

Non-spherical particle sub-models in comprehensive modelling of combustion systems

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Summary

1. Biomass and waste combustion: the problems
2. Comprehensive modelling of biomass co-firing: hierarchical approach.
3. Non spherical particles: open issues and characterisation/validation needs
4. Some examples and conclusion





Shape and Bulk of Biomass Energy



Rice Husk



Corn Waste



Palm Waste



Wooden Chip



Wooden Chip



Sugarcane



Straw

**Refuse Derived
Fuel (RDF)**





Biomass-waste energy utilisation

- Direct combustion and co-combustion
- Gasification
- Pyrolysis

Different operating conditions (T, tr, HR)



Pulverized systems

Fluidized beds

Fixed beds

10-100 μm

0.5 -5 mm

1-10 cm

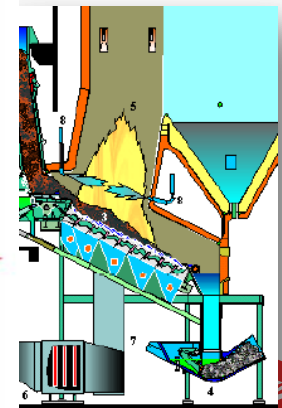
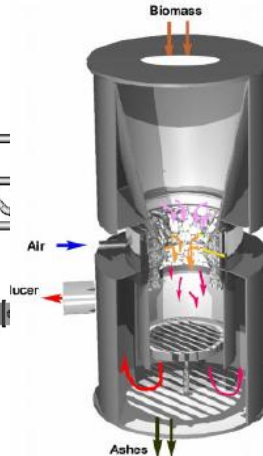
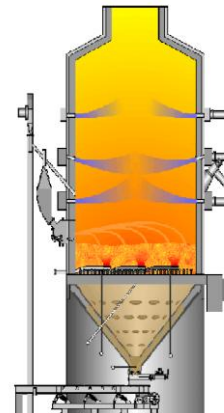
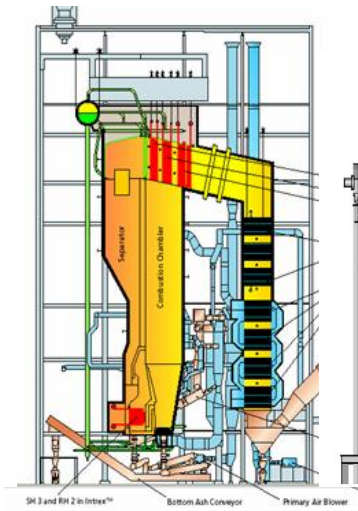
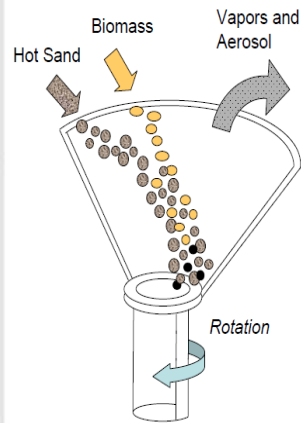
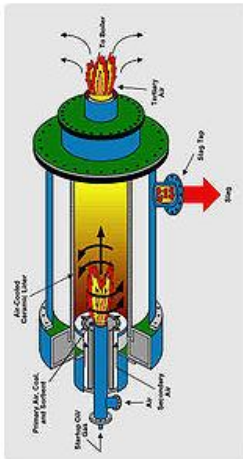
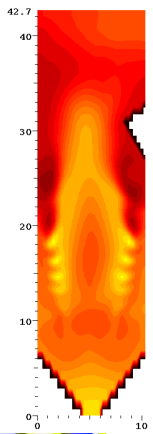
Cyclone boilers
Rotative cones

Bubbling beds

Grates

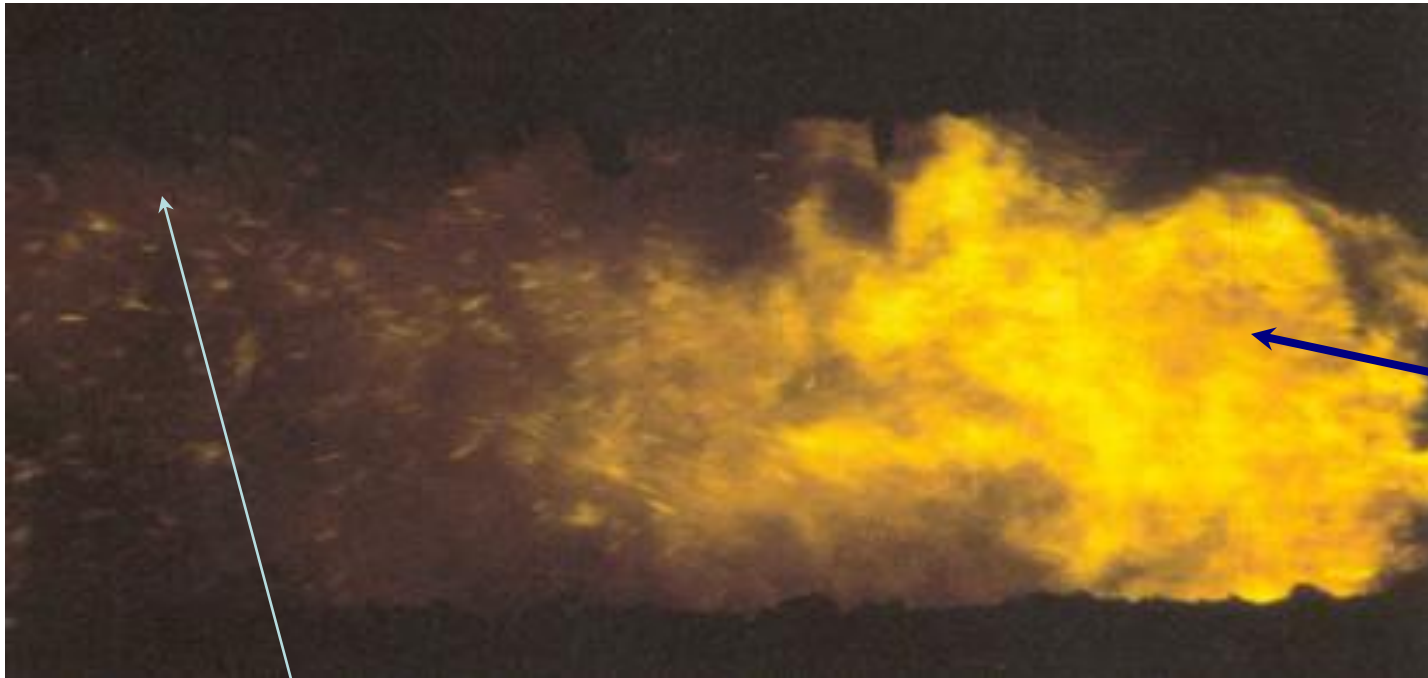
Particle size

Thermal severity
turbulence





Structure of a Coal-Straw flame



- High volatile bituminous coal
- Short Flame

- Burning straw particles

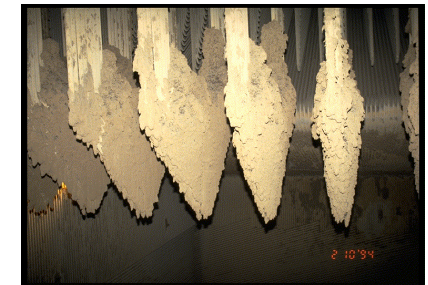
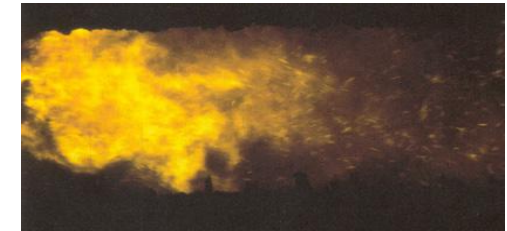
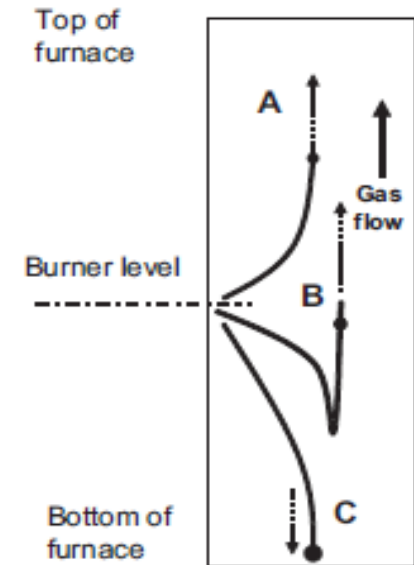
Shredded straw





Combustion of biomass-wastes: problems

- Particle trajectories → different residence times
- Less optimal particle size distribution than coal → different burn out times
- Incomplete burn out in combustion chamber
 - Local higher C and CO levels, at evaporator wall tubes:
 - corrosion risk
 - Increased slagging risk
 - Post-combustion at SH level
 - Too high T at SH → even there slagging risk
- Higher risk for flame impingement (longer flames)
- Large amount of unburned wood in ash hopper
- Local higher heat fluxes





Comprehensive coal/biomass combustion modelling

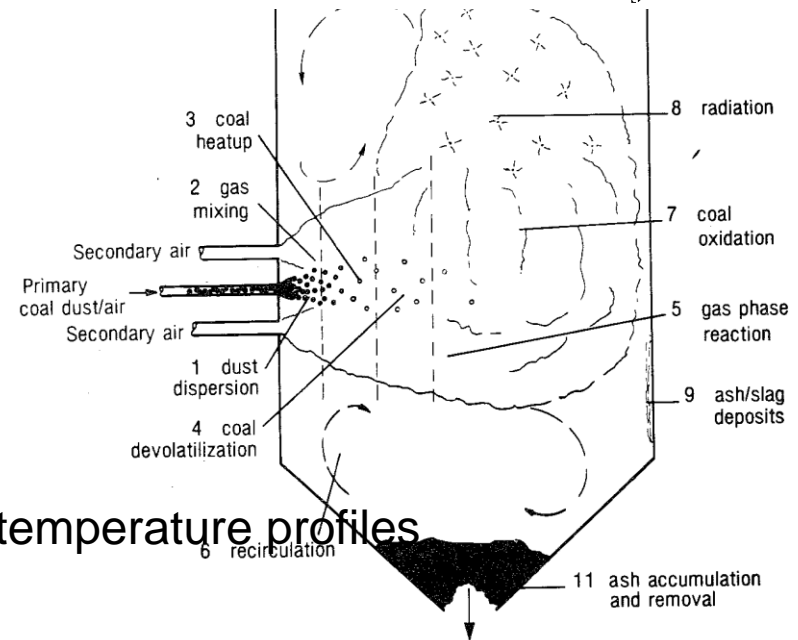
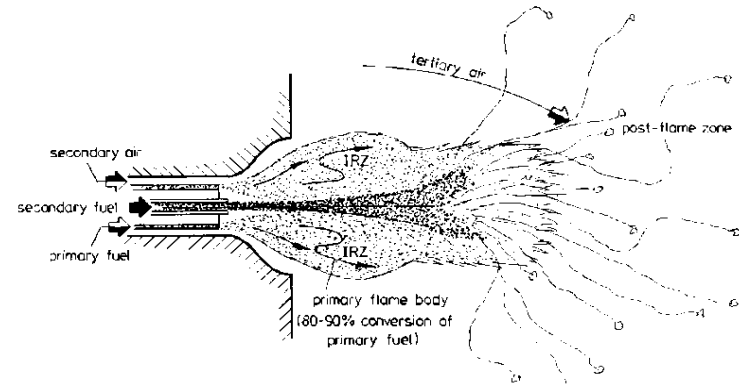
- The framework is based on **CFD** using numerical solutions of multidimensional, differential equations for conservation of mass, energy, and momentum.
- Other **submodels are coupled** within this framework to account for gaseous species mixing and chemical reactions, solid fuel particle trajectories, devolatilization and char oxidation, and radiant energy transport.
- A comprehensive model must **balance** submodel **sophistication** with computational **practicality**.
- Much of the research in this field is aimed at both improved solution techniques, and new or more “*efficient*” **submodels** able to provide practical engineering solutions.





Example- PF firing systems: sub-models

- Coal/biomass ignition/flame sub-model
 - **Solid particle trajectories**
 - **Devolatilisation**
 - Homogeneous combustion chemistry
- **Char burnout sub-model**
- Heat transfer sub-models
 - Radiant zone
 - Convection zone
- **Ash partitioning sub-model**
 - **Deposition**
 - Trace metals
- Combustion by-products
 - NO_x , SO_x , Hg chemistry, particulates
- Integrated furnace model
 - Calculation of heat transfer, species, temperature profiles in all furnace



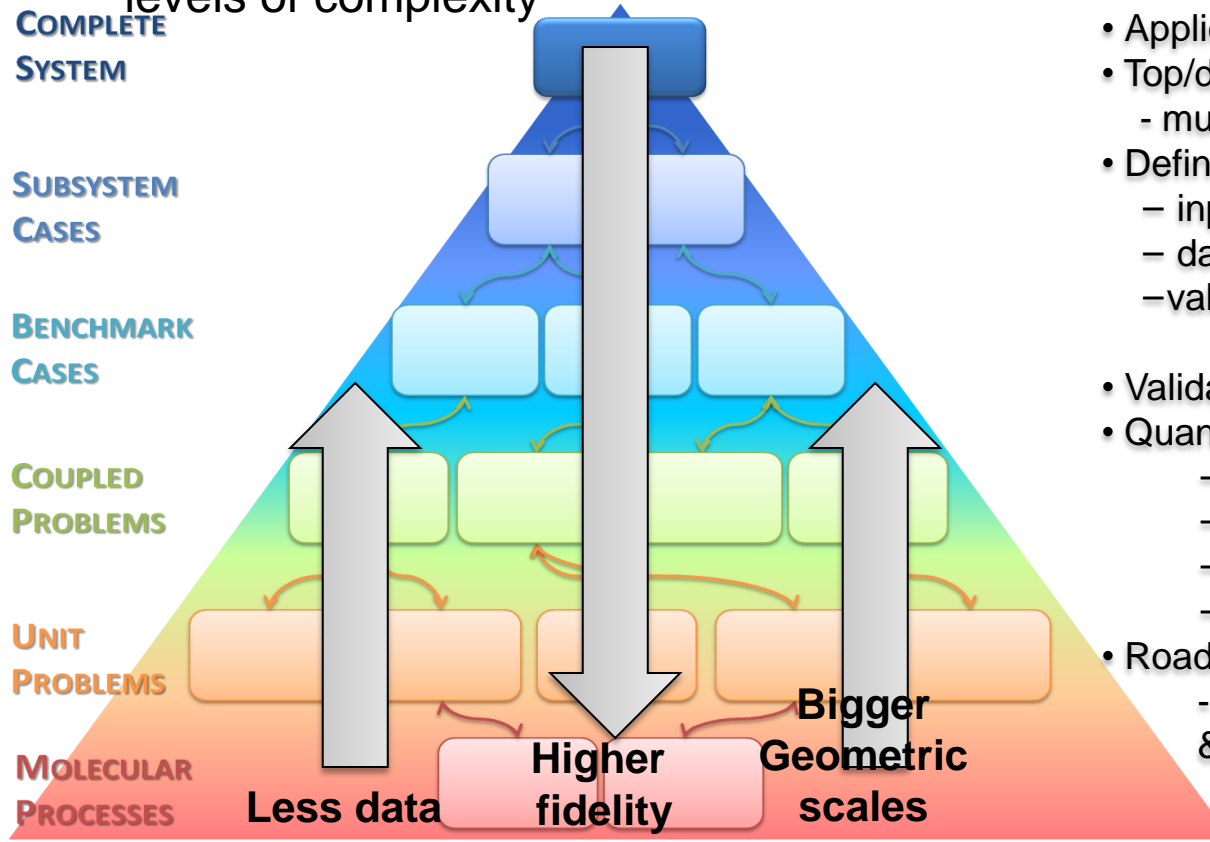


Achieving predictivity in comprehensive modelling

(see: Oberkampf, Trucano, *Prog. Aerosp. Sci.* 38 (2002) 209-272)

- Hierarchy strategy

- Identify range of experiments, possible separation of coupled physics and levels of complexity



- Application driven:
- Top/down:
 - multi to single-physic codes
- Definition of each brick:
 - inputs/ outputs
 - data: experiments & simulations
 - validation analysis
- Validation in each brick
- Quantifiable sensitivities
 - input parameters
 - b.c.'s
 - models
 - numerics
- Roadmap:
 - dynamic selection of experiments & models





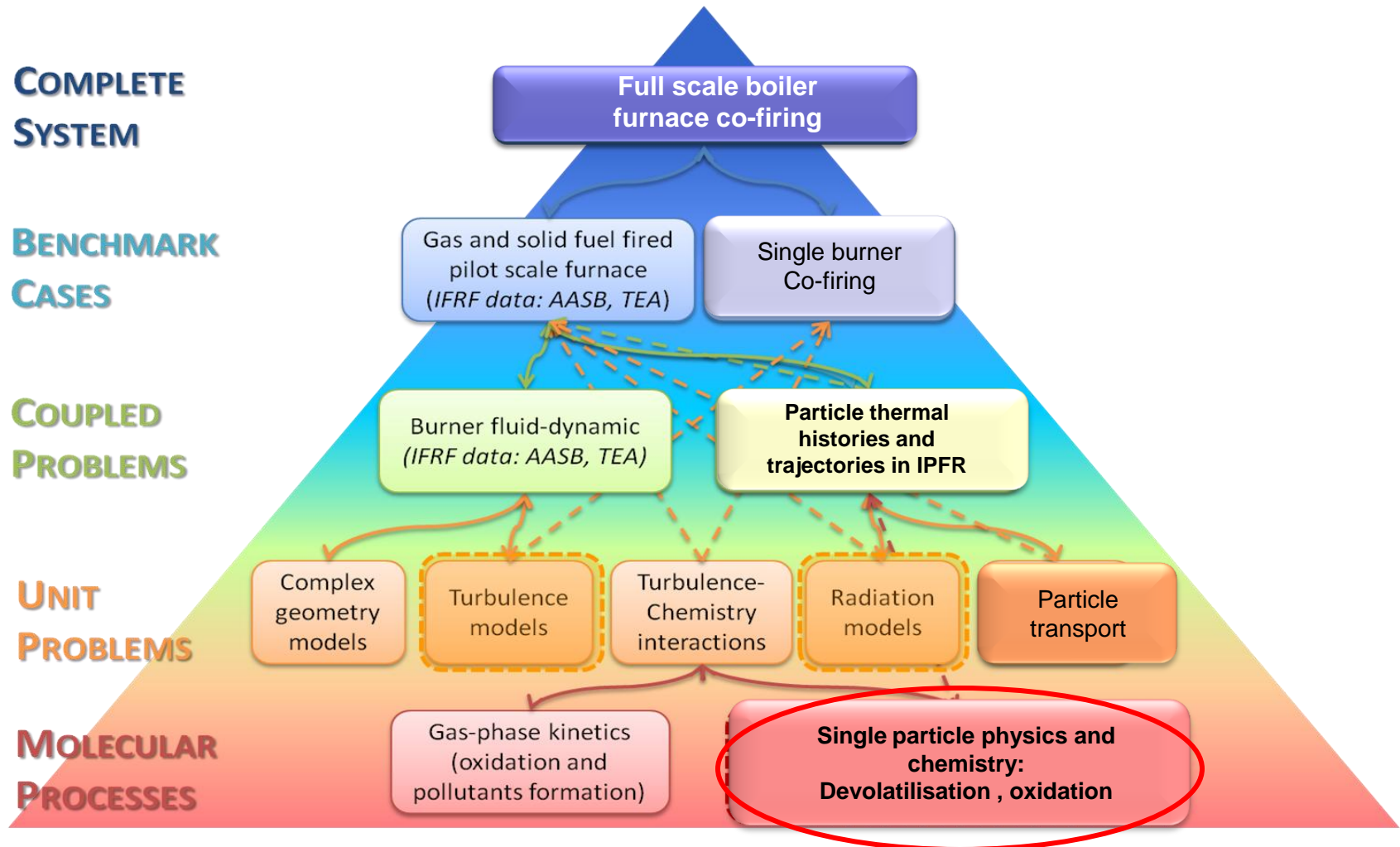
Non spherical particles issues

- Current models used to predict the motion of pulverized coal particles rely on a **spherical assumption**, which may deviate significantly from reality for the case of bio-dust.
- Qualitative observations suggest that pulverized **straw/biomass particles are highly nonspherical** (flake-like, rod-like), greatly enhancing the surface area, compared to a sphere, which represents the minimum in terms of surface-to-volume ratio.
- Clearly this affects the **motion, heating and surface reactions of a biomass particle** and appropriate modeling choices have to be taken to improve the design for co-firing of biomass in utility boilers.



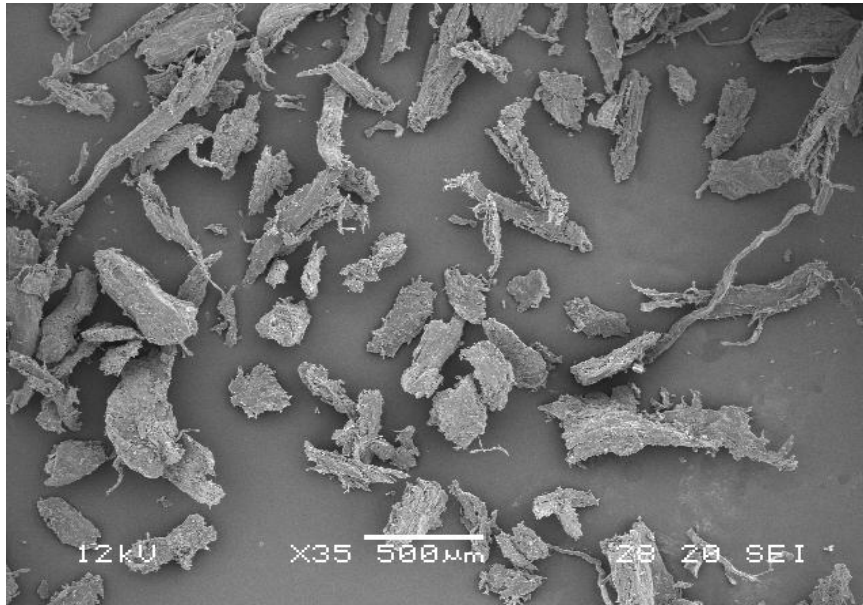


V&V hierarchy applied to biomass co-firing

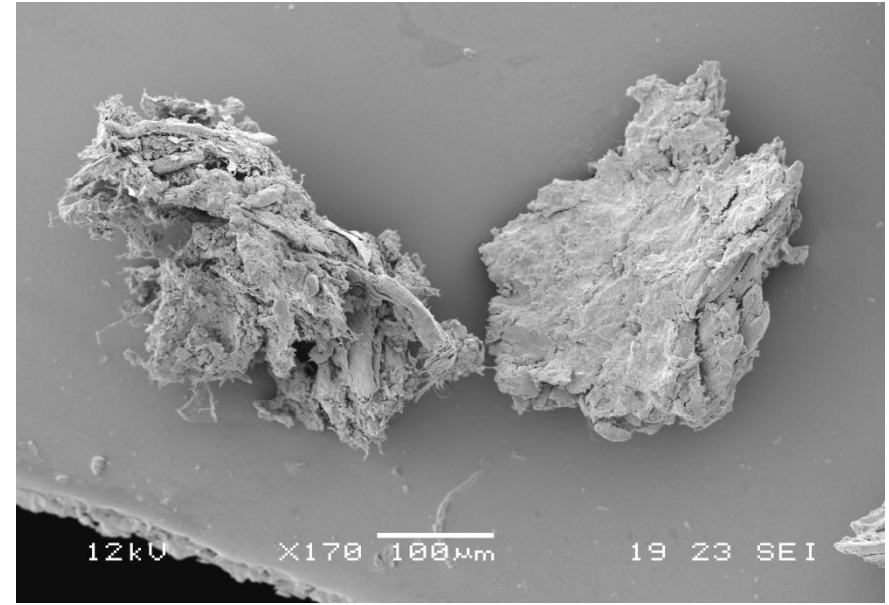




Particle size distribution- morphology



SEM images of wood particles evidencing the heterogeneous nature of the fuel



SEM images of olive residue evidencing the heterogeneous nature of the fuel

Depend on fuel nature and preparation (grinding) process

definition of suitable and representative parameters:

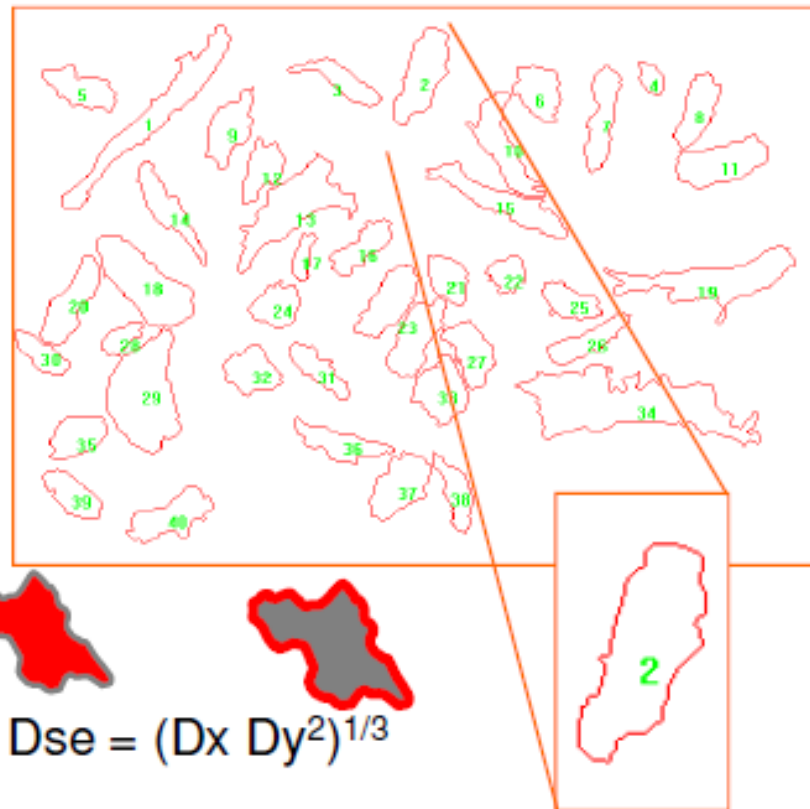
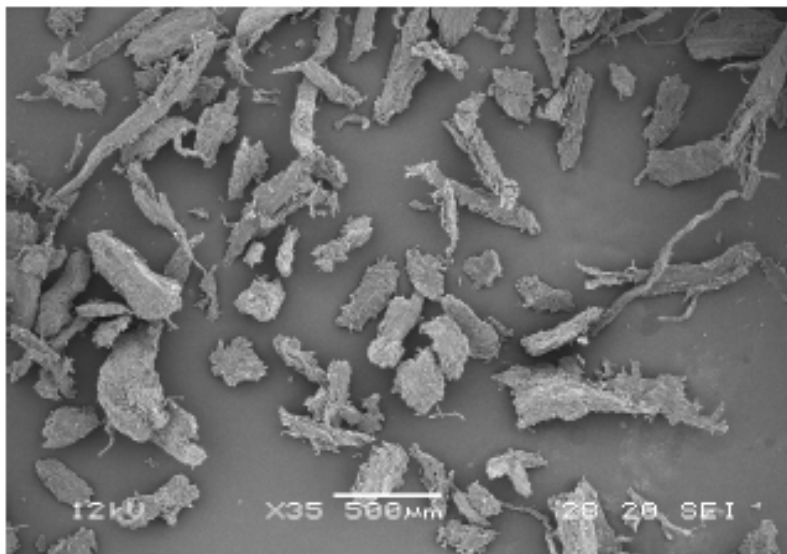
- size (e.g. equivalent spherical diameter), PSD
- shape (e.g. roundness),
- other geometrical parameters (perimeter/area, fractality)





Ground biomass PSD and morphology by image analysis

SEM images + image analysis S/W: quantitative analysis (samples of 300-350 particles)



Definitions:

size equivalent spherical diameter
 shape: roundness $SF = p^2 / 4\pi A$



$$D_{se} = (D_x D_y^2)^{1/3}$$

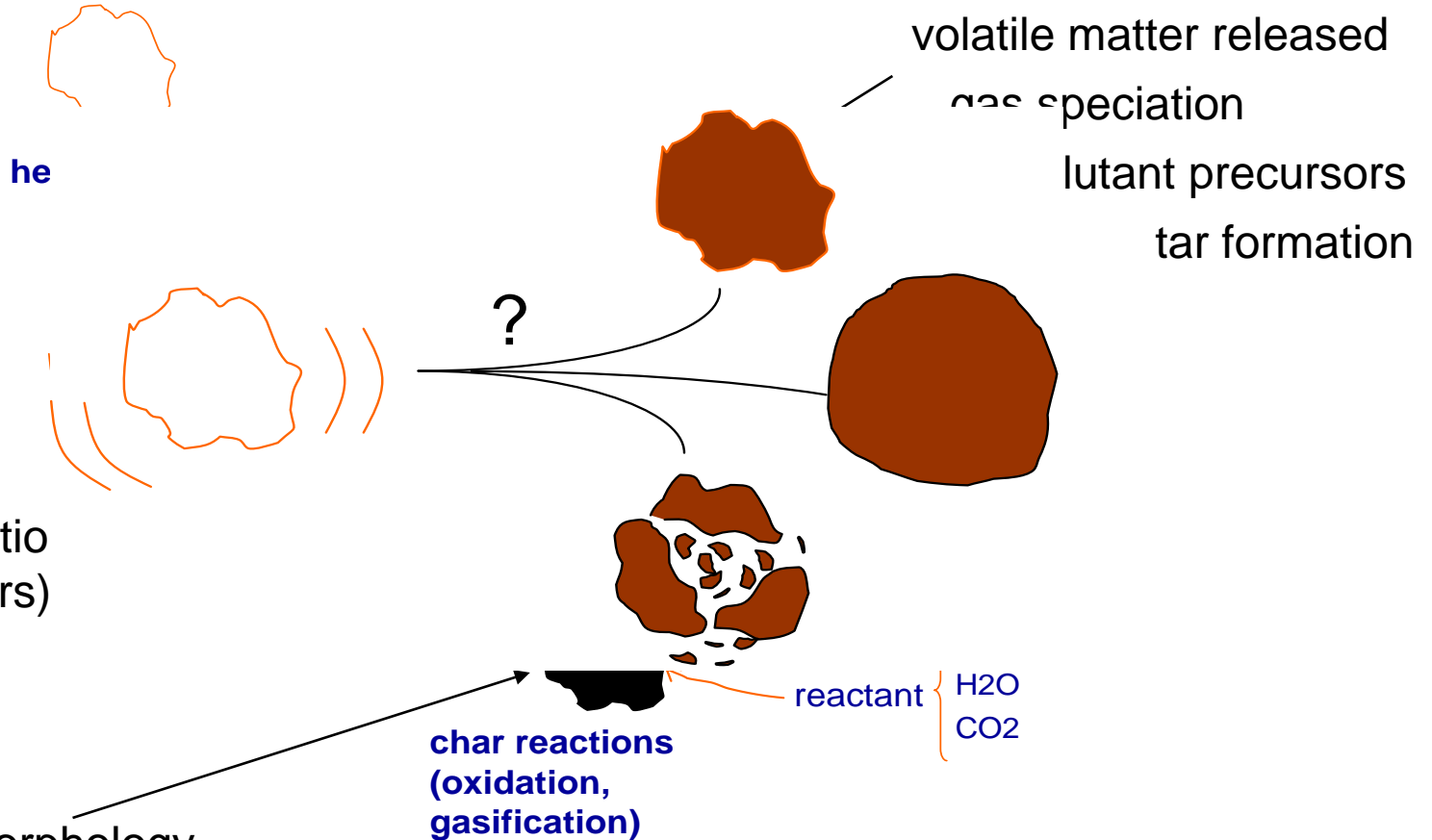
E. Blagini et al. - Characterization of high heating rate chars of biomass fuels
 32nd International Symposium on Combustion





Focus on devolatilization: needs

Basic step for:
combustion
gasification
oxyfiring



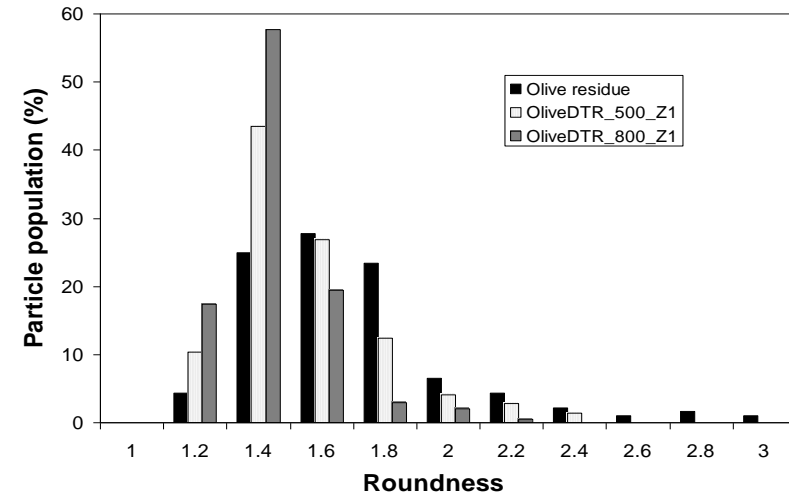
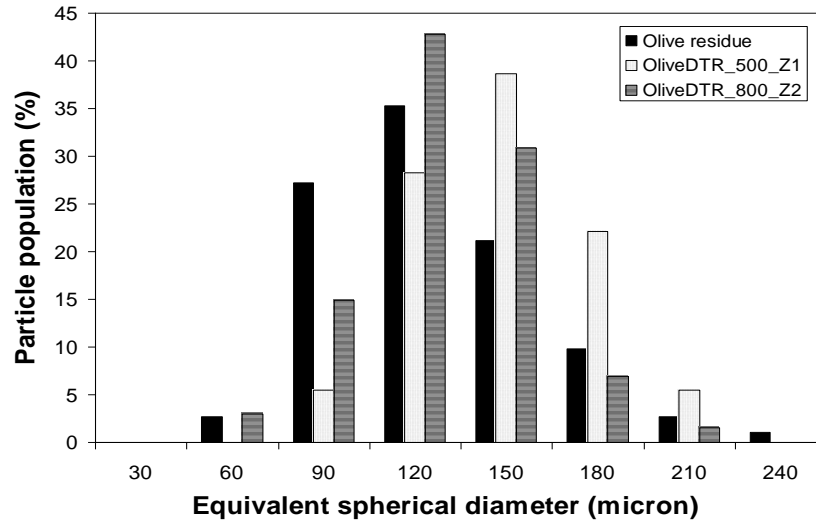
time of devolatilization
(kinetic parameters)

reactivity
size and morphology
physical properties
(density, cp, HV, porosity, SA)

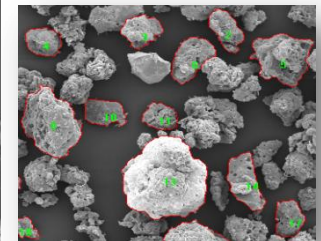
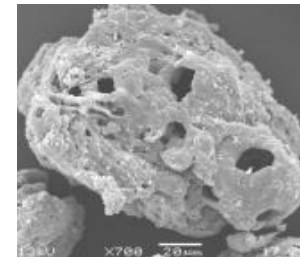
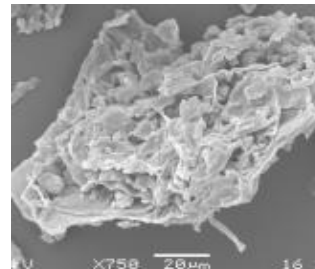




Effect of devolatilisation on PSD: olive residues

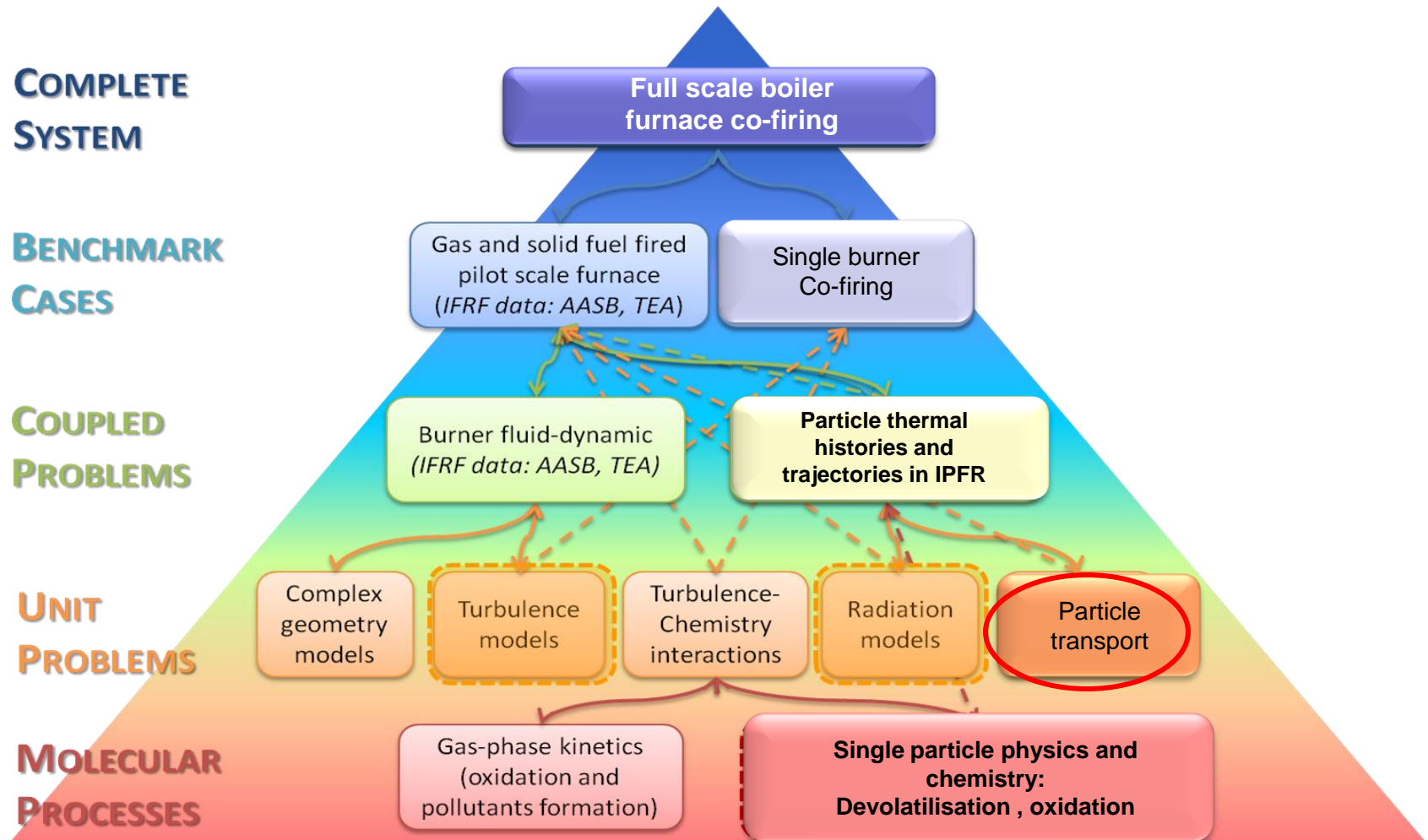


Olive Cake





V&V hierarchy applied to biomass co-firing





Particle transport

- **Effect of non-sphericity on the particle motion**

- Usually available in commercial CFD codes through a modification in the steady state drag coefficient based on the sphericity factor (e.g. Haider and Levenspiel, 1989).

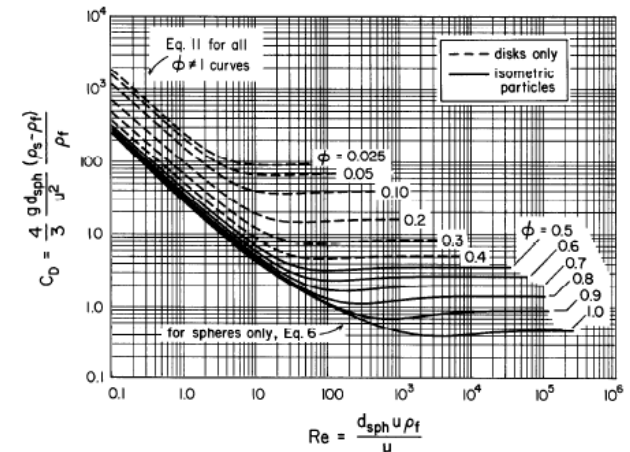
$$C_D = \frac{24}{Re_p} \left(1 + b_1 Re_p^{b_2} \right) + \frac{b_3 Re_p}{b_4 + Re_p}$$

$$b_1 = \exp(2.3288 - 6.4581\psi + 2.4486\psi^2)$$

$$b_2 = 0.0964 + 0.5565\psi$$

$$b_3 = \exp(4.905 - 13.8944\psi + 18.4222\psi^2 - 10.2599\psi^3)$$

$$b_4 = \exp(1.4681 - 12.2584\psi + 20.7322\psi^2 - 15.8855\psi^3)$$



- **Effect of non-sphericity on wall collisions**

- Lack of available models





Particle transport and turbulence

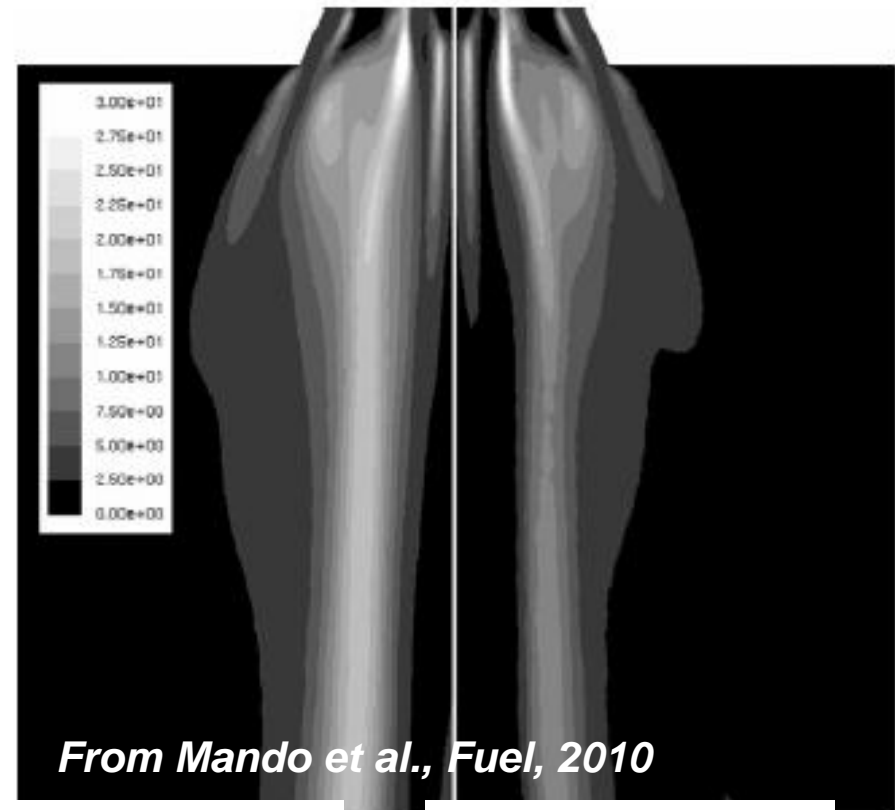
- **Effect of non-sphericity on turbulence modulation**

- Pulverized biomass particles are generally bigger and more elongated than coal particles
- Lack of validation of existing turbulence modulation models.
- Usually not available in commercial CFD codes → need for model implementation (UDF)

$$S_{kp} = \frac{\alpha \rho_p}{\tau_p} \left(|\bar{u}_i - \bar{u}_{pi}|^2 + \overline{u'_{pi} u'_{pi}} - 2k \right)$$

- EXAMPLE
- The presence of straw particles attenuates the turbulence.
- Even though straw particles are larger, the shape of the particles increases their drag coefficient and thereby decrease the slip/terminal velocity which is the essential to produce additional turbulent kinetic energy

Distribution of k
in a CHP unit fed
with pulverised
straw



From Mando et al., Fuel, 2010

No modulation

Modulation





Particle heating

- **Effect of non-sphericity on particle heating.**
 - available models in commercial CFD codes are usually based on the spherical assumption, so that it would be necessary to develop some efficiency factor based on particle sphericity to correct the convective and radiative heat transfer (Mandø et al., 2010).
 - For convective heat transfer we can use correlations developed for cylinders or disks.

Cylinders at low Re

$$Nu = W_0(Re)Pr^{0.33} + W_1(Re),$$

where

$$W_0 = \begin{cases} 0.46271 \exp(1.01633(\log_{10}(Re)) + 0.5121(\log_{10}(Re))^2), & 10^{-2} \leq Re \leq 3.14, \\ 0.597(Re/\ln(1/Re))^{1/3}, & Re < 10^{-2}, \end{cases}$$
$$W_1 = \begin{cases} 0.10666 \exp \left(\begin{array}{l} 0.41285(\log_{10} Re) + 0.43847(\log_{10} Re)^2 \\ +0.1915(\log_{10} Re)^3 + 0.01802(\log_{10} Re)^4 \\ -0.005225(\log_{10} Re)^5 \end{array} \right) & \\ 0.0917 & Re < 10^{-2} \end{cases}$$

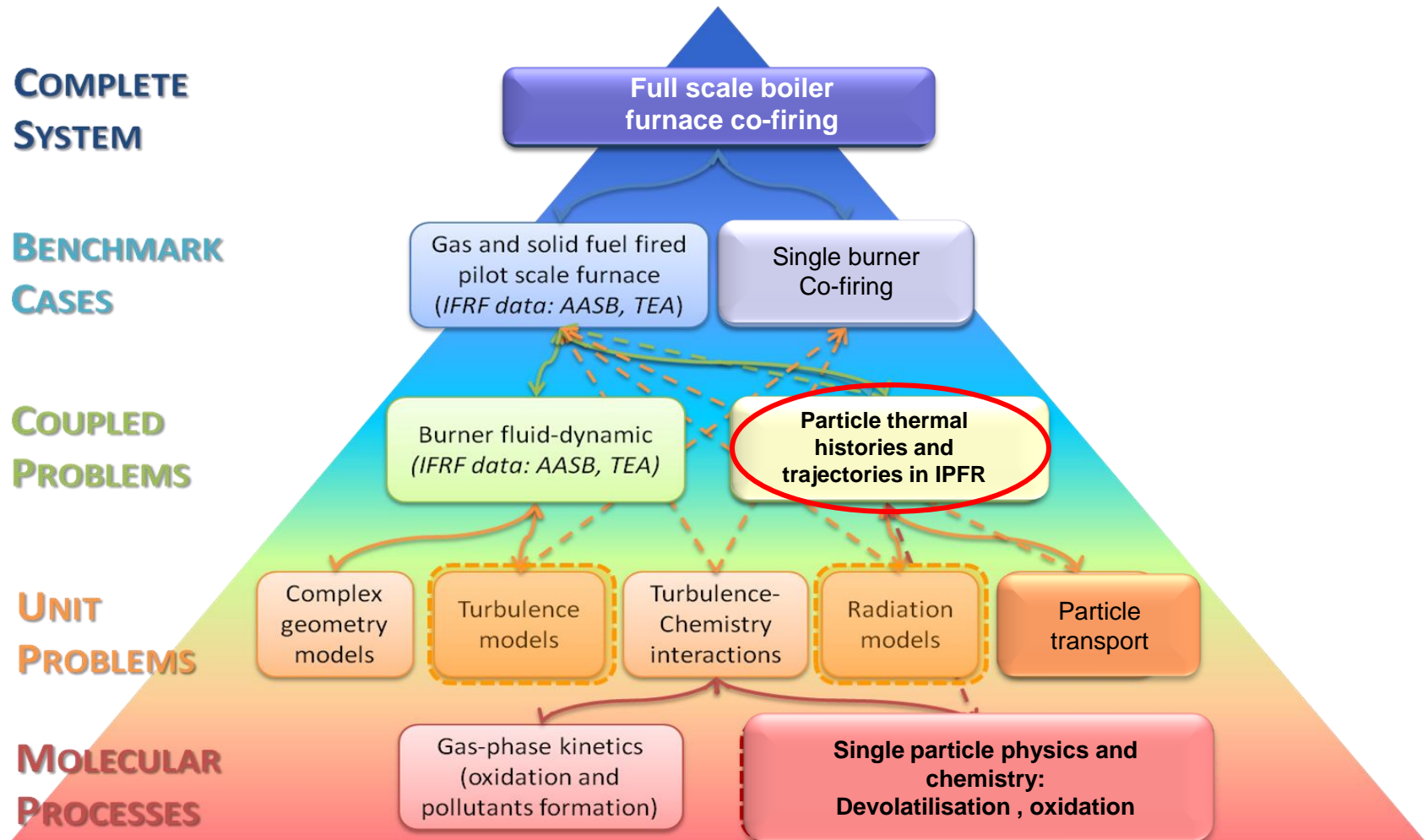
Flat disks

$$Nu = 0.644Re^{0.5}Pr^{0.33}$$



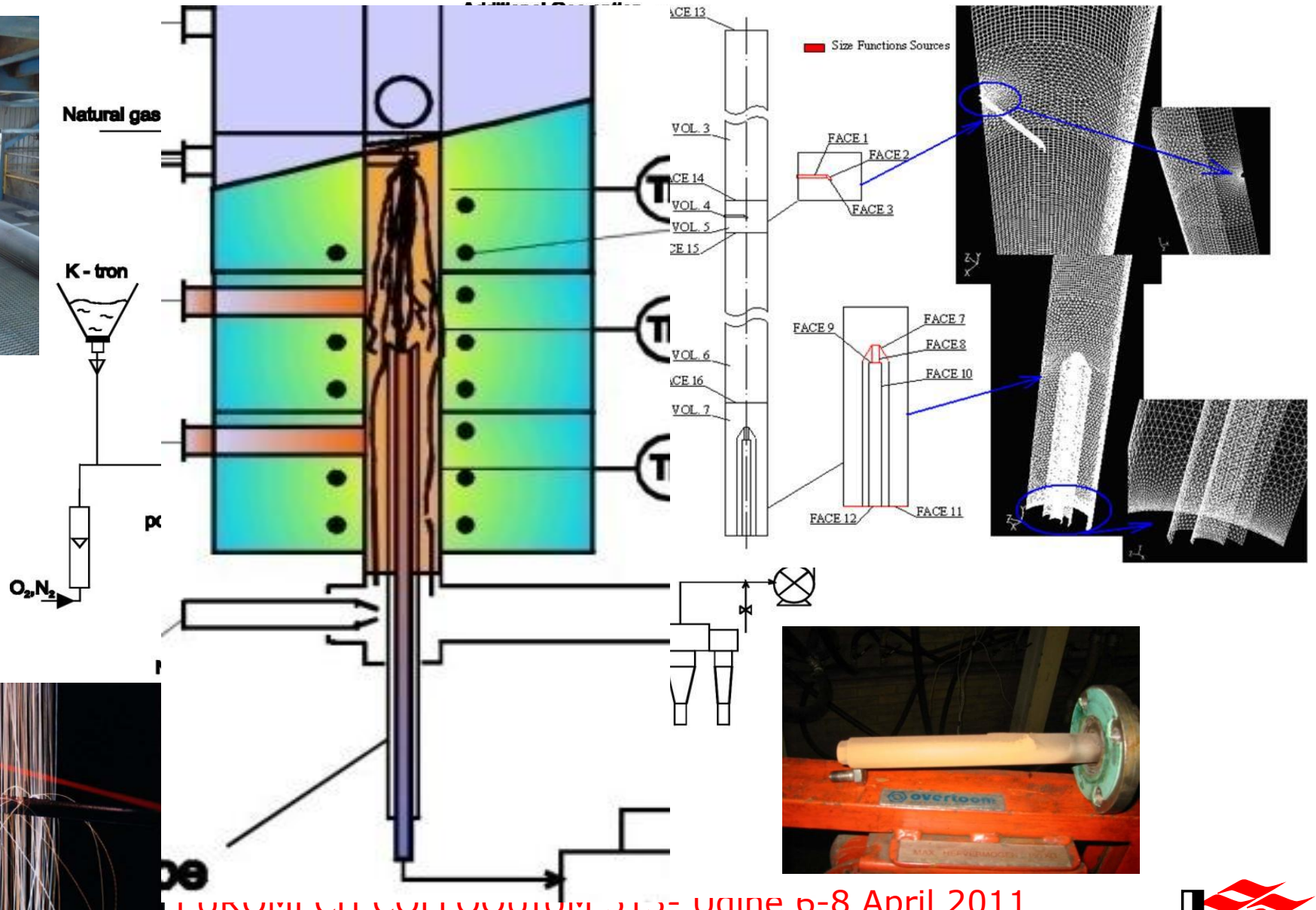


V&V hierarchy applied to biomass co-firing





IFRF Isothermal Plug Flow Reactor





Testing sub-models in IPFR

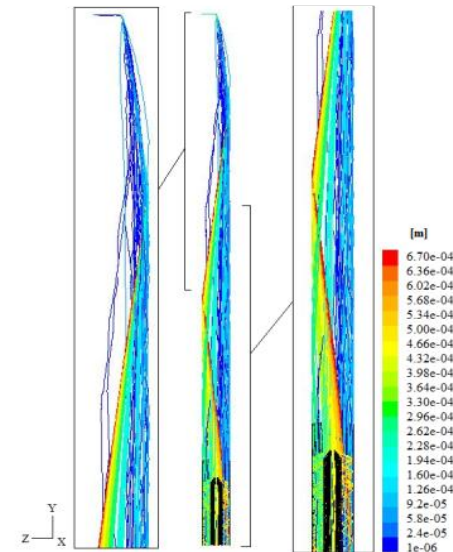
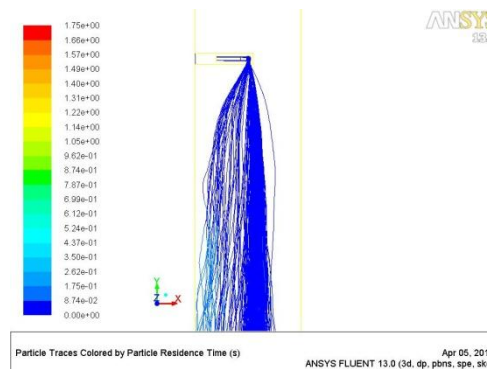
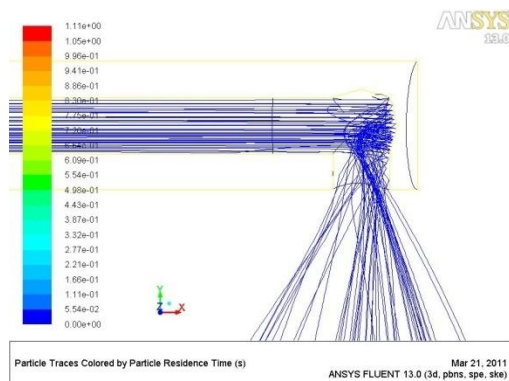
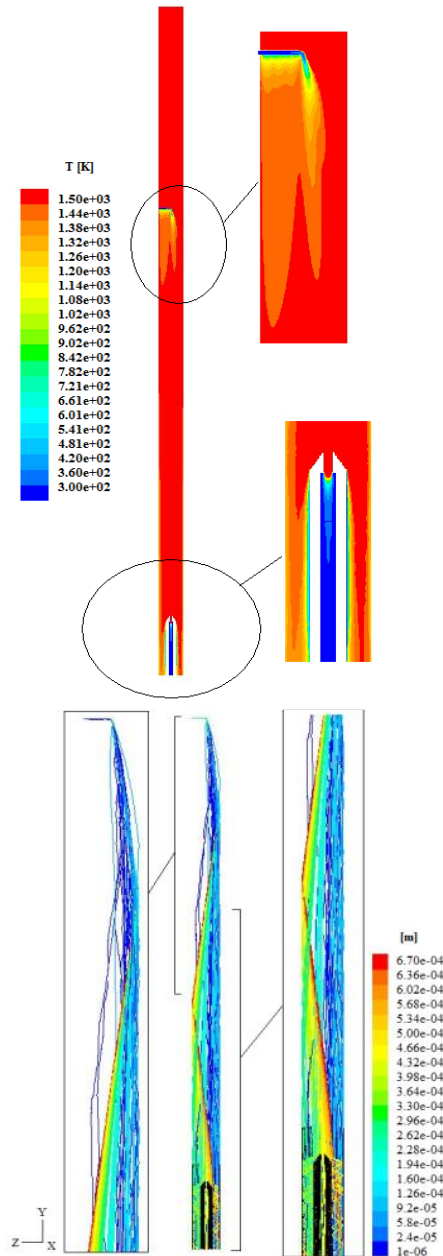
First level: No particle in gas flow :

- probes presence effect on hot gas fluid-dynamic and temperature
- the effect in changing gas carrier velocity and composition
- the effect of feeding probe shape

Second level: unreactive particles

Inert solid particles feeding to analyse spread characteristics and particles trajectories.

- Collection efficiency is assessed

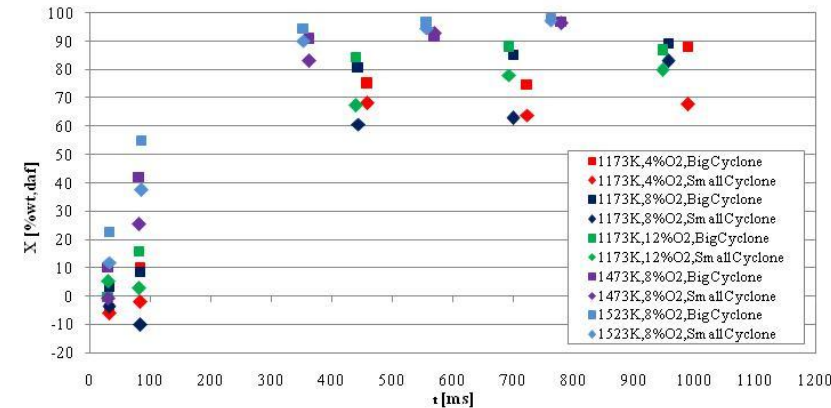
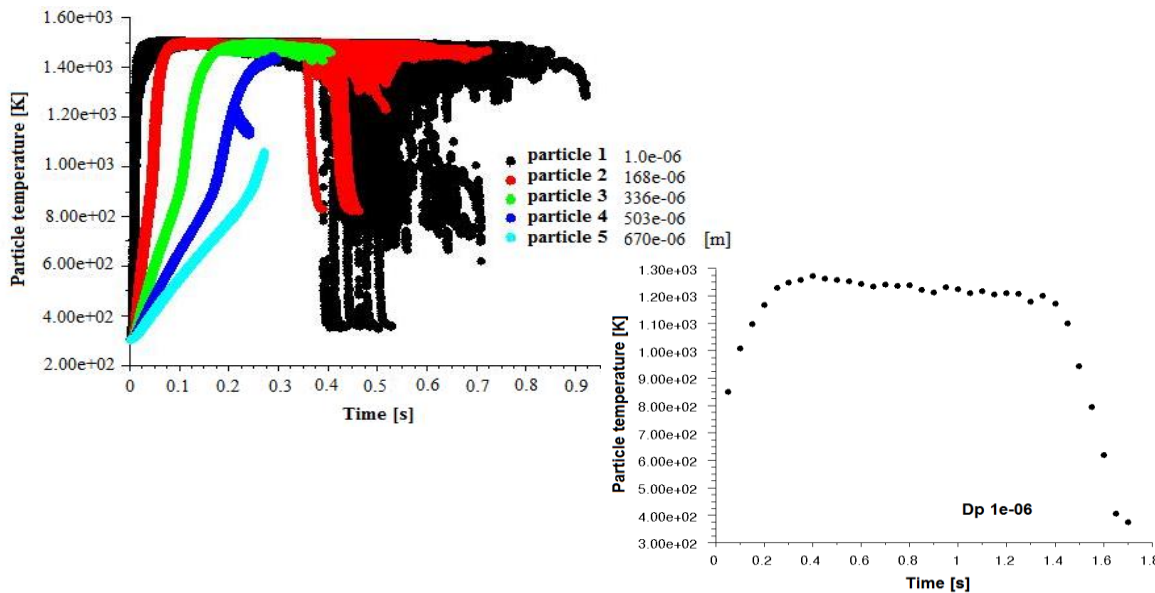




Testing sub-models in IPFR

Third level: Reacting particles numerically injected to analyze devolatilization and char combustion phenomena

Single size classes and a Rosin-Rammler size distribution (5 size classes): particle conversion is evaluated



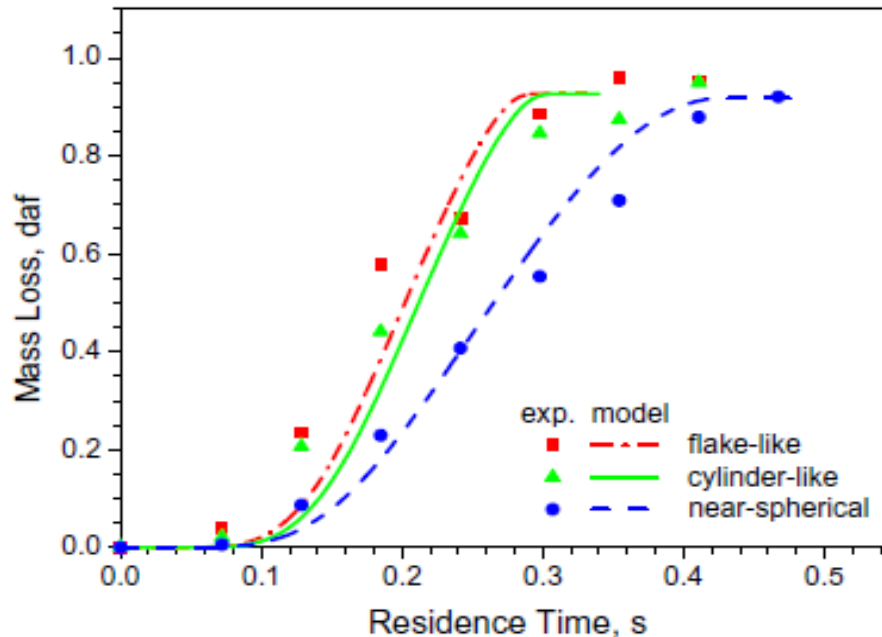
NOMINAL TEMPERATURE: 1100°C



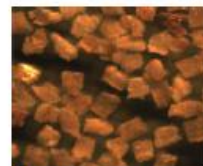


Devolatilisation kinetics

- ***Effect of non-sphericity on devolatilization kinetics***



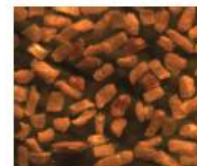
The near-spherical particle loses mass more slowly compared with the other two shapes, while the flake-like particle devolatilizes slightly faster than cylinder-like particle



(a) flake-like particle



(b) cylinder-like particle



(c) near-spherical particle



(d) poplar samples





Char conversion: burning rates

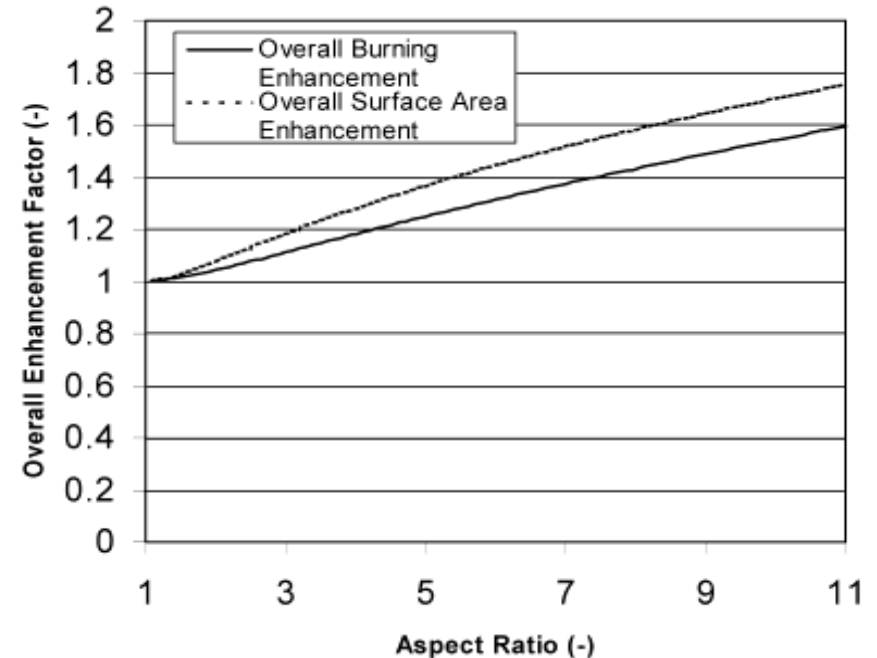
- **Effect of particle non-sphericity on burning rates**

- **BURNING ENHANCEMENT FACTOR** compared to a sphere with the same diameter

$$\Theta = \frac{0.3\psi + 0.7}{\psi} \quad \frac{dm_p}{dt} = -q\Phi_{en}A_p$$

- Based on observations from Gera et al. (2002) who found that the increase in surface area of a cylindric switchgrass particle was larger than the increase in the overall burning rate.

From Gera et al., Energy & Fuels, 2002



Calculated sphericity factor and burning enhancement factor if the aerodynamic properties are to be similar to a 60 μm coal particle.

d_p (μm)	ψ	Θ
200	0.34	2.4
300	0.12	5.7
600	0.03	23





Co-firing burner modelling

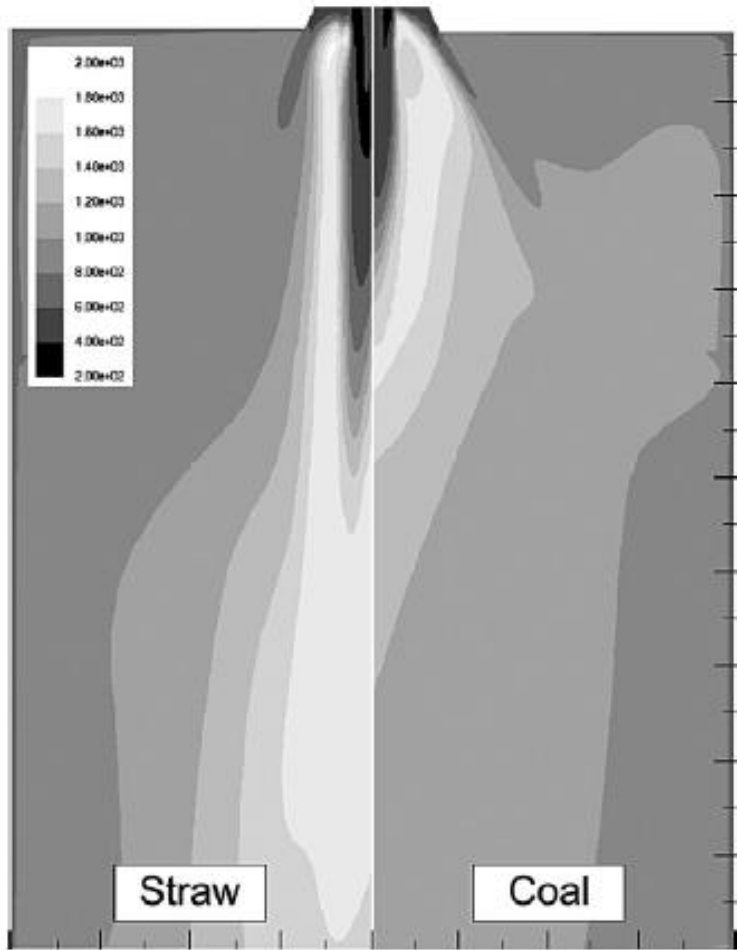
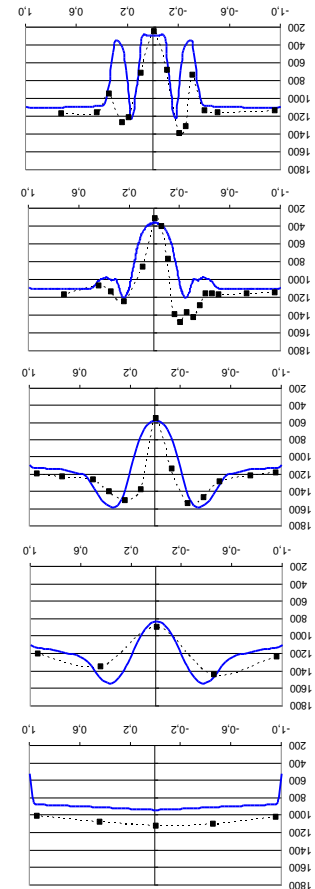
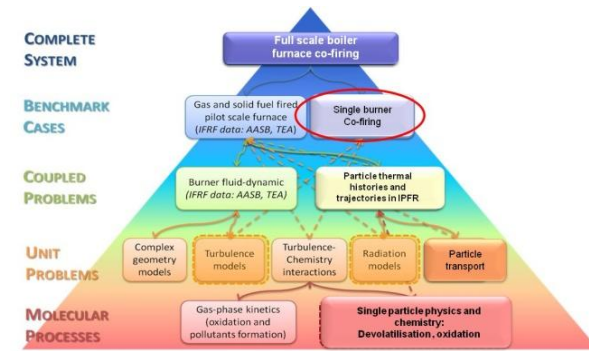


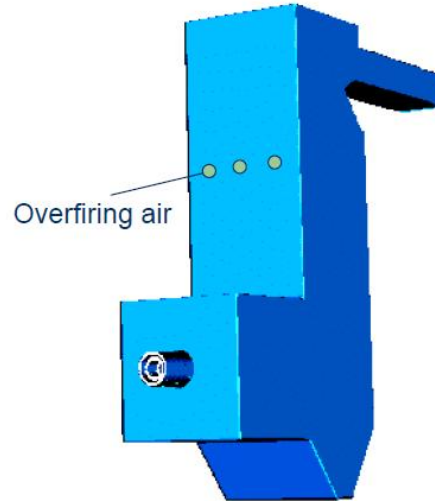
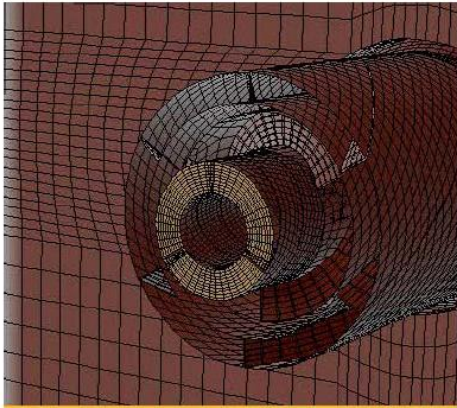
Fig. 6. Contours of temperature [K] on horizontal half plane. Grid: 4×10 m.



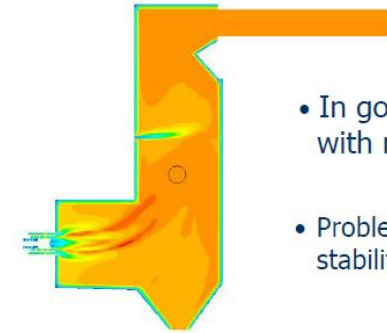
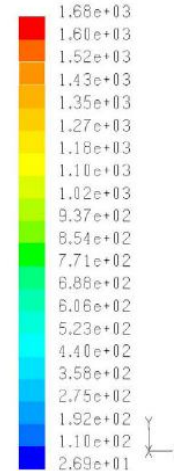


Comprehensive modeling of wood combustion: practical engineering solutions

Single Burner Furnace



Predicted Temperature – wood combustion



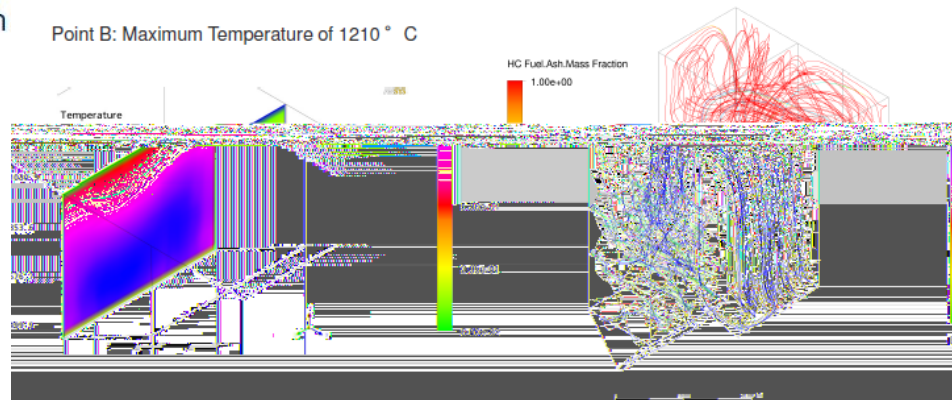
- In good agreement with measurement
- Problem of flame stability

Detailed triple-staged low-NC computational mesh

Temperature Profile

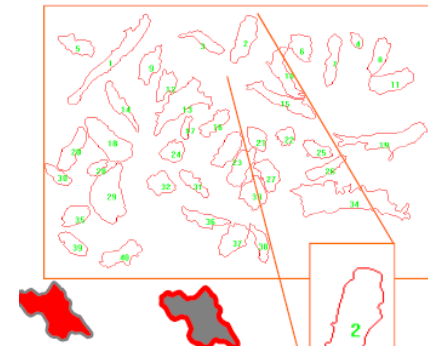
Point B: Maximum Temperature of 1210 ° C

Flow of Ash Particles

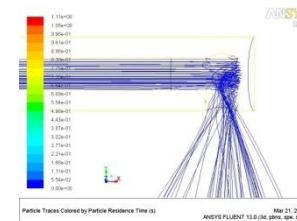


Concluding remarks (1)

- Biomass is strongly non-uniform fuel: particles are not spherical and their sizes, shapes and thermochemical properties are also strongly non-uniform.
Detailed characterisation needed.



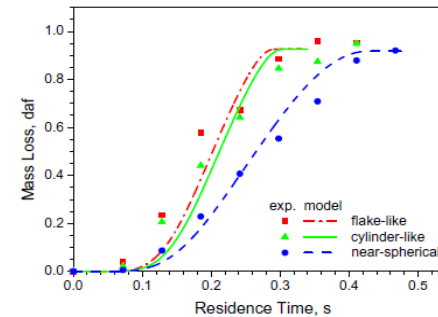
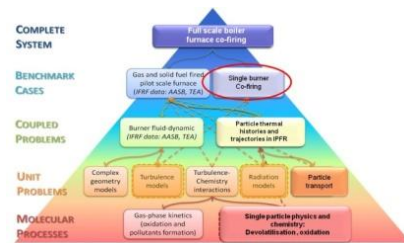
- Biomass/secondary fuel behaviour needs to be treated with specific **sub-models** to achieve predictivity: **non sphericity effects should be taken into account**
 - Particle transport and turbulence effects
 - Wall collision: slagging/shredding of deposits
 - Heat transfer: T vs time history
 - Effects on devolatilisation/oxidation





Concluding remarks (2)

- **Hierarchical approach** in comprehensive code validation is needed to assess the importance of non-sphericity both in single phenomena and in coupling effects -



- Comprehensive combustion codes are now potentially able to account for specific fuel properties (and their distribution as well) and to include detailed descriptions of different phenomena (including non-sphericity) but **prediction is still a challenge**





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