DEVELOPMENT AND QUALIFICATION OF PROCEDURES FOR THE CHARACTERIZATION OF SOLID FUELS IN CONVENTIONAL, COFIRING AND OXYFUEL COMBUSTION

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Introduction

There is constantly a raising need for wide and reliable data on solid fuel properties among utility operators, manufactures and scientists. Indeed the more stringent environmental legislation and the tendency towards the use of fossil and renewable fuels for electricity generation makes solid fuel combustion characterization of current interest. There are required parameters and indices for the assessment of fuel behavior, detailed fuel properties for utility designing, wide spectra of well-described experimental results for model validation in combustion, cofiring and oxyfiring systems. A qualitative description of solid fuel combustion should include detailed information about pyrolysis rate, devolatilization products (gas speciation, tar and soot formation) and the rate of char combustion. Additionally, information on the effect of burner design and operation on these parameters is needed. Experimenters should develop qualified methods for decoupling the main steps, studying them with sufficient accuracy and providing a limited number of significant parameters to allow modelers to simulate and optimize the process.

The main objective of this paper is to define procedures providing qualified data for quantitative prediction of operational/design parameters of industrial-scale combustion systems through Computational Fluid Dynamics simulations. Utilities and research needs are:

- fuel properties for enhancing flexibility of utilization;
- prediction of their impact on performance (e.g. efficiency, emission, corrosion, slagging);
- definition of quick and easy-to-use indices for design and operation;
- tools for predicting the behavior of heterogeneous fuels and blends;
- need of more sophisticated and detailed data/properties for predicting process performances and validating models.

Validation is an essential part of model development and this is done through:

- definition of parameters and model settings,
- collection of “in-flame” data,
- “ad hoc” experiments for sub-models,
- databases for fuel properties and fuel models.

Development of procedures for solid fuel characterization

Typically, fuels are characterized on a lab scale by the use of "traditional" analyses (see Table 1), useful for fingerprinting and comparing the fuel with others. Additional analyses can be performed on solid fuels to give more information and useful parameters: ash fusion; FTIR; maceral, NMR and chemical analysis. The evaluation of physical properties (size, shape, density, surface area, porosity, specific heat, conductivity, emissivity) is also important. All these properties should be defined for fuel and char particles as average and representative values in a preliminary approach. However a distribution of values can be more appropriate for advanced models that can study the population of different dimensional classes [1]. Size, shape, swelling factors and their distributions can be obtained. Variations may depend on the heterogeneous nature of the fuel, particle-to-particle differences, pretreatments (e.g., grinding and sieving).

Table 1. Activities of the virtual Solid Fuel Characterization Laboratory.

Solid Fuel Characterization Laboratory			
Unit	DICCISM-UNIPI	IFRF	CPR
Expertise	Experimental characterization on a Lab scale	Experimental characterization on a pilot scale	Data elaboration and model development
Activities	• Traditional analysis (ultimate, proximate, ash, heat value, morphology) • Devolatilization tests (FTIR) • Pyrolysis tests, tar and char analysis • Development of CFD models as diagnostic tools	• Sample preparation (milling, sieving) • Char preparation • High temperature and heating rate tests in IPFR (devolatili-zation, char oxidation, oxyfiring) • Solid Fuel DataBase	• Elaboration of exp. data • Model development • Kinetic models for devolatili-zation and char oxidation, structural models

The use of data obtained in mild conditions of temperature and heating rate, like those programmed in "traditional" lab scale apparatuses, is unsuitable for large scale plants applications. The effect of the operating conditions is not negligible, e.g., the volatile matter released during the devolatilization of coals and biomass fuels in drop tubes can be up to 30% higher than that measured in the proximate analysis [2]. Therefore, experimental procedures which utilize advanced facilities, that more closely simulate the actual combustion environment, should be used to test solid fuels. There is a general lack of quantitative information collected in reactors which operate in these conditions. Also uniform methodologies with the use of such apparatuses are not shared and standardized. Qualified procedures for solid fuel characterization are desired for providing useful parameters for large scale applications (advanced models, plant design and optimization) focusing on similar conditions of temperature, heating rate and residence time.

Expertises and specific activities in the Pisa group are listed in Table 1. Protocols for each activity have been developed to assure reliable data by verifying the

repeatability of the tests and reducing the experimental errors. Besides traditional lab-scale apparatuses, a pilot scale drop tube (Isothermal Plug Flow Reactor IPFR) is used to give conditions similar to those of large scale furnaces.

Equipment

The IPFR (Fig.1) is a drop tube (4.5 m total length x 0.15 m inner diameter) with fuel particles fed pneumatically at a certain height through one of the 19 lateral ports along the tube, the heating system is formed of electrical resistances (54 kW) along the tube and hot gases from the 60 kW burner at the top section of the reactor, solid residues and product gas are quenched at the bottom of the reactor and sampled on the collector probe for online and offline analyses. The high temperature (1400 °C) and heating rate (10^4 °C/s) of IPFR in the new asset of Livorno (IT), the qualification activities (upgrading of specific components and diagnostic tests) and the experimental procedures make it a superior facility for providing data and parameters for advanced models of pulverized fuel combustors as well as innovative plants (e.g., oxyfiring and gasification). The qualification of the IPFR is a continuous in-progress activity consisting in improving the reactor characteristics, verifying the performance and validating the reliability of data obtained. For instance, activities to eliminate or mitigate possible non-homogeneous points in the temperature gradients inside the reactor have been carried out or programmed, like mass flow controller check, electrical heater improvement, automatic regulation of carrier gas mix. This was done because the isothermal conditions of the reactor are a crucial issue to provide reliable data for combustion related investigation. Also the interpretation of the raw results requires some discussion on the balance of macro-products, that hardly closes, and the effective thermal history of solid particles, that may differ significantly from the nominal conditions of the reactor. Some protocols on that are discussed below.

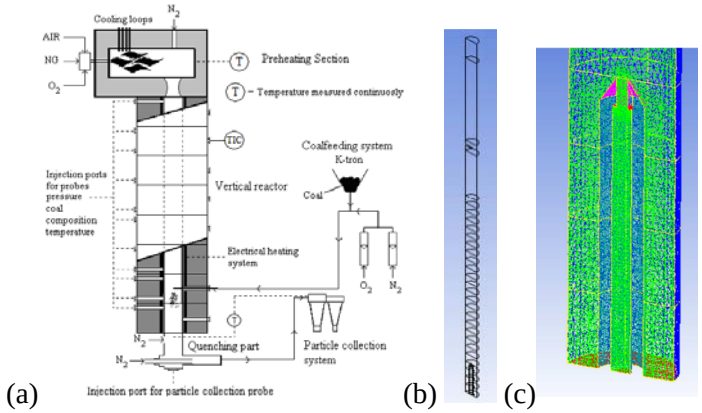

Figure 1. Sketch of the IPFR reactor (a), CFD model (b) and grid details (c).

Development of CFD model as a diagnostic tool

The CFD model was developed with Ansys 13, using the software ICEM for the grid generation and Fluent for the fluid dynamics simulations. Since the plane symmetry of the IPFR, it was chosen to model half of it, as shown in Fig. 1b-c. A preliminary grid independency study was carried out, leading to an unstructured grid with about 901000 elements.

Different levels of simulations were carried out as illustrated in the sketch of Figure 2:

- Single-phase runs (no coal feeding).
- Two-phase runs with non reactive particles
- Two phase runs of devolatilization and char oxidation.

The single-phase runs were used to understand the injection probe fluid-dynamics and the IPFR operations in terms of inner temperatures. Indeed temperature predictions were compared with measurements at different axial level in the reactor The non reactive two phase runs were aimed at assessing the effect of different modeling parameters on the particle trajectories. Finally the two-phase reactive runs were compared with devolatilization and char oxidation experiments. A post-processing tool was developed on purpose in order to extract from a single simulation conversion data at different location of the sampling probe.

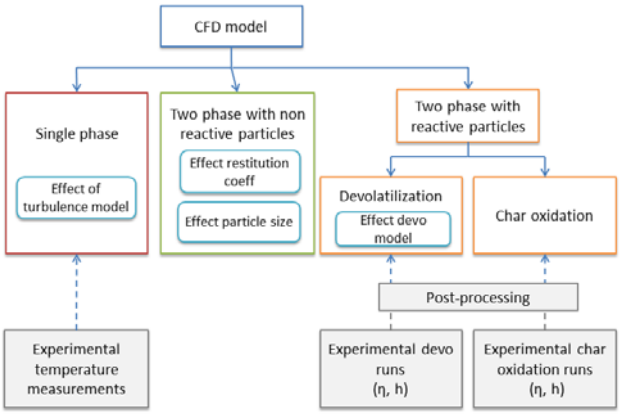

Figure 2. Scheme illustrating the CFD procedures.

Description of protocols

Protocol of conversion

The most common way to evaluate the conversion from devolatilization and char oxidation tests in drop tubes is to assume that a tracer remains constant during the test and uniformly distributed within the sample. If ash can be assumed thermally stable the ash tracer method can be applied. Otherwise, some elements (e.g., titanium that is a thermally stable element) can be used as tracers (see scheme in Fig.3). To avoid contamination of char samples with soot and condensed tar slightly oxidizing conditions can be used in pyrolysis tests (see also [3]). The characterization of solid fuels as received may be difficult because of its heterogeneity and the unexpected behavior of the smallest fractions (fines), that may concentrate ash in them. The fuel preparation (sieving) is then fundamental and narrow size ranges of particles should be studied. In all cases the quantification

of errors (from ash disomogeneity, fragmentation phenomena, vaporization and element ejection, see [4]) is fundamental.

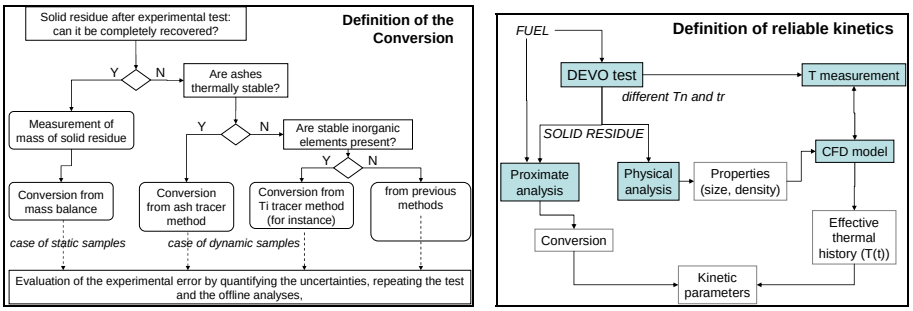

Figure 3. Protocol schemes for evaluating the conversion and the effective thermal history for kinetic elaboration in IPFR.

Protocol of the effective thermal history and elaboration of kinetics

Conversion data obtained for devolatilization and char oxidation tests in IPFR can be programmed under different nominal temperatures and residence times in the reactor. The High Temperature Volatile Matter released can be obtained, as well as kinetics at high temperature and heating rate. The physical properties of the fuel and solid residues are used as described in Fig.3, to evaluate the effective thermal history of the particles during the test by adjusting the CFD model of the IPRF. Kinetics can be obtained after choosing a suitable submodel:

- a single first order reaction model can be used in a preliminary step, because it is generally inaccurate to represent the conversion in all conditions, but it is recommended for its simplicity and to give indication of reaction time;
- lumped models (e.g., two steps reactions like Kobayashi model [5]) can be used to give a more accurate approach and predict the Volatile Matter released in different conditions (see example in Fig. 4);
- structural models (e.g., the Advanced Biomass and Coal Devolatilization model [6]) are more complex but give a detailed description of the entire range of conversion.

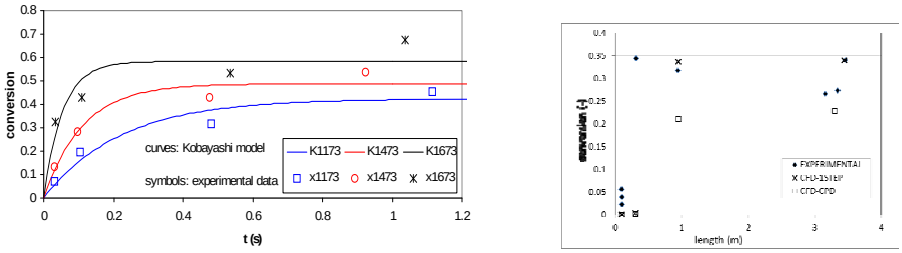

Figure 4. (a) Comparison of IPFR devolatilization results (under different reactor temperatures, expressed in K) of a SA coal and fit results with a two steps model; (b) comparison of CFD and experimental conversion data for devolatilization.

Fig. 4b shows a comparison of predicted and measured conversion coal of devolatilization at 900°C.

Discussion and conclusion

Innovative processes (Oxy-fuel, flameless, gasification) and new fuels (biofuels, wastes) are a challenge for mathematical modeling. Submodels accounting for solid fuel particle devolatilization and char oxidation, particle size and shape variations, tar/soot formation and oxidation, fate of ash and heteroatoms (N, S) should be developed and coupled in a comprehensive CFD model that must balance the sophistication, introduced by the submodels, with the computational capability. It is therefore desirable to provide reliable and qualified parameters for model validation in combustion, cofiring and oxyfiring systems. A comprehensive and detailed characterization of solid fuels can be performed in the Solid Fuel Characterization Laboratory, ranging from lab to pilot scale facilities, simple to complex models. Procedures for elaborating reliable and qualified indexes and model parameters have been developed and shared between experimenters and modelers. Some protocols and examples have been described in this paper.

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