EUROMECH COLLOQUIUM 513:

Dynamics of non-spherical particles in fluid turbulence

Università degli Studi di Udine

Numerical Modeling of Char Particles Segregation in Entrained-Flow Slagging Gasifiers

Fiorenzo Ambrosino[1,4], *Andrea Aprovitola*[2],

Francesco Saverio Marra[2],

Fabio Montagnaro[3], *Piero Salatino*[4]

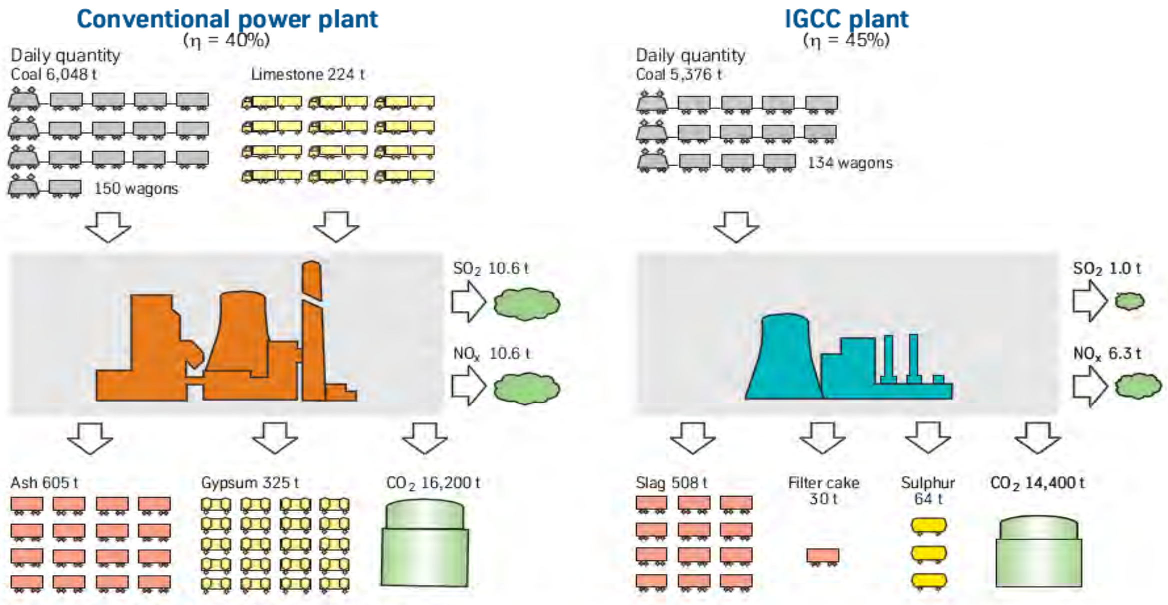
1. **ENEA** - Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile, CR Portici, Piazzale Enrico Fermi 1, 80055 Portici (Italy)
2. **Istituto di Ricerche sulla Combustione**, Consiglio Nazionale delle Ricerche, Via Diocleziano 328, 80124 Napoli (Italy)
3. **Dipartimento di Chimica**, Università degli Studi di Napoli Federico II, Complesso Universitario del Monte di Sant’Angelo, 80126 Napoli (Italy)
4. **Dipartimento di Ingegneria Chimica**, Università degli Studi di Napoli *Federico II*, Piazzale Vincenzo Tecchio 80, 80125 Napoli (Italy)

ISTITUTO DI RICERCHE SULLA COMBUSTIONE

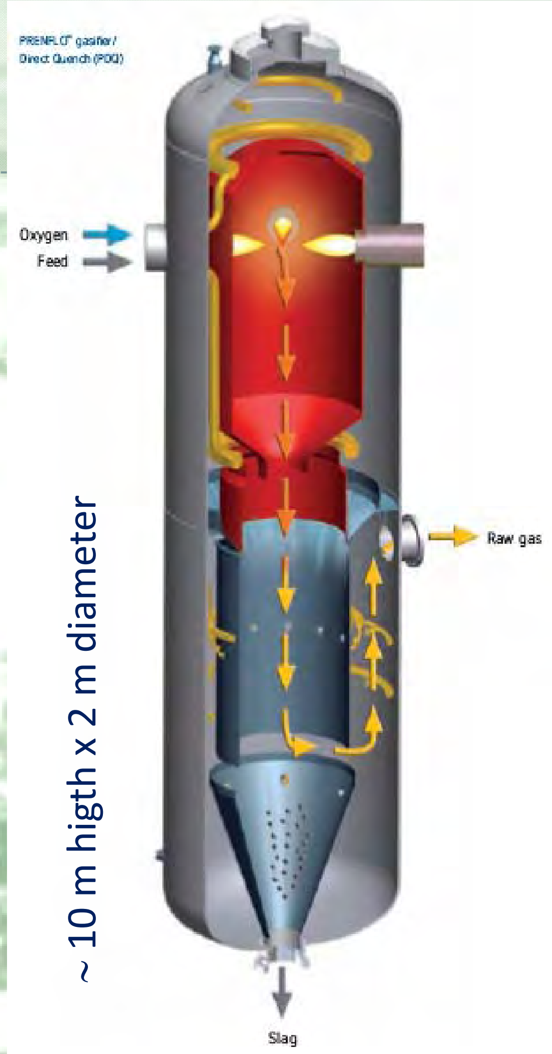
CONSIGLIO NAZIONALE DELLE RICERCHE

Coal Gasification

- Coal is widely adopted worldwide and does not will last for at least two centuries.
- Need to adopt new combustion technologies to lower environmental impact and raise efficiency: oxy-fuel combustion.
- IGCC power plants are flexible and prone to CCS.



Basis: Coal with 73% C, 1.2% S, 10% ash, LHV 25 MJ/kg



- Feeding pulverized coal and oxygen, very pure syngas ($H2 + CO$) is produced.
- Impurities are mainly collected in the slag forming at the confining walls due to the deposition of particles driven by a swirled turbulent flow.
- Factors affecting efficiency are very difficult to control.

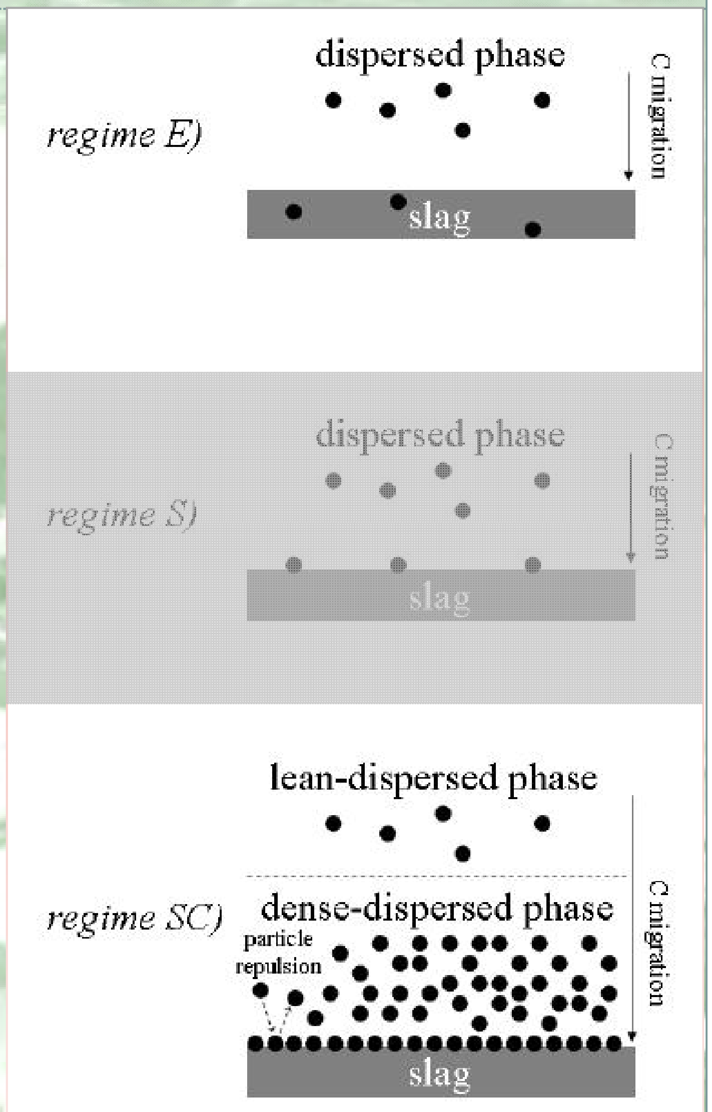
Char-Wall interaction

Swirled flow aid to eliminate impurities (ash) but also migrate unburnt coal particles (char) towards the wall.

A simple 1D model has highligthed that a very high migration of particles towards the walls occurs.

Mechanisms of particle-wall interaction can be very complex and are affected by the regime of particle accumulation *[Montagnaro e Salatino, 2010]:*

- **E)** ***Entrapment***
  not desidered for combustion efficiency
- **S)** ***Segregation***
  not likely
- **SC)** ***Segregation and coverage***
  likely and desired: long residence time



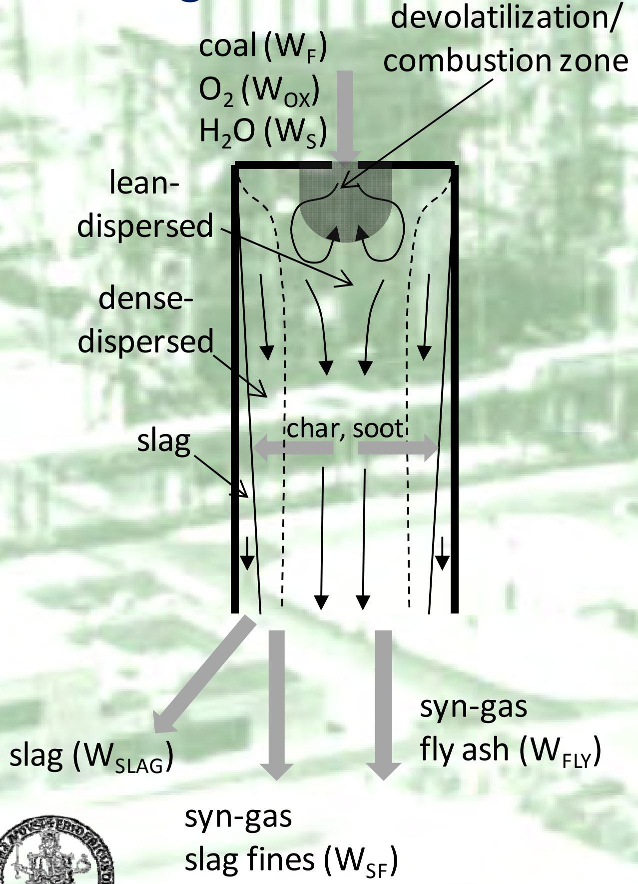
Is regime E or SC that occurs in a gasifier ?

Experimental Evidence

Two streams of slag collected in the Puertollano gasifier (Spain):

1. Slag
2. Slag fines

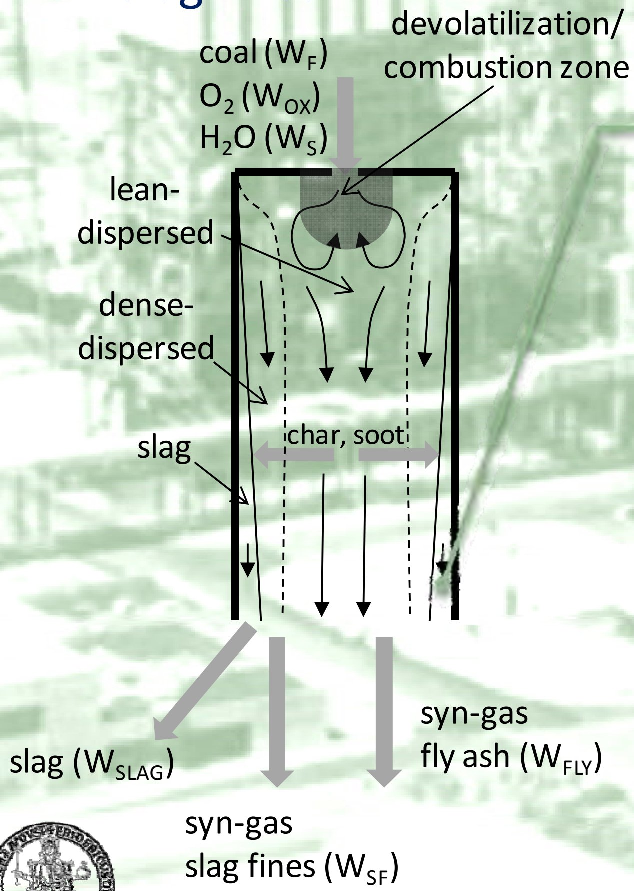
At a first look, elemental analysis on slag did not highlight the presence of carbon

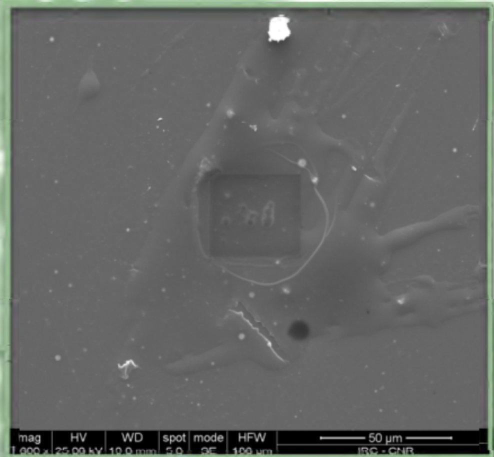


Experimental Evidence

Two streams of slag collected in the Puertollano gasifier (Spain):

1. Slag
2. Slag fines





SEM micrographs for the **cross-sections** of: a selected zones of slag particles magnfication=1600×).

Different results were obtained by SEM-EDX of Slag:

- Inorganic fraction (Si – Al): 47.5%
- Carbon: 9.3% (in segregated form: carbon content in the darker region as high as about 50 %).

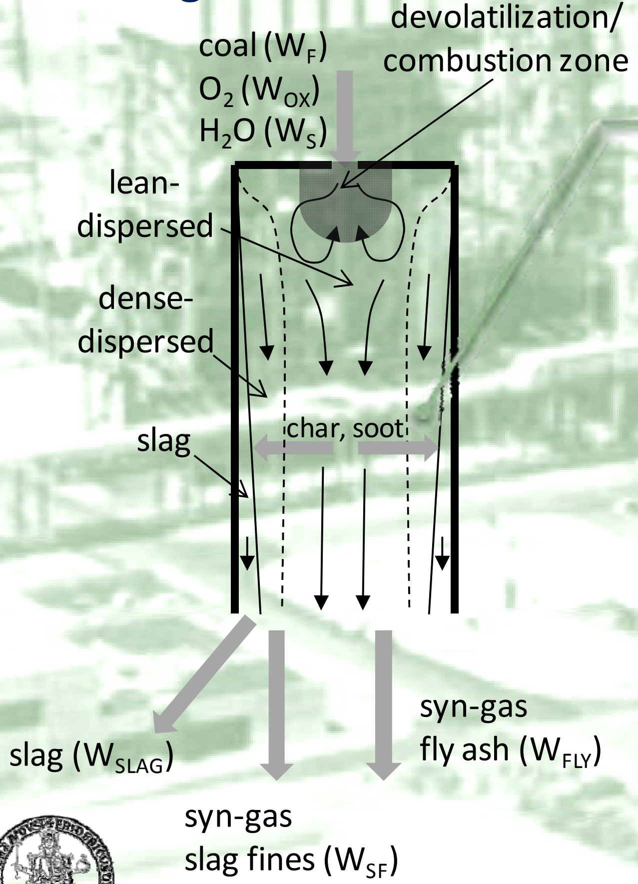
Relevance of carbon entrapment into the slag fraction

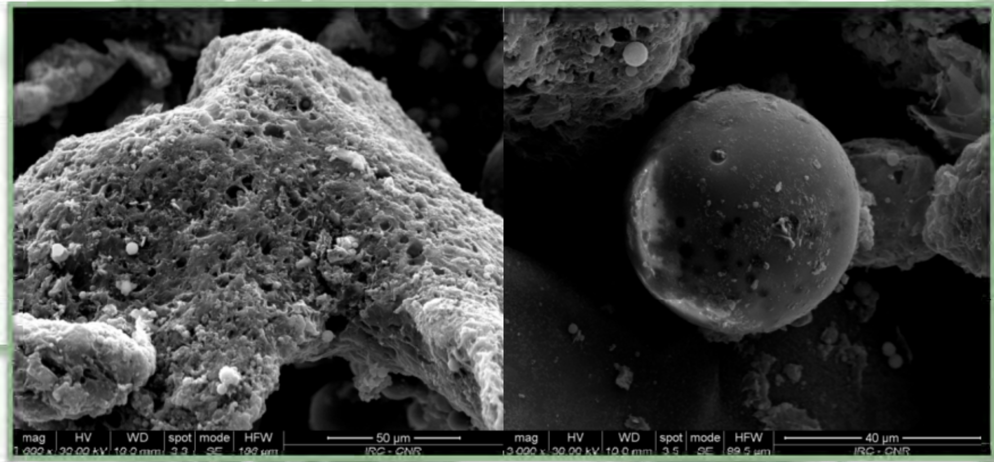
ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Experimental Evidence

Two streams of slag collected in the Puertollano gasifier (Spain):

1. Slag
2. Slag fines





SEM micrographs for different whole slag fines particles: left porous (magnification=1600×); right dense (magnfication=3000×).

Results obtained by SEM-EDX of slag fines particles:

- Porous (left) or compact (right) structure
- Porous particles: Carbon 85% (unreacted char)
- Dense particles: Carbon 15 % - Si+Al 34 % (intermediate properties between porous slag fines and coarse slag)
- Particle size ~ 100 μm - Particle density ~ 1000 kg/m^3

Relevance of the establishment of a dense-dispersed phase

Numerical Simulation – aim and scope

Existing numerical codes implement comprehensive models of the gasifier for design purposes. Mostly based on Euler RANS for the gas phase and DEM for the solid phase .
Correlations are adopted to predict coal pyrolisis, char devolatilization, volatiles combustion and particle deposition rates on the wall.

All the closures are based on empirical models.

Existing models of particle deposition rates take into account only the possibility of a **sticky/non sticky impact**, that leads to the establishment of a disperse-entrapment regime, making impossible to predict the devolatilization in the dense segregated region characterized by long residence times.

Scope of this study is to develop a model for the ***prediction*** *of the mechanism leading to the occurrence of the segregation and coverage regime.*

Detailed simulations (LES-LPT) of the particle laden flow are too CPU demanding at the full size of the gasifier. Therefore a multilevel approach is proposed to identify computationally practicable configurations able to represent the actual particle-wall interaction into a gasifier.

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulation – multilevel approach

Level 0

1 D model help to establish order of magnitude of particle deposition rates and physical characteristics (size and density) of particles that reach the wall.

Level 1

URANS model of the full gasifier at proper particle load helps to identify characteristic regions of the near wall zones where the behaviour of particle – wall interaction shows clearly identifiable features.

Level 2

Detailed Large Eddy Simulations of a very simplified models, where the previously identified features can be reproduced, are adopted to conduct parametric investigation and identify the driving mechanisms of particle-slag interaction.

This study is at an initial stage: only preliminary results are shown, relevant to cases chosen mostly for proper validation.

Numerical Simulation – Software platform

OpenFOAM
The Open Source CFD Toolbox

- Open Source CFD libraries and codes
- Based on the Finite Volume method for the gas phase
- Written in Object Oriented C++
- Parallel by MPI standard
- A wide network of developers is establishing worldwide, especially in the academic community

Lagrangian Particle Tracking provided by the **SolidParticleCloud class**

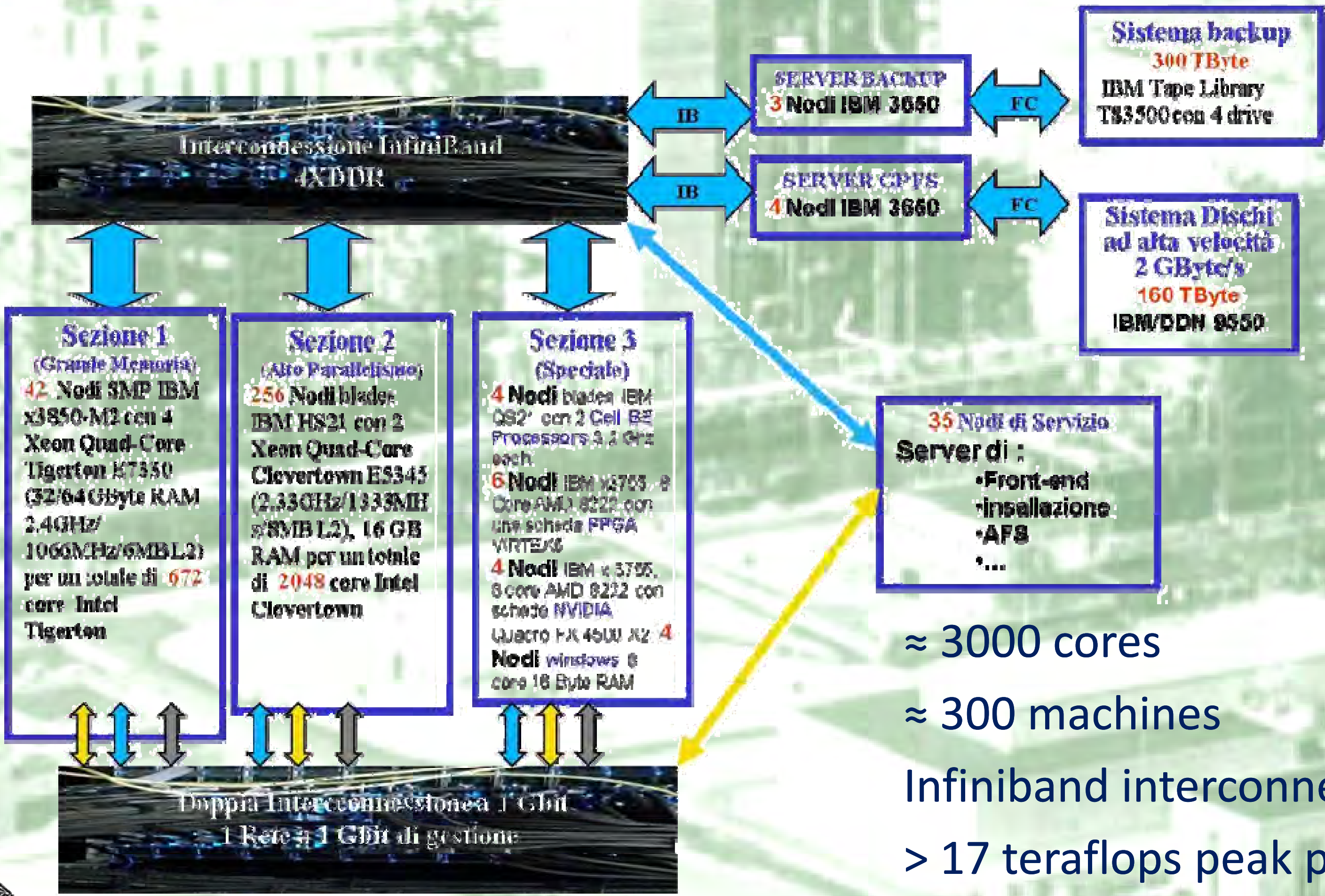
- 1 way coupling
- Forces: drag, weight and bouyancy
- Simple particle-wall interaction

Needs to be further developed !

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulation – Hardware platform

ENEA-CRESCO High Performance Computing Centre



≈ 3000 cores

≈ 300 machines

Infiniband interconnection

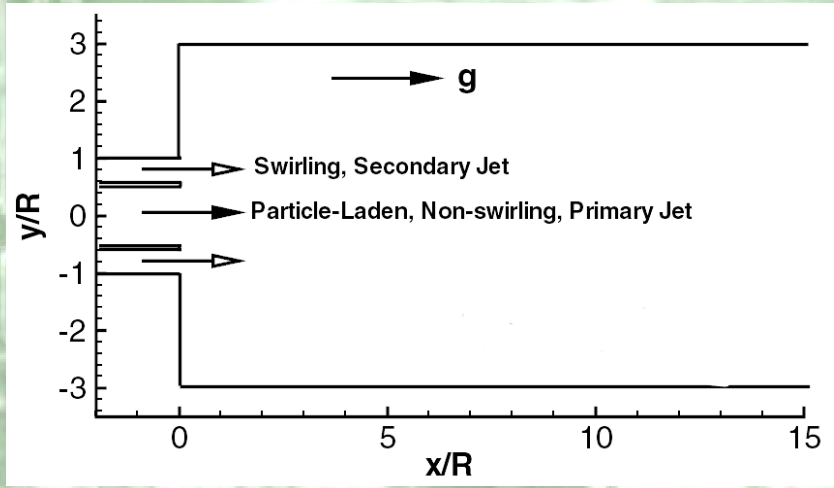
> 17 teraflops peak performance

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulation – URANS of the gasifier

Gasifier prototype: Sommerfeld and Qiu
[Sommerfeld e Qiu, 1993]

- *Provides a good data set of experimental results useful for validation*
- *Validation data also available from detailed LES simulation [Apte et al., 2003]*



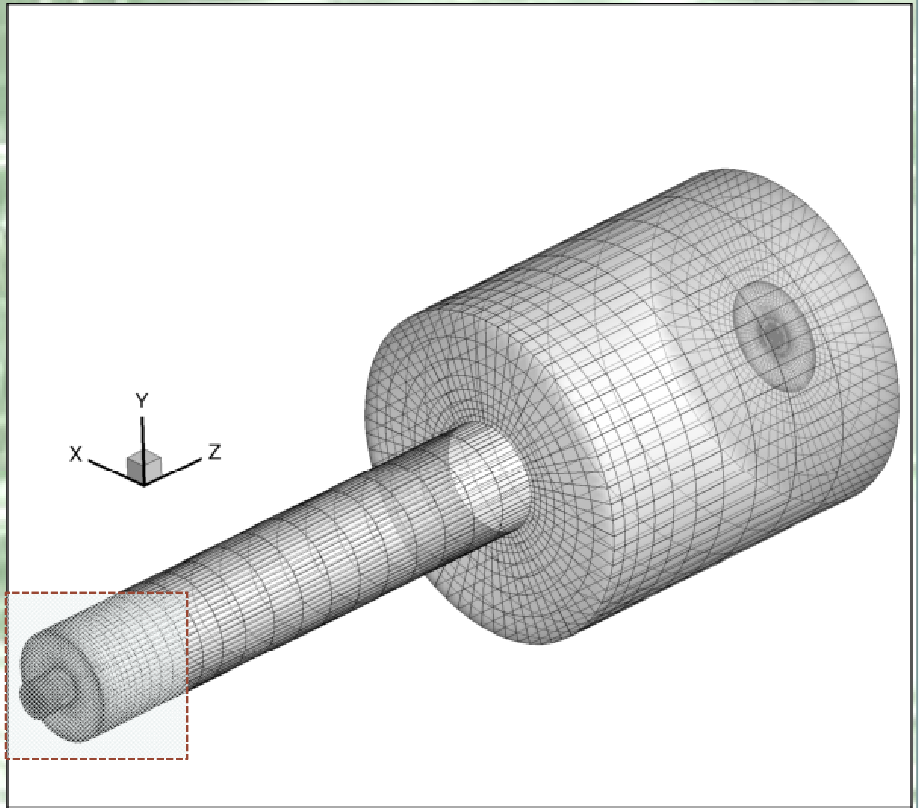
Main parameters
$R = 0.096$ m, $L = 1.5$ m, $R_{ref} = 0.032$ m (outer annulus)

Gas phase*: Ambient air, $U_{ref} = 12.89$ m/s, $Re_{ref} = 26200$, Swirl number = 0.47*

Particle *phase: average $D_p = 0.45$ μm, Particle loading ratio = 0.034 (about 10^6 particles in the domain)*

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulation – URANS of the gasifier



Gas Phase

Fully compressible averaged Navier-Stokes flow model equations aiming to a prompt generalization to variable density flows.

$\kappa - \omega$ SST model *[Menter et al., 2001]*, adequate to capture the vortex core

2nd order schemes in both time and space, PISO procedure for continuity closure

3D computational mesh:
multi-block and structured, composed of about 150000 cells

Particle phase

1-way coupling, only Drag and Gravity force

Track to Face algorithm for LPT
[Mc Pherson et al, 2009]

About 250000 **parcels** in the domain

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulation – URANS of the gasifier

Gas Phase

Fully compressible averaged Navier-Stokes flow model equations aiming to a prompt generalization to variable density flows.

$\kappa - \omega$ SST model *[Menter et al., 2001]*, adequate to capture the vortex core

2nd order schemes in both time and space, PISO procedure for continuity closure

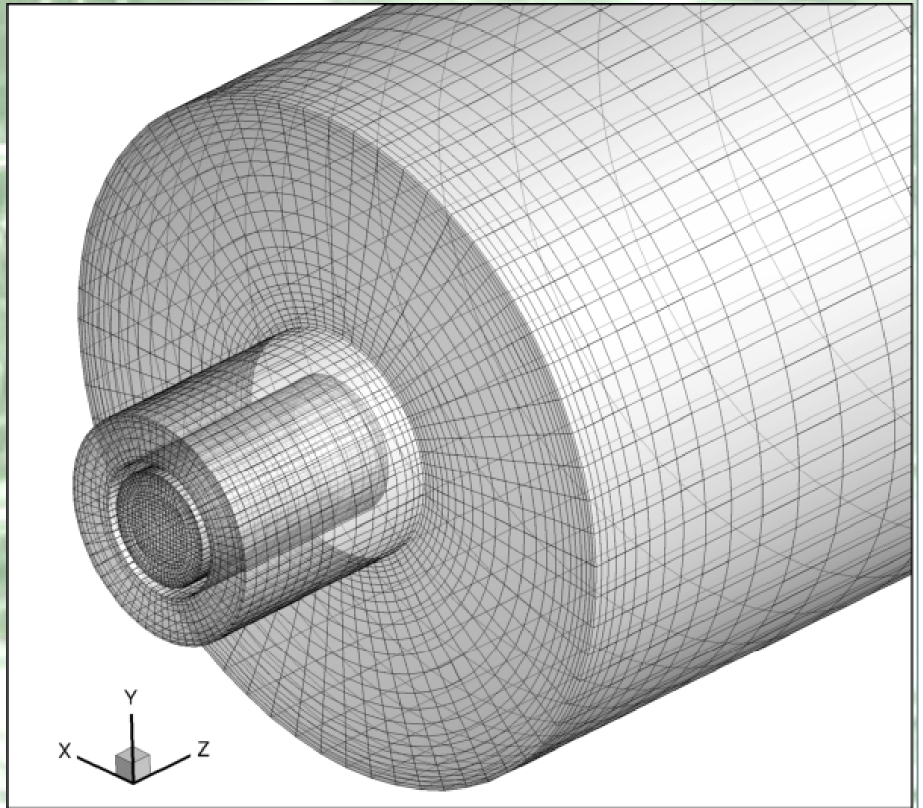
3D computational mesh: multi-block and structured, composed of about 150000 cells

Particle phase

1-way coupling, only Drag force included

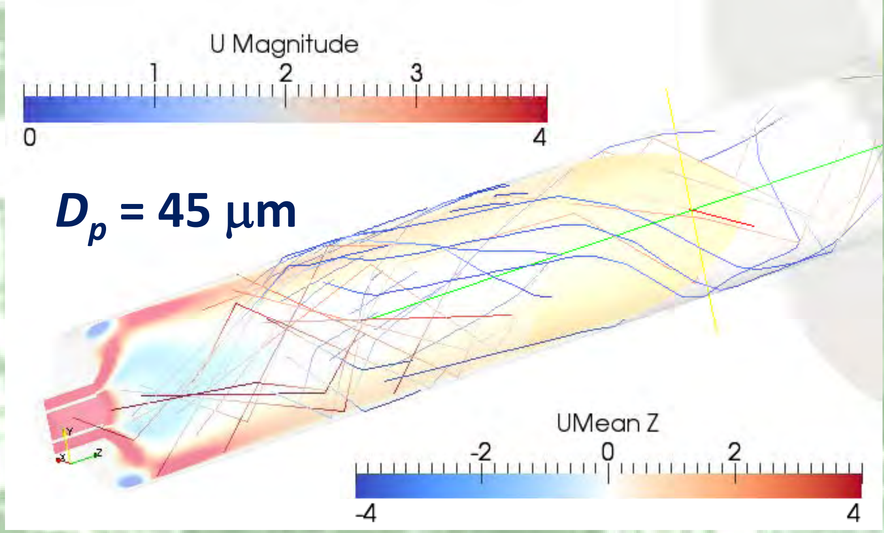
Track to Face algorithm for LPT *[Mc Pherson et al, 2009]*

About 250000 **parcels** in the domain



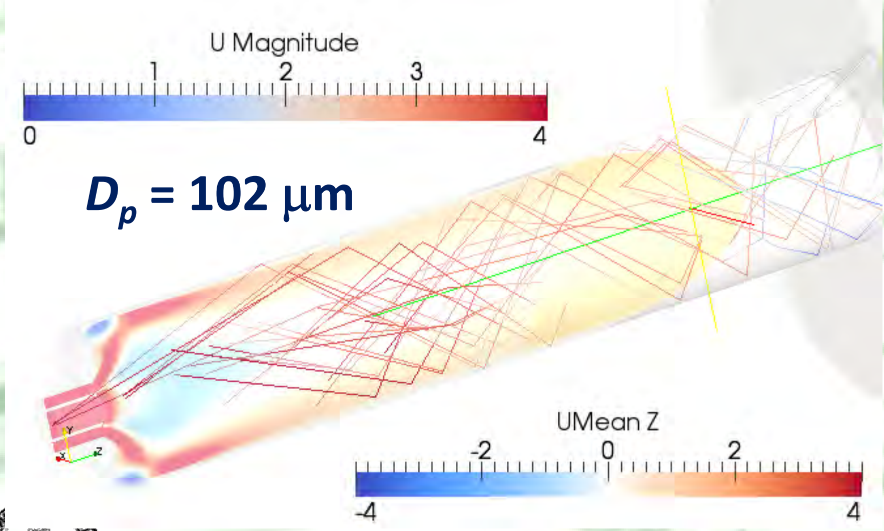
ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

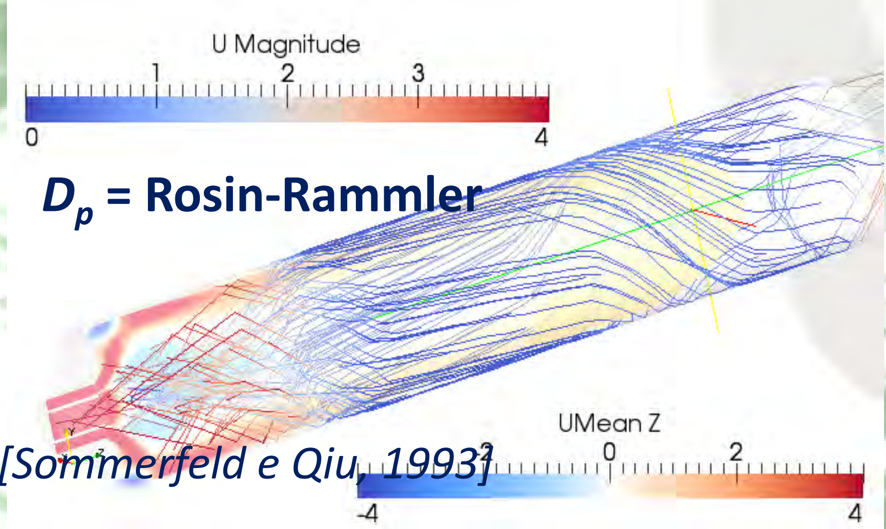
Numerical Simulations Level 1 - Results



Particle pathlines coloured by particle velocity and superposed to the axial velocity flood contours in the midplane section.

Essential particle motion features captured

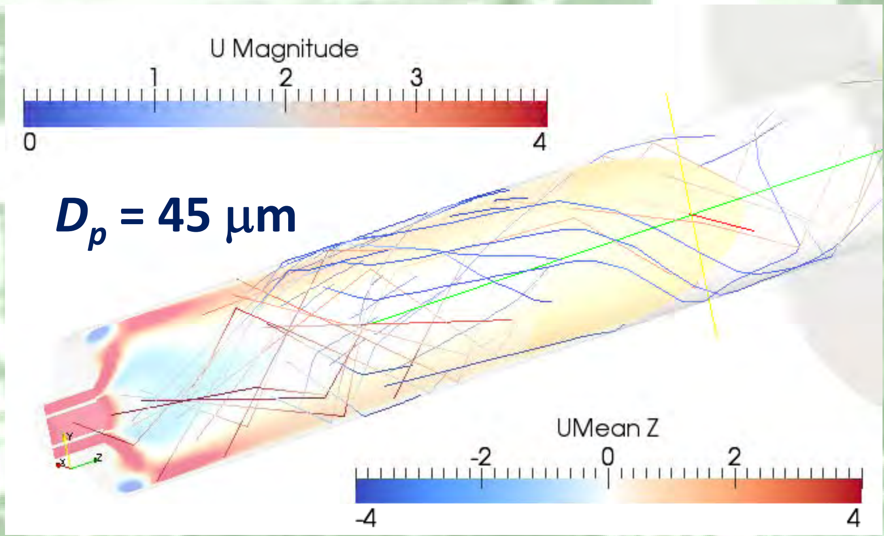


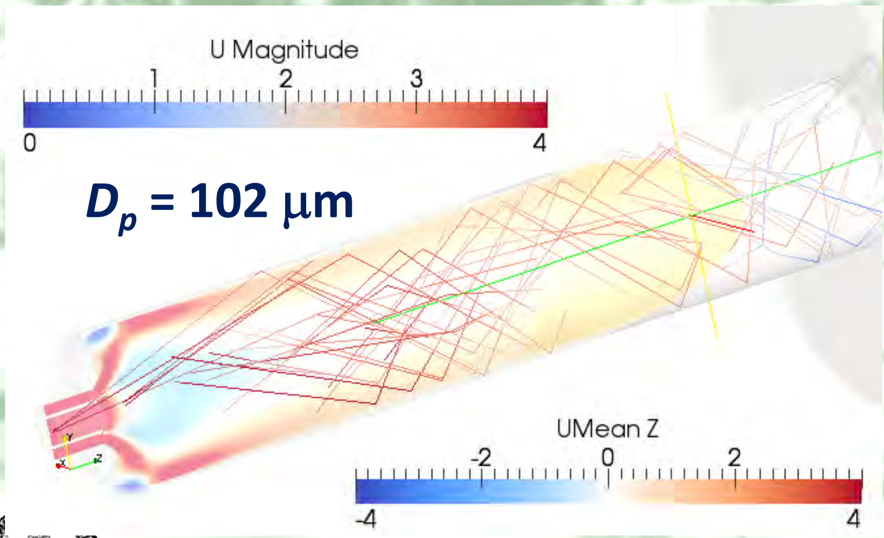


[Sommerfeld e Qiu, 1993]

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

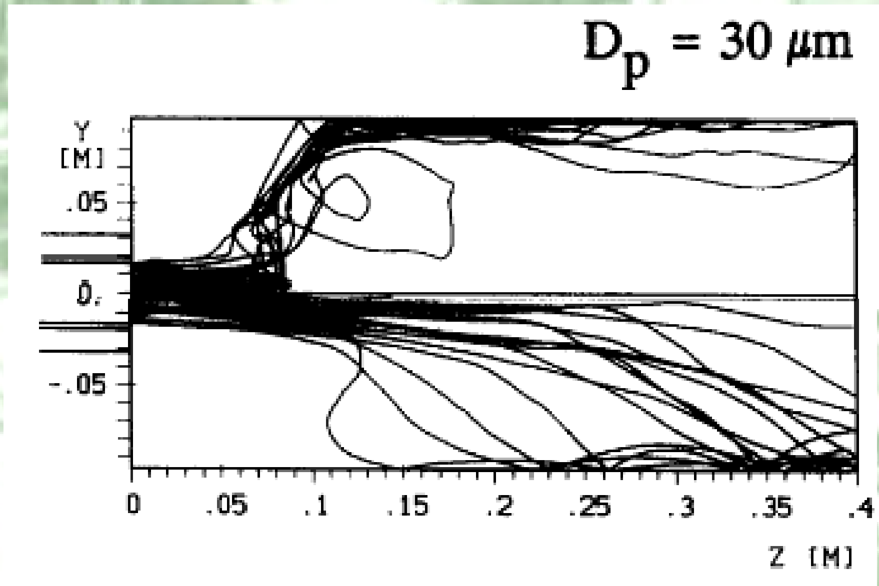
Numerical Simulations Level 1 - Results





Particle pathlines coloured by particle velocity and superposed to the axial velocity flood contours in the midplane section.

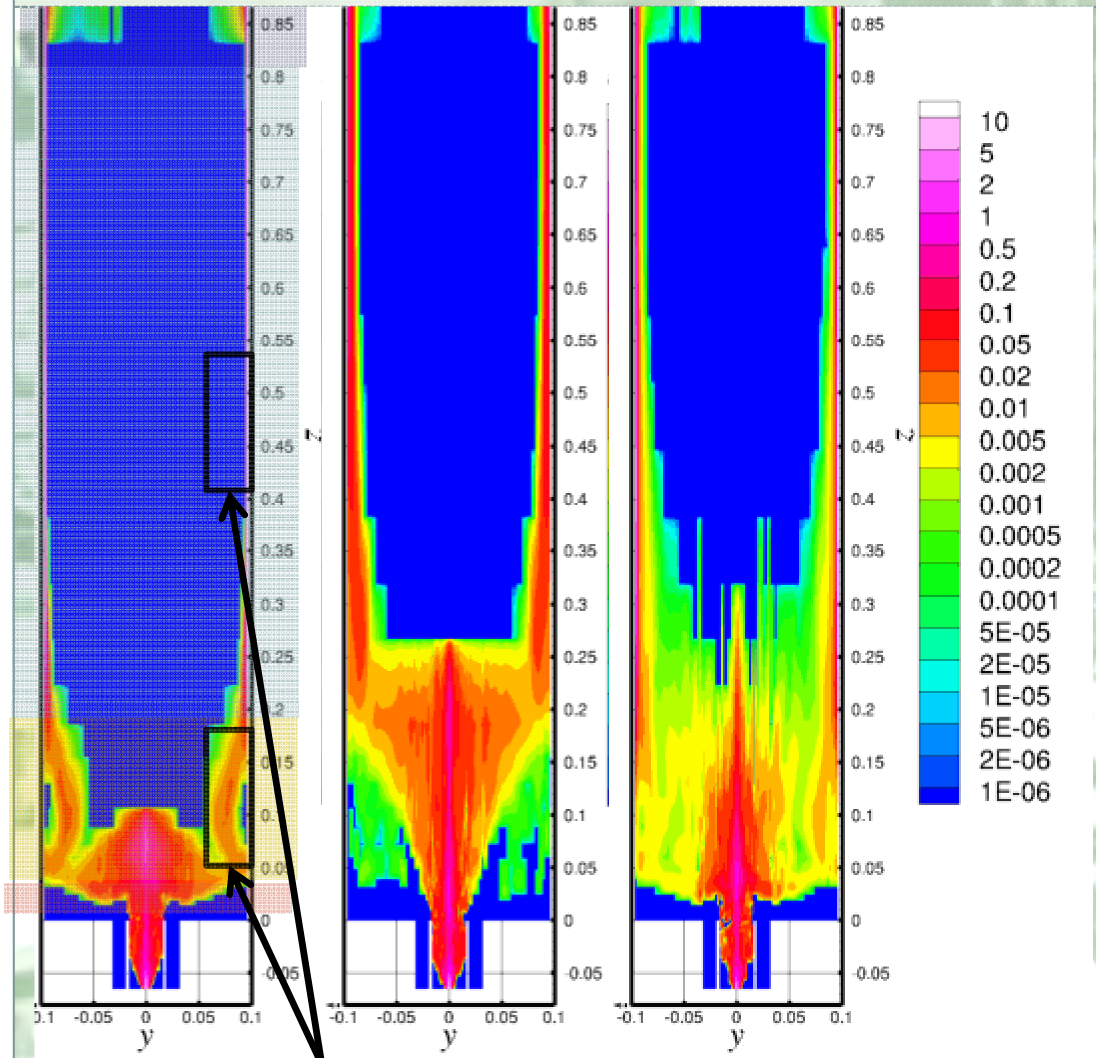
Essential particle motion features captured



[Sommerfeld e Qiu, 1993]

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Numerical Simulations Level 1 - Results



Volumes for LES simulations.

Average particle concentration (21 samples from 8 to 10 s)

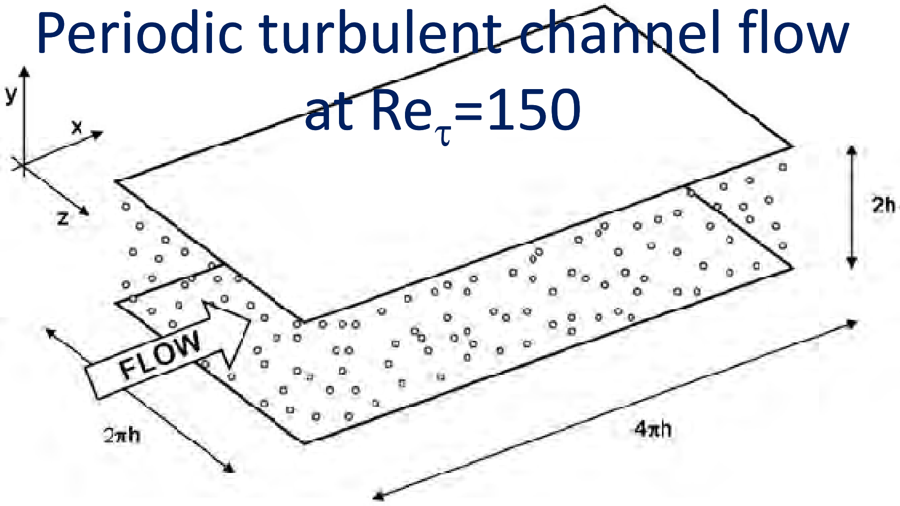
<u>4 distinct regions identified:</u>

1. Low number of impacts
2. High inertia impacts
3. Parallel to the wall particle flow
4. Lifted particles flow

Aimed at extract data about the flow and particle velocities in regions near the wall, particle impact velocities, particle load, etc.

LES of particle laden boundary layers

Periodic turbulent channel flow at Re_τ=150



Aim and scope:

- An almost obliged step for validation
- Sensitivity of particle accumulation at the wall upon different wall characteristics (molten slag treated as inelastic surface, $\varepsilon < 1$)
- Possibility of incipient formation of one among **E**, **S** or **SC** regimes.

<u>Gas Phase</u>

Fully compressible filtered Navier-Stokes equations aiming to a prompt generalization to variable density flows. Pressure force and work added in momentum and energy eq.

Localized dynamic model LDKM SGS closure, that solves an additional equation for the SGS turbulent kinetic energy *[Menon et al. 1995]*

2^{nd} order schemes in both time and space, PISO procedure for continuity closure

<u>Particle phase</u>

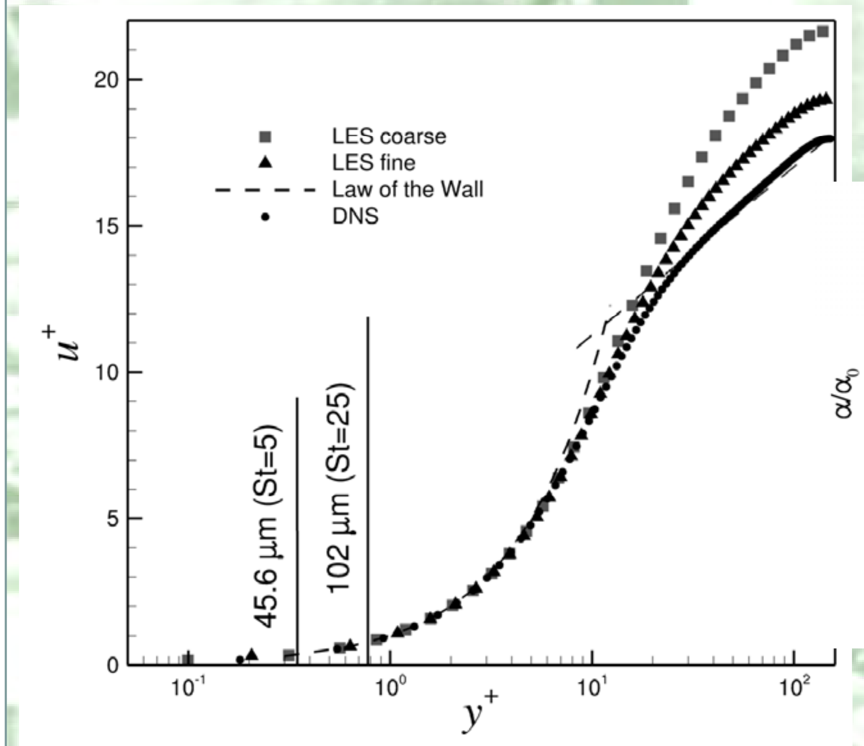
1-way coupling, only Drag force included

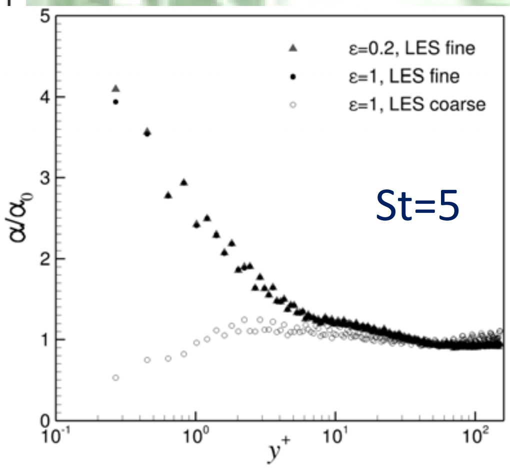
Track to Face algorithm for LPT *[Mc Pherson et al, 2009]*

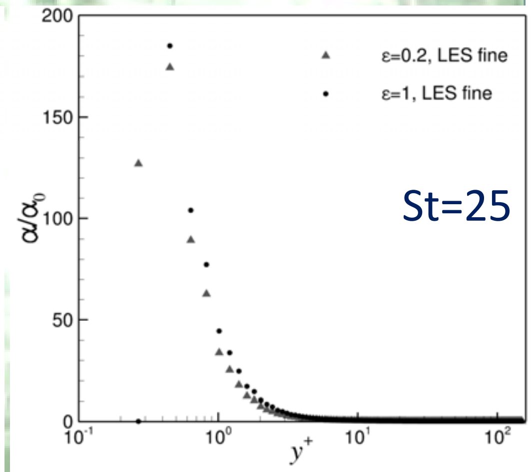
100000 **particles** in the domain

Setup similar to Marchioli et al. (2008)

LES of particle laden boundary layers flow







3D computational mesh:

Grid refinement sensitivity analysis:

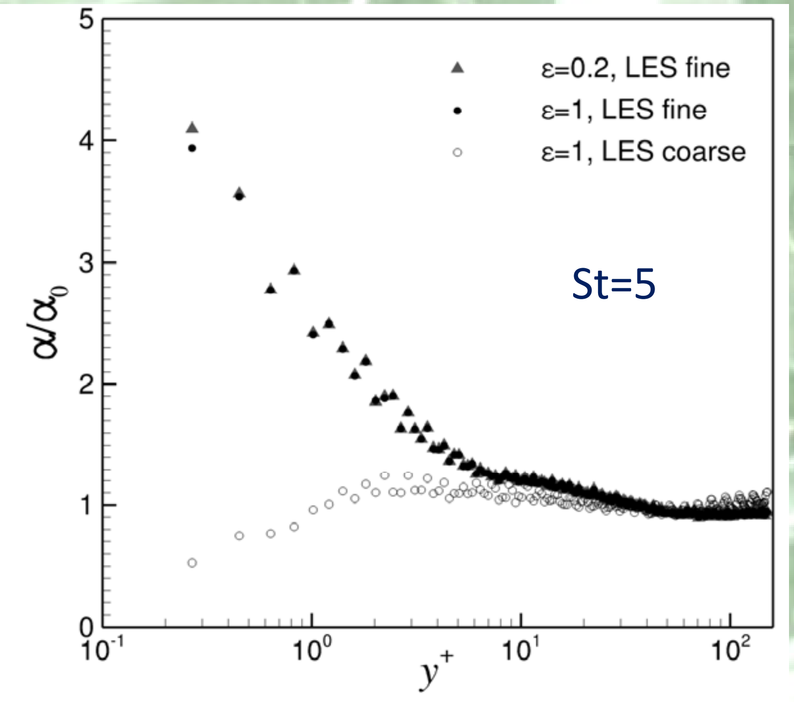
32x32x64 coarse or 48x48x96 fine

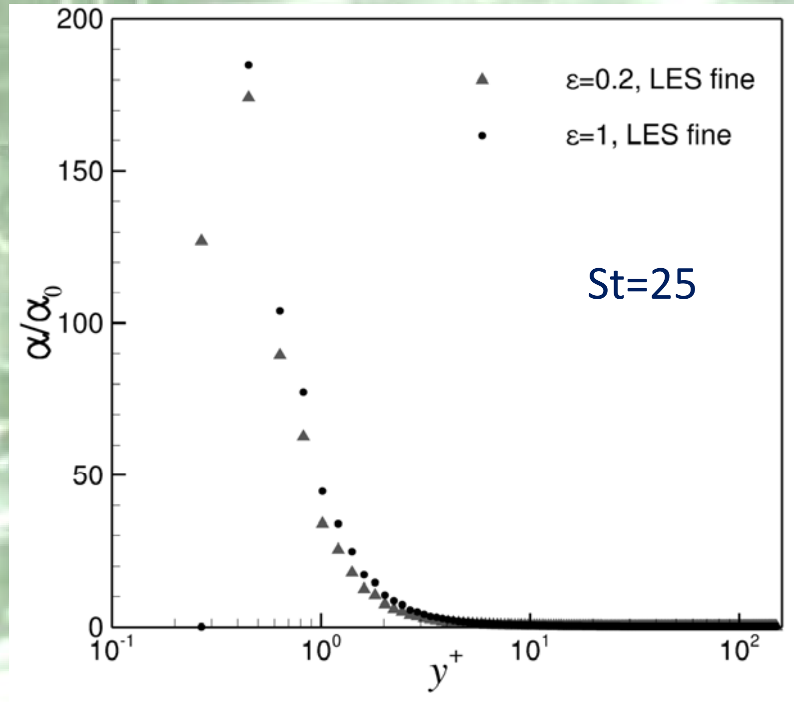
Variable restitution coefficient ε to simulate the presence of slag/covered slag:

Very weak dependence upon ε

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

LES of particle laden boundary layers flow





3D computational mesh:

Grid refinement sensitivity analysis:

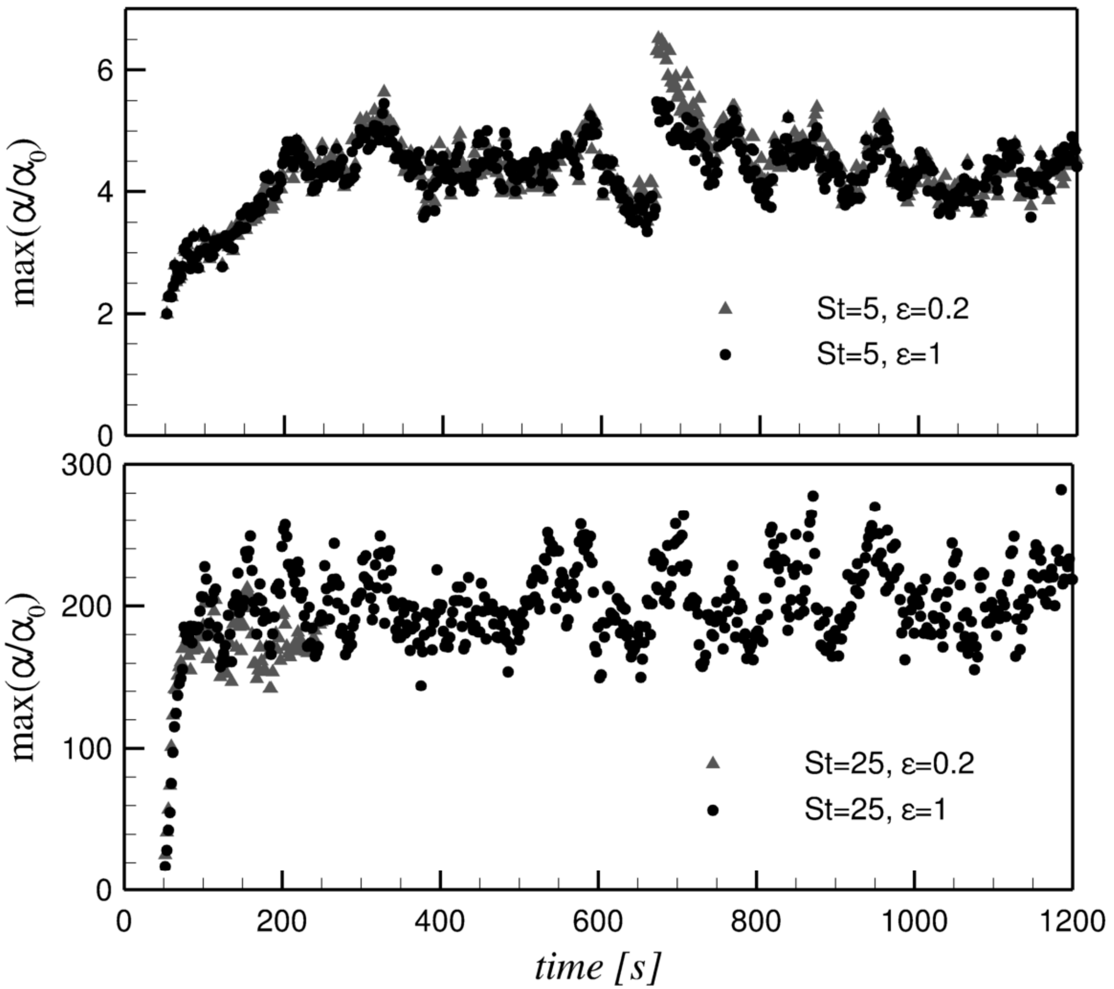
32x32x64 coarse or 48x48x96 fine

Variable restitution coefficient ε to simulate the presence of slag/covered slag:

Very weak dependence upon ε

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

LES of particle laden boundary layer flows

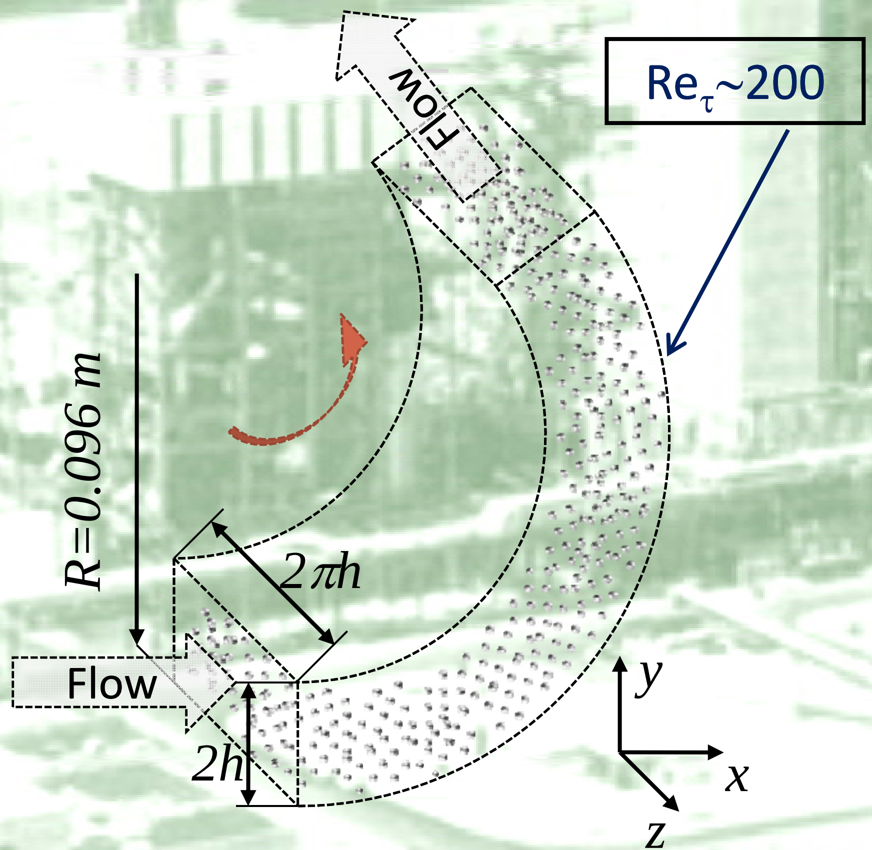


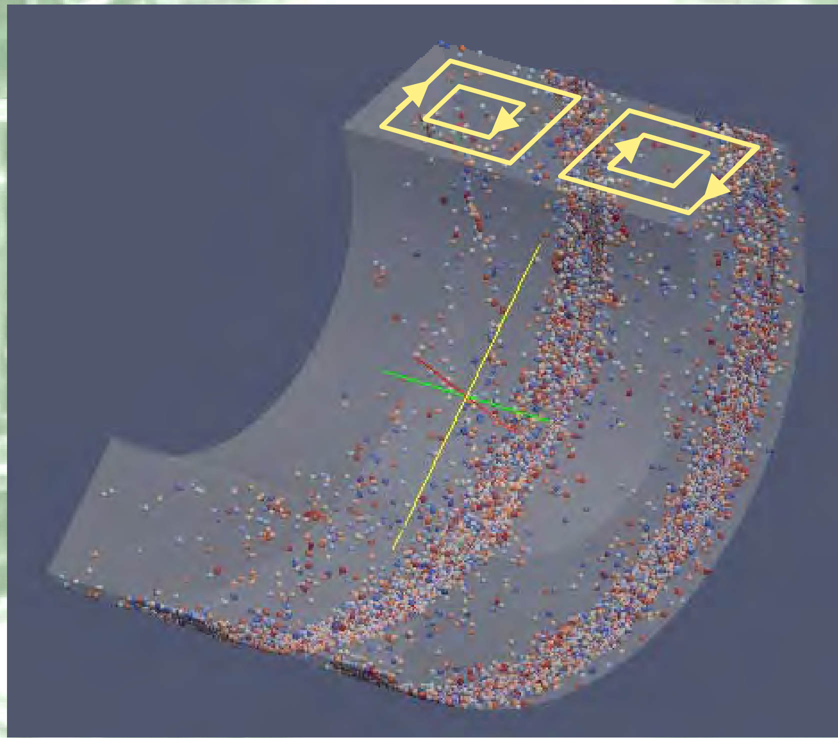
- The phenomenon is mostly driven by turbophoresis: particles have very low impact velocity.
- The accumulation of particles near the wall is not affected by wall properties
- The accumulation of particles near the wall takes a very long time, not comparable to the residence time of particles of few seconds in gasifiers.

Maximum normalized particle concentration averaged along the homogeneous directions vs time

LES of particle laden boundary layer swirled flows

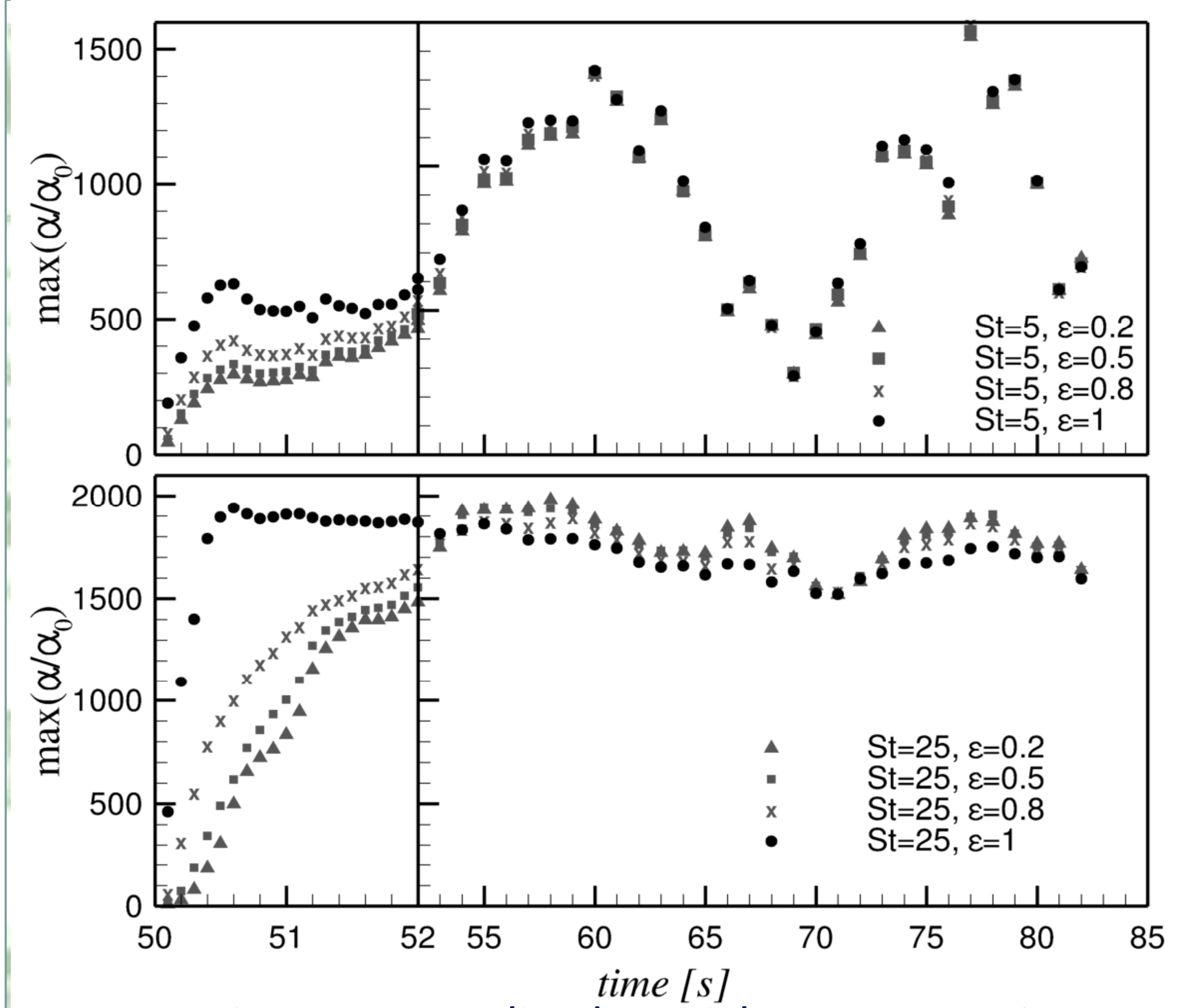
Periodic turbulent curve channel flow (rotating Couette flow)





Impact under condition of **non parallel average flow** is essential to properly reproduce the fate of particles in highly swirled flows

LES of particle laden boundary layer swirled flows



Maximum normalized particle concentration averaged along the homogeneous directions vs time (first 2 s enhanced)

- Satistically (almost) steady state conditions reached in times comparable with the residence time into a gasifier;
- wall properties affect the accumulation of particles during the transient phase;
- Two different behaviors of the transient phase varying ε.

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE

Conclusions and Future work

Conclusions

- A multilevel procedure (Exp → 1D → 3D-URANS → 3D-LES) has been established to investigate the fate of particles into slagging gasifiers;
- Need of accuracy improvements for smaller particles;
- Preliminary results allow to identify some conditions where the surface property of slag play a role

Future work

- The particle clustering lead to high level of concentration, claiming for the inclusion of a full 4-way coupling approach.;
- Char particles are not spherical; inclusion of a stickiness model also needed;
- Char particle in the dense layer have to burn to complete carbon conversion, leading to a variable gas/solid ratio: inclusion of combustion models and variable density flow.

Thank you for your kind attention

ISTITUTO DI RICERCHE SULLA COMBUSTIONE
CONSIGLIO NAZIONALE DELLE RICERCHE