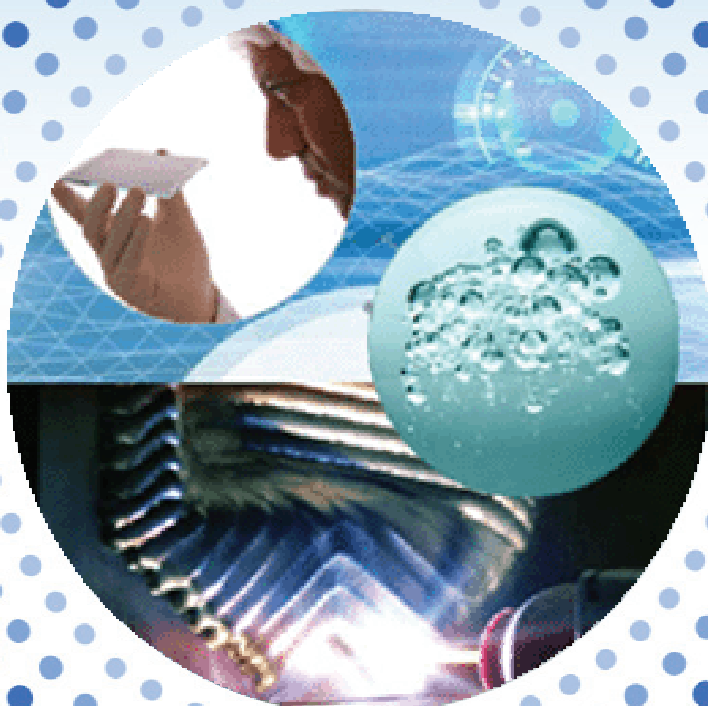
On-going developments in Code_Saturne® for modelling oxycombustion processes



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Saturne User’s Club

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Outline

- Combustion and energy supply

- Fossil fuels and oxycombustion

- Requirements for oxyfiring vs. air firing

- Adapting Code_Saturne® to oxy-combustion

- First tests of the combustion model (axisymmetrical pulverised coal jet flame)

- Conclusions and future work

Combustion

- **Combustion** is a "complex sequence of exothermic chemical reactions between a fuel and an oxidant accompanied by the production of heat or both heat and light".

- In the large majority of the real world uses of combustion, the oxygen (O_2) oxidant is obtained from the ambient air and the resultant flue gas from the combustion will contain nitrogen:

Methane combustion : $CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2$ + heat

-As can be seen, when air is the source of the oxygen, nitrogen is by far the largest part of the resultant flue gas.

Combustion

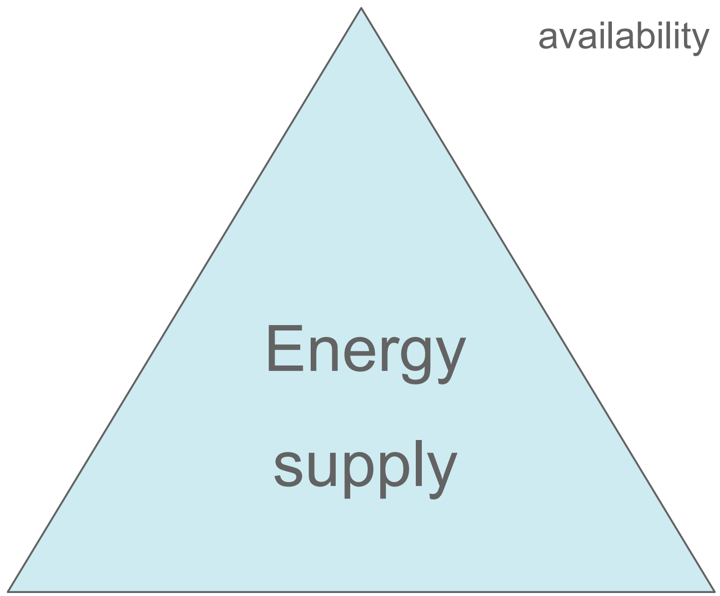
- In reality, combustion processes are never perfect or complete. In flue gases from combustion of carbon (as in coal combustion) or carbon compounds (as in combustion of hydrocarbons, wood etc.) both unburned carbon (as **soot**) and carbon compounds (**CO** and others) will be present. Also, when air is the oxidant, some nitrogen can be oxidized to various nitrogen oxides (**NO_x**). Sulphur and nitrogen are present in coal and can be oxidized to various oxides (**NO_x**, **SO_x**).

$$\text{coal} + \text{air} \rightarrow \text{carbon dioxide} + \text{water vapour} + NO_x + SO_x + \text{soot} + CO + \text{ash}$$

Energy supply

security of energy supply

availability (long and short term)



competitiveness

Not only costs but also related to its degree of supply security and environmental adavantage

environmental acceptability

Regarding all stages (from production through transportation to utilization)

Combustion of fossil fuels

- security of energy supply
- competitiveness
- environmental acceptability

Emissions :

particulates → respiratory health

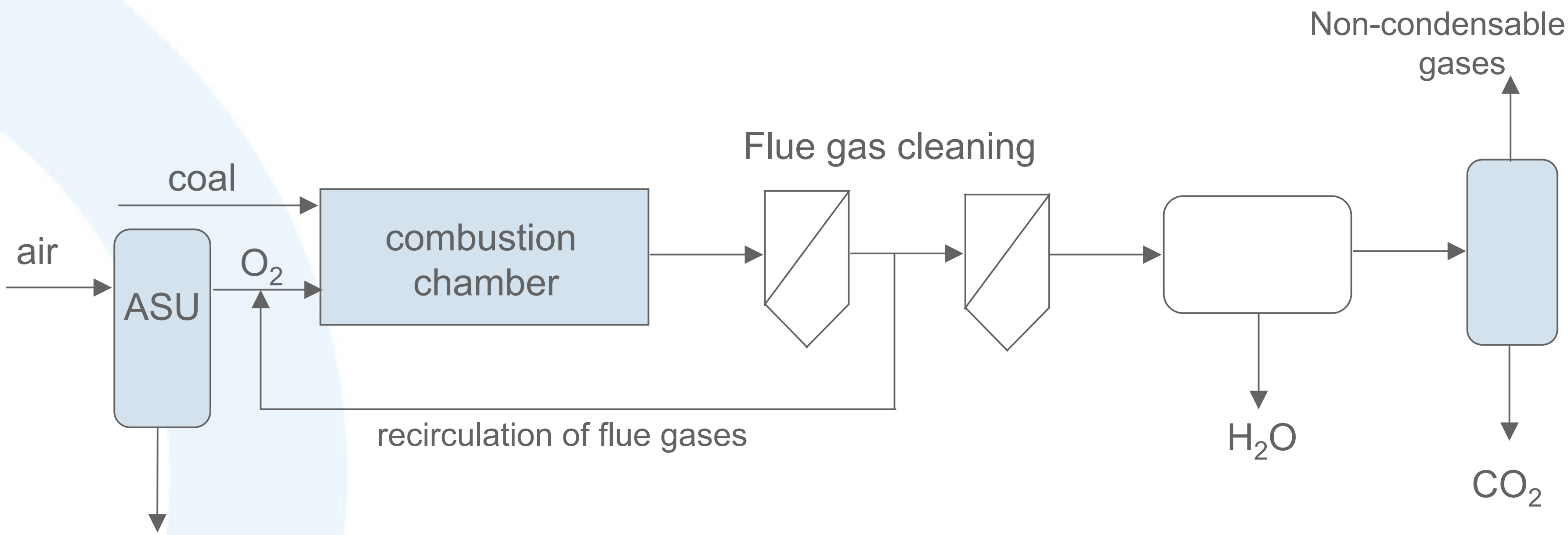
NO_x, SO_2 → acid rain

CO_2 → greenhouse effect

CO_2 capture and storage (CCS)

- Precombustion
    - Air separation
    - Gasification
- Postcombustion
    - CO_2 capture from flue gases (CO_2 absorbents)
- Oxycombustion
    - Air separation
    - Combustion with pure oxygen

A *clever* environmental solution : Oxycombustion



- Almost no emission to the atmosphere (Particulates, NO_x, SO_x, CO_2)

Context and motivations

-In the frame of CO_2 capture technologies EDF favours oxycombustion as the most promising option for coal power plants in the mid-term perspective

- CFD simulations is an important tool for the optimisation and better design of a boiler. Code_Saturne® is EDF's Open Source CFD solution for 3D fluid dynamics and combustion calculations.

Introduction

Requirements for oxyfiring vs. air firing

- Different flue gases atmosphere: **higher CO_2 and H_2O concentrations**

- Radiative properties f(CO_2 , H_2O)
- Heat capacities: Cp_{CO2}, Cp_{H2O} > Cp_{N2}
- Chemical reactions:

Heterogeneous reactions:

$C_{(s)} + CO_2 \rightarrow 2CO$

$C_{(s)} + H_2O \rightarrow CO + H_2$

Homogeneous reactions:

$CO + H_2O \rightarrow CO_2 + H_2$

(Water-gas shift reaction)

$CO_2 \leftrightarrows CO + \frac{1}{2}O_2$

Introduction

Requirements for oxyfiring vs. air firing

- Devolatilization

  - Higher mass loss under CO_2 atmosphere rather than under N_2 atmosphere (DTF measurements)

- Char combustion

  - Heterogeneous reactions with CO_2 and water vapour:

$$C_{(s)} + CO_2 \rightarrow 2CO$$

Already implemented

$$C_{(s)} + H_2O \rightarrow CO + H_2$$

Future developments

-Flue gas recirculation

  - Increase in water vapour content
  - Flue gas mass flow rate

Adapting Code_Saturne® to oxy-combustion

- Enhancement of the algorithm for the kinetics to equilibrium in $CO_2 \leftrightarrows CO + ½O_2$ reaction

- Implementation of the heterogeneous oxidation of char by CO_2

- Possibility to deal with different oxidizers in the inlet conditions (air, oxygen, flue gases)

- Future developments :
    - Implementation of the heterogeneous reaction with water vapour
    - Evaluation of the assumptions between kinetic and diffusive limitations

Adapting Code_Saturne® to oxy-combustion

- Combustion models:

- Gas phase reactions:

$$CH_{X1} + O_2 \rightarrow CH_{X2} + H_2O$$ (low temperature devolatilization)

$$CH_{X2} + O_2 \rightarrow CO + H_2O$$ (high temperature devolatilization)

$$CO + \frac{1}{2}O_2 \leftrightarrows CO_2$$

-Heterogeneous reactions:

$$C_{(s)} + \frac{1}{2}O_2 \rightarrow CO$$

$$C_{(s)} + CO_2 \rightarrow 2CO$$

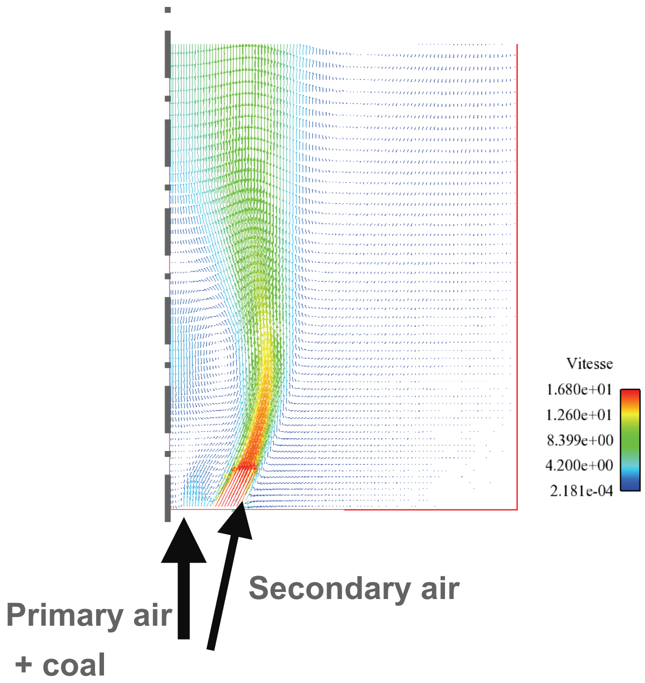
New features for oxy-combustion

First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- Simple geometry: a cylinder, which allows axisymmetrical treatment and therefore reduces to 2D case (15000 cells) for a 1,20 m long combustion chamber

- New reactions and kinetics in the combustion model have been tested for several configurations:

  - Air firing
  - Nitrogen replaced by CO_2 (same volumetric proportions as in air)
  - Nitrogen replaced by CO_2 (same mass proportions)
  - Oxy-combustion similar conditions (with recycled gases)



First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- New features in the combustion model where tested one-by-one in order to quantify the importance of both reactions.

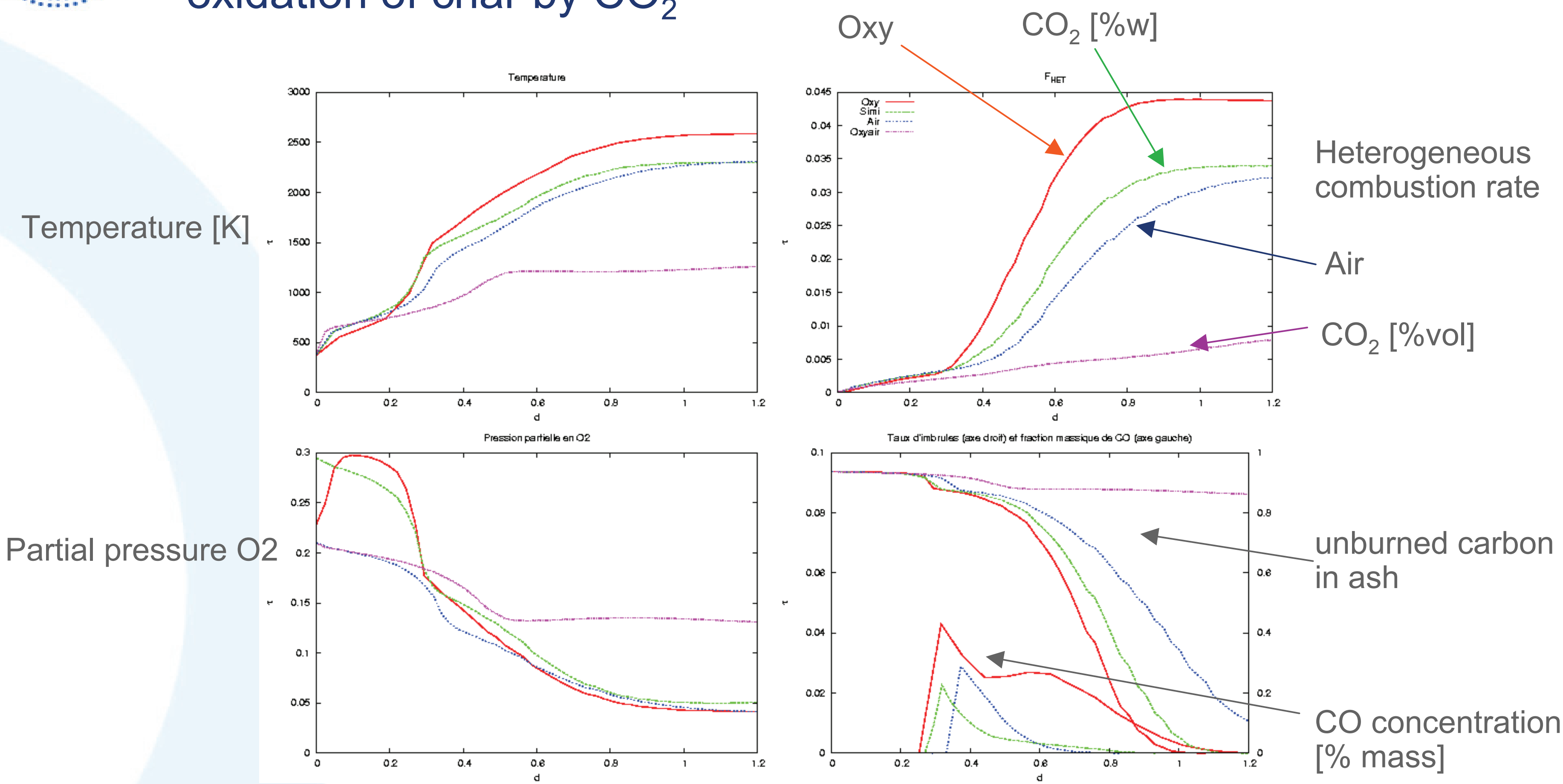
	$CO + 1/2O_2 \leftrightarrows CO_2$	$C_{(s)} + CO_2 \rightarrow 2CO$
Case A	instantaneous kinetics $\rightarrow$	not used
Case B	global kinetics $\leftrightarrows$	not used
Case C	global kinetics $\leftrightarrows$	taken into account

First tests of the combustion model in an axisymmetrical pulverised coal jet flame

- Inlet conditions for the 4 types of flame:

	Air	CO2 [%w]	CO2 [%vol]	Oxy
Primary oxidant	Air	O_2+2,39 CO_2	O_2+3,76 CO_2	O_2+0,3N_2+0,7H_2O+2,4CO_2
Secondary oxidant	Air	O_2+2,39 CO_2	O_2+3,76 CO_2	O_2+0,2N_2+0,5H_2O+1,2CO_2
Primary mass flow [kg/s]	1,9E-3	1,9E-3	1,9E-3	1,9E-3
Secondary mass flow [kg/s]	9,3E-3	9,3E-3	1,05E-2	6,7E-3
Coal mass flow [kg/s]	9,0E-4	9,0E-4	9,0E-4	9,0E-4

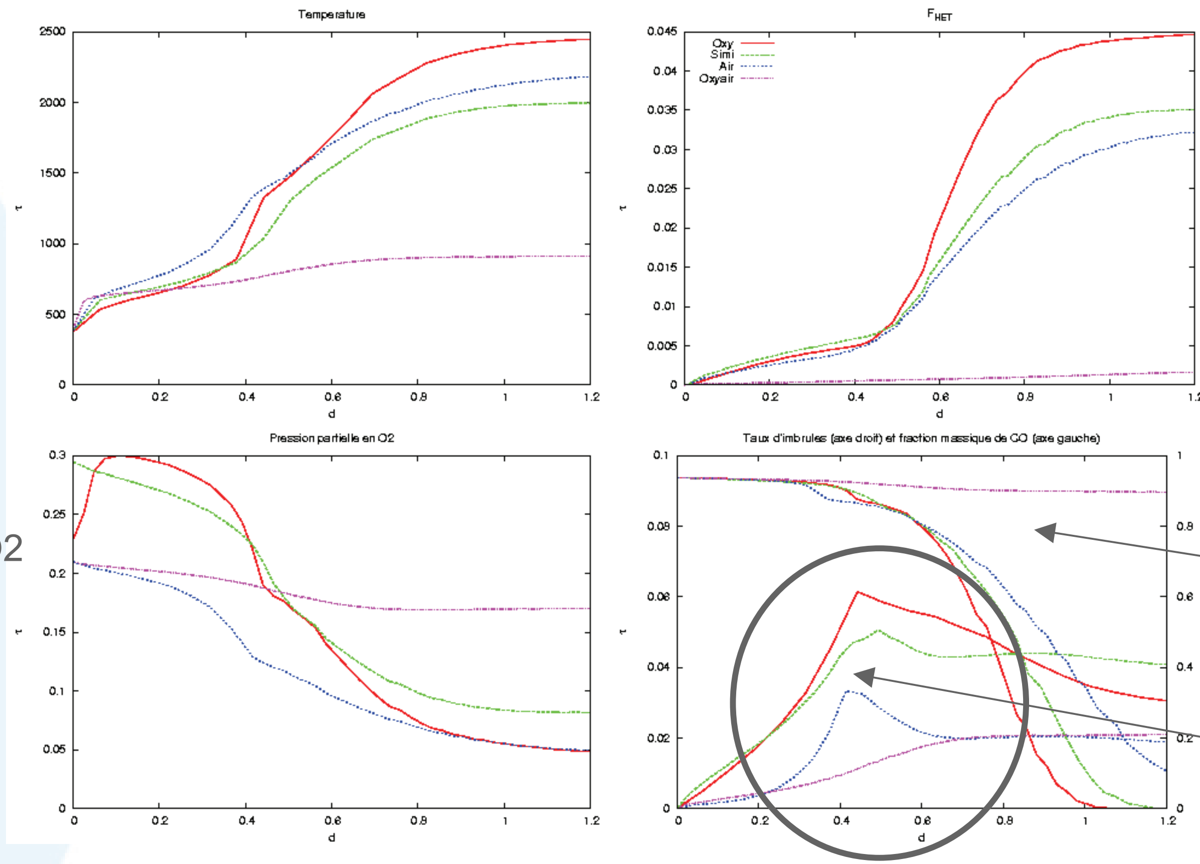
Case A : Instantaneous kinetics for CO/CO_2 and without oxidation of char by CO_2



Case B : Global kinetics for CO/CO_2 and without oxidation of char by CO_2

Temperature [K]

Partial pressure O2



Heterogeneous combustion rate

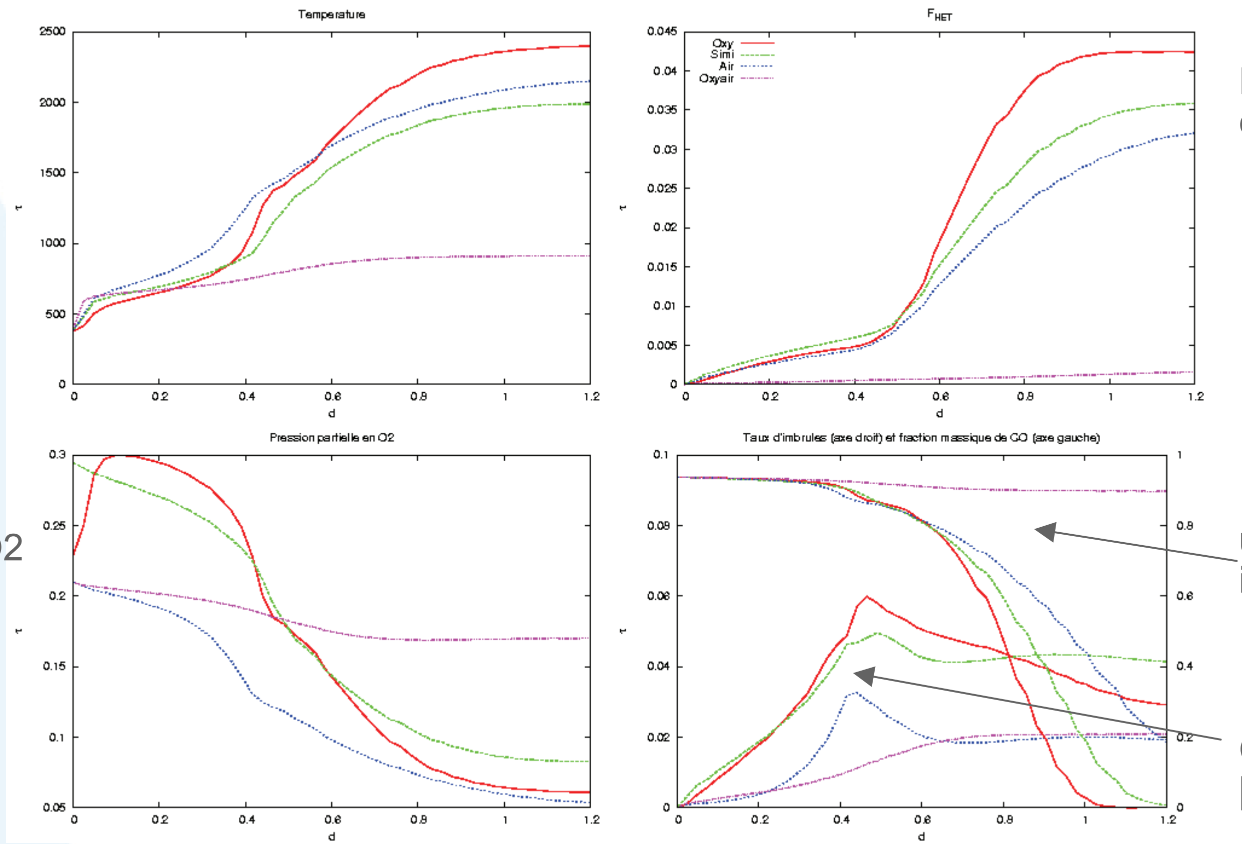
unburned carbon in ash

CO concentration [% mass]

Case C : Global kinetics for CO/CO_2 and taking into account the oxidation of char by CO_2

Temperature [K]

Partial pressure O2



Heterogeneous combustion rate

unburned carbon in ash

CO concentration [% mass]

Conclusions :

- First developments in the combustion model for Code_Saturne® have been successfully adapted in order to model oxy-combustion processes.

- Several flames have been used to test the different models one-by-one.

- A very different combustion behaviour has been observed when air is no more the diluting gas. CO_2 (vol.) leads to incomplete combustion because of the high dilution and decrease of temperature. Nevertheless combustion in CO_2 (mass) atmosphere is more efficient than air firing. Finally, under oxy-combustion conditions, the quantity of diluted gases being definitely lower, combustion is more effective than in the case of combustion in air.

- Taking into account or not the kinetics of CO oxidation seems to have more influence on the results than the heterogeneous reaction of CO_2 and char. However, the kinetics used here do not correspond to any real case of combustion of a specific coal. It will be advisable to get realistic values for this kinetics from experiments in Drop Tube Furnaces.

Future Work :

- Due to the high water vapour content in recycled flue gases in oxy-combustion processes, the heterogeneous gasification of char by water vapour should be studied:

  $C_{(s)} + H_2O \rightarrow H_2 + CO$

- Regarding combustion regimes, due to the fact that all different reactants (O_2, H_2O and CO_2) not have the same reactivity towards carbon in the char, the assumption of similar regime (bulk-surface diffusion, pore diffusion or reaction control) could be not correct.

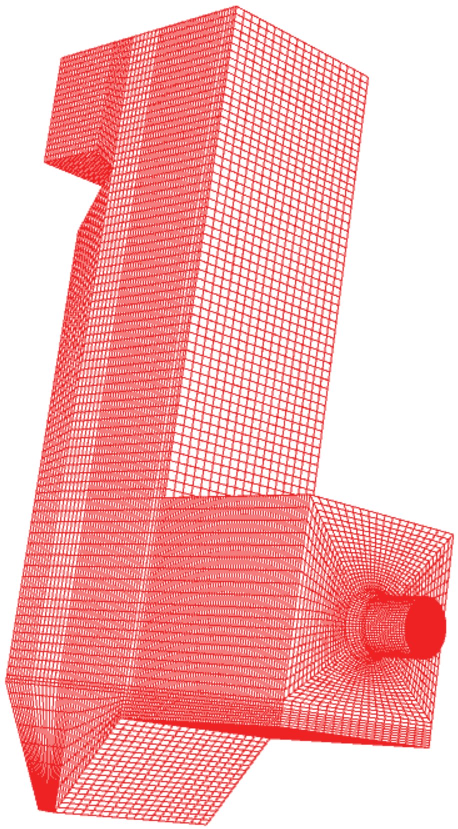
- It is likely that high temperature gasification with H_2O or CO_2 is kinetically controlled, or in the transition region, while the O_2 reaction with carbon is in the diffusion-controlled regime at the same temperature.

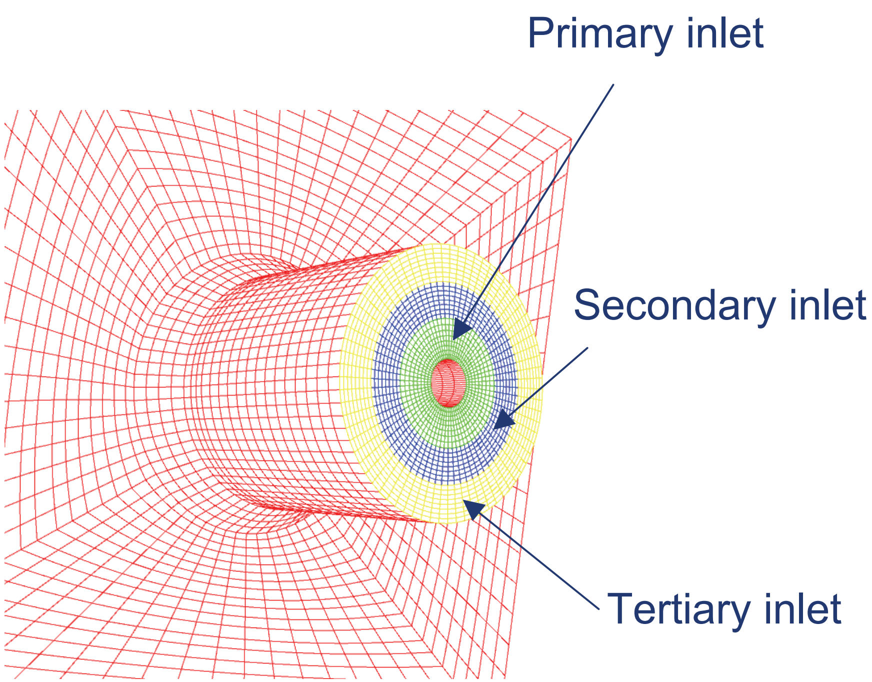
- For the purpose of model validation we take part in projects involving oxifiring facilities (Oxycoal, IFRF)

Practical example :
Modelling the E.ON UK's 1 MWth CTF with Code_Saturne®

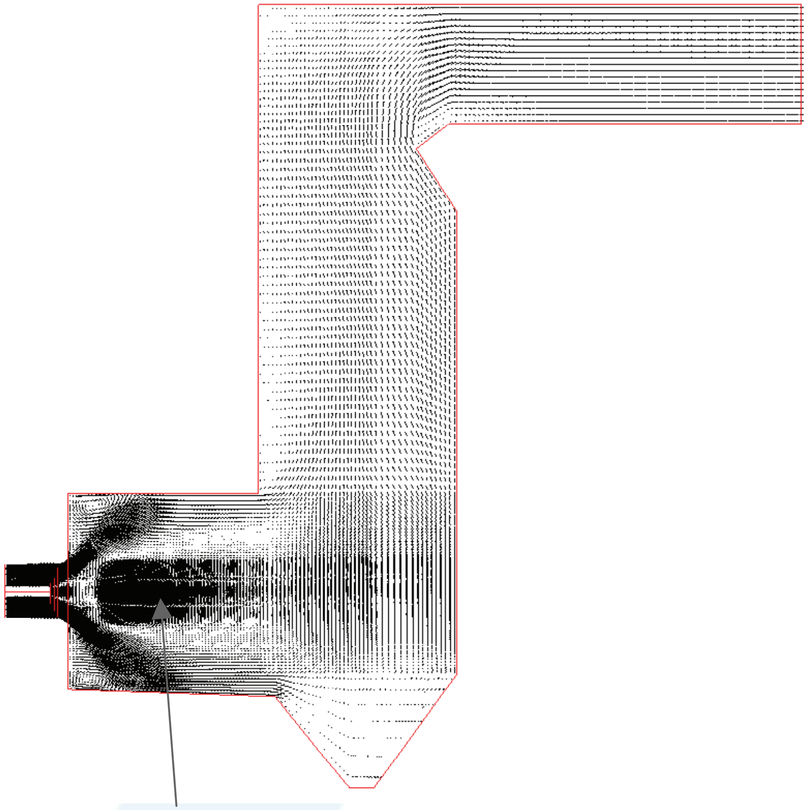
- Calculations made in frame of the british project *Oxycoal*

- 500 000 cells

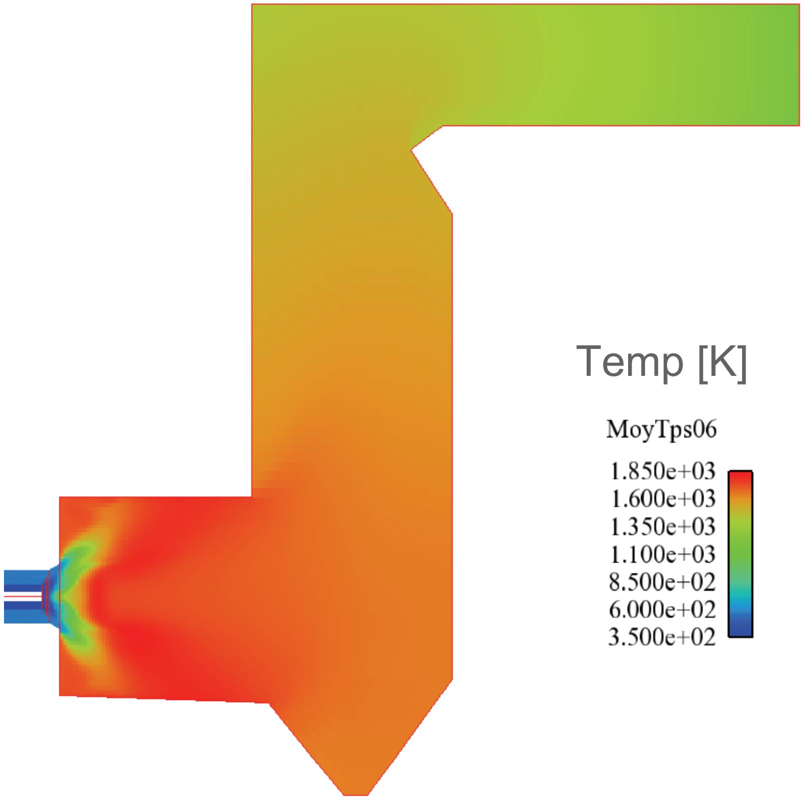




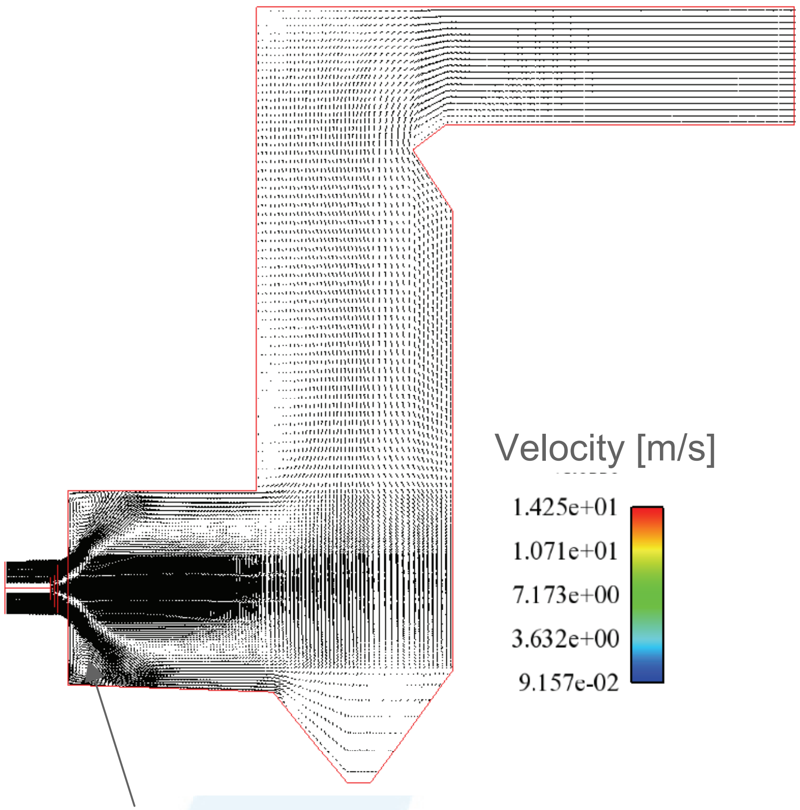
Velocity and temperature in middle plane (air firing)



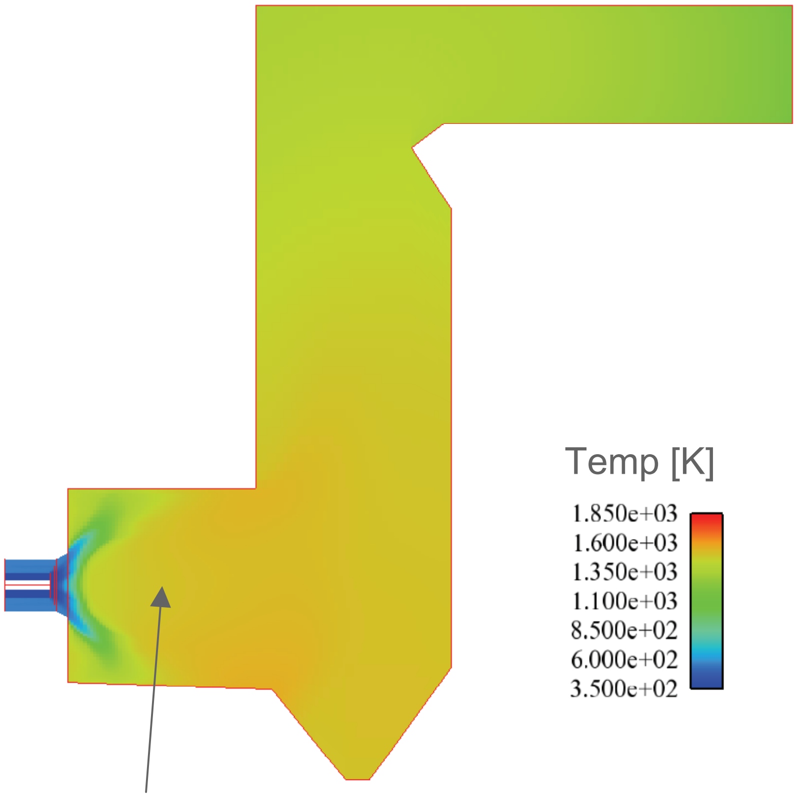
Large internal recirculation zone



Velocity and temperature in middle plane (oxy firing)



Smaller external recirculation zones



Lower temperature and flame shifted