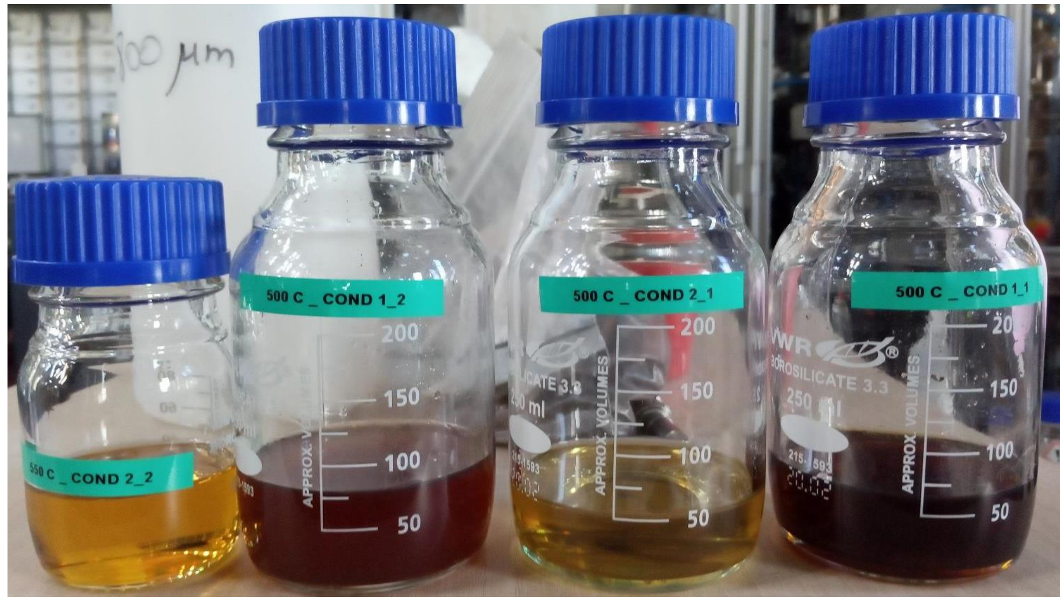
Challenges		Possible Solutions
Quantifying the liquid production rate	→	• Online sampling and analysis with injecting the IS
Collecting all the produced liquid	→	Modifying the condensers (Packing or S&T condenser)

Liquid Products Analysis









Thanks

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UCL Université catholique de Louvain
Chimie Lille ÉCOLE NATIONALE SUPÉRIEURE DE CHIMIE
Interreg France-Wallonie-Vlaanderen UNION EUROPÉENNE EUROPESE UNIE

Acknowledgements

Interreg France-Wallonie-Vlaanderen
UNION EUROPÉENNE EUROPESE UNIE
PSYCHE

Avec le soutien du Fonds européen de développement régional
Met steun van het Europees Fonds voor Regionale Ontwikkeling

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