UNIVERSITY OF AMSTERDAM

RESEARCH PRIORITY AREA SUSTAINABLE CHEMISTRY

The role of sustainable (aviation) fuels in the energy transition

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Our focus: Engineering sustainable processes

1

Petroleum/petrochemical processes

2

CO$_2$ activation

3

Biomass to chemicals/fuels/materials

4

Renewable energy

5

Water treatment

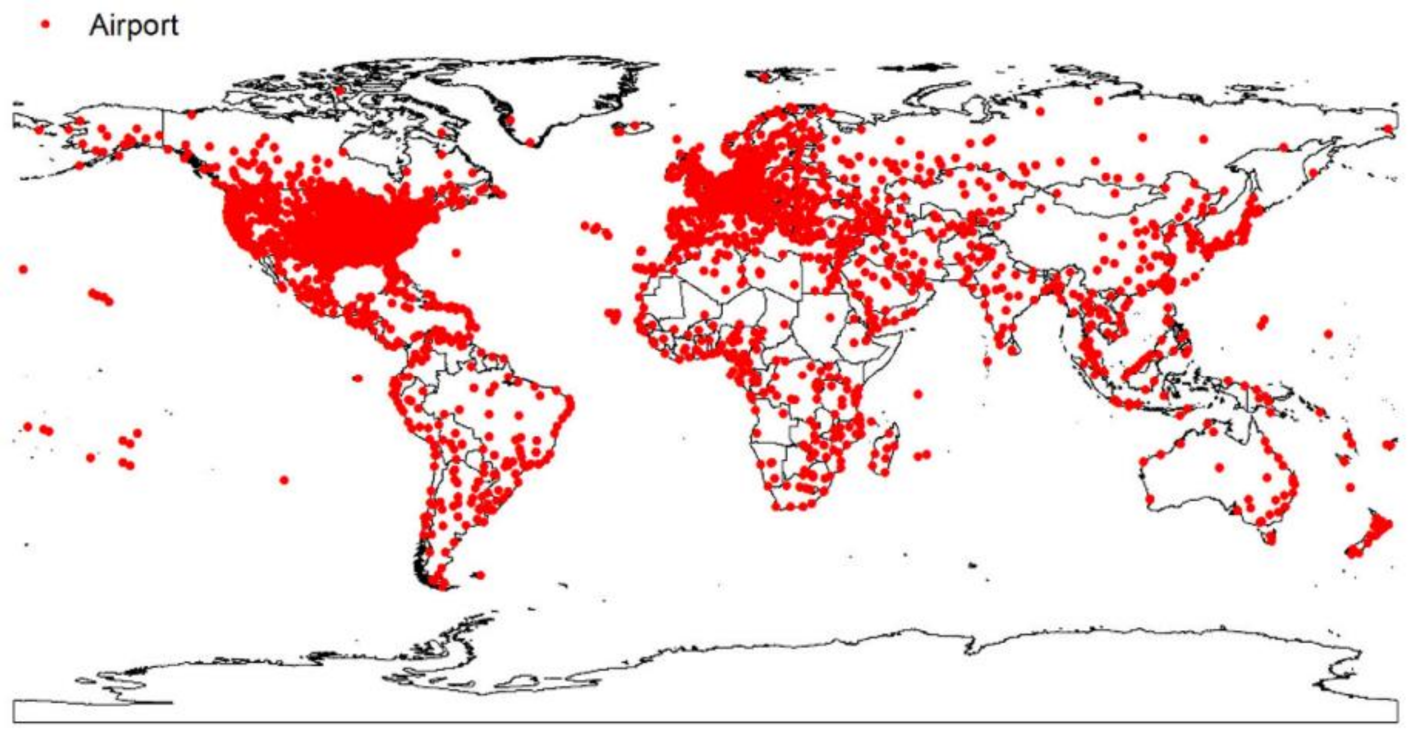
6

Sustainable coatings

7

Lower alkane activation

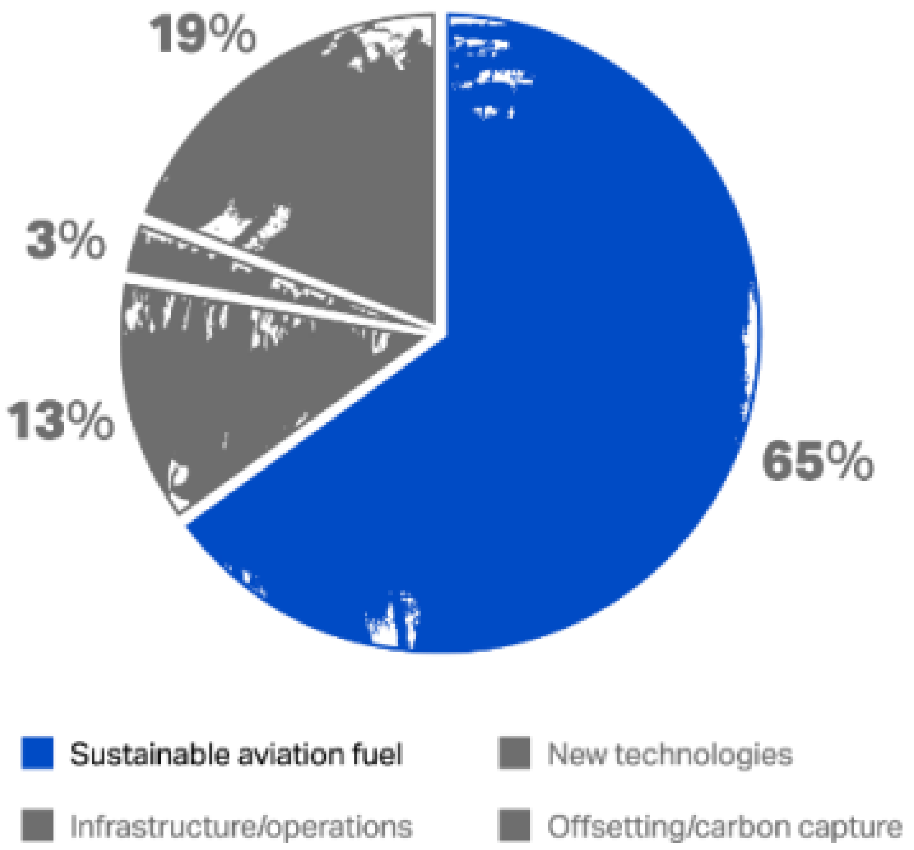
Aviation Industry



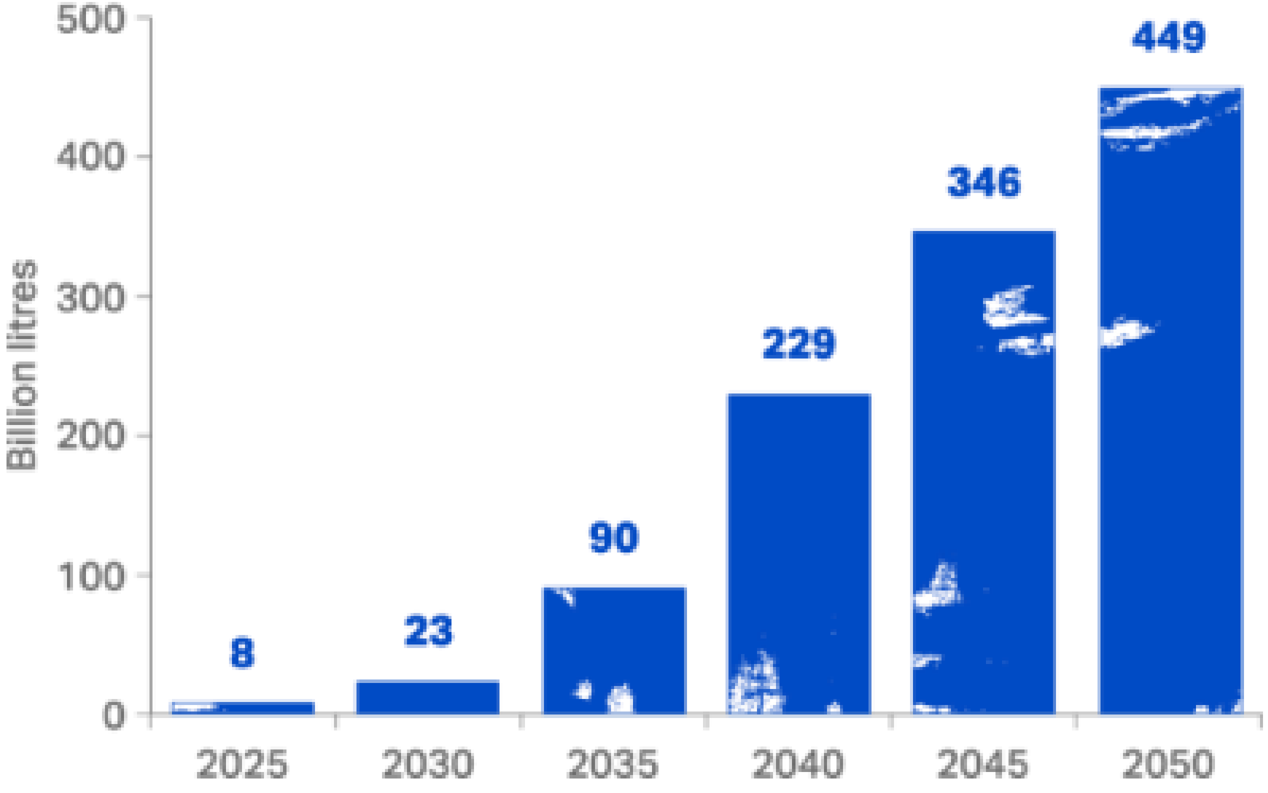
- 57 million jobs
- USD 2.2 trillion in global GDP.
- 2035: 7.2 billion passengers through the world’s major airports
- twice the number of passengers in 2016
- > 3 billion tons of GHG emissions by 2050
- 4 times greater than the 2015 baseline (0.78 billion tons).

Air Transport Action Group (ATAG)

Contribution to achieving Net Zero Carbon in 2050

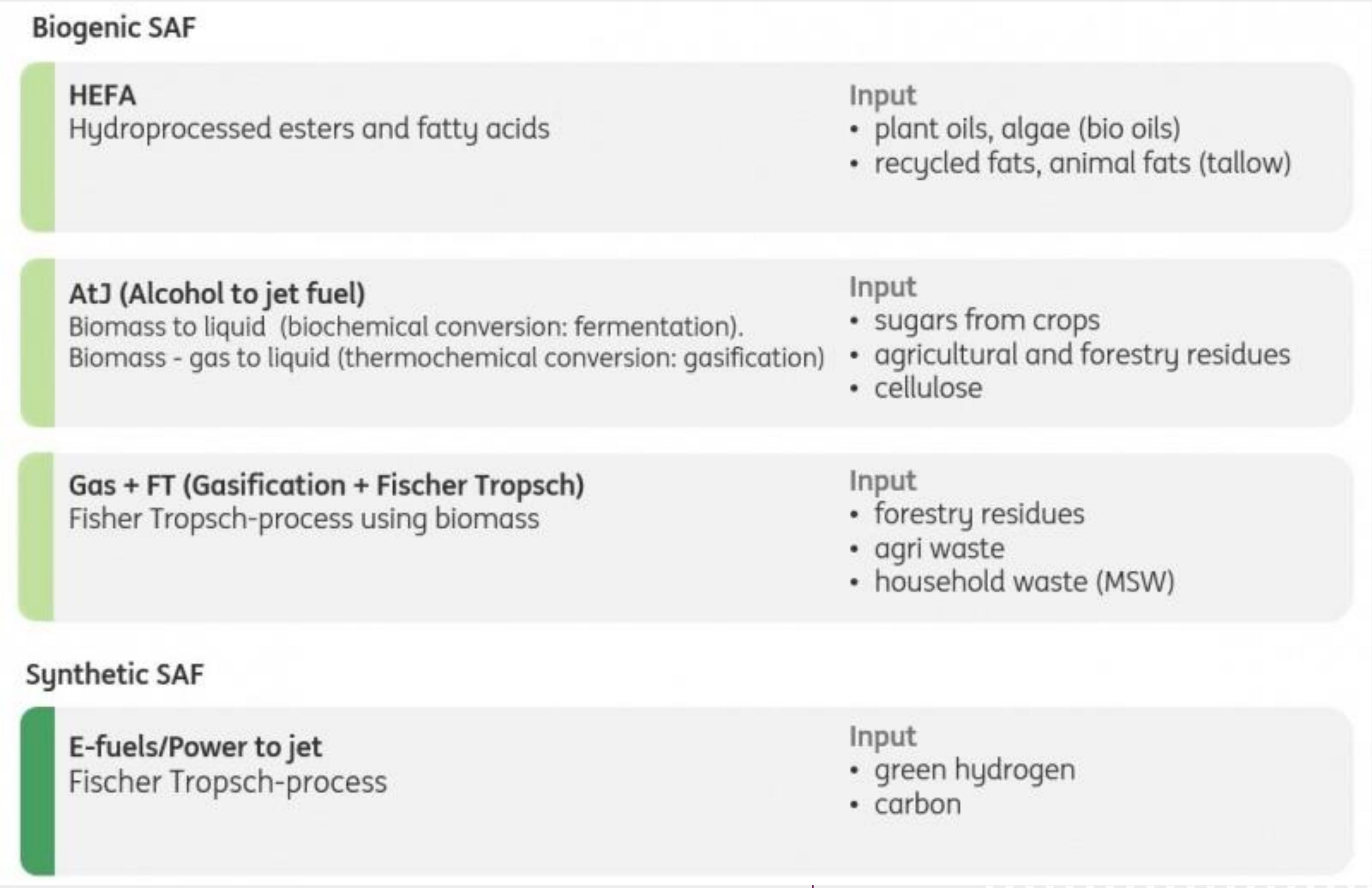


Expected SAF required for Net Zero 2050



	2025	2030	2035	2040	2045	2050
Regional & short haul **< 1,500 km** c.20% of industry CO_2	SAF	SAF	Electric or Hydrogen combustion and/or SAF	Electric or Hydrogen combustion and/or SAF	Electric or Hydrogen combustion and/or SAF	Electric or Hydrogen combustion and/or SAF
Medium haul **1,500-4,000 km** c.30% of industry CO_2	SAF	SAF	SAF	SAF	SAF	SAF potentially some hydrogen
Long haul **> 4,000 km** c.50% of industry CO_2	SAF	SAF	SAF	SAF	SAF	SAF

Available options



Biogenic SAF

HEFA
Hydroprocessed esters and fatty acids

Input
- plant oils, algae (bio oils)
- recycled fats, animal fats (tallow)

AtJ (Alcohol to jet fuel)
Biomass to liquid (biochemical conversion: fermentation).
Biomass - gas to liquid (thermochemical conversion: gasification)

Input
- sugars from crops
- agricultural and forestry residues
- cellulose

Gas + FT (Gasification + Fischer Tropsch)
Fisher Tropsch-process using biomass

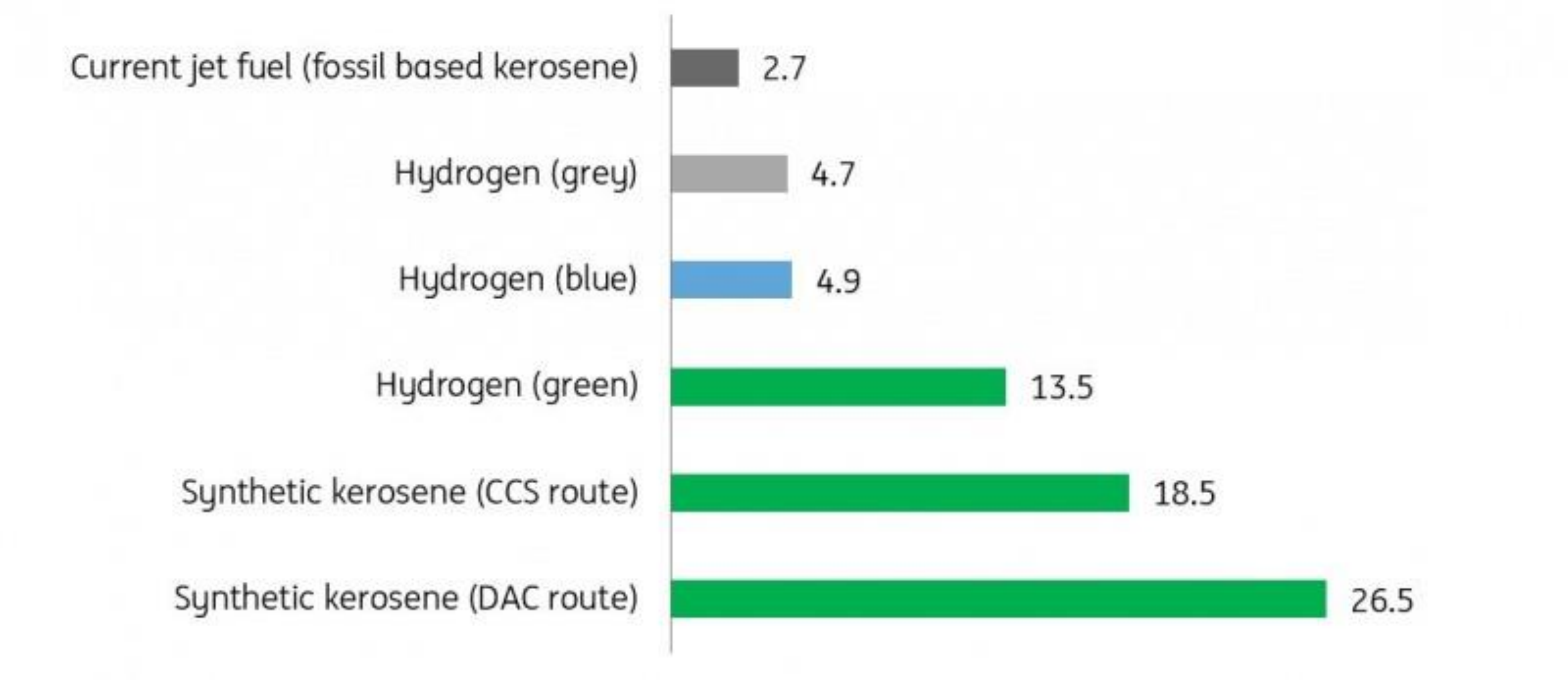
Input
- forestry residues
- agri waste
- household waste (MSW)

Synthetic SAF

E-fuels/Power to jet
Fischer Tropsch-process

Input
- green hydrogen
- carbon

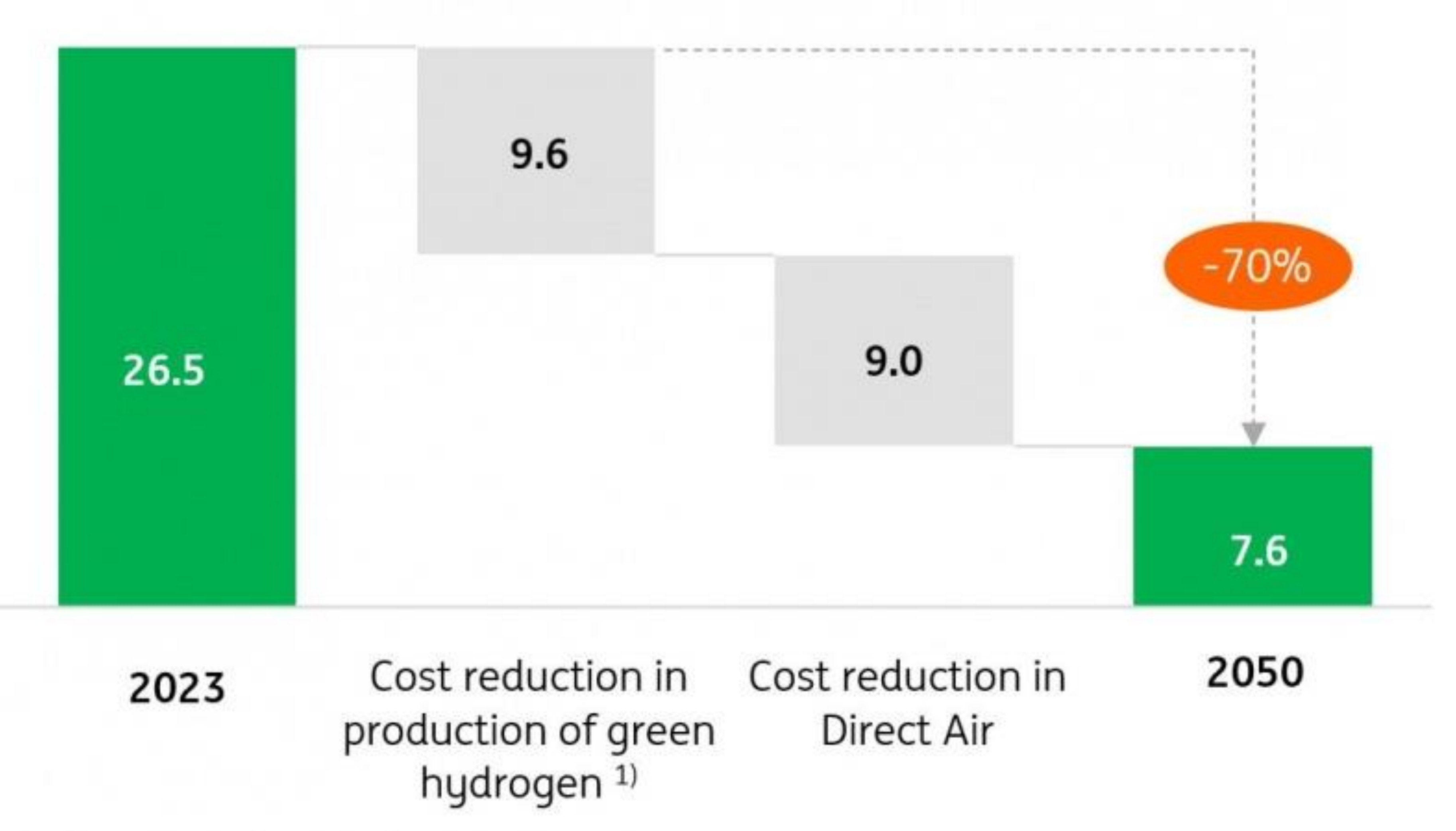
Synthetic SAF



Unsubsidised cost of kerosene and synthetic fuel in euro cents per seat per kilometre

Source: ING Research

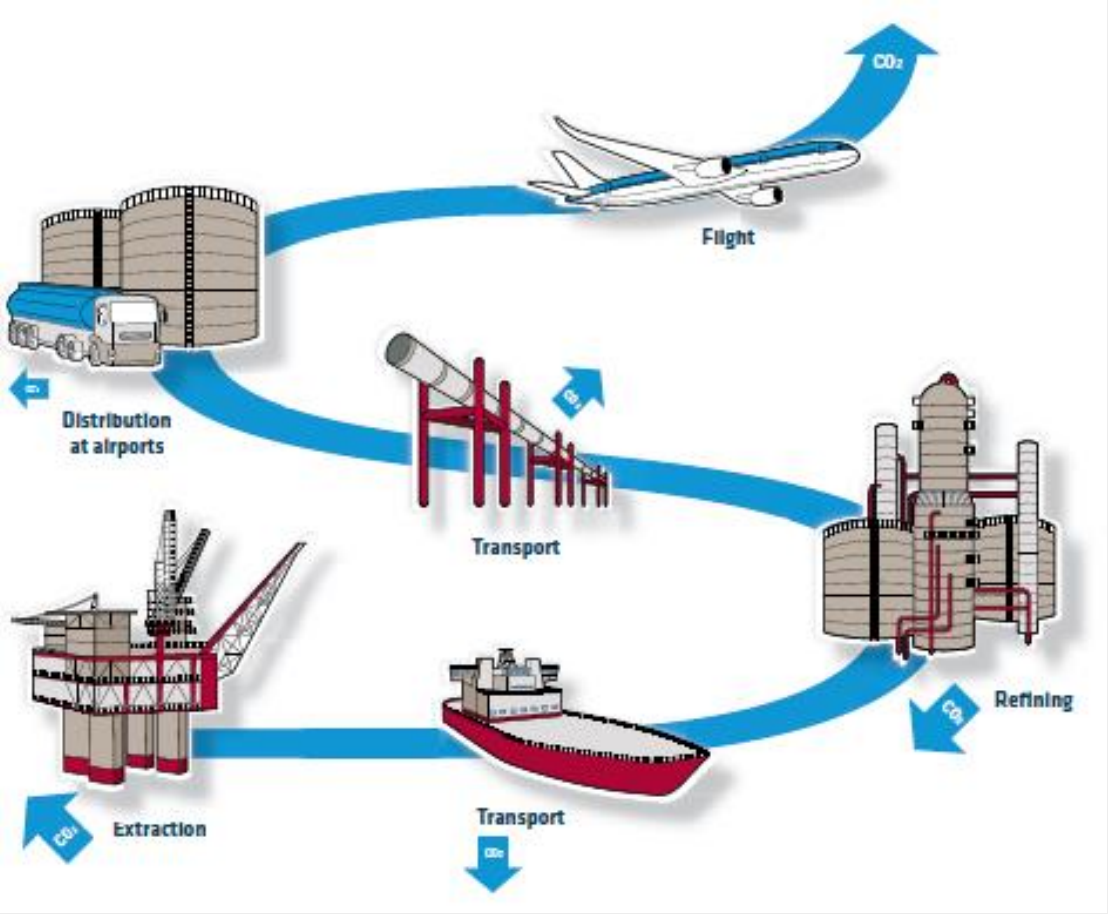
Synthetic SAF



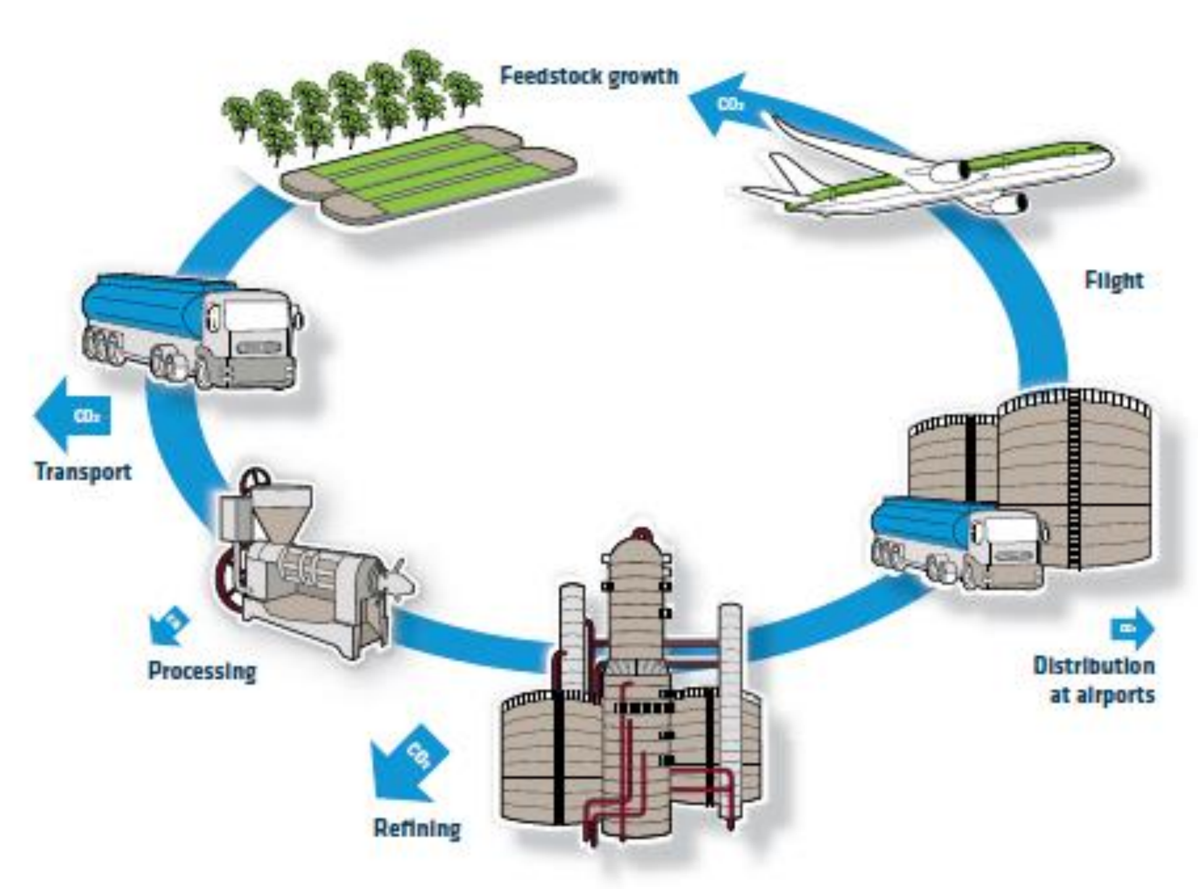
Source: ING Research

Sustainable jet fuel from Organic waste

Carbon lifecycle diagram: fossil fuels



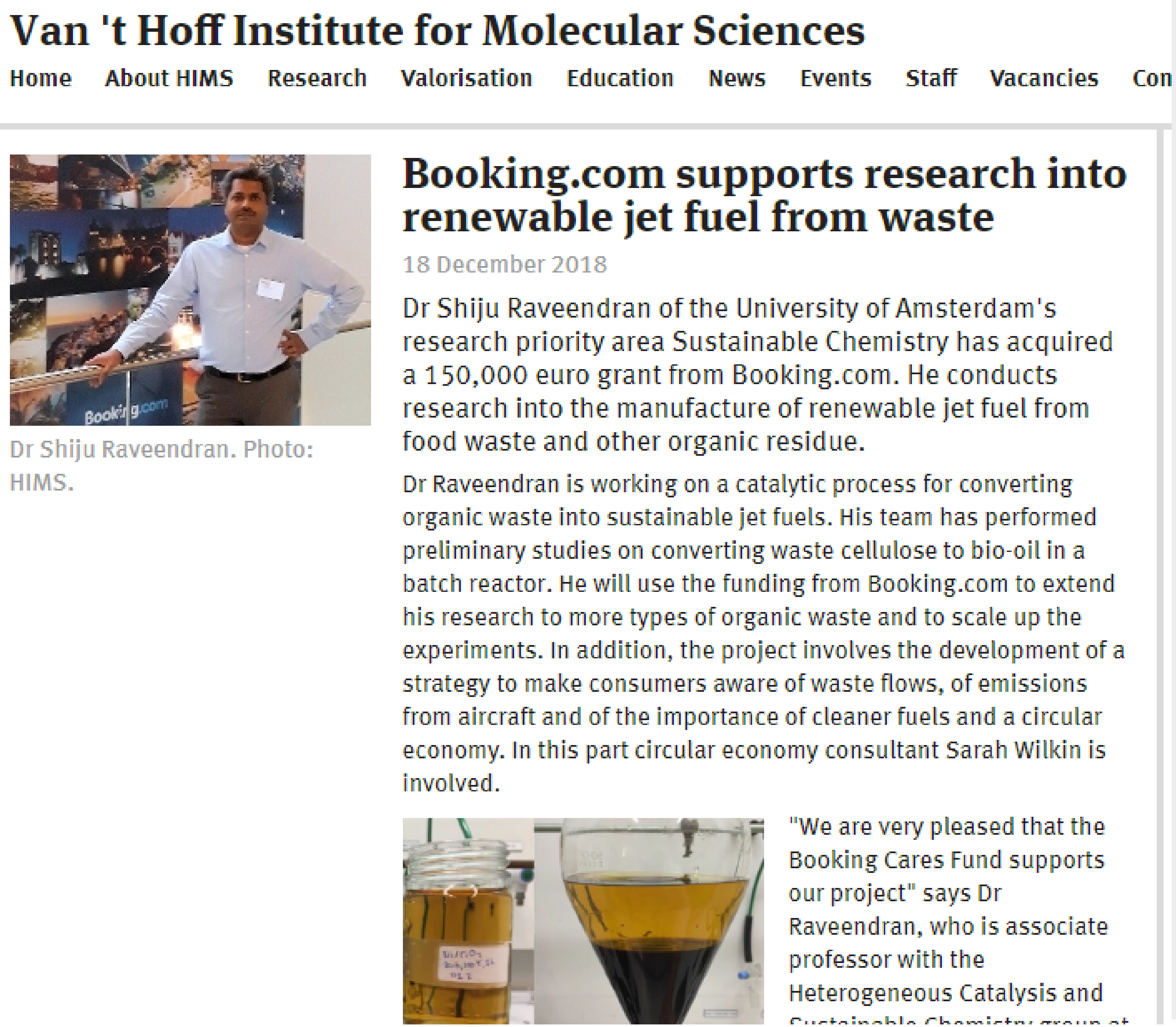
Carbon lifecycle diagram: Sustainable aviation fuel



- Uncertain costs of green hydrogen and synthetic kerosene by 2050.
- Uncertain factor: oil price in a net-zero economy.
- Polluting jet fuel is very cheap and green alternatives are expensive.
- Room for policymakers to intervene by taxing dirty technology or subsidising clean technologies.
- Without such policies, the use of synthetic fuel is unlikely to take off in aviation making it impossible for the sector to reach net zero by 2050.
- But the technologies need to be ready….

SAF may not fly without policy support…

Renewable jet fuel from Organic waste



Van 't Hoff Institute for Molecular Sciences

Booking.com supports research into renewable jet fuel from waste

18 December 2018

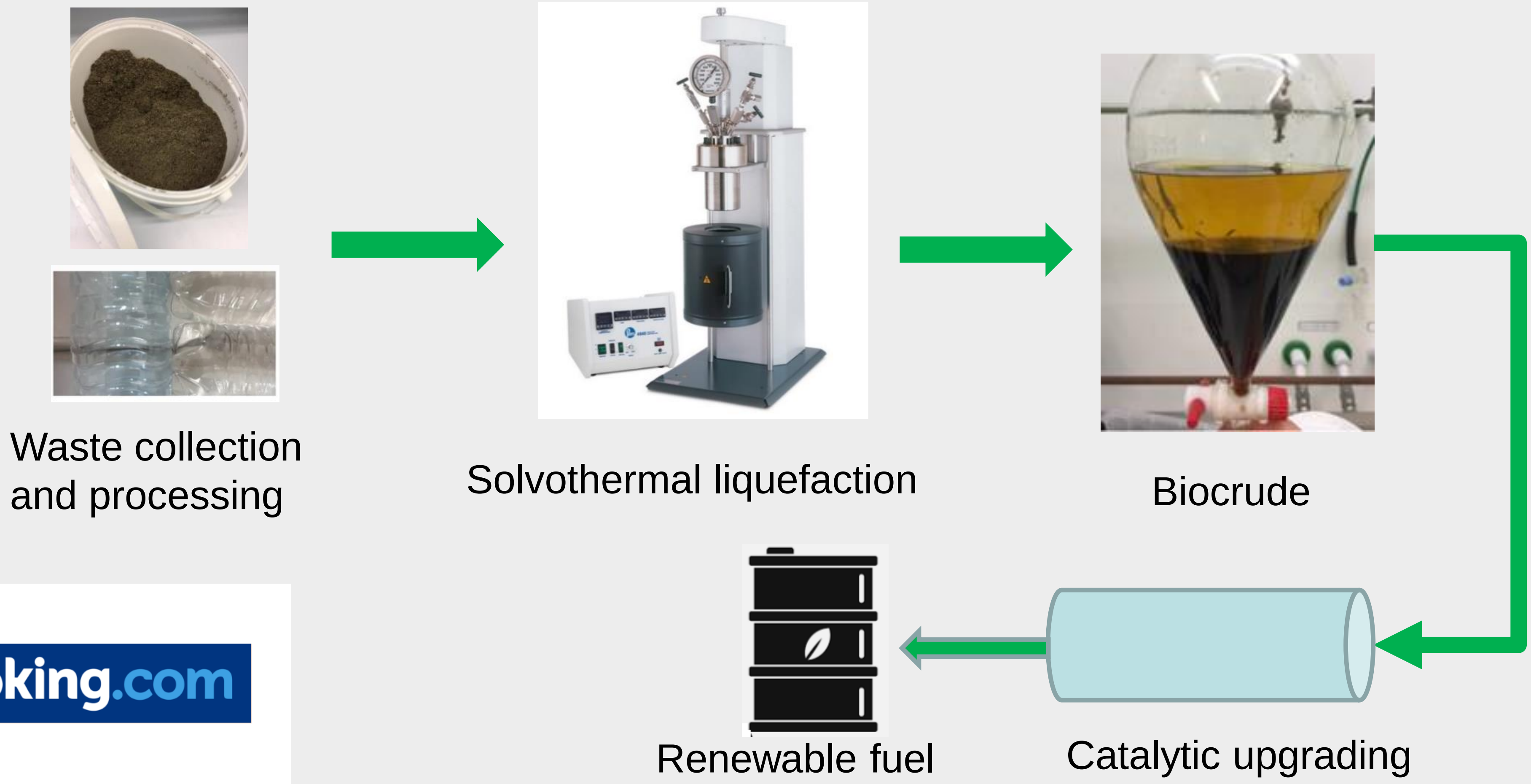
Dr Shiju Raveendran. Photo: HIMS.

Dr Shiju Raveendran of the University of Amsterdam's research priority area Sustainable Chemistry has acquired a 150,000 euro grant from Booking.com. He conducts research into the manufacture of renewable jet fuel from food waste and other organic residue.

Dr Raveendran is working on a catalytic process for converting organic waste into sustainable jet fuels. His team has performed preliminary studies on converting waste cellulose to bio-oil in a batch reactor. He will use the funding from Booking.com to extend his research to more types of organic waste and to scale up the experiments. In addition, the project involves the development of a strategy to make consumers aware of waste flows, of emissions from aircraft and of the importance of cleaner fuels and a circular economy. In this part circular economy consultant Sarah Wilkin is involved.

"We are very pleased that the Booking Cares Fund supports our project" says Dr Raveendran, who is associate professor with the Heterogeneous Catalysis and

Hydrothermal Liquefaction

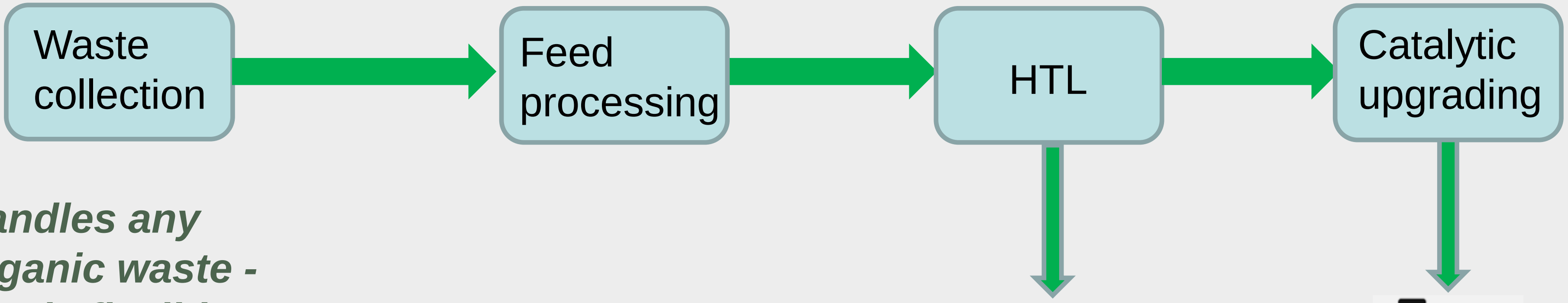


Booking.com

Q8 Research

- J. Mors, N. R Shiju, The synthesis of biooil using ambient pressure liquefaction of organic waste, *Sustainable Chemistry for Climate Action*, 100013, **2023**.
- S Shirazimoghaddam, I Amin, JA Faria Albanese, N R Shiju, Chemical Recycling of Used PET by Glycolysis Using Niobia-Based Catalysts, *ACS Eng. Au*, 3, 1, 37–44, **2023.**

Hydrothermal Liquefaction



Handles any organic waste - Feed –flexible Technology *(food waste, food processing waste, Agro waste, manure, industrial waste, mixed non-recyclable plastics)*

Recovery of Carbs, Proteins

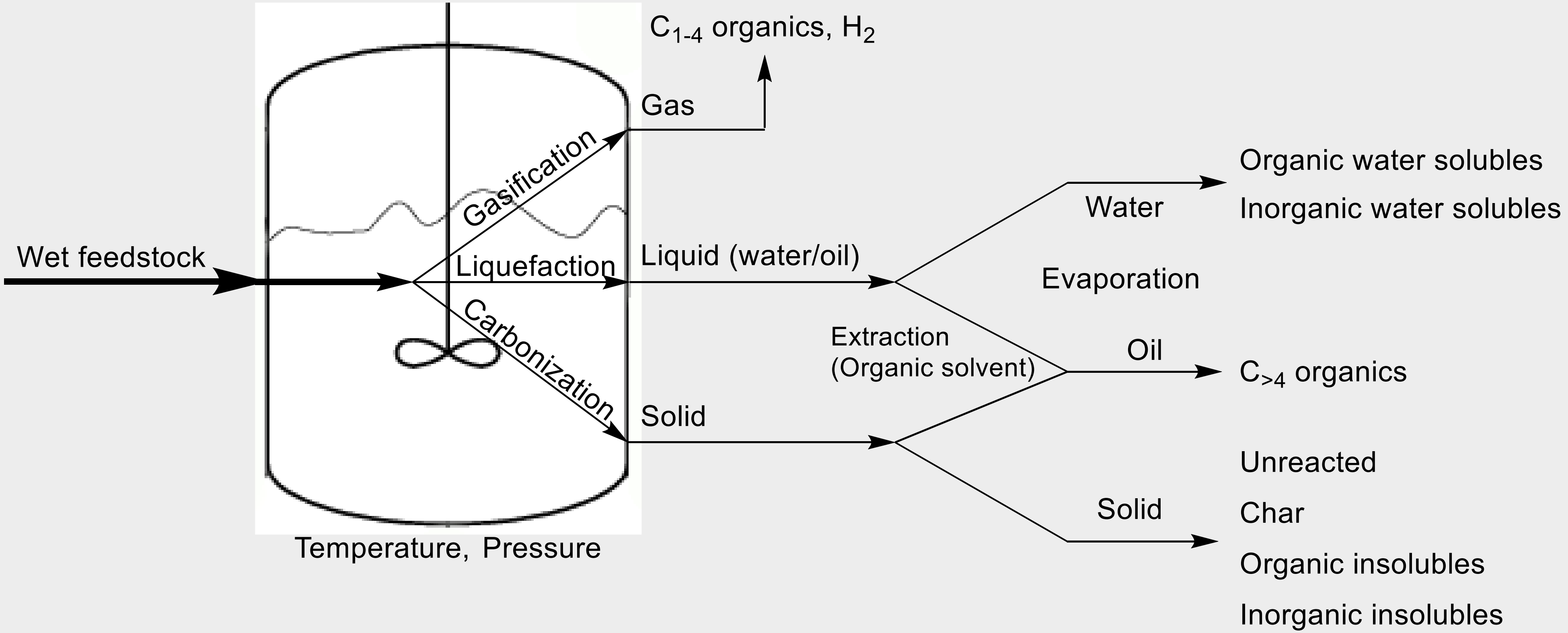
Renewable fuel

Energy efficient*: Uses water in waste as a reactant and recovers mineral-rich water. No need of drying wet waste*

Drop-in renewable crude as product: *Energy-dense liquid crude, compatible with petroleum crude. Can be processed in existing refining infrastructure. No change required in engine technology.*

Fast process –minutes to hours

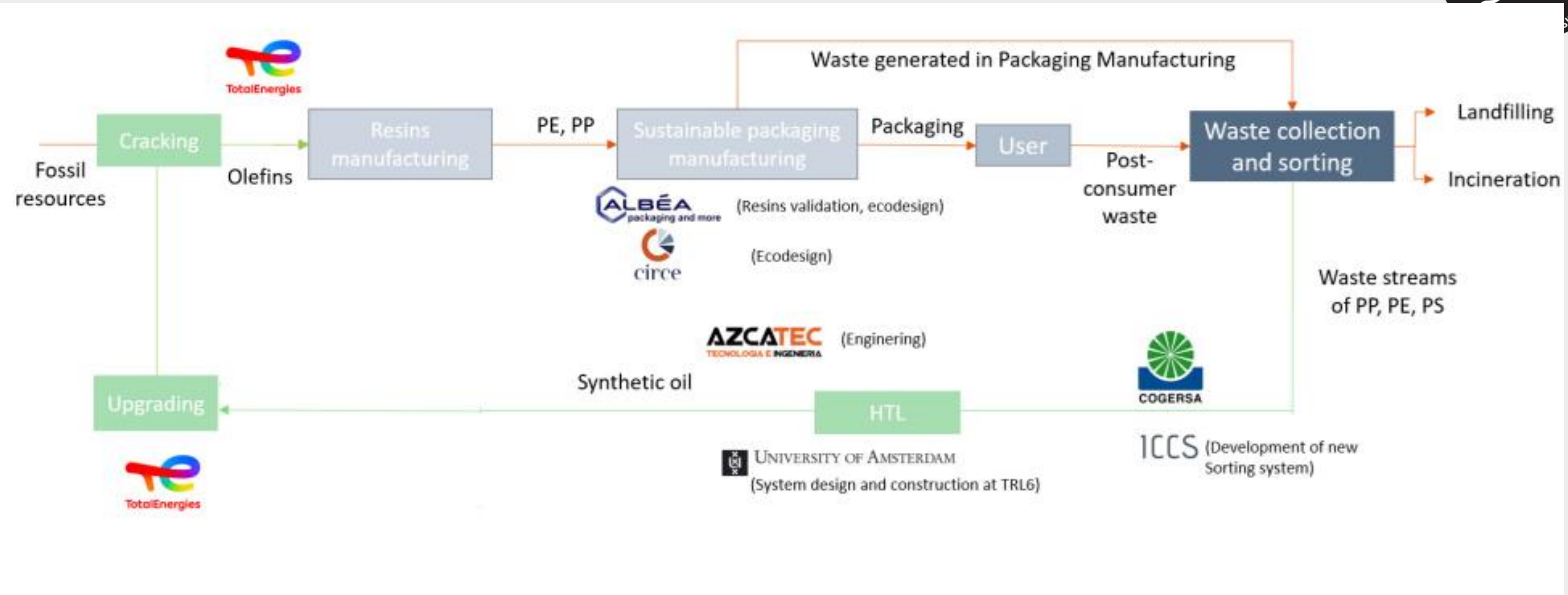
Liquefaction Technology



- A. K. Panda, A. Alotaibi, I. V. Kozhevnikov, N. R. Shiju, Pyrolysis of Plastics to Liquid Fuel Using Sulphated Zirconium Hydroxide Catalyst, *Waste and Biomass Valorization*, 11, 6337–6345, **2020.**
- Hydrothermal Liquefaction of Plastics: a survey of the effect of reaction conditions on the reaction efficiency.

Matthijs Justin Boel and N. Raveendran Shiju, *Reaction Chemistry and Engineering*, under review.

Liquefaction for chemical recycling of plastics


TotalEnergies

Fossil resources

Cracking

Olefins

Resins manufacturing

PE, PP

Sustainable packaging manufacturing

Waste generated in Packaging Manufacturing

Packaging

User

Post-consumer waste

Waste collection and sorting

Landfilling

Incineration

ALBÉA packaging and more (Resins validation, ecodesign)

circe (Ecodesign)

Waste streams of PP, PE, PS

AZCATEC TECNOLOGIA E INGENIERIA (Enginering)

COGERSA

Synthetic oil

Upgrading

HTL

TotalEnergies

UNIVERSITY OF AMSTERDAM (System design and construction at TRL6)

ICCS (Development of new Sorting system)

PLASTICE

https://plastice.eu/

European Commission

Horizon Europe

Overall: 20 million Euros

UvA: Lab scale studies, Process technology (basic and detailed engineering)

Grant Agreement N° 101058540

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Plastics recycling by Liquefaction

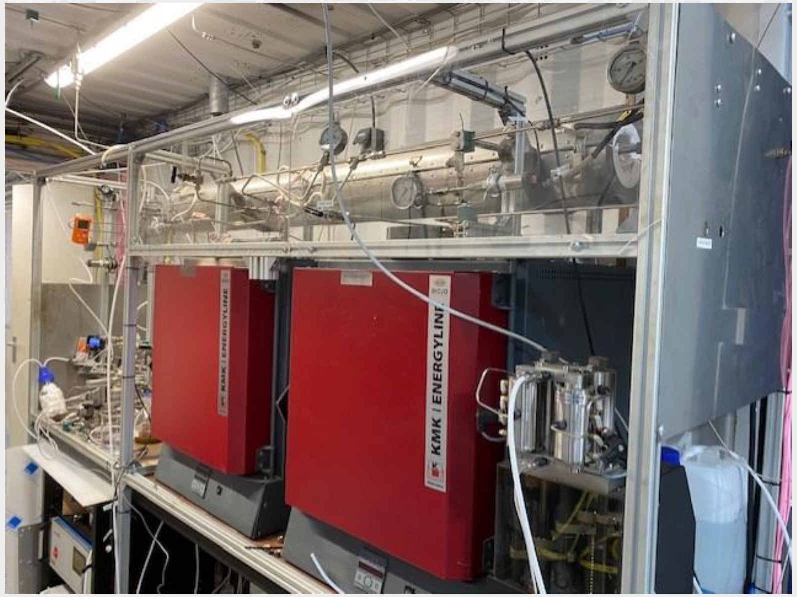
Waste collection → Feed processing → **HTL** → oil

oil → Upgrading Cracking → Monomers → Polymers

oil → Upgrading → Synthetic oil

PLASTICE

Reactors



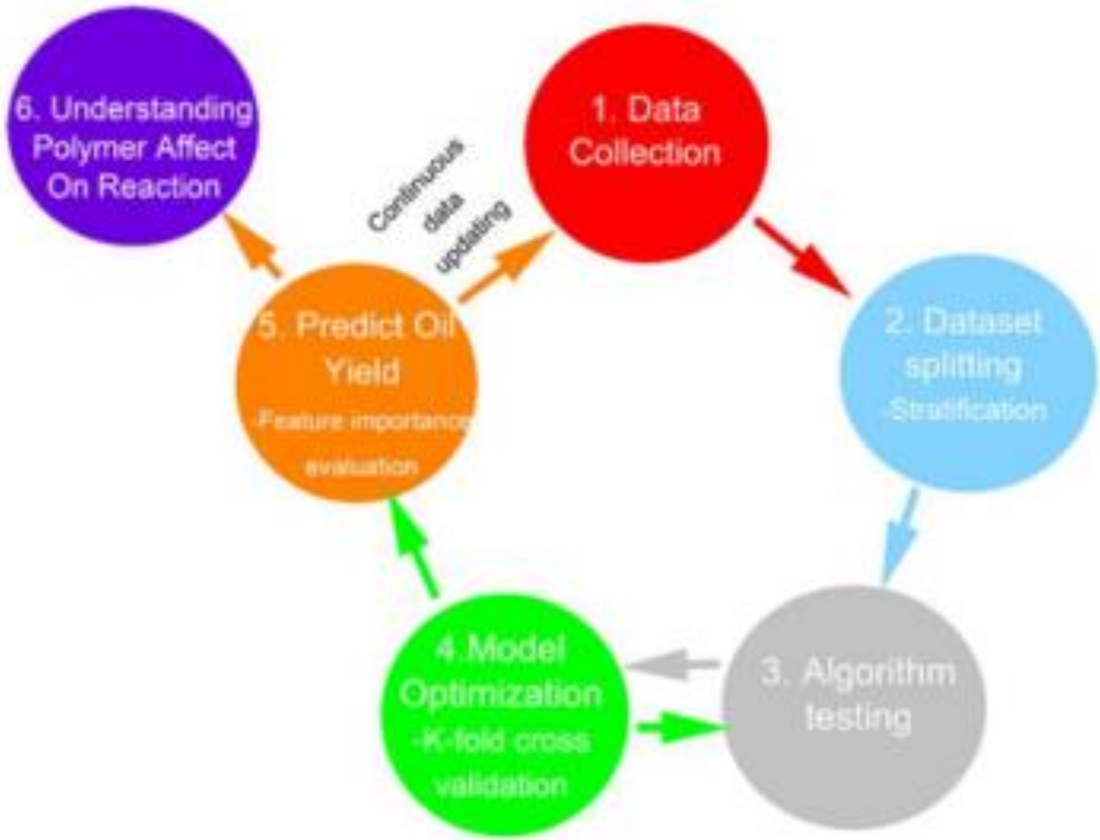
Extrusion (first step)

Mix feedstock with water
Pump with a flow rate of
6 ml/min

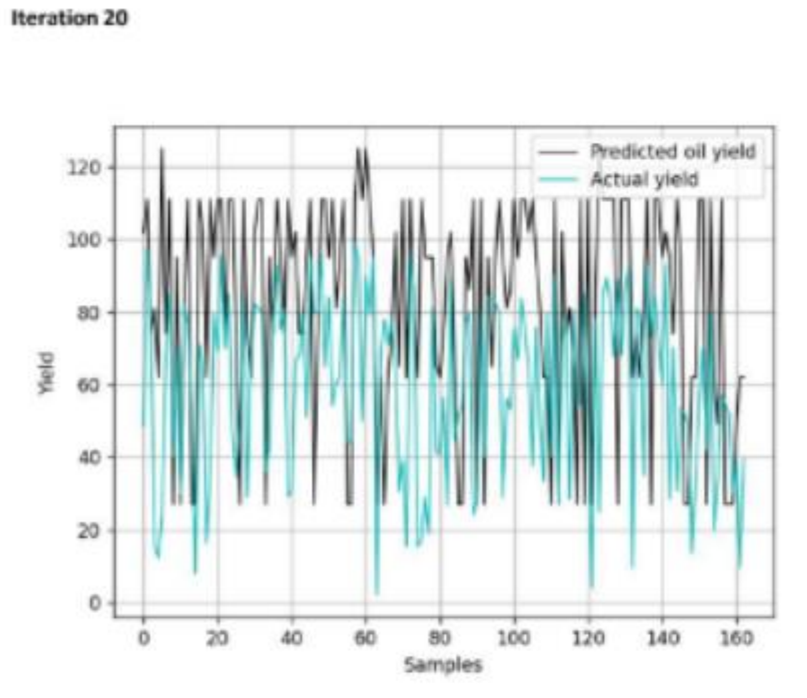
Continuous Flow Reactor
620 °C and 220 bar

AI/ML to help liquefaction

Figure 1



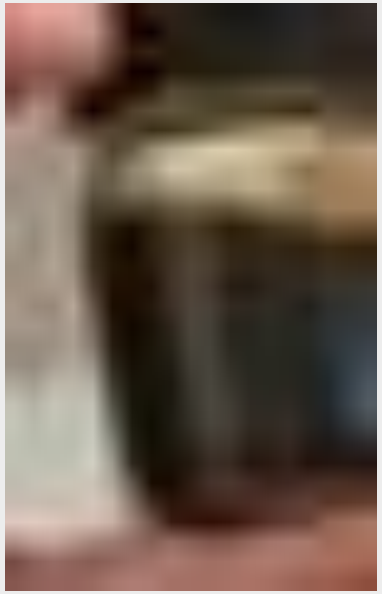
eXtreme Gradient Boosting (XGBoost) algorithm

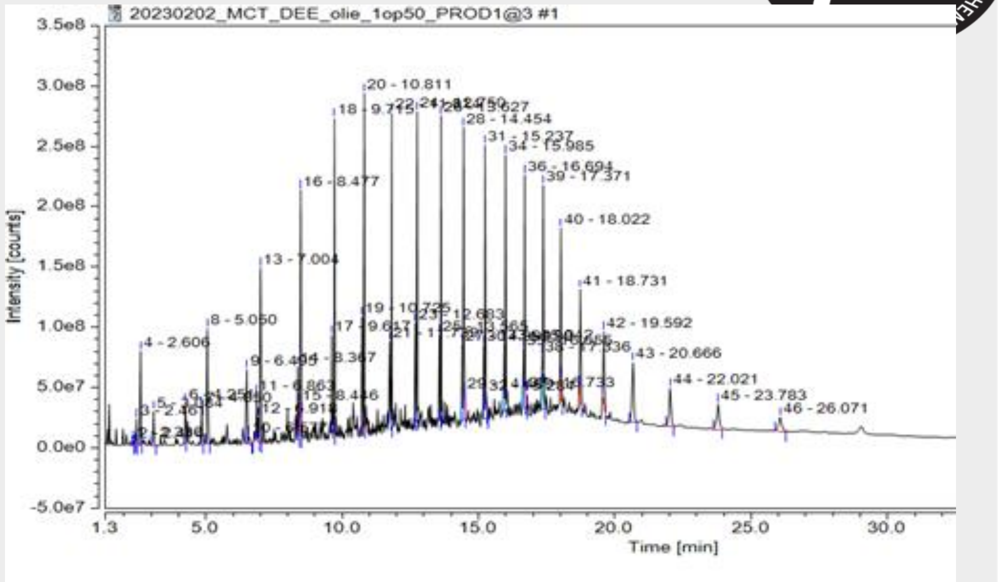


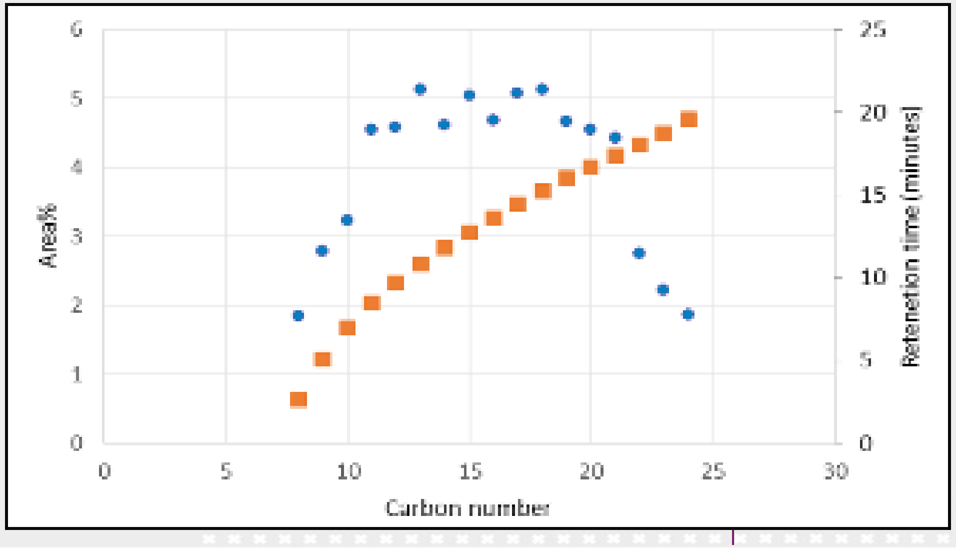
Mean absolute error (MAE) value of 9.1


Before Organic Chemistry
After Organic Chemistry
Argon mix
Nitrogen mix

Plastics recycling by HTL



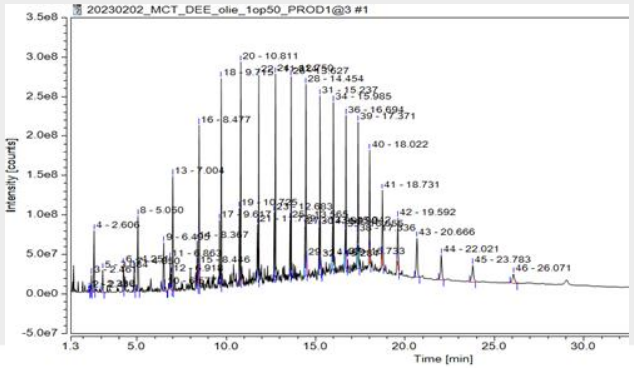




- By optimizing conditions, high oil yields were obtained.
- Depending on the feedstocks, the composition can slightly vary.
- Oil, gas and char fractions depend on the feedstock, reaction conditions and additives.

Composition of oil and gas

No.	Peak Name	Retention Time min
1	hexane	2,336
2	Cyclopentane, 1,2-dimethyl-, cis-	2,414
3	Heptane	2,461
4	Cyclohexane, methyl-	2,606
5	Cyclobutene, 2-propenylidene-	3,084
6	Cyclopentane, 1-ethyl-3-methyl-, cis-	4,251
7	Octane	4,850
8	Benzene, 1,3-dimethyl-	5,050
9	Cyclohexene, 1,6-dimethyl-	6,495
10		6,577
11	p-Xylene	6,863
12		6,918
13	heptane	7,004
14		8,367
15	Decane	8,446
16	undecane	8,477
17	Dodecane	9,617
18	Cyclopentane, 1-methyl-2-(4-methylpentyl)-, trans-	9,715
19	Dodecane	10,725
20	1-Tridecene	10,811
21	Pentadecane	11,739
22	10-Heneicosene (c,t)	11,814
23	Tetradecane	12,683
24	E-2-Hexadecacen-1-ol	12,750
25	Pentadecane	13,565
26	Acetic acid, chloro-, hexadecyl ester	13,627
27	Hexadecane	14,399
28	cis-13-Eicosenoic acid	14,454
29	1-Hexadecanol, 2-methyl-	14,489
30	Tetradecane, 2,6,10-trimethyl-	15,190
31	cis-Vaccenic acid	15,237
32	1-Hexadecanol, 2-methyl-	15,284
33	Tetradecane, 2,6,10-trimethyl-	15,942
34	ocdecane	15,985
35	nonadecane	16,655
36	Octadecanal, 2-bromo-	16,694
37	17-Pentatriacontene	16,733
38	Eicosene	17,336
39	Eicosane	17,371
40	uncosane	18,022
41	docosane	18,731
42	tricosane	19,592
43	tetracosane	20,666
44	pentacosane	22,021
45	hexacosane	23,783

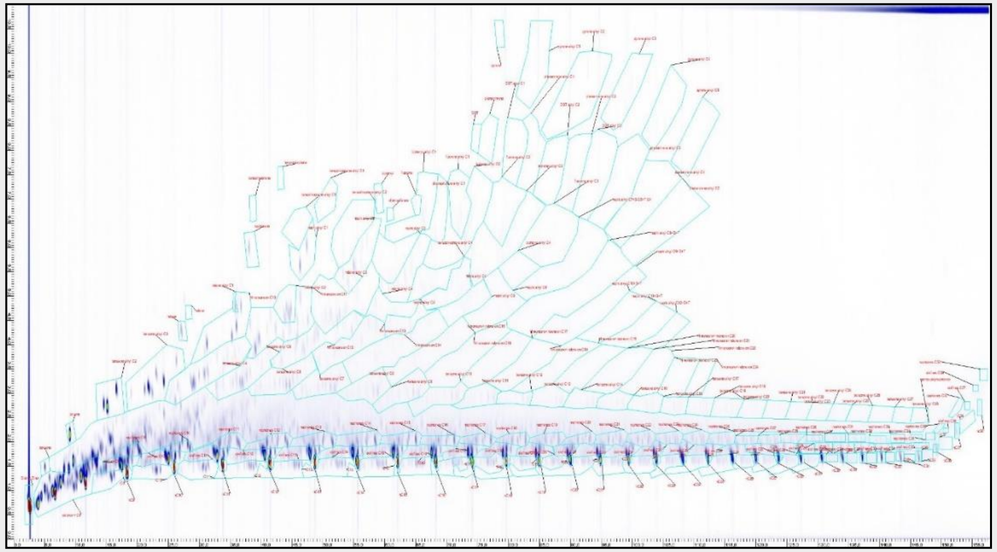


Gas

Component	detector	vol%
Hydrogen	TCD	4,57
Argon	TCD	28,15
CO	TCD	0,31
CO_2	TCD	2,04
Methane	TCD	15,20
Methane	FID	15,30
Ethane/ethylene	FID	23,33
n-C3	FID	11,63
Propylene	FID	2,32
Acetylene	FID	0,74
Iso-Butane	FID	2,17
n-Butane	FID	0,00
trans-2-Butene	FID	0,33
iso-Butylene	FID	0,19
cis-2-Butene	FID	0,15
iso-Pentane	FID	0,11
n-Pentane	FID	0,37
total		**91,81**

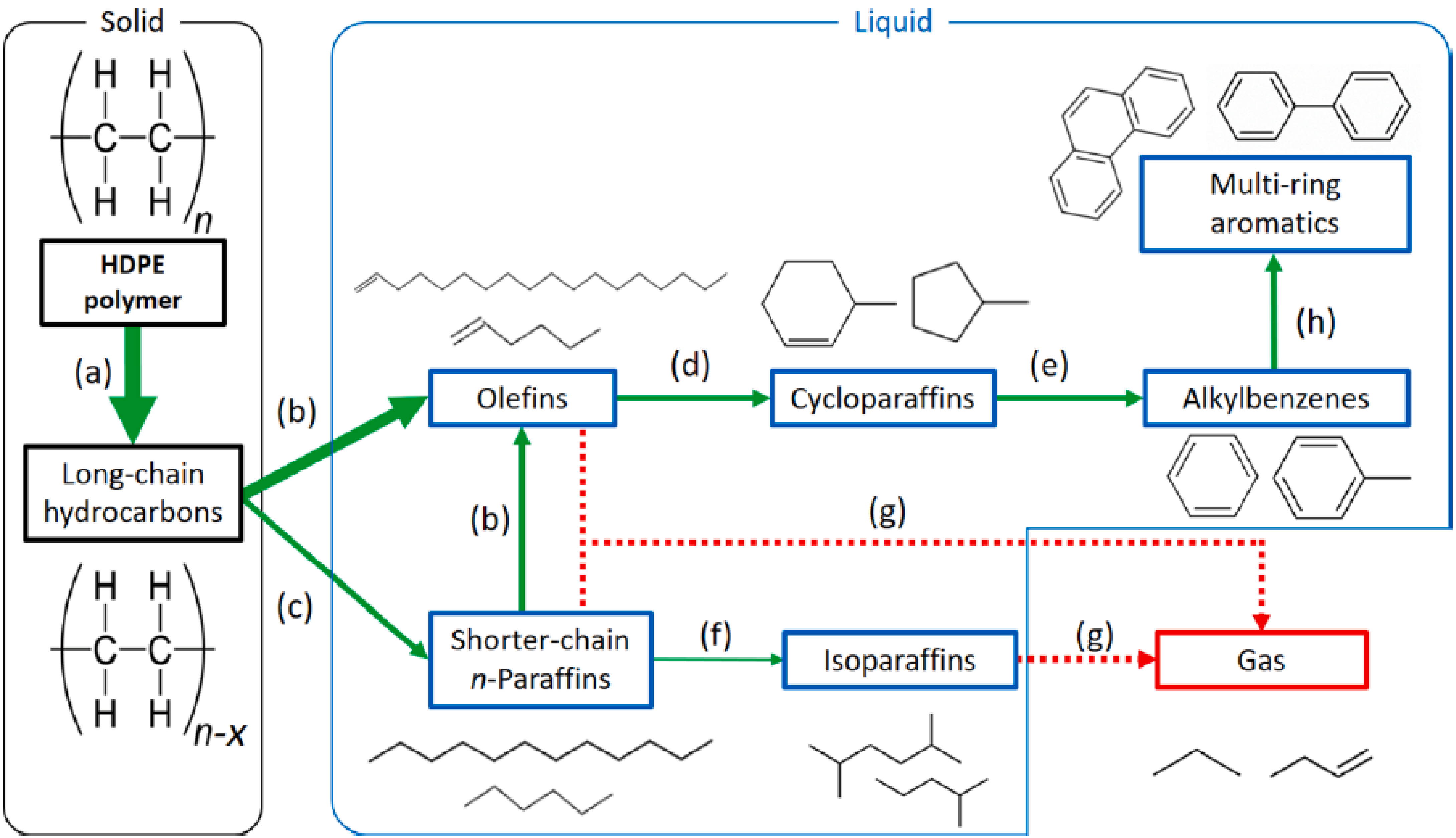
Mainly safe products. Small amounts of CO, CO_2

Oil from HDPE



Mono aromatics contain			
	877078	883548	886549
Benzène	0,10	0	0,12
Toluène	0,60	0.04	0.76
m/p-Xylène	0,16	0.17	0,68
o-Xylène	0,10	0.09	0,33
Styrène	0	0	0.02
Para Cymène C10H14	0	0.01	0,03
TOTAL	1,11	0.36	2.23

	877078	883548	886549
FAMILY	% m/m	% m/m	% m/m
Normal and iso-paraffins	27.01	35.52	33.75
Olefins	21,55	32.22	27.80
Mono naphthènes	12,6	16.37	15.58
Poly naphthènes	14,34	8.64	7.94
Mono aromatics	8,06	6.95	12.45
NMA	3,50	-	-
Di aromatics	1,05	0.30	2.25
Tri aromatics	0,0	0.0	0.08
Tetra aromatics +	0,0	0.0	0.11
Non identified	0,01		0.03
Other < C9	11.70		
TOTAL	99.81		99.80



Solid

HDPE polymer

(a)

Long-chain hydrocarbons

Liquid

(b)

Olefins

(d)

Cycloparaffins

(e)

Alkylbenzenes

(h)

Multi-ring aromatics

(c)

Shorter-chain *n*-Paraffins

(b)

(g)

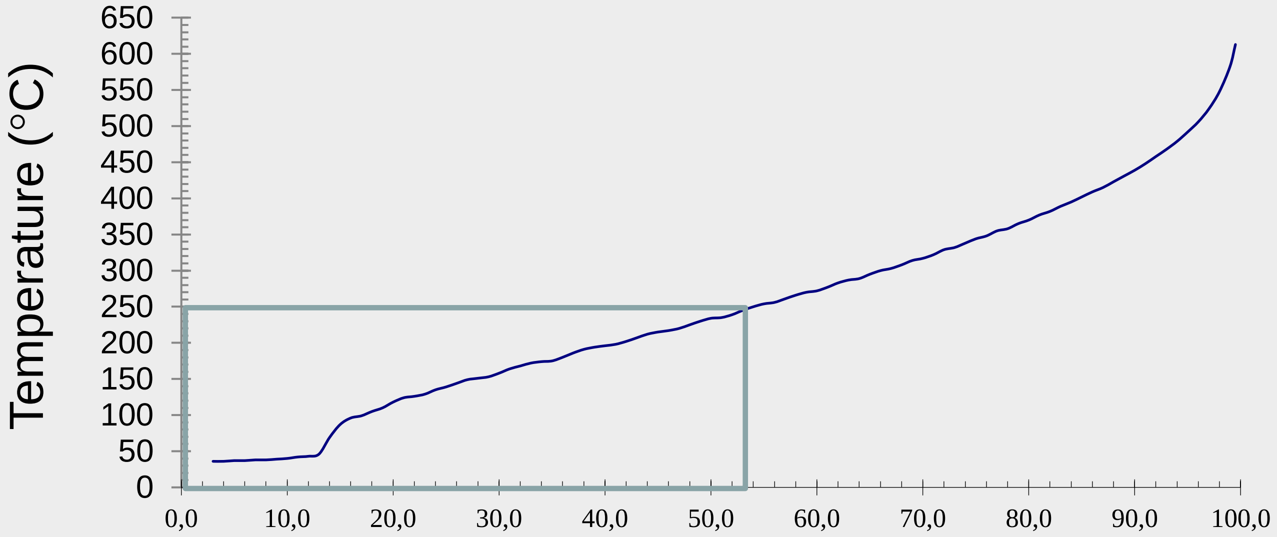
(f)

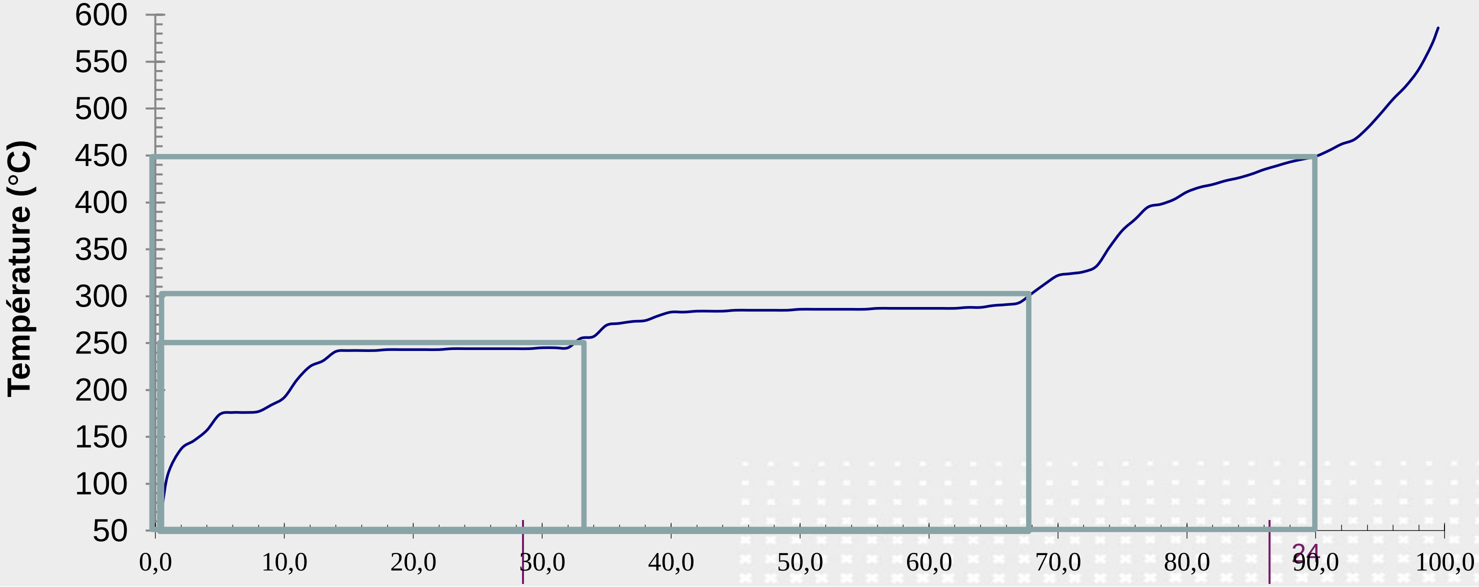
Isoparaffins

(g)

Gas

Simulated Distillation





Analysis for inorganic species

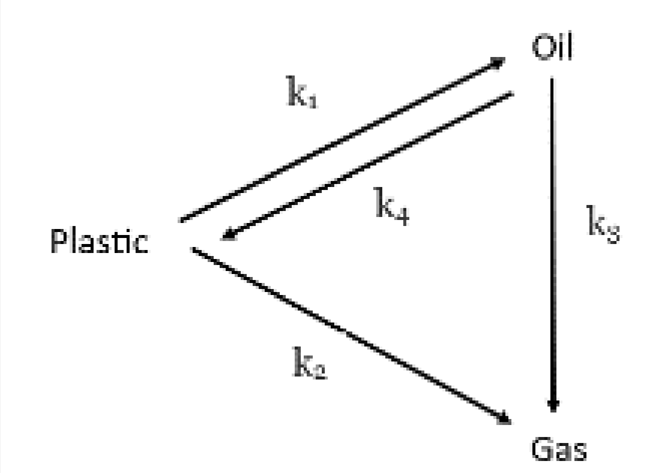
Oil
K, Ca, Cr, Fe, Ni, Cu, Zn, Ag, Cd, Co
S, Cl

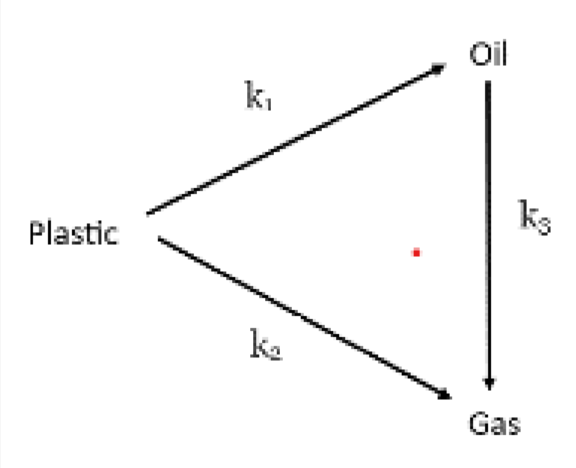
Water
Cr, Fe, Ni
S, Cl

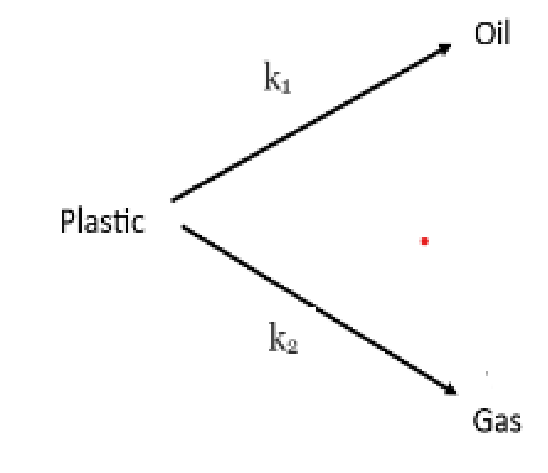
Char
K, Ca, Cr, Fe, Ni, Cu, Zn, Ag, Cd, Co
S, Cl
Si, P, Ti, V, Mn, As, Rb, Sr, Zr, Mo, Rh, Sn, Ba, Pb

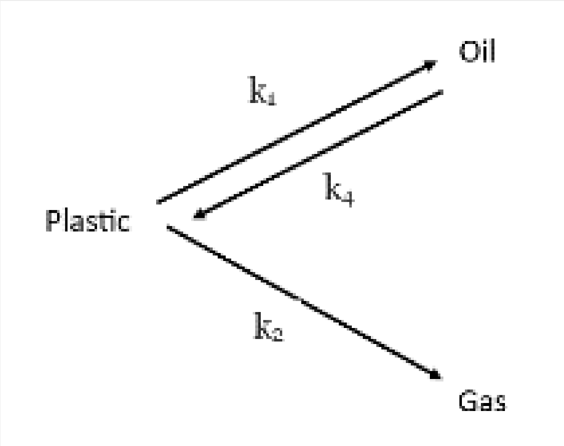
Kinetic models

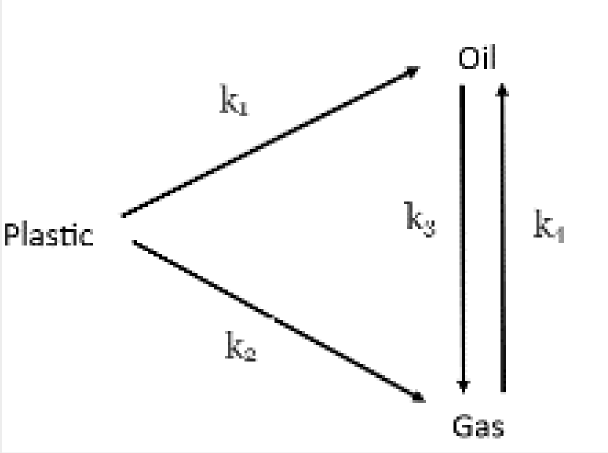
Model 2

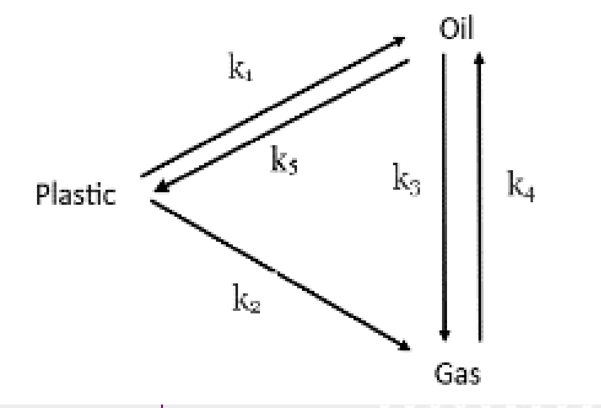


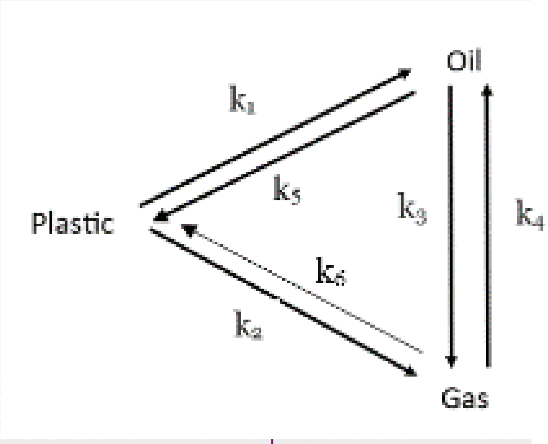






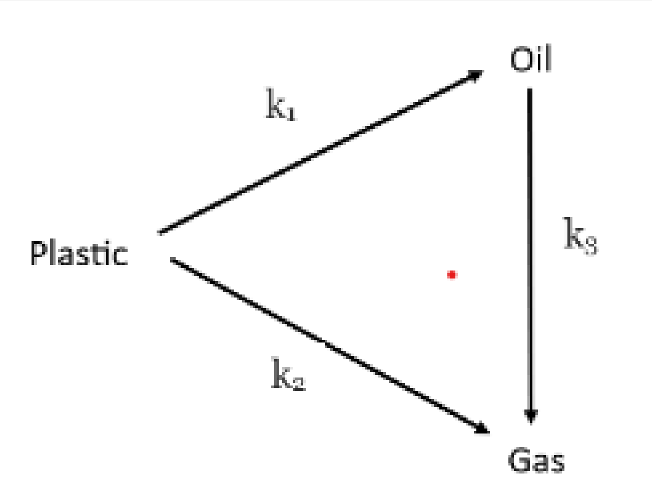


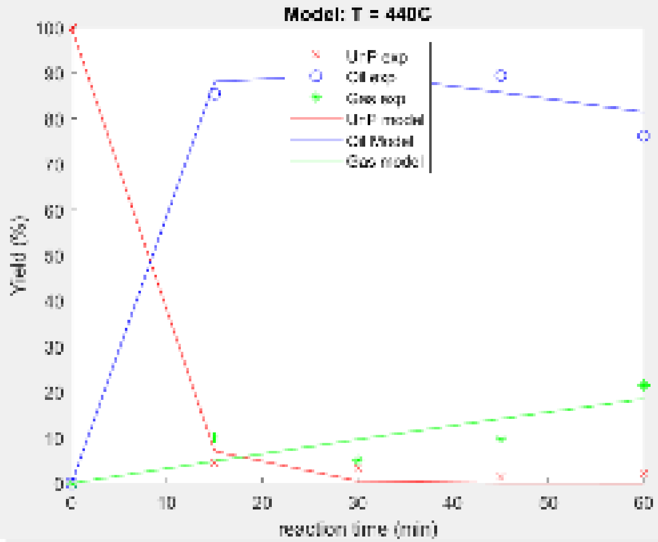


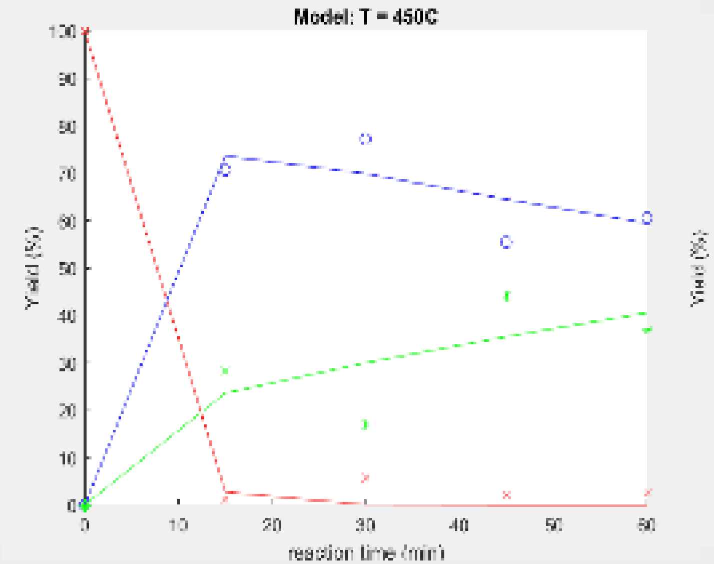


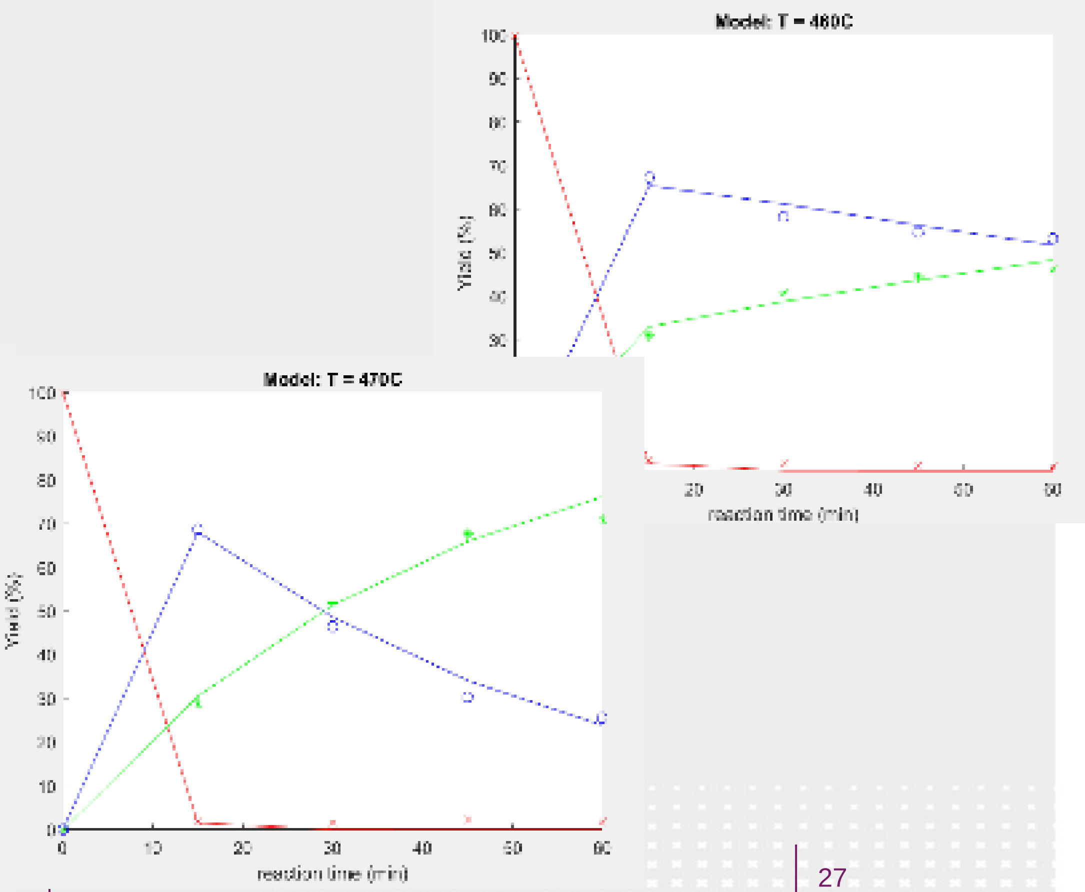
Model 2

Temperature	K1	K2	K3
440	0.1742	0.0031	0.0034
450	0.1929	0.0468	0.0054
460	0.1955	0.0802	0.0056
470	0.2555	0.0257	0.0237









Modeling using kinetic parameters from model 2

2-dimensional, unsteady, incompressible, single phase, and laminar flow

$$\nabla\cdot(\rho u) = 0$$

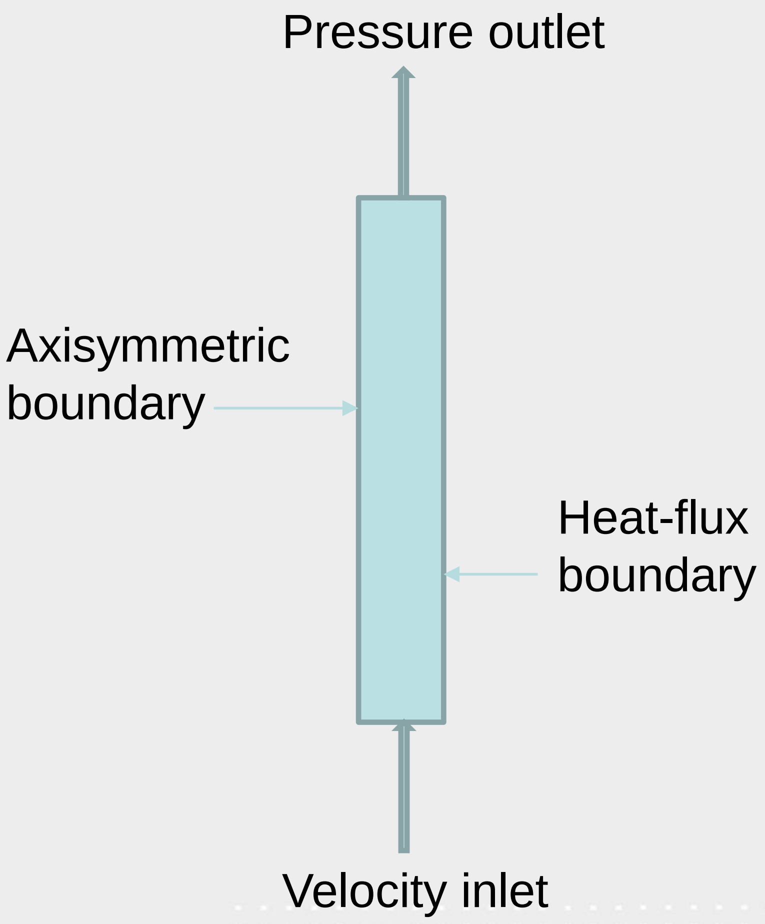
$$\rho\frac{\partial u}{\partial t} + \rho(u\cdot\nabla)\,\mathrm{u} = \nabla\cdot[-pI + \mu(\nabla\,\mathrm{u} + (\nabla\mathrm{u})^{\mathrm{T}})]$$

ρ, μ, and u are the density, viscosity, and velocity of the fluid
p = pressure

Governing equation for energy

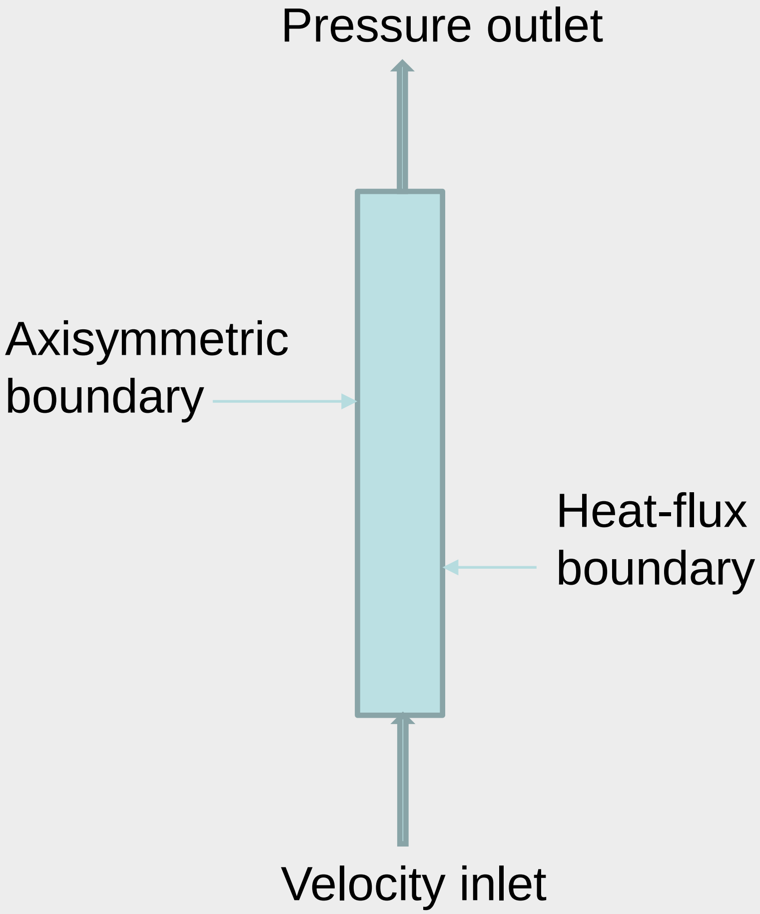
$$\rho C_p\left(\frac{\partial T}{\partial t} + (u\cdot\nabla)T\right) + \nabla\cdot(-k\nabla \mathrm{T}) = Ua(T_{ext} - T)$$

T = temperature of the slurry fluid inside the reactor
T_{ext} = external temperature.
C_p = specific heat
k = thermal conductivity of the fluid
U = the heat exchange coefficient.



Modeling using kinetic parameters from model 2

2-dimensional, unsteady, incompressible, single phase, and laminar flow.



Transport equation for each species:

$$\frac{\partial}{\partial t}(\rho\omega_i) + \nabla\cdot(\rho\omega_i u) = -\nabla\cdot J_i + R_i$$

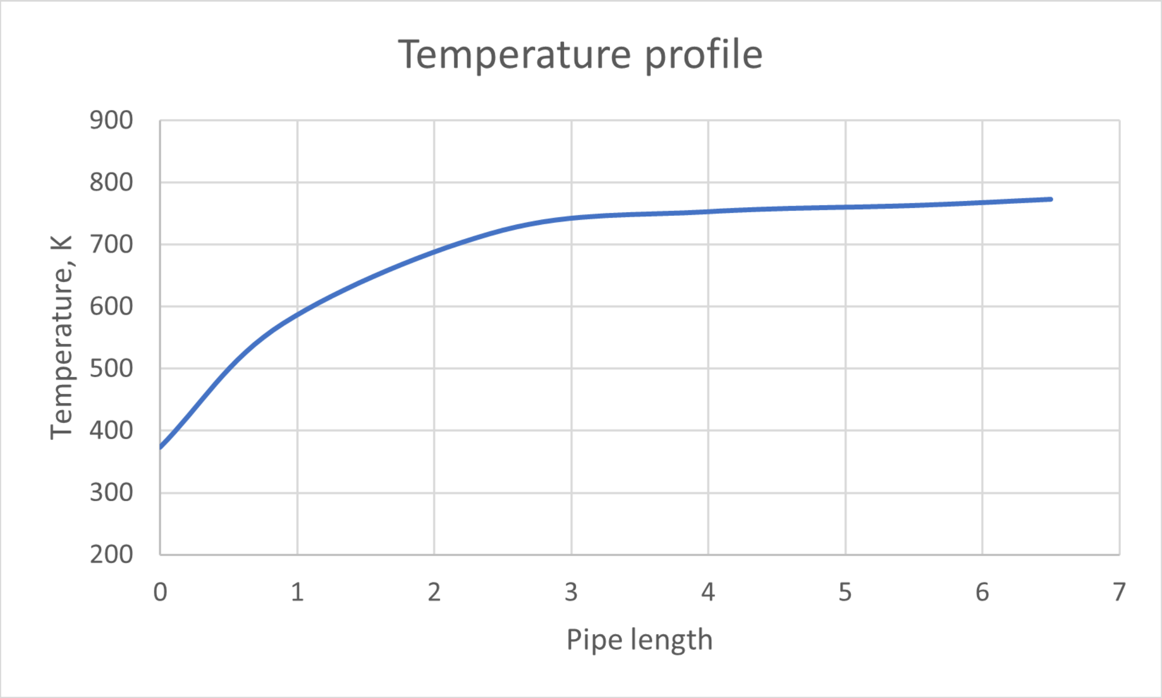
Diffusion flux (mixture averaged diffusion model)

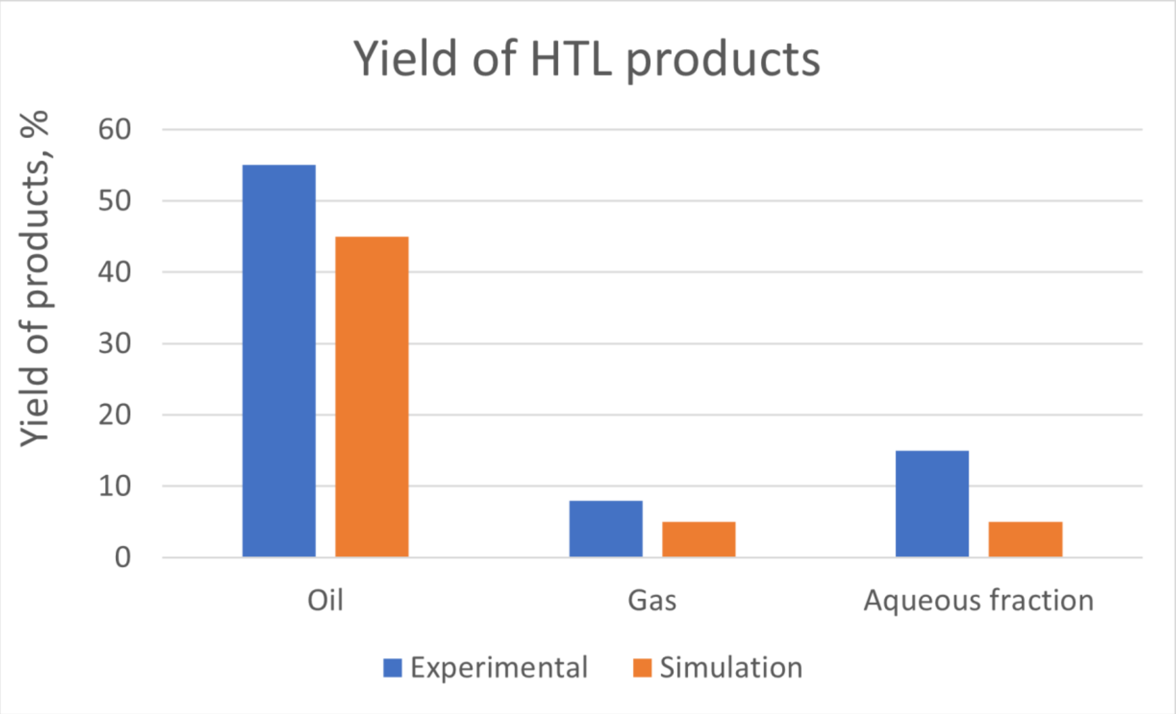
$$J_i = -\left(\rho D_i^m \nabla\omega_i + \rho\omega_i D_i^m \frac{\nabla M_n}{M_n}\right)$$

ω_i = mass fraction of species,
J_i = diffusion flux of species,
i and R_i = net production of species
i due to chemical reaction.

Diameter of reactor = 9.5 mm; Length of reactor = 0.2 m Reaction time 15 min; Slurry feed rate = 1–4 ml/min Slurry concentration = 15 wt%

Yield of products-experimental vs simulation

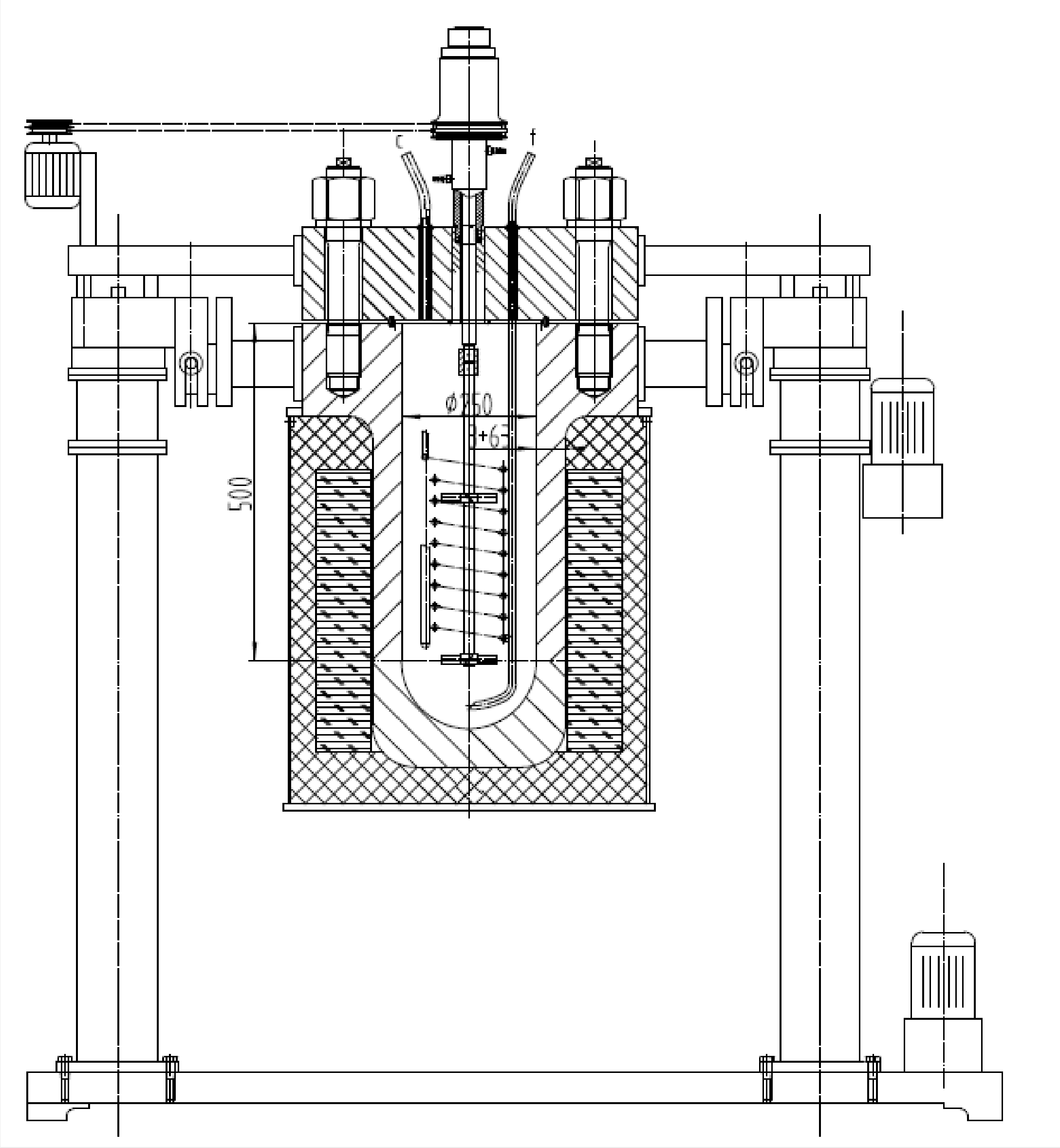




Process parameters used: inlet temperature: 300 K; residence time: 1 min; reaction temperature: 673 K, Pressure = 180 bar.

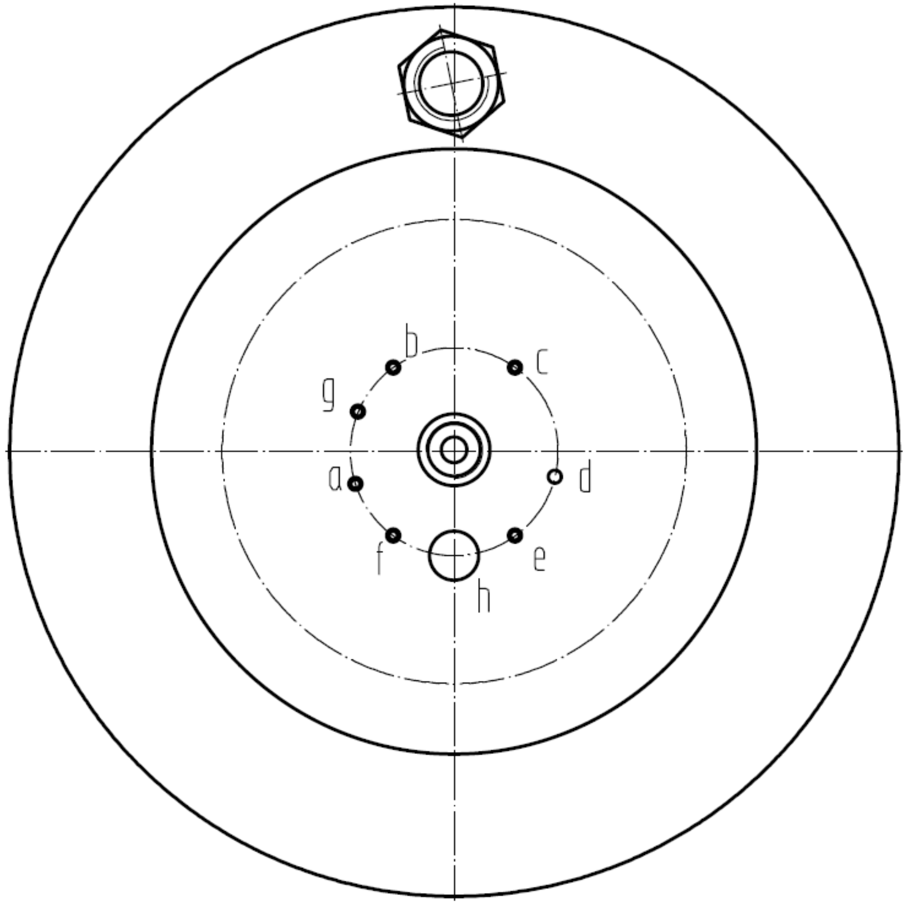
- 2-dimensional, lumped kinetic model and a single phase fluid flow
- Reaction kinetics for HTL is not easy

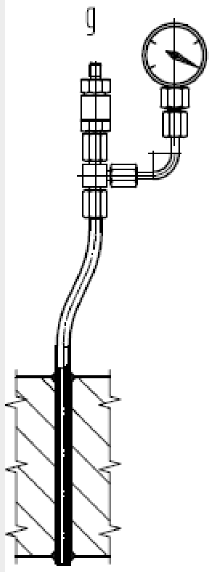
Batch reactor design



Technical parameters	
Work pressure, MPa	30
Work temperature, °C	500
Design pressure, MPa	35
Design temperature, °C	550
Material	SS304 with SS316 liner
Working volume, m^3	
Heat exchange area	
Bursting disc open pressure, MPa	35
Mixing type	Paddle
Motor power, KW	
Mixing speed, r/min	0-500
Corrosion allowance, mm	

Top view

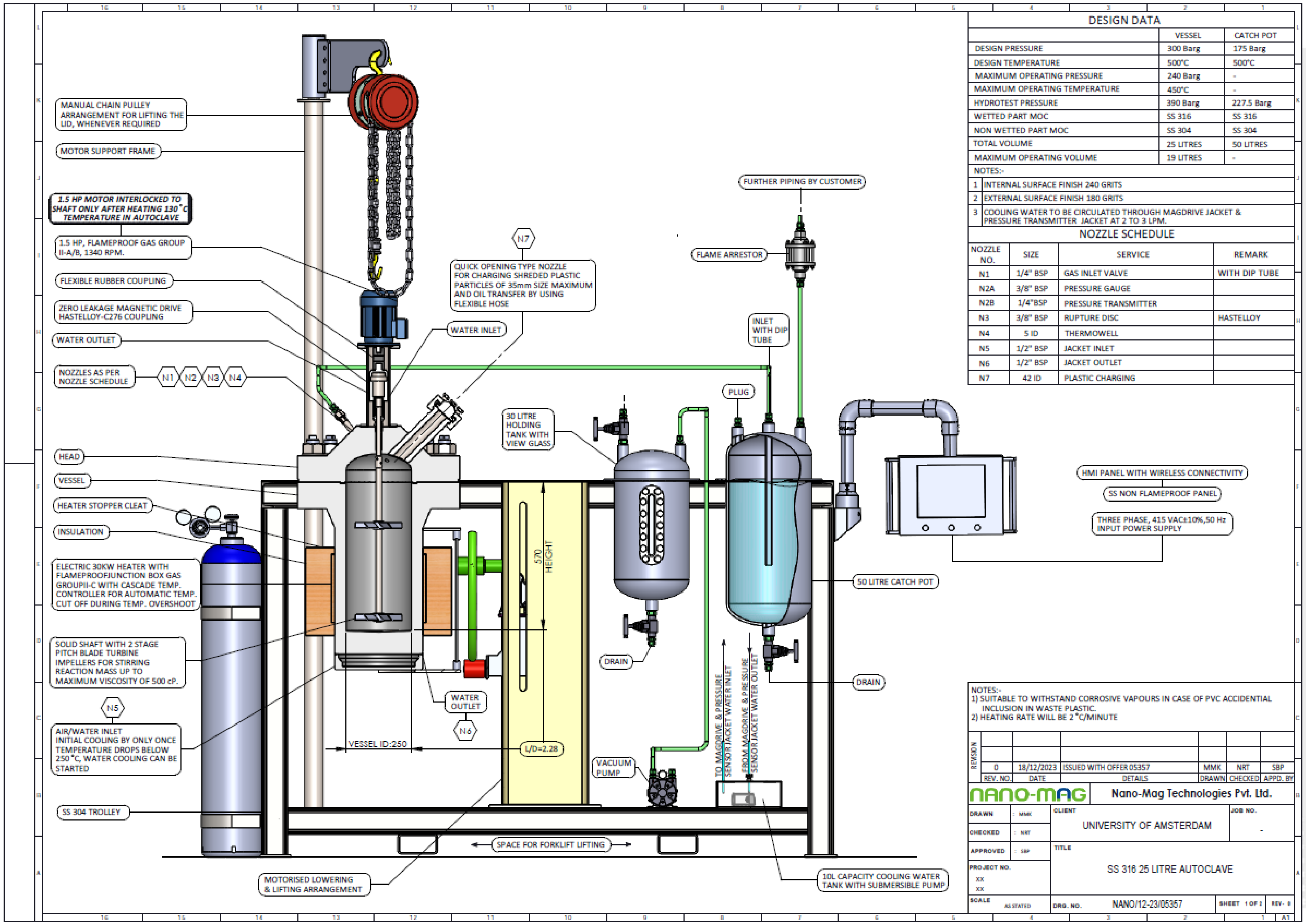




Nozzle pipe table

No	Size	Usage
a	∅ 12	Vent port
b	∅	Bottom insert
c	∅	Coil inlet port
d	∅	Gas inlet port
e	∅	Thermowell
f	∅	Coil outlet port
g	∅	Pressure gauge/burst disc
h	DN20	Solid feeding port

Intermediate Scale-up-same performance?



DESIGN DATA

	VESSEL	CATCH POT
DESIGN PRESSURE	300 Barg	175 Barg
DESIGN TEMPERATURE	500°C	500°C
MAXIMUM OPERATING PRESSURE	240 Barg	-
MAXIMUM OPERATING TEMPERATURE	450°C	-
HYDROTEST PRESSURE	390 Barg	227.5 Barg
WETTED PART MOC	SS 316	SS 316
NON WETTED PART MOC	SS 304	SS 304
TOTAL VOLUME	25 LITRES	50 LITRES
MAXIMUM OPERATING VOLUME	19 LITRES	-

NOTES:-

1. INTERNAL SURFACE FINISH 240 GRITS
2. EXTERNAL SURFACE FINISH 180 GRITS
3. COOLING WATER TO BE CIRCULATED THROUGH MAGDRIVE JACKET & PRESSURE TRANSMITTER JACKET AT 2 TO 3 LPM.

NOZZLE SCHEDULE

NOZZLE NO.	SIZE	SERVICE	REMARK
N1	1/4" BSP	GAS INLET VALVE	WITH DIP TUBE
N2A	3/8" BSP	PRESSURE GAUGE	
N2B	1/4"BSP	PRESSURE TRANSMITTER	
N3	3/8" BSP	RUPTURE DISC	HASTELLOY
N4	5 ID	THERMOWELL	
N5	1/2" BSP	JACKET INLET	
N6	1/2" BSP	JACKET OUTLET	
N7	42 ID	PLASTIC CHARGING	

NOTES:-
1) SUITABLE TO WITHSTAND CORROSIVE VAPOURS IN CASE OF PVC ACCIDENTIAL INCLUSION IN WASTE PLASTIC.
2) HEATING RATE WILL BE 2 °C/MINUTE

REVISION					
0	18/12/2023	ISSUED WITH OFFER 05357	MMK	NRT	SBP
REV. NO.	DATE	DETAILS	DRAWN	CHECKED	APPD. BY

NANO-MAG Nano-Mag Technologies Pvt. Ltd.

DRAWN : MMK	CLIENT UNIVERSITY OF AMSTERDAM		JOB NO. -
CHECKED : NRT			
APPROVED : SBP	TITLE SS 316 25 LITRE AUTOCLAVE		
PROJECT NO. XX XX			
SCALE AS STATED	DRG. NO. NANO/12-23/05357	SHEET 1 OF 1	REV- 0

Thank you!

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