Alternative combustion techniques using organic fuel:
case studies with CFD

Project Introduction
RETROFEED

RETROFEED – Implementation of a Smart RETROfitting Framework in the Process Industry towards its Operation with Variable, Biobased and Circular FEEDstock

- ✓ Topic: H2020-CE-SPIRE-05-2019
- ✓ IA action
- ✓ Total investment: 15.454.951,88€
- ✓ EU Funding: 9.912.915,33€
- ✓ Duration 48M (November 2019 – October 2023)

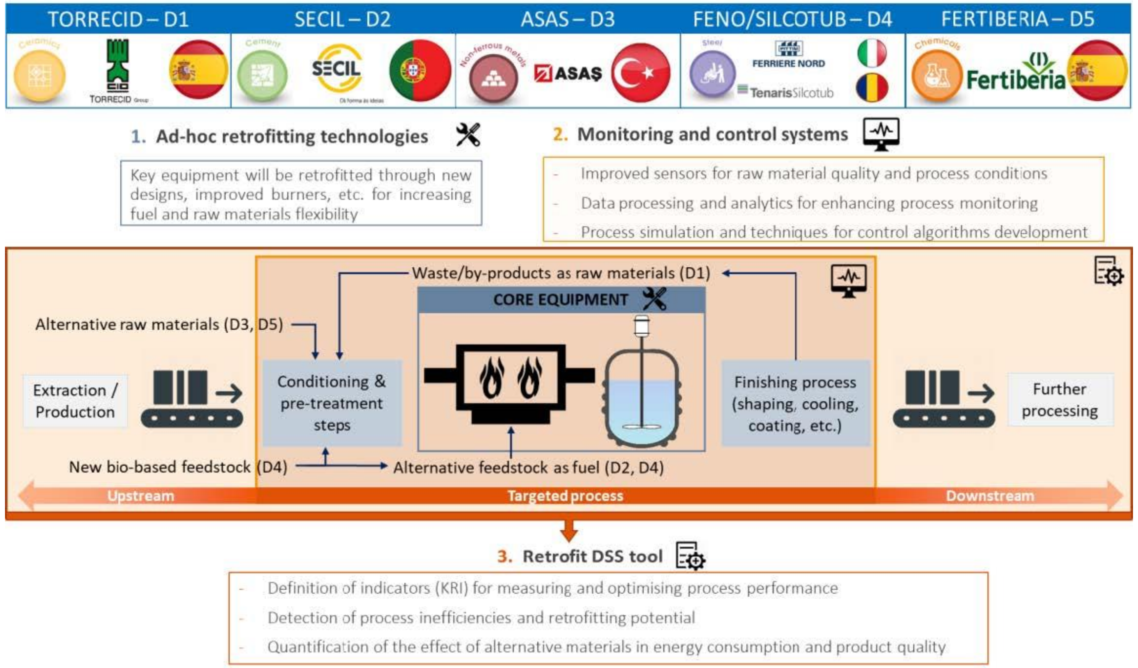
Project Introduction

Main objective

RETROFEED main objective is to:

- **enable the use of an increasingly variable, bio-based and circular feedstock in process industries through the retrofitting of core equipment,** the implementation of an advanced monitoring and control system, and providing support to the plant operators by means of a DSS covering the production chain.
- This approach will be demonstrated in **five Resource and Energy Intensive Industries REIIs (ceramic, cement, aluminium, steel, and agrochemical).**

Project Introduction
Overall concept



1. Ad-hoc retrofitting technologies

Key equipment will be retrofitted through new designs, improved burners, etc. for increasing fuel and raw materials flexibility

2. Monitoring and control systems

- Improved sensors for raw material quality and process conditions
- Data processing and analytics for enhancing process monitoring
- Process simulation and techniques for control algorithms development

3. Retrofit DSS tool

- Definition of indicators (KRI) for measuring and optimising process performance
- Detection of process inefficiencies and retrofitting potential
- Quantification of the effect of alternative materials in energy consumption and product quality

- ✓ Core equipment retrofitting
- ✓ Improving M&C system
- ✓ Development of new sensors
- ✓ Development of Digital Twins
- ✓ Development of Decision Support Systems
- ✓ TRL 7 solutions

Project Introduction

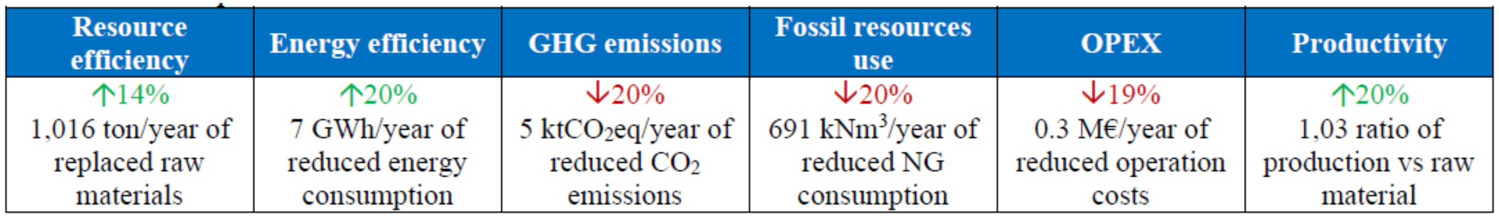
Direct impacts

- Increasing the resource and energy efficiency of the targeted processes by 20%;
- Decrease GHG emissions through retrofitting by at least 30%;
- Decreased utilisation of fossil resources in the process industry of at least 20%;
- Reduced OPEX by 30% and increased productivity by 20%;
- Effective dissemination of major innovation outcomes to the current next generation of employees of the SPIRE sectors, through the development, by education/training experts, of learning resources with flexible usability. These should be ready to be easily integrated in existing curricula and modules for undergraduate level and lifelong learning programs.

Expected impacts on industries

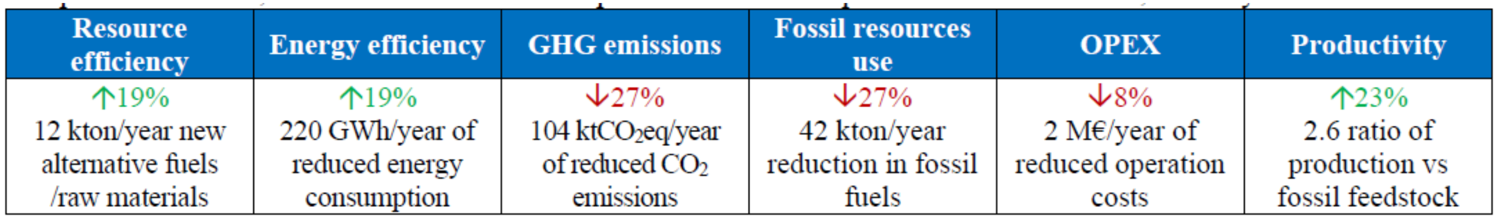
Efficiency metrics definition

Cement and concrete



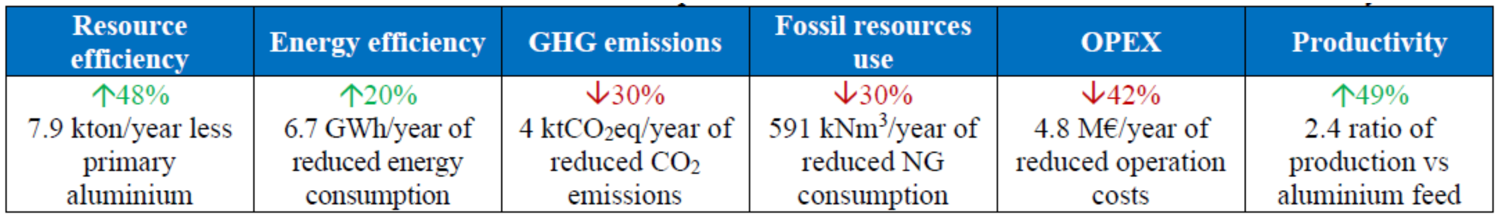
Resource efficiency	Energy efficiency	GHG emissions	Fossil resources use	OPEX	Productivity
↑14% 1,016 ton/year of replaced raw materials	↑20% 7 GWh/year of reduced energy consumption	↓20% 5 ktCO$_2$eq/year of reduced CO$_2$ emissions	↓20% 691 kNm^3/year of reduced NG consumption	↓19% 0.3 M€/year of reduced operation costs	↑20% 1,03 ratio of production vs raw material

Ceramic and glass



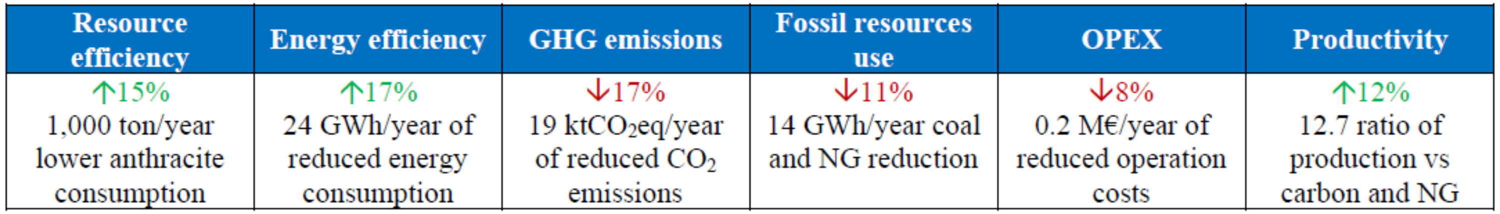
Resource efficiency	Energy efficiency	GHG emissions	Fossil resources use	OPEX	Productivity
↑19% 12 kton/year new alternative fuels /raw materials	↑19% 220 GWh/year of reduced energy consumption	↓27% 104 ktCO$_2$eq/year of reduced CO$_2$ emissions	↓27% 42 kton/year reduction in fossil fuels	↓8% 2 M€/year of reduced operation costs	↑23% 2.6 ratio of production vs fossil feedstock

Aluminum



Resource efficiency	Energy efficiency	GHG emissions	Fossil resources use	OPEX	Productivity
↑48% 7.9 kton/year less primary aluminium	↑20% 6.7 GWh/year of reduced energy consumption	↓30% 4 ktCO$_2$eq/year of reduced CO$_2$ emissions	↓30% 591 kNm^3/year of reduced NG consumption	↓42% 4.8 M€/year of reduced operation costs	↑49% 2.4 ratio of production vs aluminium feed

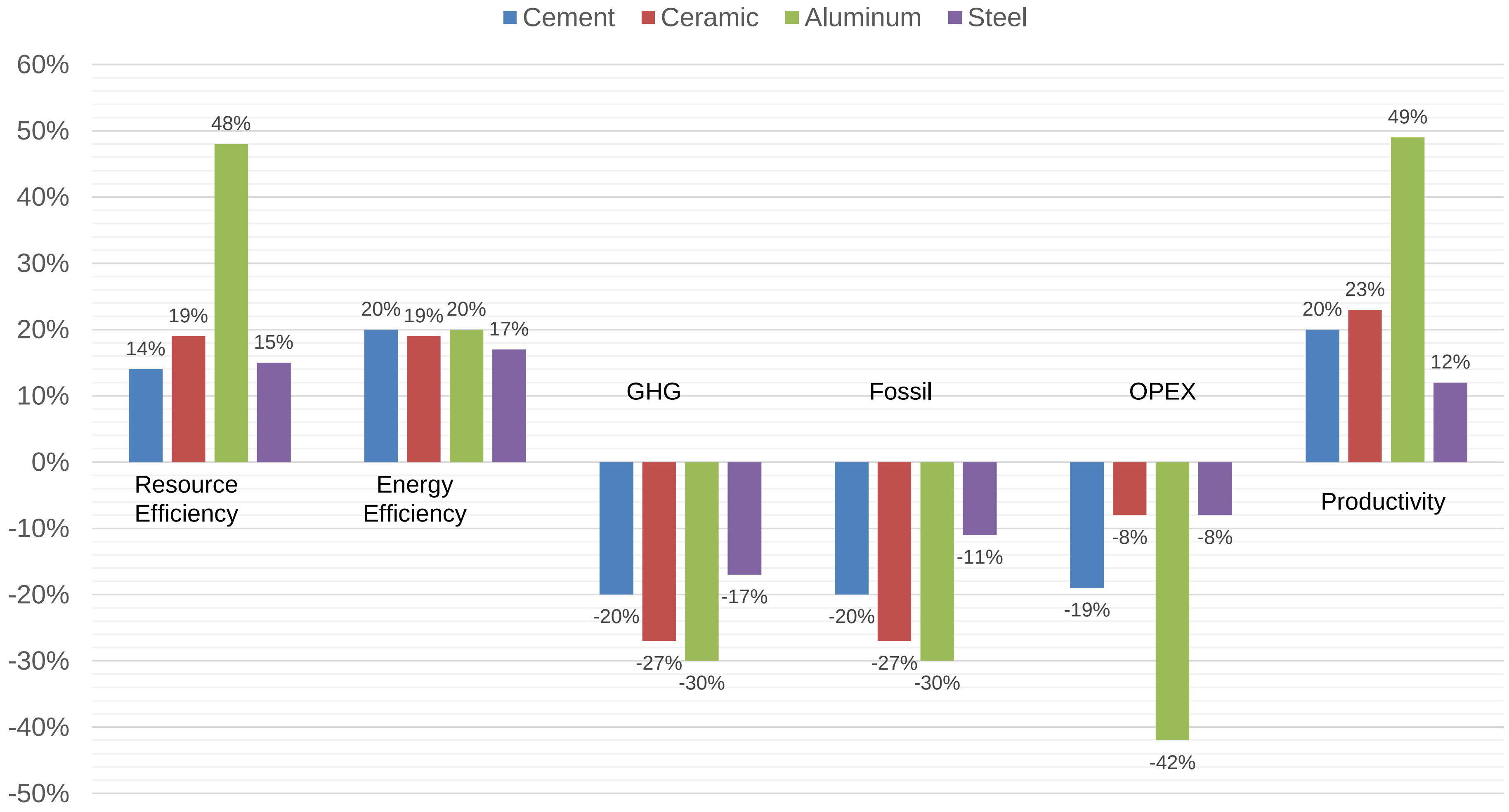
Steel



Resource efficiency	Energy efficiency	GHG emissions	Fossil resources use	OPEX	Productivity
↑15% 1,000 ton/year lower anthracite consumption	↑17% 24 GWh/year of reduced energy consumption	↓17% 19 ktCO$_2$eq/year of reduced CO$_2$ emissions	↓11% 14 GWh/year coal and NG reduction	↓8% 0.2 M€/year of reduced operation costs	↑12% 12.7 ratio of production vs carbon and NG

Expected impacts on industries

Efficiency metrics improvement



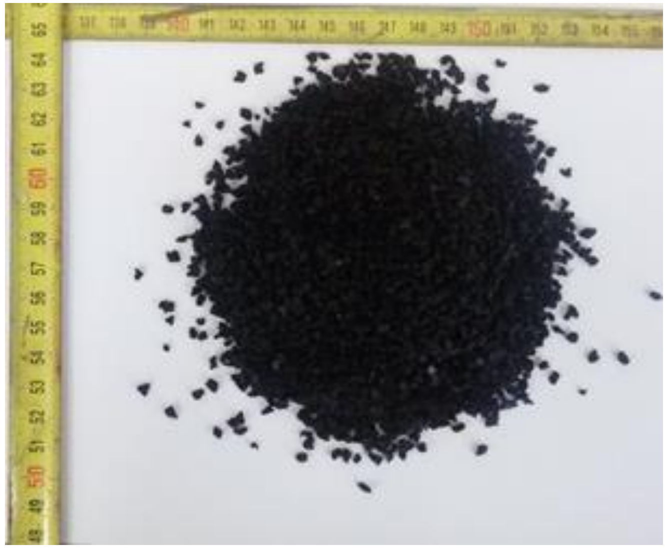
Materials

Plastic Grains

The performed analysis:

- Elemental analysis
- Heating value
- Proximate analysis
- Thermogravimetric analysis

Granulated tires



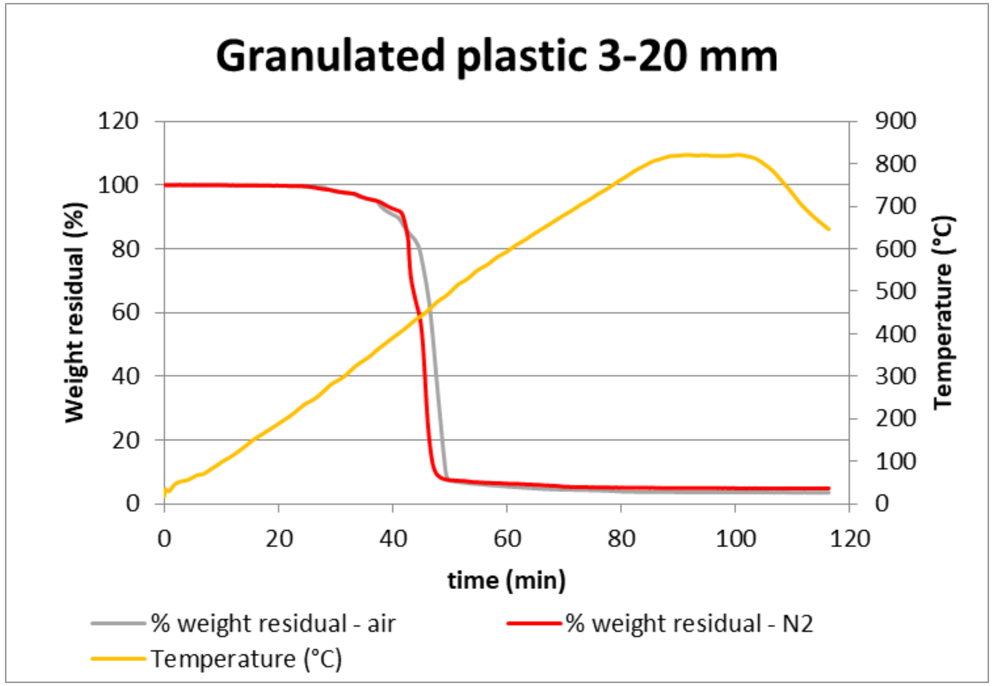
Materials

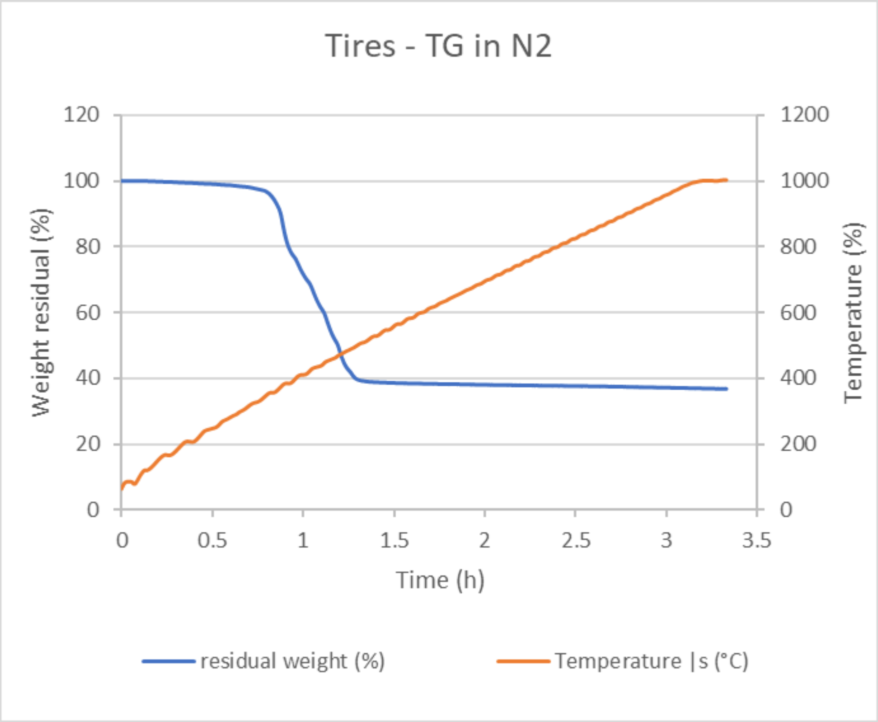
Proximate and Elemental analysys

	EOL tires	Plastic (I.Blu)
PCS (MJ/kg)	34-36	32
S (%)	1.5-2.0	0.03
H (%)	8.2	10
N (%)	1.3-2.0	1
C (%)	78-80	65-70
O (%)	<1	-
Cl (%)	-	0.35
Volatile matter (%)	63-35	88
Ash (%)	8-10	8-10
Fixed carbon (%)	25-27	1.5
Moisture (%)	2.3	1.8
Density (kg/m^3)	1000	400
Physical appearence	grain	grain

Materials

Proximate and Elemental analysys



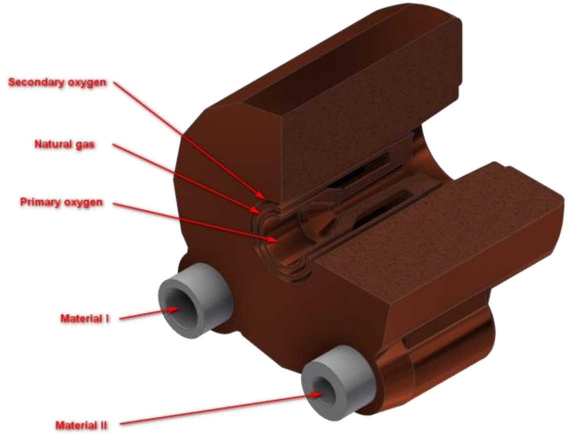


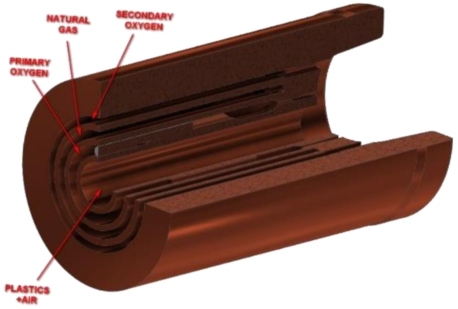
Plastic is chosen

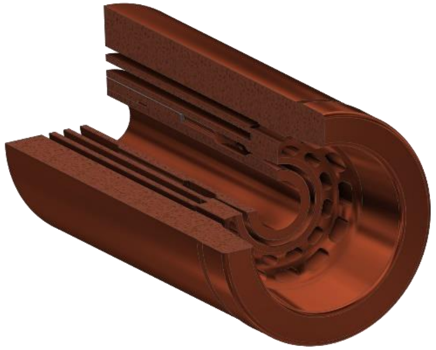
Tests - reference

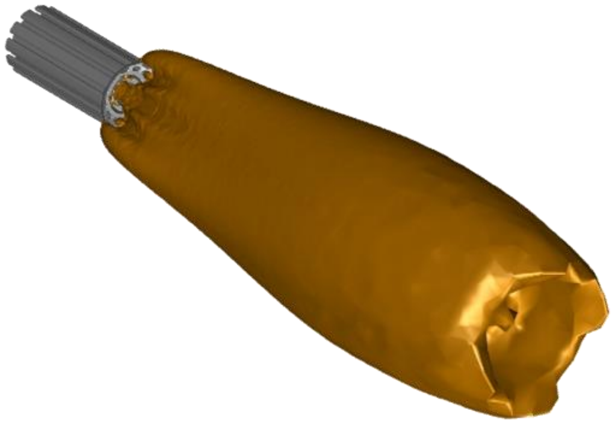
- ✓ Check on behaviour as burner/injection

Item	**Unit**	**Reference**	**Burner**	**Injector**
Primary oxygen flow	Nm3/h	300	600	1200
Natural gas flow	Nm3/h	250	100	100
Secondary oxygen flow	Nm3/h	300	600	120
Primary oxygen pressure	bar(g)			11
Natural gas pressure	bar(g)		0.5	0.5
Secondary oxygen pressure	bar(g)		3.5	1.2
Plastic particles flow	kg/min		10	20
Plastic particles average size	mm		2	2
Compressed air flow via plastics supply line	Nm3/h	0	150	200



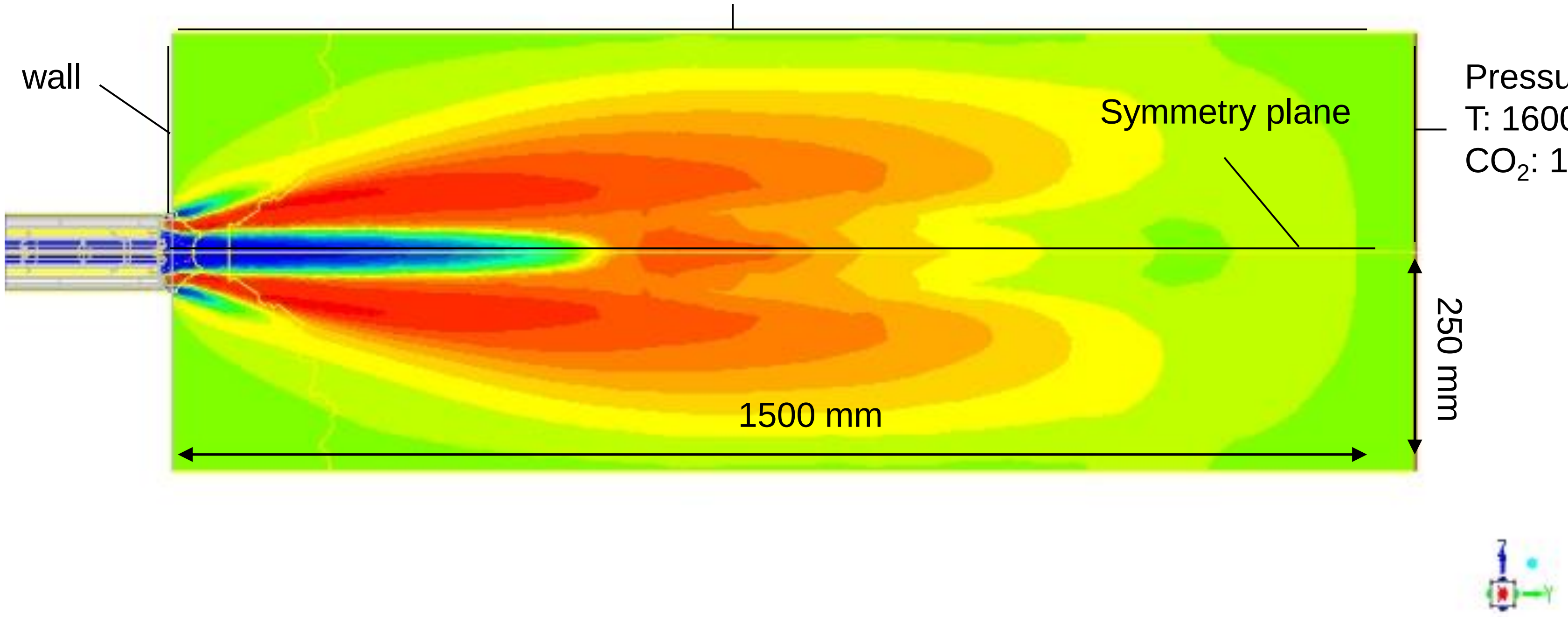






Burner & Injector Mode
Mesh & CFD conditions

- ✓ 600,000 cells



Pressure outlet
T: 1600 C°
CO_2: 100%

wall

Symmetry plane

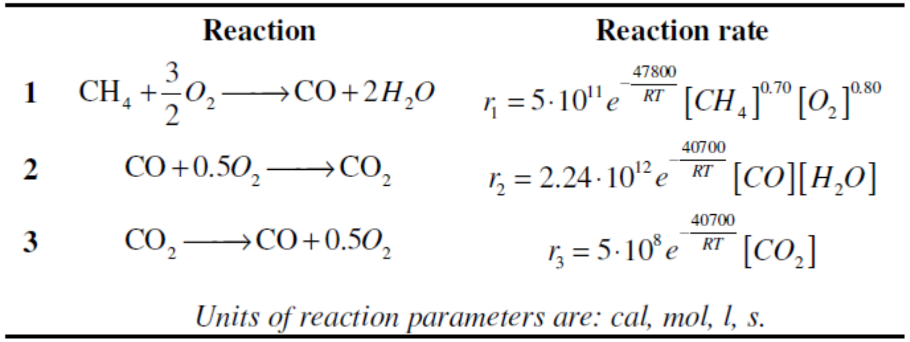
Pressure outlet
T: 1600 C°
CO_2: 100%

Plastic		
D	2	mm
volatiles	80%	w/w

Inlet Temperature: 25°C

Kinetics

Westbrook-Dryer mechanism (WD).



	Reaction	Reaction rate
1	$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$	$r_1 = 5 \cdot 10^{11} e^{-\frac{47800}{RT}} [CH_4]^{0.70} [O_2]^{0.80}$
2	$CO + 0.5O_2 \longrightarrow CO_2$	$r_2 = 2.24 \cdot 10^{12} e^{-\frac{40700}{RT}} [CO][H_2O]$
3	$CO_2 \longrightarrow CO + 0.5O_2$	$r_3 = 5 \cdot 10^{8} e^{-\frac{40700}{RT}} [CO_2]$

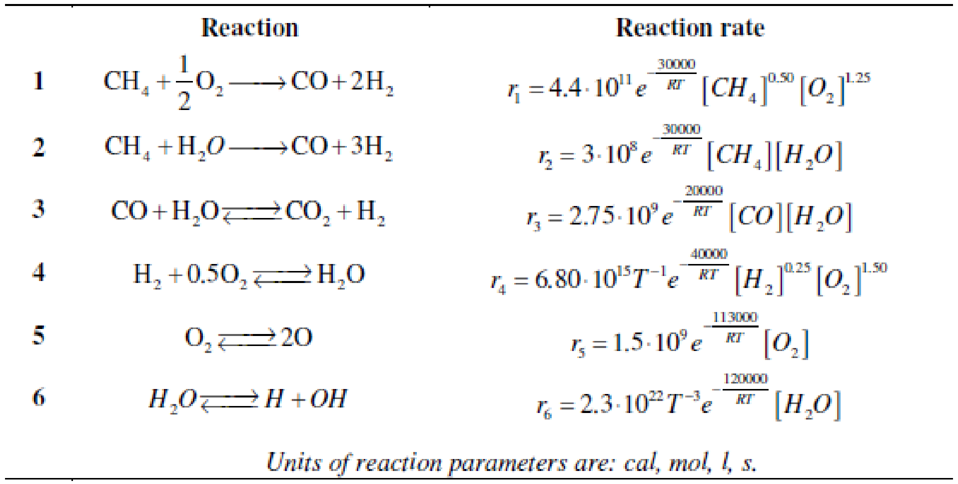
Units of reaction parameters are: cal, mol, l, s.

Table 1. Westbrook-Dryer mechanism (WD).

Turbolence – chemistry coupling:
Eddy Dissipation Concept (EDC)

Frassoldati et al. 2009, Simplified kinetic schemes for oxy-fuel combustion

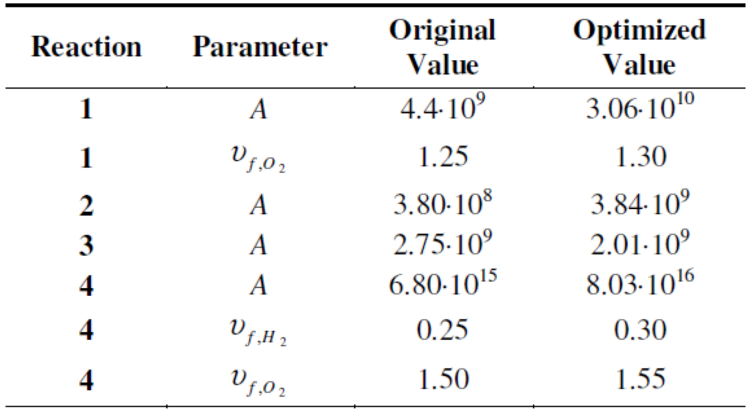
Jones-Lindstedt mechanism with dissociation reactions (JL-R).
Optimized parameters



	Reaction	Reaction rate
1	$CH_4 + \frac{1}{2}O_2 \longrightarrow CO + 2H_2$	$r_1 = 4.4 \cdot 10^{11} e^{-\frac{30000}{RT}} [CH_4]^{0.50} [O_2]^{1.25}$
2	$CH_4 + H_2O \longrightarrow CO + 3H_2$	$r_2 = 3 \cdot 10^{8} e^{-\frac{30000}{RT}} [CH_4][H_2O]$
3	$CO + H_2O \rightleftharpoons CO_2 + H_2$	$r_3 = 2.75 \cdot 10^{9} e^{-\frac{20000}{RT}} [CO][H_2O]$
4	$H_2 + 0.5O_2 \rightleftharpoons H_2O$	$r_4 = 6.80 \cdot 10^{15} T^{-1} e^{-\frac{40000}{RT}} [H_2]^{0.25} [O_2]^{1.50}$
5	$O_2 \rightleftharpoons 2O$	$r_5 = 1.5 \cdot 10^{9} e^{-\frac{113000}{RT}} [O_2]$
6	$H_2O \rightleftharpoons H + OH$	$r_6 = 2.3 \cdot 10^{22} T^{-3} e^{-\frac{120000}{RT}} [H_2O]$

Units of reaction parameters are: cal, mol, l, s.

Table 3. Jones-Lindstedt mechanism with dissociation reactions (JL-R).

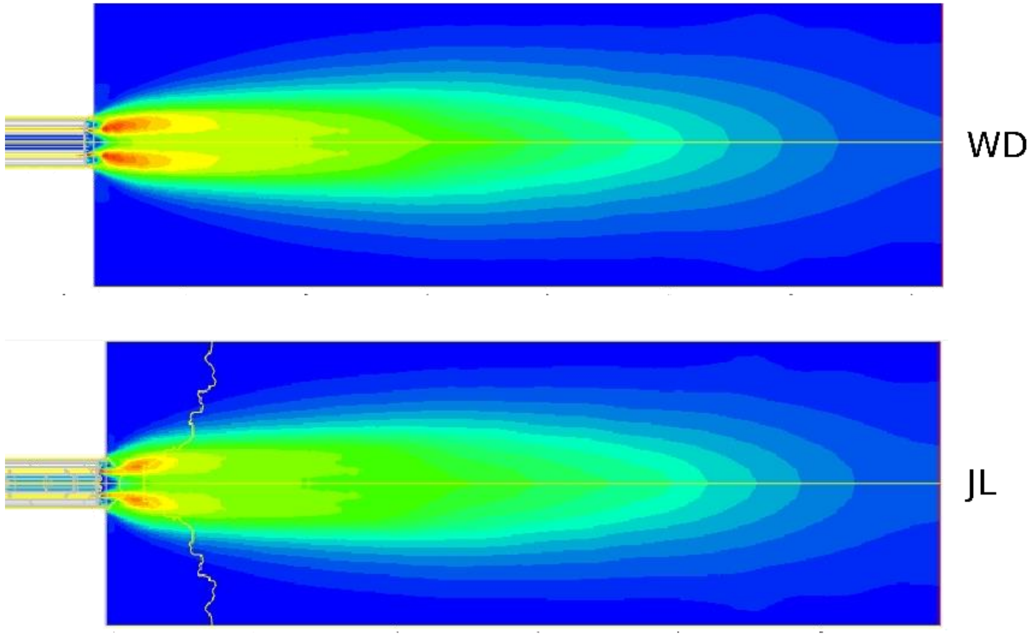


Reaction	Parameter	Original Value	Optimized Value
1	A	$4.4 \cdot 10^{9}$	$3.06 \cdot 10^{10}$
1	υ_{f,O_2}	1.25	1.30
2	A	$3.80 \cdot 10^{8}$	$3.84 \cdot 10^{9}$
3	A	$2.75 \cdot 10^{9}$	$2.01 \cdot 10^{9}$
4	A	$6.80 \cdot 10^{15}$	$8.03 \cdot 10^{16}$
4	υ_{f,H_2}	0.25	0.30
4	υ_{f,O_2}	1.50	1.55

Table 4. Modified Jones-Lindstedt mechanism for oxy-fuel combustion.

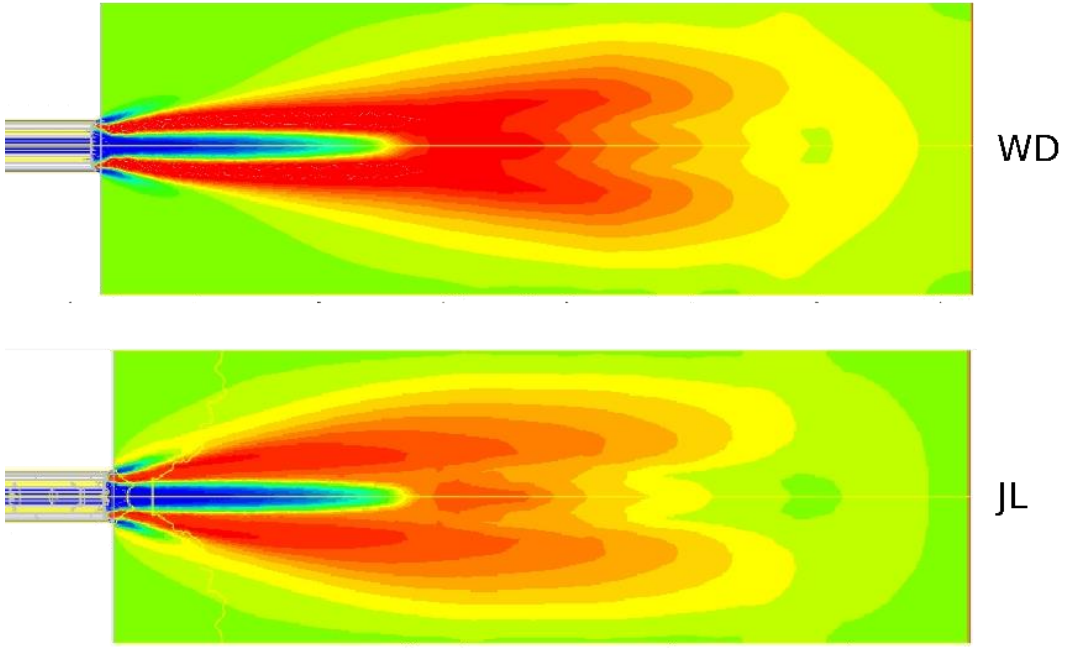
Kinetics comparison

Velocity



No big differences in Velocity field.

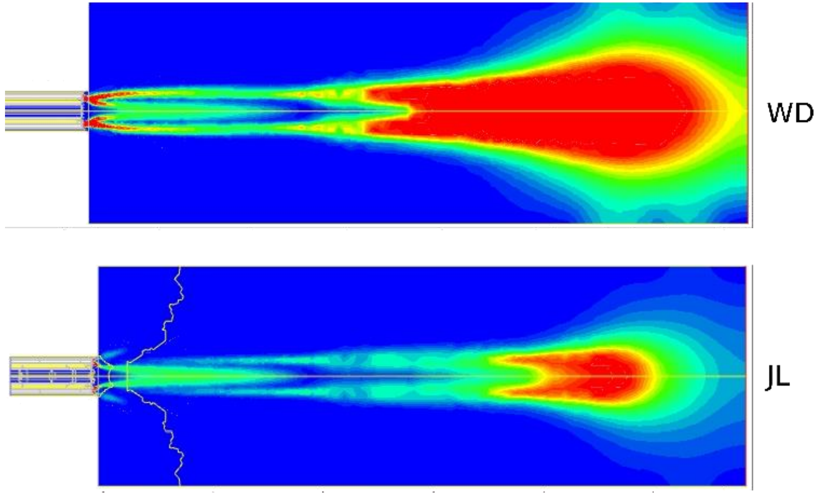
Temperature



High T zone is larger in WD simulation, because it underestimate CO production and overestimate total combustion of CH_4 to CO_2.

Kinetics comparison

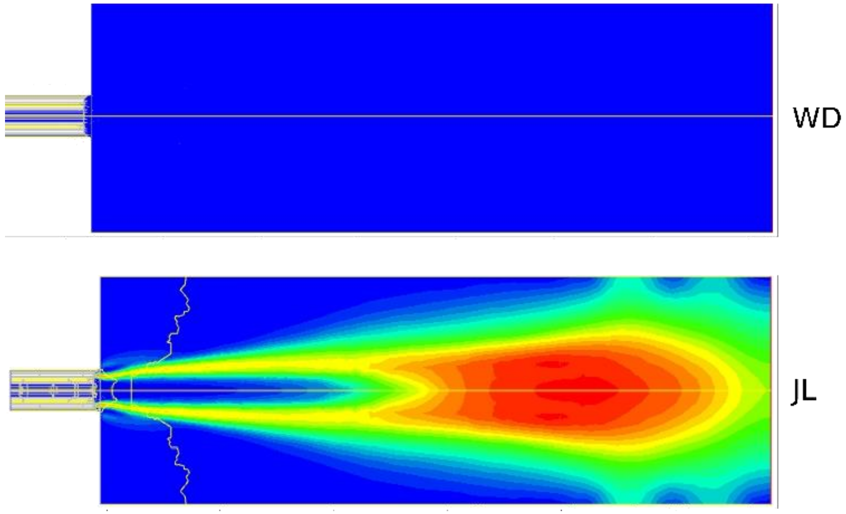
CH_4



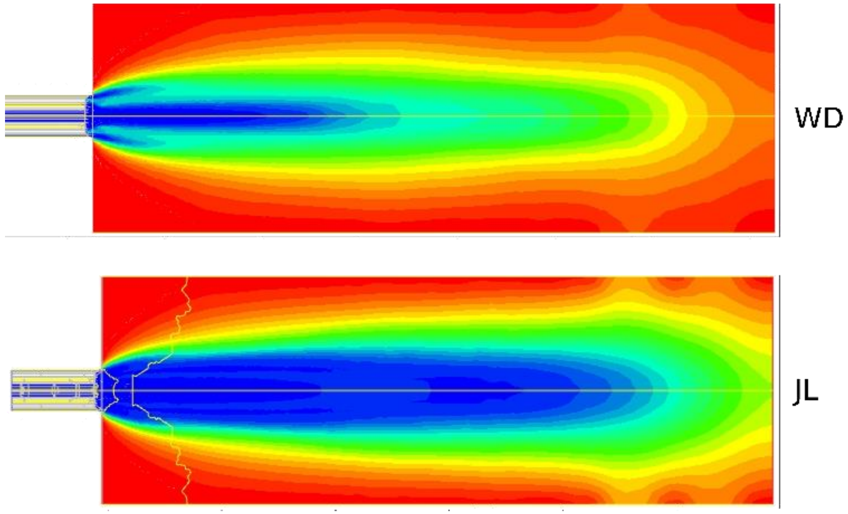
For WD scheme: underestimate of CO and overestimate of CO_2.

CH_4 released as volatile species in these preliminary simulations

CO

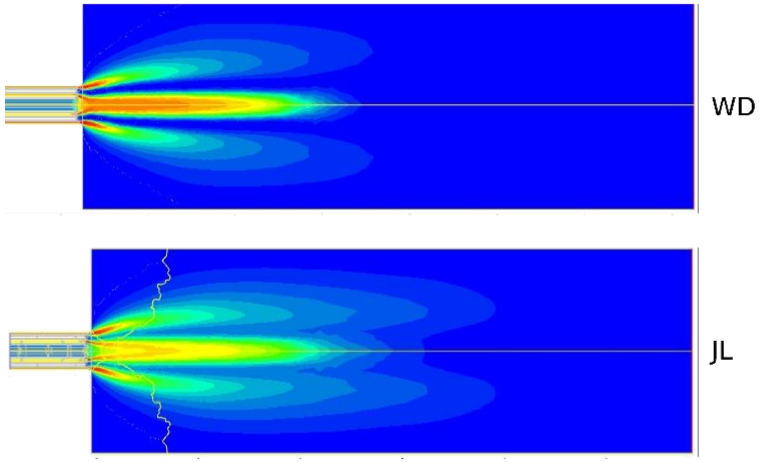


CO_2



Kinetics comparison

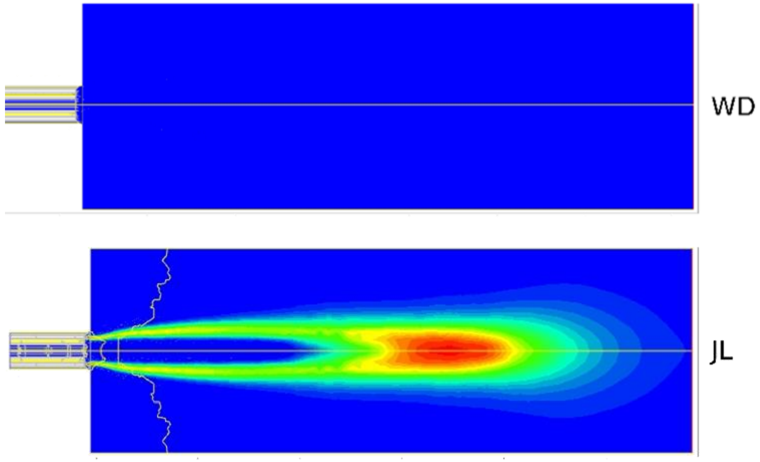
O_2



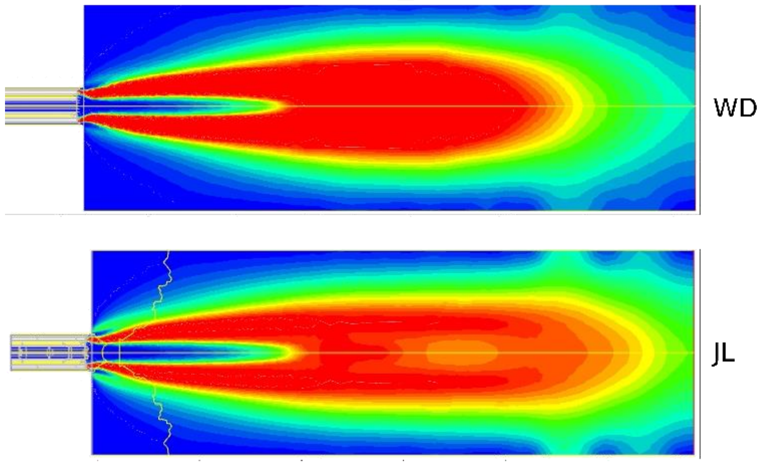
For WD scheme: H_2 is not considered.

For JL scheme: combustion of H_2 is considered

H_2



H_2O



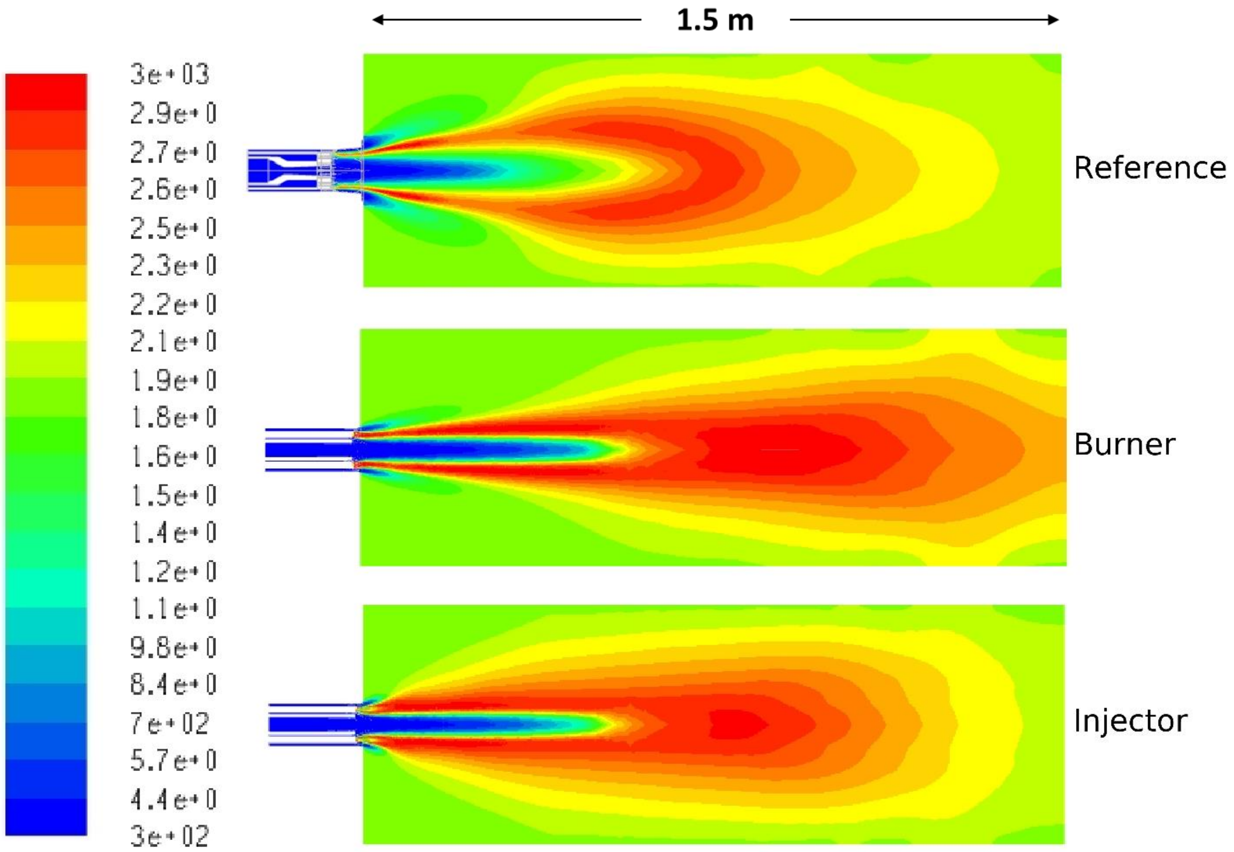
Burner & Injector Mode Simulation issues

- ✓ **Reference mode** was simulated using Jones-Lindstedt mechanism (dissociation reactions (JL-R) and optimized parameters) and eddy dissipation/finite rate (ED/FR) for turbolence – chemistry coupling

- ✓ **Burner mode** was simulated using an empirical mechanism and Eddy Dissipation Concept (EDC) for turbolence – chemistry coupling

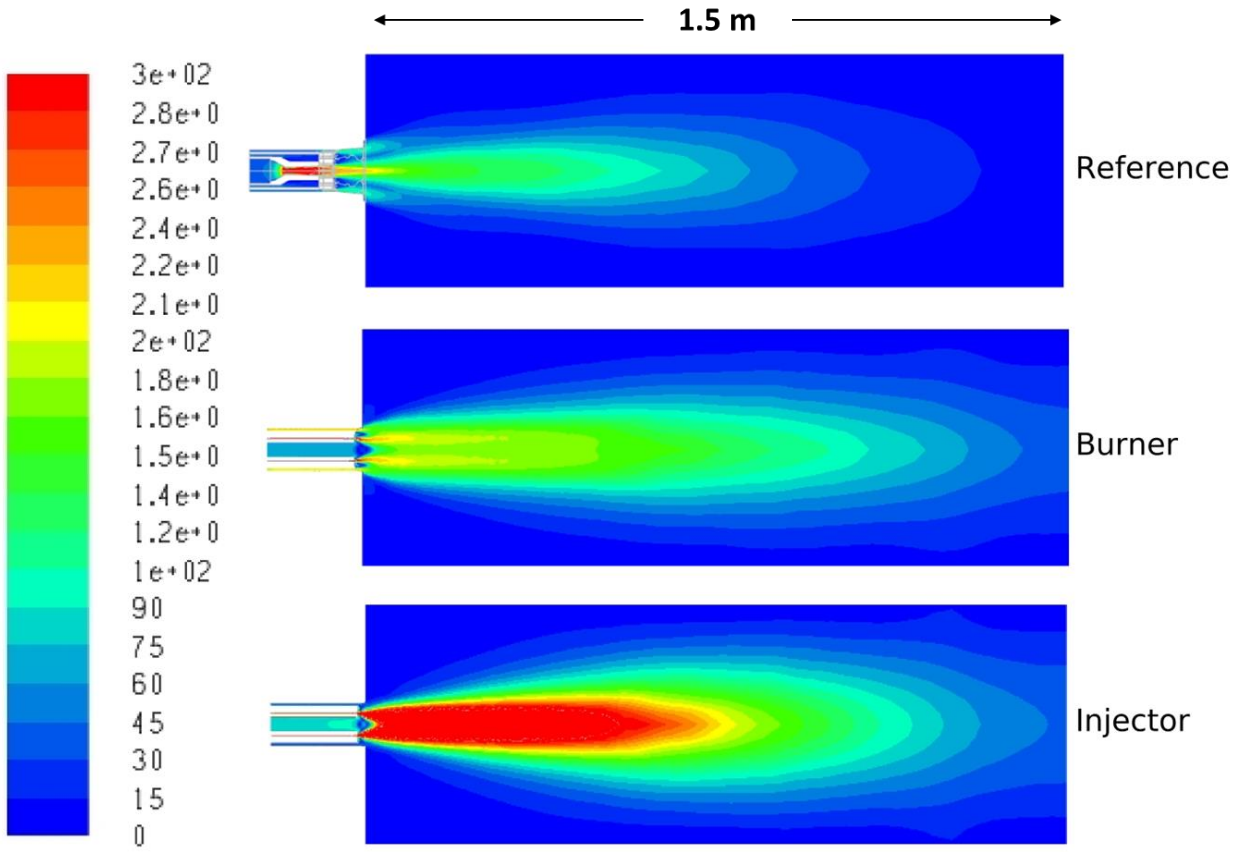
- ✓ **Injector mode** was simulated using an empirical mechanism and Eddy Dissipation Concept (EDC) for turbolence – chemistry coupling

Results - Temperature Field [K]



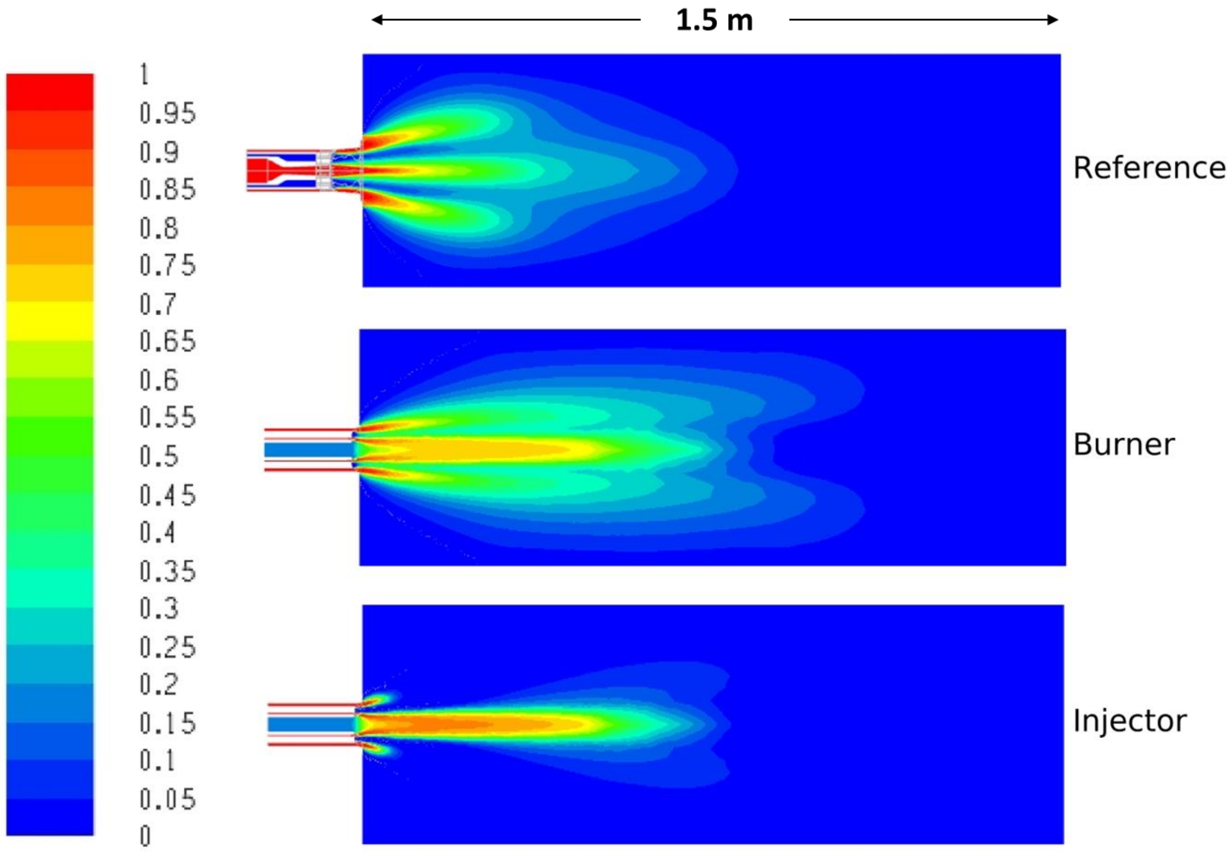
Using plastic particles enlarge the high temperature zones

Results - Velocity [m/s]



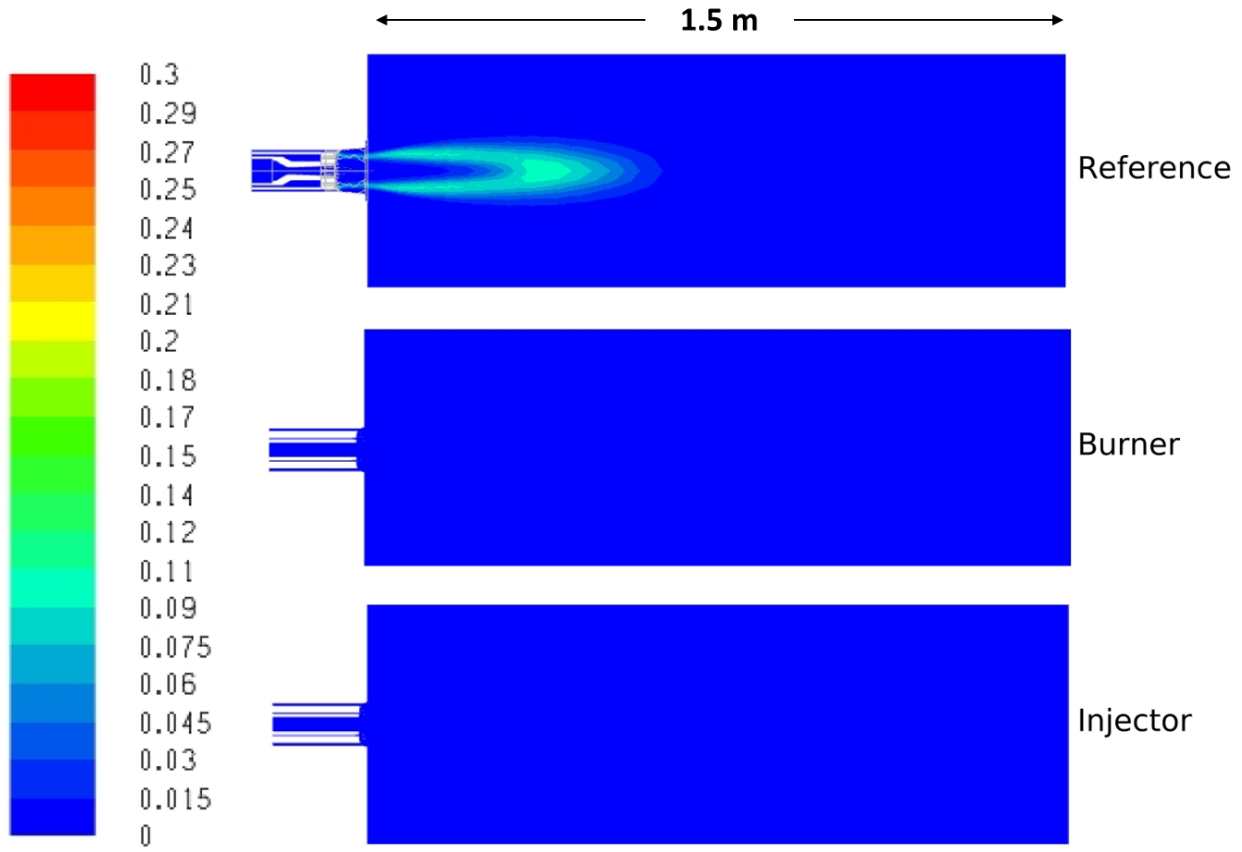
Using plastic particles enlarge the high velocity zones.
Especially in the Injector mode

Results - O_2 [vol/vol]



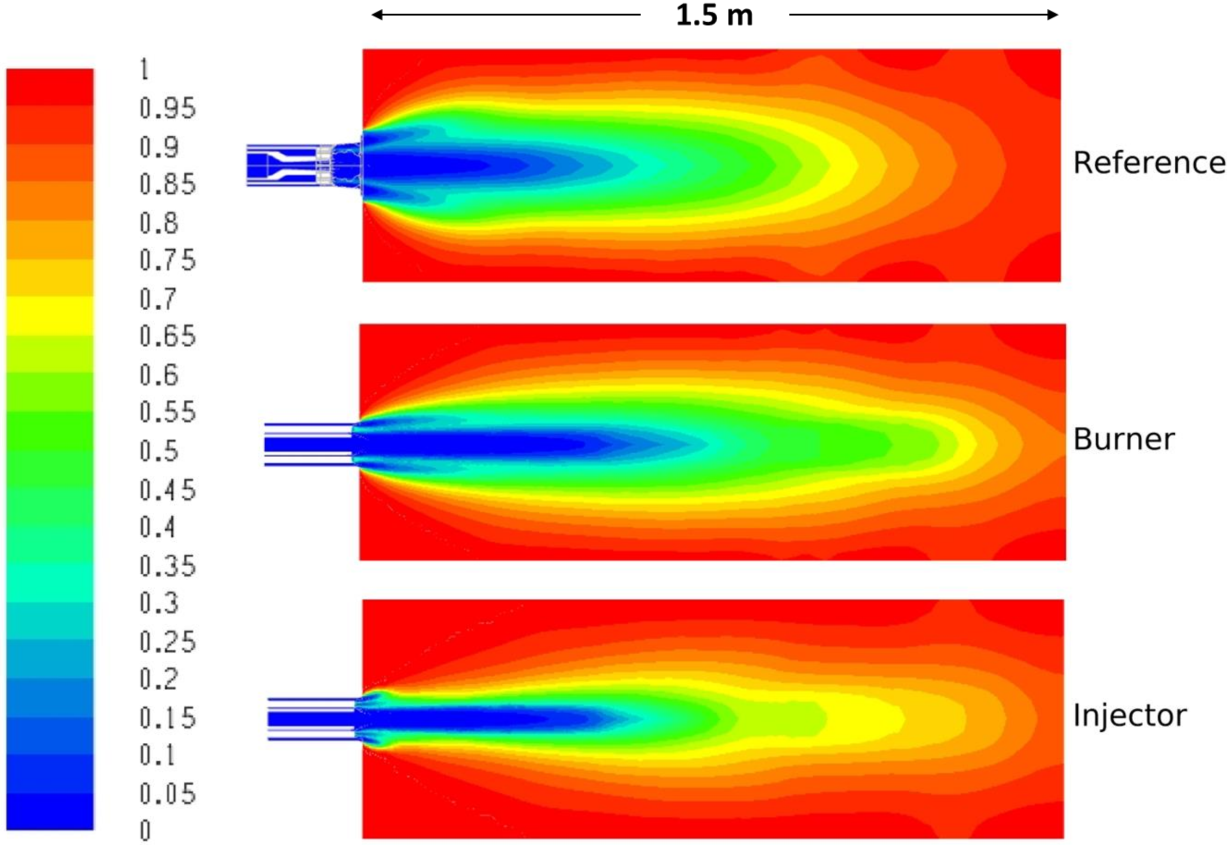
O_2 consumption are comparable among all cases

Results - CO [vol/vol]



Injector and Burner mode were simulated using a W-based mechanism and CO formation is underestimated

Results - CO$_2$ [vol/vol]



CO$_2$ results are the same for all cases.
(Flame is placed in a 100% CO$_2$ environment)

Conclusion

Preliminary CFD simulation pointed out plastic as combustible able to obtain flames similar to methane

Next step:
Plant trial

dissHEAT

RINA