VALIDATION OF OXY-FUEL COMBUSTION MODELLING VIA PILOT AND SEMI-INDUSTRIAL FURNACE TESTS

C. Galletti*, G. Coraggio, L. Tognotti*,****

leonardo.tognotti@diccism.unipi.it

* Dipartimento di Ingegneria Chimica, Chimica Industriale e Scienza dei Materiali, Università di Pisa, Pisa, Italy

** International Flame Research Foundation, Italy

Abstract

The modeling through computational fluid dynamics of oxy-combustion experimental tests in the semi-industrial furnace Fo.Sper equipped with the low NOx TEA-C burner is discussed with particular highlight on the approach. Since the complex geometry of the burner, a modeling strategy has been adopted to diminish the CPU time and thus make the simulatiosn affordable. The model aims at validating different sub-models (turbulence, radiation/spectral, kinetics) for the cases under investigation through the comparison of predictions and in-flame measurements of temperature and chemical species.

Introduction

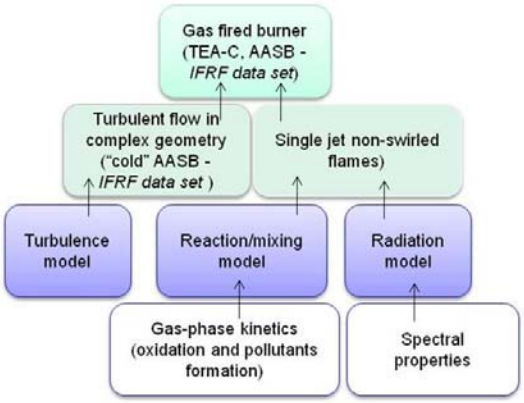
It is acknowledged that Computational Fluid Dynamic (CFD) could be an effective tool for the development of oxy-combustion at the industrial scale; however the use of CFD for the investigation and design of combustion systems faces some problems related to lack of rigorous validation of CFD models especially for the case of CO2-enriched atmosphere. This issue is very important as CFD sub-models for turbulent combustion (combustion models, kinetic schemes, spectral models) have been generally developed for air-combustion cases. Indeed one of the main research topic in oxy-combustion is the development of suited models for CO2-enriched atmosphere

CFD simulations at the industrial scales are computational demanding so that simplified models have to be generally adopted for the chemistry and radiative properties treatment. Global oxidation mechanisms are used, however they have been validated for conventional combustion. The substitution of CO2 to N2 in oxy-combustion may change the relevance of different elementary reactions thus changing the global rates 0. Andersen et al. 0 evaluated the performance the two-step mechanisms of Westbrook and Drier 0, WD, and the four-step mechanism of Jones and Lindstedt 0, JL, for predicting a plug flow reactor in both air and oxy-conditions. These global models are largely employed in conventional combustion simulations. The authors found that the prediction of CO levels was strongly unsatisfactory, so that suggested modification of the CO/CO2 reaction subset. Improved predictions were obtained especially for the WD mechanisms. Moreover

the authors recommend the use of finite rate approaches, such as the Eddy Dissipation Concept, to model the turbulence-chemistry interaction. Similarly Frassoldati et al. 0 optimised the JL scheme for oxy-fuel combustion by performing calculations in laminar counter-flow diffusion flames.
It is worth noting that most of the sub-models are tested on lab-scale devices, numerically and/or experimentally. However there is need of validating them directly at the largest scales were different effect may arise.
To this purpose IFRF is investigating both numerically and experimentally oxy-combustion flames in semi-industrial systems following the Verification & Validation approach 0 0.
In the present work, CFD simulations of experiments conducted with a low NOx burner installed in the FoSper furnace, a replica (placed at the ENEL experimental facility of Livorno, Italy) of the IFRF furnace n.1, in both air and oxy-fired conditions 0 are performed with the software Fluent 6.3. by Ansys Inc.. So far the furnace has represented a reference case for a number of modelling activities with commercial and in-house codes during the last years. However, no formalized procedures have been provided in such studies, for the assessment of the level of agreement between experiments and simulations.

Verification and Validation approach

The approach followed is fully described in recent IFRF Reports [8]. The concept is based on the proper Design of Experiment (DoE), that is necessary for developing a joint experimental and modeling activity. In other words, in planning semi-industrial scale campaigns, one should try to answer the following questions before to design the experimental matrix: what data and information is needed for modeling, and what is needed for validation? Within the validation activity, we want to quantify the level of agreement between the experimental data and computational results with quantifiable metrics and taking into account uncertainty in the experiment and in the model.



The validation activity can be performed at different levels of complexity that can be derived from the complete system through the construction of hierarchies which decompose the system of interest into levels of decreasing complexity. The construction of hierarchies can also help in designing validation experiments (see the example in figure for oxy-natural gas tests in furnace #1).
The errors associated to experiments (intrinsic, statistical errors, measuring position) have been discussed in [8]. The modelling approach should take into account the

existence of "scenario" uncertainties (heat fluxes/temperature at the furnace wall), the complexity of the burner that needs grid reduction strategies (numerical solution error), the proper choice of kinetic and radiation submodels (modeling uncertainties), and finally some criteria of comparing experimental results and model predictions (validation metrics: quantitative evaluation of agreement between experiments and model predictions).
In the following the application of the validation approach is described on the experimental campaigns on air and oxy-fuel combustion with NG in Fo.Sper furnace equipped with a low NOx burner, TEA-C[9].

Experimental facilities [9]
The Fo.Sper furnace has an internal square cross-section of 2 x 2 m, is approximately 6.25 m long and is made of 11 independently water-cooled refractory-lined sections. Seven cooling loops are used to extract sufficient energy from the combustion chamber to maintain a temperature history comparable to a radiant section of a full-scale boiler operating with air. The TEA-C is a Low NOx burner used in industrial utility boilers; to allow the testing on the Fo.Sper furnace, a reduced dimension prototype of 3MW thermal power was used. In this prototype air feeding is done by a wind-box with a vertical entrance, the air goes into the burner through two separate ducts called secondary and tertiary both having an axial movable swirler and a damper that controls the flow rate distribution. The primary duct, positioned on burner axis, provides the air/coal mixture to the combustion chamber with pulverized coal experiments (not considered in the present studies). It is equipped by an internal axial swirler and a nozzle which makes a separation between coal rich and lean jets in order to enhance the in-flame NOx reduction effect. The primary air flow is maintained active even with NG configurations. For the NG firing operation, 8 lances inject the fuel through nozzles having two holes with an axis which forms a 45 degrees angle with the burner axis.

Numerical model
The numerical model was developed with Fluent 6.3 by Ansys Inc. The grid was created with the software Gambit. Due to the burner/furnace symmetries, just one quarter of the furnace was modeled in order to decrease the CPU time of the simulations. A fluid domain were used fro the burner and the furnace, whereas the cooling loops were modeled as solid domains with a square cross section of perimeter equals to the circular section of the real loops. This was made in order to allow setting heat extraction BCs from the cooling loops, thus using available measurements on heat flux.
Due to the complexity of the burner much effort was devoted to the optimization of the grid. In particularly, two domains were chosen:
- a *complete domain*, in which the burner was represented in all details;
- a *reduced domain* in which the burner was "cut" by representing just a portion of the secondary and tertiary ducts.

The idea is to perform preliminary runs on the complex domain in isothermal conditions an thus to use obtained velocity an turbulence profiles to set proper BCs at the primary an tertiary duct inlets on the reduced domain.
Grid independency studies were applied to both domains. The complex domain leaded to an hybrid grid consisting of 4.5M cell, whereas the reduced domain leaded to 3.4M cells. The grids, which are both hybrid and show
special refinements near the burner, are depicted in Figure 2.

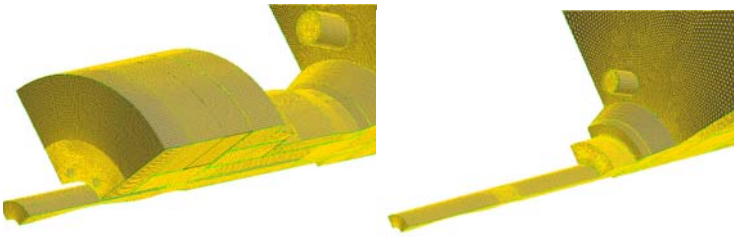


Figure 2. Details of the grids for the (a) complete and (b) reduced domains.

Physical models and validation procedure
In the framework of oxy-combustion experiments in the Fo.Sper furnace, important validation aspects regard:
- the geometry, due to the complexity of the burner;
- the choice of the turbulence model, due to the presence of swirled flows;
- the choice of the combustion model/kinetic mechanisms;
- the choice of radiation/spectral models.

Moreover some boundary condition (BCs) have to be properly set as not directly available from the experimental campaign. This is the case of air leakage, which unavoidably occurs when retrofitting existing air-fired furnaces to oxy-fired conditions. The amount of air leakage is reconstructed by performing mass balance on the system based on the flue gas composition, however uncertainties still exists on the location of the air leakage. It is assumed that air leakage is fed with the primary and secondary recycled flue gases stream. Logically, this procedure has to be validated.
For the BCs at the walls two options were investigated: a wall temperature profile (and emissivity) from measurements and an heat flux obtained from an energy balance on the overall furnace.
According to the above points, a modeling program was defined and this is illustrated in the scheme of Figure 3. This consisted mainly of 4 steps:

1) In the first step, isothermal tests in air (with velocity measurements) were used to analyze the suitability of specific turbulence models. The standard k-e turbulence model was compared to the SST k-w model and to the Reynolds Stress models, which are more suited for the for the swirled flows under investigations. The simulation of such tests was performed with the complete domain.

2) In the second step, BCs from gaseous combustion experiments (mass flow rates, species concentrations and temperatures) were used to set non reacting simulation with the complete geometry.
3) In the third step, the same simulations of step 2 were performed on the reduced geometry. To do that, velocity, temperature, species mass fractions and turbulence characteristics profiles were extracted from the simulations of step 2 as set as BCs to the inlets of the secondary and tertiary ducts. If such approach is correct, velocity profiles inside the furnace obtained with simulations of steps 2 and 3 should coincide.
4) In the fourth step gas combustion tests are simulated with the reduced domain. Inlet BCs are obtained from previous step. Different conditions are considered: air-fired and oxy-fired with R = 0.69, even though the case with R = 0.61 is planned for the near future. Simulated results are compared with available measurements of temperature and species concentrations inside the furnace. The NG fuel is modeled as a mixture of CH4, C2H6, C3H8, N2, CO2.

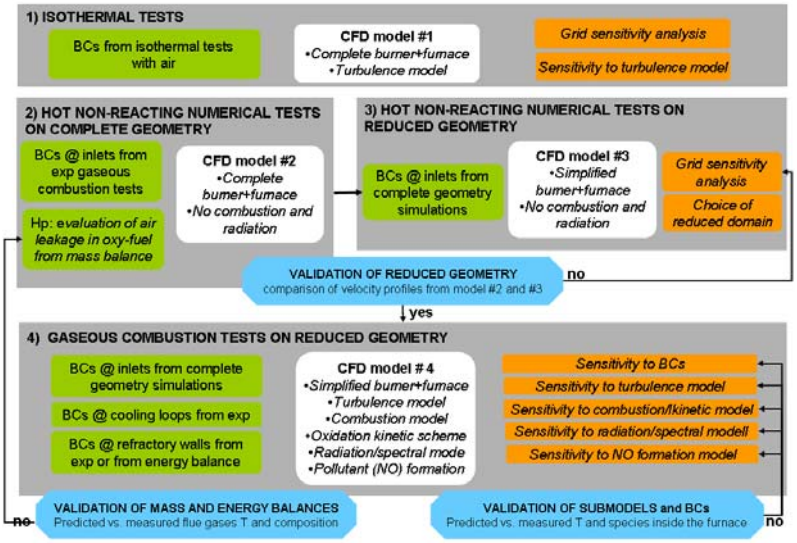


Figure 3.

The global kinetic mechanism of Westbrook and Drier 0 consisting of fuel oxidation (CH4, C2H6, C3H8) to CO and subsequently oxidation of CO to CO2 is employed and will be denoted as WD. The modified version of such mechanism for the oxy-combustion case proposed by Andersen et al. 0 is also tested and will be denoted as WDoxy.
Different turbulence/chemistry interaction models were used: the Eddy Dissipation Model (EDM) 0 the Eddy Dissipation Concept (EDC) 0 and a combined Eddy Dissipation/Finite Rate model (ED/FR). In the EDM model the chemical reactions are governed by turbulent mixing so that reaction rates are expressed as a function

of the turbulent characteristics. To account chemistry effect, in the ED/FR model, both a mixing rate and an Arrhenius rate, based on the mean properties, are evaluated and the smallest one is chosen as the mean reaction rate for the reacting species. However, the ED/FR model can handle only global kinetic mechanisms, being the turbulent rate the same for all the reactions. According to EDC, combustion occurs in regions ("fine structures") of the flow where the dissipation of turbulent kinetic energy takes place; such regions are treated as perfectly stirred reactors (PSR) and their characteristics are provided by a step-wise energy cascade model. EDC allows accounting more detailed schemes. The P1 radiation model is employed with spectral properties evaluated through the WSGG model available in Fluent 6.3u. It is well known that WSGG parameters have been derived for air combustion cases so in future it is planned to vary such parameters as proposed for instance by Johansson et al.
The second order discretization scheme was applied. To help solution convergence, such a scheme was initialized on results obtained with a first order scheme. Convergence was ensured by all residuals below 10^-5, except for the continuity equation for which residuals were of about 10^-4. Moreover the stabilization of physical quantities was monitored at different location inside the furnace. The level of agreement between experiments and prediction is evaluated through the use of error validation metrics.

Results and Discussion

Validation of reduced domain

Firstly the reduced domain (see scheme of Figure 3) was validated through comparison of velocity profiles obtained at different axial distances in the furnace with the completed domain. Figure 4 shows such comparison for the axial velocities. It can be noticed that the agreement is satisfactory, thus allowing operating with the reduced domain in order to decrease the computational time.

Effect of BCs, combustion model, kinetics and radiation model

As far as reacting runs are concerned, simulations highlighted the importance of setting proper BCs based on experimental data. In particular simulations were made with the EDM combustion model whose performance will be discussed in the following sections. Temperatures predicted with the hypothesis on the heat flux were strongly over predicted, far from the furnace axis, thus indicating wrong BCs at the refractory walls. It should be said that predicted flue gas temperatures were in agreement with measured ones, thus indicating that the energy balance was correct. The knowledge of a temperature profiles along the furnace walls lead to a strong improvement of predictions. Therefore wall temperature measurements are very attractive for validating the numerical model.

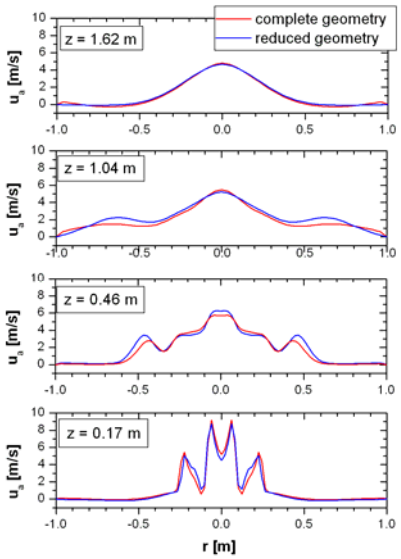


Figure 4. Comparison of axial velocity profiles predicted with the reduced and complete domains at different distances from the burner quarl.

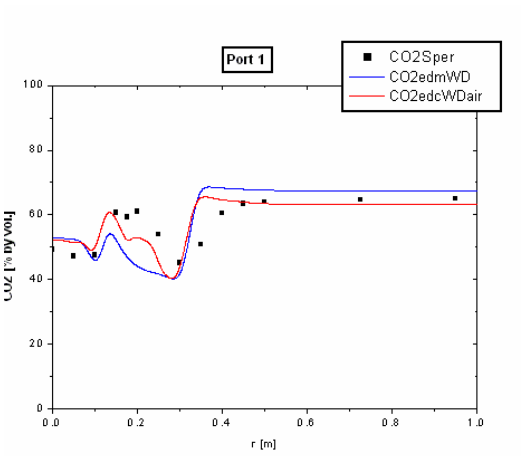
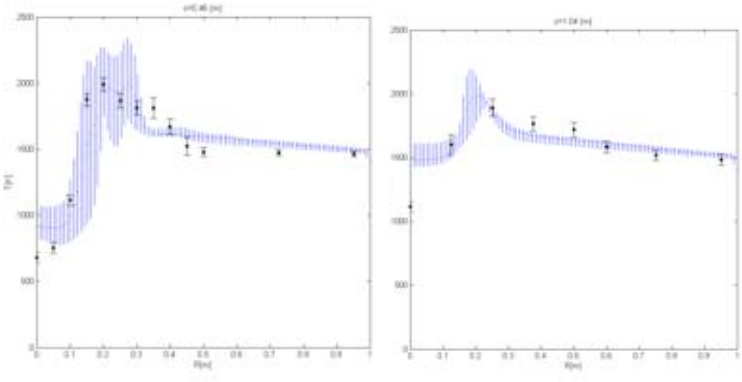


Figure 5. Comparison between radial profiles of measured of CO2 with those predicted with two different combustion models and kinetics.

Figure 5 compares the measured radial profiles of CO2 with those predicted with two different combustion models. It can be noticed that temperature measurements at the first port (z = 0.17 m) show well defined peaks indicating a flame front: such peaks are not detectable by the EDM combustion model. Figure 6 finally compares temperature profiles at two in-flame ports, including the modeling and experimental uncertainties.The work has shown that the turbulence/chemistry interaction treatment plays a major role in determining the temperature and species flow field, thus indicating the inadequacy of fast chemistry approaches. A satisfactory agreement was found between experimental and predicted temperatures, CO2 and O2 profiles. Great discrepancies were found



on CO, and this may be due to the poor capability of global schemes such as the WD schemes. Slightly better results were obtained with the WD scheme modified for oxy-fuel conditions by Andersen et al. 0, however future work will consider more kinetic schemes and will concentrate on pollutant emissions.
The validation procedure faces some criticism, when applied to semi-industrial devices, especially because scale of the burner/furnace requires significant demanding grid. so that efforts are needed in order to optimize the computational time. Other issued not shown in the present paper regard the air leakage unavoidably occurs when retro-fitting existing air-fired furnaces in oxy-combustion. Provided that the amount of air leakage can be reconstructed from available measurements on the flue gas composition by performing a mass balance, the location of the air leakage cannot be known precisely and have to be assumed.

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