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COLLOQUIUM I

Pollutants Formation and Reduction

I - 1

Innovative Regeneration Strategy for a Soot Trap Coupled to a TPOX Reformer

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This work investigates an innovative idea to remove soot from inside a syngas mixture which doesn't contain oxygen, produced by TPOX (Thermal Partial Oxidation) reforming and used to feed a SOFC (Solid Oxide Fuel Cell).

The basic purpose behind this study is to increase the lifetime of the SOFC, obviously later to avoid aerosol's emissions in the environment. Soot is in fact poisonous for the Fuel Cells and its presence at the anode of the FC is undesirable.

Experimental tests are here proposed in order to show the possibility to gasify particles using directly gases into the reformed mixture (CO_2 and H_2O first of all), without any oxygen addiction, leading the system to very high temperatures up to 800°C.

The results obtained are very promising, showing relatively fast gasification of soot produced and retained by the filter. Some evidences are shown in this article too, in order to prove the theory hypothesised, monitoring the gases at the inlet and the outlet of the trap.

The main goal of this study was to propose a new concept to remove soot applicable to systems based on the Fuel Cell technologies or other fields using syngas as vector of energy (e.g. biomass gasification). More experiments are however necessary to clarify better the kinetic of the reaction.

I - 2

Catalytic Soot Combustion via Earth Alkaline Doped Ceria

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The catalytic activity of cerium oxide towards the combustion of carbonaceous materials at low temperature has been widely investigated, mainly in the area of diesel soot emission control. Catalysts suitable for promoting low temperature combustion of carbonaceous materials may indeed be applied in the traps designed for the abatement of diesel particulate, which is one of the most harmful pollutants emitted by diesel engines. In literature it is also well know as the CeO_2 decrease its catalytic property in a relatively short time of use. To stabilize the catalyst during a longer period towards solid carbonaceous materials oxidation, the cubic lattice ceria was doped by earth alkaline metals like: Ba, Ca, Sr, Mg. The work explains the role of earth alkaline doping into the basic material lattice with a XRD and BET analysis. The catalytic activity of the doped catalysts, before and after a specific ageing protocol, was investigated with the TPC test and the activation energy was calculated for each reaction using the Starink method after DSC runs at different heating rate.

I - 3

Characterization of Particulate Emissions from Common Rail Diesel Engine

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The loading of a DPF entails the need of trap regeneration by particulate combustion, whose efficiency and frequency are somehow affected by the way soot is deposited along the channels. Great efforts are thus spent to improve the understanding of the filtration process of DPFs, aimed at obtaining a deeper insight into the relationship between engine performance and filter loading so as to take advantage of this insight for DPF design and optimization purposes. Small lab-scale 300 cpsi DPF samples were loaded downstream the DOC in an ad hoc designed reactor capable of hosting 5 samples with part of the entire flow produced by an automotive diesel engine at the 2500x8 BMEP operating condition, selected to be representative as one of the critical engine points of the NEDC. Soot layer thickness was estimated by means of FESEM observations after sample sectioning at progressive locations, obtained through a procedure defined not to affect the distribution of the soot inside the filter and to enable estimation of the actual soot thickness along the channel length. This is a pre-requisite to get suitable data for the validation of the DPF models required for trap design and optimisation.

I - 4

Investigations into the Formation of Soot Particles

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Empirical intermolecular potentials and a 'basin-hopping' optimization scheme are used to investigate the formation of soot particles from clusters of polycyclic aromatic hydrocarbon (PAH) molecules. Accurate intermolecular binding energies for small PAH molecules obtained from *ab initio* SAPT(DFT) calculations are compared with empirical intermolecular potentials parameterized from experimental data. Basin hopping geometry optimization of PAH clusters based on a simple Lennard-Jones plus point charges model combined with image projection to simulate TEM images reveals structures which are not dissimilar to those found by experiment.

I - 5

Perturbations Studies on Incineration of Sewage Sludge Spiked with Chlorinated Hydrocarbons

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Upset conditions occurring during the incineration are generally responsible of the production of intense emissions, which can continue until the perturbation persists. These conditions are due to instantaneous alteration of the composition of the feed stream or modification of the combustion chamber parameters (temperature, oxygen availability) and are responsible in the formation of products of incomplete combustion (PICs). A laboratory study was performed aimed at investigating the formation of hazardous organics during puffs formation during incineration of sewage sludge. Puffs production was simulated by means of an instantaneous injection of a surrogate organic mixture (SOM), constituting of 20% of toluene, 25% of chlorobenzene and 55% of tetrachloroethene, before or after the first thermal chamber.

Results evidenced that (i) many chlorine containing-compounds are formed, being their abundance dependent on the SOM injection point, (ii) among the chlorine-containing PICs there are aliphatic as well as aromatic compounds, (iii) the destruction of SOM components is dependent on the SOM injection point up to the reactor temperature of 700°C while above such a temperature it is independent from the injection point and (iv) benzene is a typical PIC from sludge combustion and its abundance is highest in the temperature range of 700-800°C. Finally, the laboratory investigation confirmed that perturbations are responsible of the appearance in the emissions of a spectrum of organic contaminants whose presence is strictly correlated with the destruction.

I - 6

Charge Distribution of Flame-Generated Nanoparticles

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We measured the size and charge distributions of incipient nanoparticles in ethylene-air laminar premixed flames below the onset of soot. We found that the measured fraction of positively and negatively charged particles was equal and well-predicted by the Boltzmann distribution, which depends only on size and temperature. In flames that produce a unimodal size distribution (SD) that does not show significant growth, the temperature of the Boltzmann charge distribution that best fits the measurements is the flame temperature (1700K). Instead, in flames that eventually produce bimodal SD, larger particles have a Boltzmann charge distribution that coincides with the cooler temperatures within 1 mm of the probe surface (1200 or 1000K) while smaller particles retain their 1700 K Boltzmann charge fraction. This observation strongly suggests that the particles with a 1700 K Boltzmann charge fraction had to be formed in the flame front and could not have nucleated in the cooler region near the probe; otherwise, their charge fraction would have a cooler Boltzmann charge fraction. Also, the smaller particles do not coagulate in the cooled flame environment prior to entering the probe while the larger particles do, thus reducing their charge fraction to the temperature of their last coagulation events.

I - 7

Novel Technology for the Abatement of NO on Cu-ZSM5 Catalysts

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This paper is focused on the scale-up of a powder Cu-ZSM5 to a structured reactor for the catalytic decomposition of NO under dry and wet conditions in the temperature range 400-550°C. Cu-ZSM5 has been deposited on cordierite monoliths by dip-coating technique using colloidal alumina or silica as binders with different zeolite/binder ratios in aqueous suspension determining the parameters to obtain the best adhesion and mechanical resistance of the washcoat layer. The monolithic catalysts have been investigated by morphological (SEM), physical (BET and porosity), chemical (ICP/MS, EDX, H_2 TPR) analysis. Results have been compared with those obtained on the corresponding Cu-ZSM5 powder sample with the same copper content and Si/Al ratio in order to define the effect of the preparation procedure on the chemical and catalytic properties of copper.

Structured catalysts show a lower intrinsic activity in NO decomposition compared to the powder sample associated to the formation of inactive CuO in addition to exchanged copper. Nevertheless, they have a higher hydrothermal resistance likely related to an inhibiting effect of both silica binder and cordierite support which prevent copper migration promoted by water vapour at high temperature. This feature makes the structured catalysts more suitable for application under real conditions.

I - 8

Numerical Evaluation of Seawater Scrubbers Efficiency for Exhaust Gas Desulphurization

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The paper focuses on desulphurisation process of exhaust gas from a marine diesel engine in a wet scrubbing system using seawater. An unsteady numerical method has been created in order to quantify the amount of sulphur dioxide absorbed in a single spherical seawater droplet from flue gas. Transport equations for species inside the droplet are solved on a non-uniform computational grid. In the model is supposed that droplet and flue gas move in counter-current. Kinematics of the droplet, heat exchange and vaporisation have been considered. Sulphur dioxide penetrates into the droplet and reacts with seawater alkaline species. This process has been modelled with a global and infinitely fast reaction mechanism. Droplet evaporation implies a diameter reduction in time so, having used a grid with a fixed numbers of nodes, a numerical method has been employed in order to update species concentrations on nodes in the new positions: the computational grid is regenerated at every time step. SO_2 absorption has been studied in different conditions in the scrubbing process: flue gas temperature, flue gas velocity, starting droplet size and velocity.

I - 9

A Simplified Approach to Model Fine Particle Formation in a Annular Combustion Chamber

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The emission of particles from aircraft engines is becoming an environmental issue and many research programs have been set-up to develop cleaner aircraft propulsion technologies. In this framework, computation fluid dynamics are gaining ever more importance as a tool that can be used to verify the results of costly test measurements and even to predict them. In the present paper we report on the development of a numerical code specifically set-up for the modeling of aviation turbine now used also for the prediction of pollutant formation and emission: the AVIO in-house code Body3D. The focus of the paper is on the implementation of a simplified soot formation model that is required to be fully coupled with the radiative balance equation in order to give simultaneous computation of the temperature and soot concentration fields. The model uses a detailed kinetic mechanism of oxidation and pyrolysis of hydrocarbons coupled, through a flamelet approach, to a k-ε based fluid dynamic code. A simplified model based on the prediction of aromatic precursors by the detailed chemistry mechanism and acetylene addition is used to predict soot. The model is used to predict flow velocities, temperature and soot volume fraction in a bi-dimensional combustor which represents a section of a complete annular combustion chamber. Model results are compared with experimental results reported in the literature.

I - 10

Vapor Condensation for Particulate Abatement

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The reduction of particulate emission is among the most challenging problems of pollutant reduction research. This is due to very low efficiency of conventional separators, such as electrostatic precipitator, cyclone wet scrubber, in the collection of ultrafine particles. To increase the diameter of fine and ultrafine particles by means of condensation of water vapor on the particles themselves seems to be a promising technique for industrial applications. Although several data are present in literature in the field of meteorology, cloud physics and aerosol science on nucleation and growth of droplets on foreign nuclei, a systematic analysis of the dependence of the process on parameters relevant from industrial point of view is not yet available. As a matter of a fact, a thorough understanding of temperature, partial pressure, properties of solid nuclei, strongly affecting the characteristic time and the efficiency of heterogeneous nucleation, are still lacking. In this paper a summary of the main physical relations governing the nucleation process and the criteria used in the design and set up of an experimental apparatus, realized for the study of heterogeneous nucleation on submicronic particles in different conditions, are presented.

I - 11

Laser Desorption/Ionization Techniques in the Characterization of Combustion Related Carbonaceous Materials

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Laser desorption/ionization techniques coupled with mass spectrometry analyzers have evolved rapidly in the recent years and are currently capable of providing valuable information about the chemical composition and structure of very high molecular weight species, mainly biopolymers or synthetic polymers.

Recent advances have been done on the application of this technique to carbon-containing species relevant in combustion, however, a thorough understanding of the desorption/ionization process is important for a correct spectra interpretation and for further improvements of the technique.

In the present paper, the effect of main experimental parameters on mass ranges detectable by laser desorption/ionization techniques has been investigated for standard aromatic molecules, like polycyclic aromatic hydrocarbons (PAH), fullerenes, polyacenaphthylene (PACE) and for complex carbonaceous materials like heavy fractions of fuel oils and combustion-formed particulate.

In particular, it has been shown that laser power (or more specifically, the surface power density of the laser spot, named laser fluence) as well as the surface concentration of samples are crucial parameters controlling the highest detected molecular weight range.

I - 12

Picosecond and Nanosecond Laser Ionization For the On-Line Analysis of Combustion-Formed Pollutant

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A novel apparatus based on Time of Flight Mass Spectrometry (TOF-MS) was recently developed and successfully applied for the on-line analysis of light gases and polycyclic aromatic hydrocarbons (PAH) from atmospheric pressure combustion systems.

In this work, in order to increase the detection mass range of combustion-formed species and to reduce the parent peak fragmentation caused by hard ionization through electron impact, laser sources have been employed for ionization.

A Nd:Yag Nanosecond laser at two different wavelengths, corresponding to the forth and the third armonic (266 and 355 nm, respectively), have been used allowing to detect PAH and water clusters up to 3000 u. The water clusters allowed obtaining a calibration of the system in a molecular weight range much larger with respect to that obtained with standard molecules generally used for this purpose .

In this work, also a preliminary application of laser pulses in the picosecond range was tested in order to further reduce fragmentation and increase ionization efficiency.

I - 13

Modeling of Size Distribution Functions and Chemical Structures of Combustion-Formed Particles

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The formation of soot in combustion is a complex process involving gas-phase chemical kinetics, heterogeneous reactions on the particle surface and particle dynamics. Modeling of these processes in combustion environments has received great attention and, today, they are able to approximately simulate the concentration and size distributions of particles in many combustion conditions. Next generation models need to predict also their morphology and chemistry in order to better predict particle radiative properties and health effects.

The present paper presents a first approach to follow chemical evolution of the particles formed in premixed flames by simulating both molecular growth and H/C variation of the particles along the flame axis. A double discretization of the particle phase is performed. Carbon number ranges from 24 to $4X10^8$ whereas H/C for each carbon number ranges from 0 to 1. Twenty five sections are used in a geometric series with a carbon number ratio of two between sections. Five sections are used for H/C variation. Overall 125 lumped species for the stable form and 125 for radicals are modeled.

The kinetic mechanism has been tested to simulate slightly-sooting premixed flames of ethylene/oxygen and benzene/air for which a large set of experimental data exists.

I - 14

An Experimental and Numerical Study of Particle Inception in Slightly-Sooting Premixed Flames of Benzene and Ethylene

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Characterization of the nascent particles and of their transformation in different flame conditions is crucial to understand the mechanism of particulate formation. In rich premixed flames a bimodal particle size distribution function has been generally observed. The modal peak larger than 10 nm is generally attributed to soot, whereas the origin and evolution of the smaller particle mode, with typical size of 2-3 nm, is still controversial. Particles formation process can also depend on flame temperature or fuel composition.

The object of the present work is to perform a comparative experimental and modeling study on the effect of fuel chemical structure on particle inception in rich premixed flames. A benzene and an ethylene flame forming comparable amounts of soot have been studied by means of situ optical techniques. Modeling of flame structure and particle formation is performed by using a complete detailed scheme for gas phase and particles reactions. The experimental and model results suggest that in benzene flame particle inception is localized across the flame front and does not continue in the post-oxidation region of the flame due to the consumption of benzene and acetylene. Soot inception is related to particle aromatization followed by coagulation. On the contrary in the ethylene flame, the large presence of benzene and acetylene downstream of the flame front makes possible particle nucleation also in the post-flame zone. In this case soot inception seems to be controlled by particle coagulation more than to precursor aromatization.

I - 15

Diagnostic of Combustion Sources by means of Air Quality Analysis

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In the last years air pollution problems with PM have become more critical and atmosphere research demands a great deal of study and comparisons between emission measurements and immission concentration. In this work a coordinated approach tend to compare PM2.5/PM10 sampling and chemical analyses at the emissions with the corresponding particulate matter in the areas surrounding industrial sites.

Monitoring and chemical characterization of PM10, PM2,5 and size distribution in industrial areas influenced by stationary sources has been undertaken in order to define major sources of impact. The inorganic (metals, anions) as well as organic components of secondary aerosol have been characterized to go deeper into the relation between combustion sources and air quality.

ENI R&M has started in its sites a 24-hour PM10/PM2.5 samples collection during campaigns carried out since 2007 using low volume CEN-equivalent samplers equipped with certified PM (particulate matter with aerodynamic diameter lower than 10 and 2.5 □m) inlet. Simultaneous samples have been collected during a campaign carried out in 2008. QA/QC procedures were strictly followed in order to collect reliable data.

Difference in average concentrations as well as episodes are discussed versus primary sources and fuel usage and meteorological effects.

Fingerprinting models are also applied to the data collected in industrial areas within the program of research funded by ENI R&M. The state of the art of the study is presented.

I - 16

Pollutant Emissions from Different Burners: Synthesis of the Activity in the Last Decade

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A long term experimental investigation has been carried out by the Combustion Laboratory of the Department of Energy at Politecnico di Milano in the past, aiming to study the effect of initial fuel-air mixing on NOx and CO emissions in non-premixed natural gas flames. The present paper reports the main results on exhaust emissions characteristic of different burner typologies and attempts to explain them through the thermal and aerodynamic field measured in the flame. Pollutant emissions have been measured in non-premixed swirling flames generated with two different fuel injection strategies. Representative results have been reported and compared with those of partially premixed flames from the same burner and those of fully premixed flames from different burners. The analysis of these measurements suggests that low EINOx values can be obtained in the very lean regime for all cases, except the non-premixed swirl flame with axial injection. However, stable and safe operation of very lean flames is not easily achieved and requires careful optimization of the fluid dynamics of the burner. The results of the partially premixed configuration indicate that this strategy could be effective in reducing pollutant emissions in existing swirl burners and should be investigated more in detail and in a wider range of equivalence ratio of the central tube mixture.

I - 17

Mass Spectrometry for the Investigation of Combustion Generated Nanoparticles

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Unlike other methods, photo ionization mass spectrometry (PIMS) offers the possibility to record spectra ranging from precursor molecules in the gas phase well into the regime of young soot. In order to use this feature for the elucidation of formation mechanisms some precautions have to be considered.

(i) Combustion generated nanoparticles can be very reactive. Hence coagulation in the sampling line must be minimized by a suitable design.
(ii) Fragmentation upon laser irradiation can be severe. Therefore, only low photon fluences can be used leading to losses in sensitivity.
(iii) Due to lack of calibration substances, concentration calibration can at best be achieved by complementary methods such as DMA.
(iv) Mass discrimination in the MS can distort measured size distribution functions.

Within these limitations a variety of features could be shown for combustion generated nanoparticles by using PIMS.

- They are formed in two distinct modes, A, B.
- Mode B shows a microcrystalline structure and a work function (ionization potential) which is decreased relatively to molecules.
- It is composed of layers of pericondensed PAHs, shows virtually no growth and a low reactivity towards O_2.
- Mode A, on the other hand, exhibits a very low fragmentation threshold and allows only very small fluences for fragment free ionization.
- Inside of flames it shows a rapid growth. Towards O_2 it is very reactive.

Studies on the formation mechanism of mode A are underway.

I - 18

Atmospheric aerosol characterization in the urban area of Napoli

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A systematic study of atmospheric aerosols in the Urban area of Napoli is presented; it is based on a set of data collected over nine years (from 2000) of Lidar measurements at the Napoli lidar station (40°50' 18''N, 14°10' 59''E, 118 m asl).

The Lidar technique is able to give information about the vertical distribution and to retrieve aerosol optical properties, like backscattering and extinction coefficients, scattering ratio, angstrom exponent and lidar ratio. Measurements have been performed systematically twice a week providing information about aerosol optical properties with a final spatial resolution of 60m and a temporal resolution of 30 min. Additional measurements have been carried in order to study: -Saharan dust transport events; - complete diurnal cycles of aerosol layers and the correlation with local atmospheric circulation phenomena; - Etna volcanic eruptions; - urban and rural sites intercomparison.

The seasonal dependence of the optical parameters and of the frequency distribution of Saharan dust events has been analyzed on a statistical basis. A detailed characterization of the Planetary Boundary Layer aerosol content of natural and anthropic origin is also reported.

I - 19

Electrostatic Enhanced Water Scrubbing for Particulate Abatement in Combustion Systems - Modelling Analysis and Preliminary Design Criteria

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Water Electrostatic Scrubber (WES) represents an alternative technology for the abatement of that submicronic fraction of particulate – belonging to the so called Greenfield gap - usually hardly captured with other cleaning techniques. In this work, preliminary results on the application of a theoretical model to the description of WES processes are reported. This analysis will guide in the assessment of design and operation criteria for WES devices.

In this work the removal of coal dust from an air gas stream is firstly considered. Our model indicates that the WES collection efficiency is higher for sprayed droplets with smaller size and higher charge, while it is poorly affected by the spray injection velocity. Indeed, theoretical collection efficiencies higher than 99.5% can be achieved with a specific water consumption around 100 ml/m^3 and a contact time lower than 3 s when 100 μm water droplets are charged at the 20% of their Rayleigh limit.

These working conditions are used to evaluate the theoretical removal efficiency for the abatement of particulate in a diesel exhaust gas. In this case, removal efficiency up to 99.9% can be reached, suggesting the applicability of WES process also in the treatment of these kinds of flue gases.

I - 20

In-Situ X-Ray Scattering Studies of the Formation Dynamics of Carbon Nanoparticles in an Ethylene Flame

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In order to study details on the dynamics of particle formation in combustion in-situ , measurement techniques able to monitor particle size and structure at the atomic scale of resolution are strongly required. X-ray scattering techniques such as small-angle x-ray scattering (SAXS) and wide angle x-ray scattering (WAXS) can provide information of size and structure with high structural resolution. Since some years we have been working on developments of diagnostic tools primarily based on WAXS for particles smaller than 2 nm. The technique is now being combined with SAXS to investigate the dynamics of particle formation processes from molecules to mature soot particles. We present results of combined SAXS and WAXS measurements on an ethylene diffusion-like flame performed with a new detector. The high dynamic range and level resolution of the detection system enable also studies of transition of particles from gas-phase to condensed phase.

I - 21

Optical Properties of Particulates Collected in Rich Premixed Benzene Flames at Different Temperatures

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The UV-Visible spectroscopic features of particulates produced in premixed benzene flames, having the same C/O ratio and different temperatures, were investigated in terms of spectroscopic parameters such as the dispersion exponent and the resonance band wavelength. The particulates were caught on quartz plates inserted at selected position of the flames. By means of a simple extraction procedure it was possible to follow the relative contribution of soluble condensed species and soot particles along the flames. The spectral properties showed to be able to detect intriguing differences between soot formed in benzene and in aliphatic flames previously studied. Any effect of the flame temperature on soot structure was found demonstrating that the peculiarity of the internal structure of benzene soot is related to the influence of fuel structure.

I - 22

Study of the Evolution of Particle Size Distribution in Premixed Flames at Different Temperatures

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The evolution of soot molecular weight distribution (MW) has been studied in premixed rich flames (Φ = 2.4) burning methane and ethylene at two different flame temperatures obtained by varying the cold-gas flow velocity keeping constant the mixture composition.

Soot sampling was carried out in the soot inception region (young soot) and in the post-oxidation flame zone (mature soot). Size exclusion chromatography (SEC), coupled with on-line UV-visible spectroscopy, was performed on DCM-extract, N-methylpirrolidinone (NMP)-extract and on soot suspended in NMP for the MW evaluation. Different resolution SEC columns have been exploited in order to furnish a reliable MW distribution both in the molecular region (10-10^4 u) and in the particle-size region (10^5-10^{10} u).

The very wide MW explored (100-10^{10} u) allows monitoring of the evolution of the features of the different soot classes occurring during the soot inception and maturation processes. Insights about the effect of flame temperature on soot formation mechanism have been obtained. It was found that differences of 100 K of maximum flame temperature have a negligible effect on both spectroscopic features and MW/size distribution of soot.

I - 23

Evaluation of Optical Properties of Condensed Phases Involved in Soot Formation

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UV-visible spectra of the particulate matter caught on quartz plates were measured in sooting ethylene/air premixed flame with C/O ratio=0.77 and maximum temperature of 1792K.

The handling procedure applied on the quarz plates after the exposition in flame allowed to evaluate the relative contribution of the condensed species (dichloromethane soluble) and of the soot particles.

Optical parameters as the dispersion exponent and the position of the maximum absorbance were used to characterize the carbon particulate matter and its evolution along the carbon formation region.

Some final consideration about the dependence of these optical parameters on flame temperature and on fuel composition were made by the comparison of the results obtained in this work with those obtained in previous works.

COLLOQUIUM II

Combustion Fundamentals

II - 1

Multi-Scale Modelling and Experimental Measurements of Soot Filtration in DPFs

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The main objective of this work is to investigate the features of soot particles deposition inside the channels of wall-flow DPFs, since they are responsible for the pressure drop evolution across the filter, and they are bound to influence the dynamics of the soot oxidation process. Both experimental observations and CFD simulations were carried out.

Laboratory scale filters were loaded with a synthetic soot generator. The profiles of particles deposition inside the channels were evaluated at different axial positions, in channels from the centre to the periphery. Hence, depending on the velocity profile at the filter inlet, channels are found to experience different deposition rates. This phenomenon was investigated through two different geometries of the filter housing, one generating a strong maldistribution of the flows at the filter inlet, while the other one resulting in a much more even profile.

The obtained experimental measurements were then reproduced through a three-dimensional mathematical model based on CFD simulations: two grids at different scales were used to this end. A “single channel” grid was used to describe soot deposition into a channel of the filter, and a “full scale filter” model was adopted to compute the different inlet flows to the channels.

II - 2

Kinetic Analysis of Pd-based Methane Combustion Catalysts

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In recent years, catalytic combustion of CH_4 has been extensively studied as alternative option to conventional thermal combustion for the production of heat and energy in view of its capability to achieve effective combustion at much lower temperatures than in conventional oxidation processes, with high efficiency and reduced pollutants such as CO and NO_x.

In this paper a kinetic study on two Pd-carried catalysts is presented: 2% Pd over $NiCrO_4$ and $CeO_2{\cdot}ZrO_2$. Both catalysts were prepared by solution combustion synthesis, fully characterized and tested for CH_4 catalytic combustion. The kinetic study, carried out in a continuous recycle reactor, showed that showed that for 2% Pd/ $CeO_2{\cdot}ZrO_2$ catalyst the most suitable model fitting the experimental data was the Mars van Krevelen mechanism taking into account the concentration of molecular O_2 adsorbed on the catalyst surface, whereas for 2% Pd/$NiCrO_4$ the reaction was first order towards CH_4 concentration and the active sites for O_2 chemisorption on catalyst surface were saturated over the entire range of investigated temperatures and O_2 partial pressures. For both catalysts, the obtained activation energy values were inside the range reported for similar catalysts in literature.

II - 3

Effects of Forced Acoustic Waves onto Jet Shear Layers

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Understanding the coupling mechanisms between acousticwaves and flames have become an important issue in thedevelopment of combustion systems to reduce noise and to avoid the structural damage that such an interaction may produce. Currently little is known about the mechanisms by which the flame responds to acoustic waves.

The present numerical work was driven by previous experimental work in ENEA on laminar and weakly turbulent premixed flames. Acoustics waves, externally generated by means of a tweeter and forced against the combustion region, were observed to tilt, and even to cause lift off and complete extinction of the flame. As first numerical test, a nonreacting mixing layer is simulated, without and with coaxial acoustic forcing. The shortening of the initial laminar region is observed as in experiments. Then, numerical results about the burner experimentally studied in ENEA are shown.

II - 4

Experimental Investigation of Lean Premixed Syngas Combustion at Gas Turbine Relevant Conditions: Lean Blow Out Limits, Emissions and Turbulent Flame Speed

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Lean premixed combustion is considered the state-of-the art technology applied in stationary gas turbines for highly efficient, low-emission power generation using natural gas. Due to the increased interest in the integration of power generation with gasification processes, to CO_2 mitigation issues and use of solid fuels, fundamental combustion properties of upcoming new synthetic fuels (syngas) must be investigated.

This work presents some of the challenges modern low NO_x GTs are going to face when dealing with these new fuels, describing chemical and physical properties of various syngas mixtures and their operational parameters compared with a natural gas reference. Description of operational window in terms of lean blow out is provided at gas turbine relevant conditions. Experiments were done for preheating temperature up to 772 K, pressure up to 15 bar and different inlet velocities.

Focus of this paper is also on the turbulent flame speed (S_T), analyzed with an experimental approach. taken (flame surface area derived from laser induced fluorescence data (OH-LIF)) S_T values can be calculated based on a mass continuity approach and thus represent global consumption rates.

II - 5

Dynamic Numerical Simulation of an Enclosed Flare

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Flare systems are widely adopted to ensure the safe and proper disposal of flammable gases under not well known conditions. Because of the huge amount of gases annually released in the atmosphere through flaring, it is clear the need to provide the best performance of this kind of appliances. This work reports on the detailed modeling and numerical simulations of an enclosed flare, a configuration that is becoming to be largely adopted, since it brings a significant improvement of the combustion process. The scope is to investigate the feasibility of a dynamic model based on the LES (Large Eddy Simulation) approach despite the large size of the flame. The numerical model developed at NIST and implemented in the open source code FDS (Fire Dynamic Simulator) has been chosen for this work. In fact, large flaring flames have several similarities with large pool fires, for which FDS has been originally developed. The unsteady structures of the thermo-fluid dynamic fields, and their modifications when some of the most important operating conditions are varied, have been successfully reproduced. Results confirm the possibility to extract from these numerical simulations useful data for the optimization of geometric and combustion parameters.

II - 6

Accuracy and Flexibility of Simplified Kinetic Models for CFD applications

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The increasing detail of fluid dynamic description and the investigation of fuels different from simple methane, like diesel or jet fuels, still require simplified kinetic mechanisms to be coupled with CFD codes, despite the increasing power and memory of modern PC. This paper discusses a new and general approach of parameter estimations of multistep oxidation mechanisms, with some preliminary encouraging results.

These estimations are easily obtained from a non linear regression of data with a very effective approach. The main novelty is the possibility of a flexible definition and generation of a large set of 'virtual experimental data' carried out in different devices through a detailed kinetic scheme. In order to take into account the quite broad temperature and stoichiometry ranges of a turbulent diffusive flame, the regression analysis is performed over data applied to an appropriate set of laminar counter-flow diffusion flames, in particular with strain rates close to the extinction. These flames are assumed as a good representation of the real flame, still maintaining a simple solution, compatible with the numerical effort required by the regression algorithm. A resulting optimized mechanism of syngas oxidation, applied to turbulent jet flames, shows a significant improvement of CFD predictions in comparison with the original mechanisms.

II - 7

Kinetic Modeling of Toluene Oxidation for Surrogate Fuel Applications

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This work's aim is to present the model activity carried out by two different research groups, belonging to LLNL and POLIMI, comparing the main pathways and results, matching data carried out in different devices both for pure toluene and mixtures. This paper analyzes and highlights the main differences among two mechanisms of toluene oxidation.

In the LLNL model, the H-abstraction reactions to form benzyl are the dominant act of toluene depletion in all the conditions investigated. On the contrary, POLIMI kinetic scheme includes a significant role played by reactions on the aromatic ring and in particular the oxygen atom addition to form cresoxy radical. Despite these differences both the mechanisms are able to catch the main characteristics of toluene oxidation kinetics with a quite good comparison with several experimental data. This work is a starting point of a future synthesis of the two models toward a deeper understanding of the real mechanism and a better description of the whole process.

II - 8

A Comprehensive Kinetic Modeling of Ignition of Syngas/Air Mixtures at Low Temperatures and High Pressures

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Syngas is one of the most promising source of energy and its employment is increasing in last years because of the large availability of coal and biomass from which it is possible to produce it. In order to develop more efficient processes suitable for different combustion conditions, a study of the kinetics of ignition has been carried out by comparing models present in the literature with experimental data. All mechanisms predict the experimental data accurately for temperatures above 1000K regardless of the pressure. Below this temperature a discrepancy from experimental data is found. By a sensitivity analysis two reactions are found to be determinant in the prediction of ignition delay times: $H_2O_2+M=OH+OH+M$ and $H+H_2O_2=HO_2+H_2$. A comprehensive kinetic model is developed on the basis of literature data and tested in a wide range of temperature ($1400K<T<600K$), pressure ($1<P<18atm$) and composition of the syngas mixture. The model shows good agreement with experimental data and correctly predicts the behavior of syngas in gas turbine-like conditions.

II - 9

Modeling of Moderately Swirling Turbulent Non-premixed Flames

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Modelling of turbulent combustion requires an accurate description of turbulence-chemistry interaction in order to obtain reliable temperature and composition.

The proposed model is usually referred to as the Finite-Mode PDF or Multi-Environment model: the distribution is represented by a finite sum of Dirac delta functions, centered in some particular values of the independent variable (nodes) and weighted by some weight functions, representing the related probabilities.

The finite-mode PDF method with three environments has been applied to the simulation of moderately swirling turbulent non-premixed flames. The model has been validated with experimental data provided by the International Workshop on Turbulent Non-Premixed Flames on a bluff-body stabilized flame fuelled with mixtures of hydrogen and natural gas (1:1 vol., swirling flame with S=0.23). Finite rate chemistry was implemented, with a simple four-step mechanism for methane combustion. The method was compared to other widely used modelling tools such as the beta PDF model, with the assumption of chemical equilibrium, and the laminar flamelet model (which allows the implementation of detailed chemistry to be used in the regions where chemical equilibrium is not reached, due to aerodynamic strain). Turbulence was described by the Reynolds-Averaged Navier-Stokes (RANS) equations approach.

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II - 10

Large Eddy Simulation of Unsteady Premixed Flame Propagation Through Repeated Obstacles

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In gas explosions, the unsteady coupling of the propagating flame and the flow field induced by the presence of blockages along the flame path produces vortices of different scales ahead of the flame front. The resulting flame-vortex interaction intensifies the rate of flame propagation and the pressure rise.In this work, a Computational Fluid Dynamics (CFD) model is developed to study the unsteady premixed flame propagation around three sequential obstacles in a vented explosion chamber. The model is based on the Large Eddy Simulation (LES) technique that directly resolves the large-scale vortices and their effects on the flame surface area. To take into account the coupling between unresolved sub-grid scale (sgs) vortices and reaction rate, the combustion model by Charlette et al. (Combust. Flame 131:159-180, 2002) is employed in the context of the flame surface density approach.Comparisons between LES predictions and experimental data (Patel et al., Proc. Combust. Inst. 29:1849-1854, 2002) show a satisfactory agreement in terms of shape of the propagating flame, flame arrival times and spatial profile of the flame speed.In order to evaluate the role of the large-scale vortices, in relation to that of the small-scale vortices, on the features of the flame propagation, LES computations are also run with the effect of the sgs combustion model eliminated. The results obtained demonstrate that the large vortical structures dictate the evolution of the flame in qualitative terms (shape and structure of the flame, acceleration-deceleration step around each obstacle). Conversely, the sgs vortices do not affect the qualitative trends. However, it is essential to model their effects on the combustion rate to achieve quantitative predictions for the flame speed.

COLLOQUIUM III

HETEROGENEOUS COMBUSTION

III - 1

Catalytic Partial Oxidation of Methane with Rhodium Catalysts for Hydrogen Production

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Catalytic partial oxidation of NG for syngas production offers an excellent alternative to steam reforming. The procurement of H_2 for fuel cells, in particular in their application for the propulsion of future vehicles, presents a further driving force for a more compact syngas production technology. The present work investigated, in the WHSV range from 130 to 450 Nl h^{-1} g_{cat}^{-1}, five different fixed bed structures using two different Rh-Al_2O_3-based catalyst both loaded with 0.5% by weight of Rh: one catalyst carrying Rh on the external support surface (egg-shell), and the other one with the same load of Rh embedded into the porous support (egg-yolk).

The goal was the design of the optimal fixed bed structure, able to attain the best performances and a thermally stable system under extreme working condition.

The highest CH_4 conversion (higher than 90%) and H_2 selectivity (higher than 98%) was obtained with the fixed bed realized only with the egg-yolk catalyst in the whole range of WHSV examined. Instead the fixed bed realized only with the egg-shell catalyst denoted the worst performance, decreasing with the increase of the WHSV. The different performance of the two catalyst type was probably due to the different shape of the particles and to the Rh position on the carrier itself.

III - 2

Structural Characterisation of Coals and Coals' Pyrolysis Products

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The study aims to analyse the coal's pyrolysis products to well represent the devolatilisation process mainly in terms of characterization of tar species respect to the structure of the parent coals.

A laboratory test rig has been adopted to subject three Argonne Premium coals to a pyrolysis process. The tars and chars produced have been analysed using two different techniques: NMR and gas chromatographic technique. Two NMR instruments have been used: the solid state NMR has been used to estimate the aromaticity factor of the starting coals and the corresponding chars produced after pyrolysis at 700 °C, liquid phase NMR measurements have been used to determine the tar aromaticity. The GC determinations have been used to analyse the range of molecular weight representative of the collected tar.

A strict correlation between coal and tar aromaticity have been found. On the contrary, the final structures of chars, appear to be very similar each other and no particular differences have been shown for chars produced from coals of very different ranks.

Chromatograms have shown that tars lighter components have been produced by the pyrolysis of lower rank coals.

III - 3

Devolatilization and Combustion Regime in Gasification of Solid Fuels

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This work analyzes and discusses typical and interesting features of the kinetic modelling of biomass gasifiers. The gas solid particle interactions are described by coupling the heat and mass transport equations with a detailed kinetics of devolatilization and gasification of the solid fuel. Volatile components released by the solid fuels are involved in gas phase pyrolysis and combustion reactions described with a detailed kinetic scheme. Due to thermal diffusion resistances, this system can typically present two steady conditions: the 'cold' or the 'hot' solution, depending on the start-up policy. Two different regimes are also observed when analyzing an elemental volume of the gasifier. While small particles show moderate temperatures (1300-1400 K) and a uniform gasification, large particles can easily give rise to a partial devolatilization of the solid fuel with higher gas phase temperatures and a more complete gas-phase combustion. The presence of gasification or combustion regimes demands for careful numerical simulations. These features are relevant not only for the proper modelling of the whole gasifier but could also provide useful information for the complete analysis of the transient behaviour of industrial units.

III - 4

Mathematical Modeling of Entrained Flow Reactors

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Aim of this paper is to present and discuss a general model of entrained flow reactors. This device reaches high temperatures and flash heating rate conditions which are very useful to study the devolatilization process of different solid fuels, such biomasses, plastics, coals and solid wastes. A mathematical model is presented focusing the attention both on the description of mass and heat transfer processes at the particle and reactor scales and on the chemical characterization of solid fuel devolatilization and gas phase evolution. Several comparisons with experimental data show the capability of the model in pyrolysis conditions, while these comparisons also indicate the limit of the model to study coal ignition in combustion environments and suggest for possible model modifications and improvements.

III - 5

Characterization of Nano-Ashes generated during Pulverized Coal Combustion

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Pulverized coal combustion in air involves the emissions of fine particles, nitrogen oxides and carbon dioxide. Pulverized coal combustion in mixtures of oxygen and recirculated flue gas are being investigated to enhance energy efficiency and reduce pollutant emissions. Data regarding the size distribution function of ultrafine particles (D<100nm) generated from coal combustion in oxygen enriched conditions are still lacking. Nano-ash smaller than 30nm have been always neglected. This paper deals with the development of a laboratory reactor to study ultrafine particles formation during pulverized coal combustion. The reactor consists of an atmospheric pressure flat laminar premixed flame homogeneously doped with pulverized coal particles, monodisperse in size. It allows the investigation of the early stage of ashes formation. High resolution Differential Mobility Analysis and thermophoretic sampling for Atomic Force Microscopy techniques have been used to detect particles as small as 1nm. Results show that ultrafine particles, commonly neglected at the exhaust of coal fueled combustors, have a very high number concentration so that they cannot be neglected. Nano-ashes are the most abundant in number and they also represent a significant fraction of ultrafine ashes volume fraction.

III - 6

Thermogravimetric Study of the Decomposition of Wood Biomass Samples

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Main goal of this work is to characterize experimentally the pyrolysis of wood biomass residues. The first step in a pyrolysis study should be the characterization of the wood material in terms of its elemental composition and of a limited number of reference constituents, in particular cellulose, lignin and hemicellulose. A simplified experimental-based algorithm has been developed in order to estimate the biomass composition starting from a single TG analysis of the material, carried out at a constant heating rate. The approach is cheap and can rapidly produce results useful for further practical analysis and modeling activities of the pyrolysis process. Degradation curves of different wood biomass and mixtures of constituents were tested, always obtaining a good agreement between experimental trends of biomass and the "estimated" ones. The developed method showed an excellent agreement with experimental data during the first devolatilization step (up to about 350-400°C). This method was also able to correctly predict the remaining amount of char produced by the process. Nevertheless this study is preliminary and the proposed approach need to be probably validated for a wider range of condition and for other biomass, the results are encouraging.

III - 7

Catalytic Combustion of Methane-Air Lean Mixtures in a Bench-Scale Reverse Flow Monolithic Reactor

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Catalytic reverse flow reactors (RFR) constitute an important alternative for the treatment of hydrocarbon-air emissions. The high thermal efficiency allows the autothermal operation, even when working with cold feeds and low hydrocarbon concentrations. In the present work, the use of monolithic inert and catalyst beds is considered. This kind of beds present important advantages due to the low pressure drops, but can reduce the stability of the RFR. The study has been performed experimentally in a bench-scale RFR for the catalytic combustion of methane-air mixtures, as a test case. It has been found that the reactor operates with satisfactory results for a wide range of switching time and methane feed concentration values, two of the most relevant operating variables of RFR.

III - 8

Analysis and Modelling of Pyrolysis of Wood in Big Samples

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Pyrolysis of wood pellets was investigated by using a special experimental device which allowed to determine kinetics of total weight loss, gas and tar production. Two different heating rates, 0.05 and 1 °C/min, were considered. Dynamic and isothermal pyrolysis tests were carried out on beech and pine wood previously dried in a oven. A simple but realistic kinetic scheme was proposed and its numerical parameters were determined from the results of experimentation on beech wood. Isothermal and dynamic tests were used for this purpose. The model has been validated against the data obtained at high heating rates both from beech and pine wood. The proposed kinetic model takes in to account the presence of two different stages during pyrolysis: a first one involving only wood pyrolysis and a second one where the products not yet escaped from the solid matrix react further. The model is able to predict the influence of the heating rate on the amount of tar, gas and char produced.

III - 9

Optimization of Rh-$LaMnO_3$ Honeycomb Catalysts for Fuel-Rich Methane Combustion

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Structured catalysts with mixed Rh–$LaMnO_3$ formulation were developed for the partial oxidation of methane to syngas intended as a preliminary conversion step in advanced combustion systems such as power turbines and utility burners employing a catalytic fuel-rich approach to reduce thermal NO_x formation. Honeycomb catalysts were fully characterized by ICP-MS, BET, DRIFT, H_2-TPR and their performances were tested under self-sustained, high temperature catalytic partial oxidation reaction to assess the impact of noble metal loading. Moreover, at fixed catalyst formulation, the impact of substrate morphology and thermal conductivity was addressed by direct comparison of honeycombs with several cell densities (cordierite 200-1200 cpsi) and two solid materials (cordierite vs. SiC).

III - 10

Catalytic Combustion for Low-NO_x H_2-Fuelled GT

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Catalytic combustion is proposed as a primary mean to control NOx emissions in gas turbine systems fuelled with pure hydrogen or high H_2 content fuels. Nevertheless it has been found that hot-spot formation on the catalyst, with solid temperatures largely exceeding the adiabatic flame temperature of the feed mixture, poses serious challenges for materials durability and, in turn, strongly limits the maximum attainable temperature level of the exit gas leaving the catalytic module. In this work several active and passive strategies have been examined either experimentally or by simulations and compared with regards to their ability to reduce catalyst overheating, such as: change of catalyst morphology (cell density), variation of thermal conductivity of the substrate, presence of a diffusional barrier above the active layer, steam addition. Moreover the study has been extended to include fuel rich feed conditions to the catalytic reactor.

III - 11

The Relevance of Slag Formation and Wall Burning to Entrained-Flow Combustion and Gasification of Coal

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This paper deals with entrained-flow autothermal slagging coal gasifiers. In particular, after an overview on gasification kinetics, a conceptual analysis of the fate of coal particles which are transferred to the molten ash slag before they are completely gasified is developed. It was underlined that carbon may remain segregated at the surface of the slag layer or be embodied into the ash melt depending on the combined effect of different mechanisms, and it was only considered the establishment of a regime in which the refractory C-fraction of the char particle is not embodied into the molten layer, but adheres to its surface thus making further progress of carbon combustion and gasification possible. Further results concerning different regimes are left to a forthcoming paper. Accordingly, a simplified 1.5D model has been developed with the proper choice of operating parameters. Model results suggested that the role of the slag on late carbon conversion is significant, as carbon particles residence times in the slag are much longer with respect to those in the dispersed phase. Moreover, the extensive transfer of ash from the dispersed phase to the wall layer was observed. Syn-gas was produced with a CO/H_2 ratio slightly larger than 1. Molar fractions of H_2 (0.31) and CO (0.37) at the exhaust, and their sum on dry basis (0.82), were finally obtained.

COLLOQUIUM IV

Innovative and Non-Conventional Combustion Processes and Technologies

IV - 1

Hydrogen-Methane Blended Fuel Jet Flames: Study of Ignition and Flames Morphology

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This research work is focused on safety aspects connected with use of hydrogen as a fuel and it represents a significant starting point towards an hydrogen economy, safe and ready to be regulated by standards and codes.

In this study methane-hydrogen blends jet flames were analyzed with the aim to characterize their dimensional properties and their interactions with warm surfaces.

Tests of ignition and stability of the flame to several flow rates and different diameters of nozzles were carried out to simulate accidental losses of the system varying operating pressures. In this way pressure drops and discharge coefficients have been characterized.

Different conditions of blends ignition according to the temperature of warm surfaces with different heights as a function of the leakage of the gas from the nozzle were determined.

Images of flames in the visible, infrared and UV regions were acquired and were afterwards computed in order to estimate the length, the width and the morphologic characteristics of flames.

This work only describes the preliminary step of this research in which the visible flame morphology and the conditions of ignitions have been investigated.

The data will supply a technological base for the determination of the entity of the risk connected to unintentional releases in storage and distribution areas of hydrogen eventually mixed to methane or natural gas.

IV - 2

Production of Biobutanol by *Clostridium Acetobutylicum*

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The socio-economic scenario of the third millennium revives the interest in production of biofuel for transport purposes by fermentation processes and the butanol appears to be a promising candidate. Present contribution reports about results of a research activity aiming at investigating the feasibility of the acetone-butanol-ethanol (ABE) production by *Clostridium acetobutylicum* ATCC824, adopting biofilm reactors for the process intensification. The kinetics of the ABE production process has been assessed by free *C. acetobutylicum* in batch reactors and in a CSTR equipped with a microfiltration unit. Solutions of lactose – concentration ranging between 10 and 100 g/L - were adopted. Tests carried out under batch conditions show that: i) cells growth is constant for lactose concentration (C_L) smaller than 100 g/L; ii) the butanol specific production rate (r_B) as a function of C_L may be represented by a Monod-like kinetics; iii) the selectivity of butanol with respect to total solvents increases with C_L and stabilizes at about 72%$_W$ for C_L larger than 30 g/L. Preliminary tests carried out under continuous conditions show that the process takes advantage from the steady state operation under solventogenic conditions. The r_B is larger in the CSTR than in the STR, when compared at the same C_L.

IV - 3

Design and Preliminary Characterization of an Experimental Set-up for Nanoparticles Synthesis through Flame Spray Pyrolysis

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The Flame Spray Pyrolysis method for high temperature synthesis of nanoparticles offers a great flexibility in terms of type of precursors, flow control, purity and amount of produced material. In this work a new experimental apparatus, basically consisting of a gas-assisted spray for droplet generation is described. A precursor mixed with a liquid fuel is then sprayed inside a sustaining flame where the reaction takes place. The spray structure was initially determined using a fast digital camera and by Phase-Doppler Anemometry (PDA) in order to determine the droplet size and speed at different heights. In the preliminary tests solutions of tetraethoxysilane (TEOS) in n-hexane and of Titanium Tetraisopropoxide (TTIP) in ethanol were used to produce SiO_2 and TiO_2 nanoparticles, respectively. The materials, collected on a filter, have been synthesized and characterized by TEM and XRD analysis. The apparatus shows good stability and reproducibility of the material produced. Further tests will be devoted to the synthesis of other types of nanoparticles.

IV - 4

New Regenerative Burner for Flameless Oxidation in Radiant Tubes

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Effective combustion air preheating in high temperature furnaces makes considerable energy saving possible, but requires rigorous NOx abatement techniques. To this purpose, flameless oxidation has become increasingly popular in steel heat treatment furnaces.

Advanced technologies with small capacity burners, in particular for radiant tubes, have incorporated effective air preheating coupled with low-NOx measures using both recuperative and regenerative heat recovery principles. Design criteria for radiant tubes are briefly reviewed and a new burner + radiant tube embodiment for large industrial furnaces is presented.

IV - 5

Modelling of a Catalytic Microstructured Reactor

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In this work a good understanding and an accurate quantitative description of fluid flow, heat and mass transfer occurring in a catalytic microstructured reactor, operating at atmospheric pressure, was achieved by using a 3D model based on momentum energy and mass balances for the specie involved. Such a model was tailored on a real lab-scale reactor where the heat generated by the catalytic methane combustion sustains the catalytic methane steam reforming reactions. The contribution of the catalytic reforming reactions was modelled considering the classic Langmuir-Hinshelwood surface kinetic theory, while a power law-like expression was employed for the methane combustion kinetics.

Accurate modelling of the reactor was complicated because of the thermal dissipation across its boundaries which strongly affects the system performance: convective and conductive heat dispersions were evaluated imposing external wall temperature profiles deduced from experiments.

Validation of the model was performed through the comparison of the numerical simulations with experimental results showing that a good fitting in terms of methane conversion and hydrogen yield can be achieved imposing proper boundary conditions. Considerations in order to simulate catalyst deactivation were also performed. The estimated errors for CH_4 conversion and hydrogen yield did not exceed 15.62% and 5.5 %, respectively.

IV - 6

Experimental Investigation of a Catalytic Microstructured Reactor for Process Intensification

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This work reports on the experimental investigation of a microstructured catalytic reactor performance where simultaneous methane catalytic combustion and steam reforming occur. The reactions take place over catalytic layers deposited on the opposite faces of the same metallic slab so that combustion heat sustains the endothermic steam reforming reaction occurring on the opposite side of the slab that also separated the channels where the reactants are fed. The system may operate both in co-current (CNC) and counter-current (CTC) flow.

60% methane conversion to syngas with a 3.33 hydrogen yield was obtained when the gas mean residence time in the reforming channel was about 57 ms and the molar steam/methane feed ratio was 2.78. Oxygen-lean stream was fed in the combustion channel because higher oxygen concentration negatively affected the catalytic combustion kinetics.

Reduction in reforming catalytic activity occurred when subsequent tests were performed: such a reduction was attributed to carbon deposition on the catalytic surface whose formation resulted not strictly dependent of the H_2O/CH_4 feed ratio.

Even if a relatively high thermal dissipation strongly limited the thermal efficiency of the process, autothermal stability of the system occurred both in CTC and CNC flow patterns under the tested conditions.

IV - 7

Experimental Analysis of Mild Combustion of Liquid Fuels

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aim to retrofit a furnace, originally designed for the mild combustion of gaseous fuels, in order to realize mild combustion conditions for liquid hydrocarbons, such as n-octane, n-dodecane, and kerosene. Experiments allowed to evaluate the influence of different parameters, such as oxygen excess, air pre-heating temperature and dilution ratio (K_v) on the sustainability of mild combustion and pollutants production. Operating maps for the investigated fuels, as well as temperatures profiles inside the furnace, have been also defined. It has been found that a steady mild combustion, with very low NOx and CO emissions, can be obtained in the temperature range 840-1010°C and for K_V values higher than 1.5 for n-octane, while in the range 855-1055°C and for K_V values higher than 1.7 for kerosene. A lower temperature limit, at about 835°C, and a lower K_V limit of 2.5 have been also identified for n-dodecane.

IV - 8

Influence of Different Hydrogen/Methane Mixtures on the Operability of Small-Size Burners for Energy Production

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The focus of this study is to develop and characterize a small-size burner able to convert the thermal energy produced by the combustion of light hydrocarbons (and eventually hydrogen) in electrical energy. In particular, to obtain such a result, two catalytic burners equipped by thermoelectric modules have been developed. The first burner showed some problems to sustain the methane combustion. For this reason the development of a second burners was necessary. The improved design of the second burner allows to manage the methane combustion over a wide range of flow rates. To characterize the combustion phase, measurements of gas, wall and bulk temperatures were made, while measurements of voltage and current intensity were made to verify the power generation of the device. Experimental results showed a linear trend between the fuel flow-rates and the measured temperatures. The power output evidenced the same trends because of its proportional relationship with the temperatures difference (detected between the hot and cold side of the burner) found at the surface of the thermoelectric modules. The results of the study are very encouraging and show the feasibility of the idea, evidencing also performances comparable with other devices found in the literature.

IV - 9

Flameless Technology for Particulate Emissions Suppression

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Combustion is a great source of carbonaceous and inorganic particle emissions, even though the combustion technologies and their efficiency are improving. Flameless oxy-combustion technology provides frontier emission performances, with the most advanced Rankine+Joule Bryton high yield thermodynamic cycle. The process ISOTHERM PWR® is an innovative high temperature, pressurized oxy-combustion process recently developed. A 5 MWth demonstration unit, settled at Gioia del Colle (BA) scores more than 5000 hr of tests on different fuels, i.e. solid, non vaporizable liquid, vaporizable liquid, gas, and wastes.

In this paper, we focused our attention on the size distribution function of the particles formed during the combustion process and emitted when burning different fuels (heavy oils, wastes and coal). Different particle-size measuring techniques are used including atomic force microscopy and spectroscopic characterization of the material collected in water samples and on-line inertial classifier and SEM analysis.

IV - 10

Effects of Hot Diluted Oxidant Flow on Reactive Structures in HDDI MILD Combustion

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The typical structure of not premixed diffusion flames in standard conditions can be significantly modified whether injected flows are diluted and/or pre-heated.

The increase of dilution level up to extreme conditions could lead to the formation of mixtures not ignitable so that the oxidation processes could be sustained just in case the pre-heating temperature of one of the two flows is high enough to promote the auto-ignition of the system. Such peculiar operative conditions, typical of Mild combustion processes, identify a combustion process named Hot Diluted Diffusion Ignition (HDDI) where referred to diffusion not premixed flames.

In this work a sub-categories of HDDI, named HODO (Hot Oxidant Diluted Oxidant), is analyzed. Such configuration considers a hot pre-heated and diluted oxidant flow that inter-diffuse inside an un-diluted fuel flow at environmental temperature. The inlet temperature and the dilution degree of the oxidant flow in nitrogen as been parametrically changed in a opposed jet configuration and the structure of the reactive region has been analyzed considering the numerical temperature and heat release profiles.

The software CkemKin and its application OPPDIF have been used to perform numerical simulations.

IV - 11

PAH/VOC Abatement in Water and Hydrogen Flows at MILD Combustion Conditions

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PAH and/or VOC emission control from industrial processes is realized through several technologies such as thermal oxidation. Although such process allows for high abatement efficiencies, it requires the use of auxiliary fuel because of the low concentration of PAH in the exhaust gases. Such aspect implies the potential formation of undesirable by-products, such as NO_x. The use of high reactants pre-heating and high dilution levels, typical operative conditions of Mild Combustion processes, can overcome such problem. Furthermore the employment of water as dilutant, and/or the use of hydrogen as fuel enhancer, can increase the abatement process efficiency for their propensity to give radicals in these thermal conditions.
In this framework, the paper aims to show a preliminary numerical analysis of PAH oxidation in Mild combustion regime in system diluted with nitrogen and/or steam and in presence of small amount of hydrogen, by evaluating the auto-ignition and oxidation times.

IV - 12

Modeling of Pollutant Emissions From a Lab-scale Burner Operating in MILD Combustion

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Recently MILD combustion has received large attention because its capability to provide high efficiencies with low pollutants emissions (NO and soot). Moreover the technology is well suited for hydrogen enriched fuels as well as for some industrial byproducts.

In the present work a Computational Fluid Dynamics (CFD) model of a lab-scale burner able to operate both in flame and MILD combustion modes was developed with Fluent 6.3 by Ansys. Experiments were carried out with both CH_4 and CH_4/H_2 mixtures (40/60% by vol.). The results of the simulations are compared with measurements, performed for both flame and MILD conditions, in order to gain insight into burner operations and modelling requirements with special attention to NO formation modelling.

It was found that the inclusion of NO formation mechanisms such as N_2O and NNH (in presence of H_2) routes is mandatory for the accurate predictions of NO emissions in MILD conditions, due to the relatively low temperatures and fluctuations which make the thermal route less effective. Such mechanisms may be not available in commercial CFD codes, so they have to be implemented through bespoke subroutines. Moreover NO have to be calculated over temperature fields obtained with detailed kinetic schemes for the oxidation process.

IV - 13

NG Oxycombustion Experiences on a 3MW Test Rig Facility

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Among the techniques worldwide indicated as the most promising for the separation of CO2 from thermal generation there is the combustion in oxygen. This solution requires the replacement of the combustion air with a mixture of oxygen and recycled flue gas. Enel has recently retrofitted a 3 MWth Facility from conventional air operation to oxycombustion with recycled flue gas. The paper reports on the results of the first oxycombustion tests performed with natural gas. The primary objectives were to demonstrate the technical feasibility of the process and to examine the opportunity of retrofitting a full scale plant for CO2 capture purpose. The effect of using oxygen instead of air on heat transfer, pollutant emissions and flame stability, was evaluated. Experiments have been carried out varying the amount of gas recycled back to the furnace (Recycle Ratio) and all the results were reported to a baseline air case. Detailed in-flame measurements of temperature and gas composition have been performed in the case of conventional air combustion and in oxycombustion at two different Recycle Ratio with the aim to collect data for computer modelling validation.

IV - 14

A Novel Concept of Looping Combustion of Carbon

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A novel concept of looping combustion/partial oxidation of carbon is presented. It is based on the feature of carbons to uptake oxygen upon exposure to air at moderate temperatures. Surface oxides of carbon are eventually released as carbon oxides (CO, CO_2) as the oxidized fuel is brought to moderate-to-high temperature in an oxygen-free atmosphere. This concept is pursued to the formulation of preliminary schemes of looping combustors/partial oxidizers of carbons. The proposed process is based either on dual interconnected fluid bed reactors or on intermittent operation of a single fixed/fluidized bed reactor. In either case, carbon particles are subjected to alternated stages of oxidation (under air-blown operating conditions) and surface oxide desorption (under oxygen-free atmospheres). Operating conditions of the oxidation and desorption stages can be tuned so as to envisage alternative looping combustion/partial oxidation strategies. The basic mechanistic background underlying the proposed process is presented and discussed. The concept has been verified with experiments carried out in TG under alternated oxidation/desorption conditions.

COLLOQUIUM V

APPLIED COMBUSTION

V - 1

Reactive CFD Analysis in a cComplete Combustor Module for Aero Engines Application

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Gas turbine combustor CFD modelling has become an important combustor design tool in the past few years. Generally the numerical models are limited to the reactive flow field inside the combustor liner with the inlet mass flow rates being derived from 1D flow network analysis and used as boundary conditions for the internal-flow-only combustor CFD prediction. Although strongly coupled in reality, the two regions have rarely been coupled in CFD modelling for industrial applications.

In this paper an improved version of BODY3D CFD in-house code is described to calculate the full model combustor, from compressor diffuser exit to turbine inlet. The coupled model accomplishes the following two main objectives: (1) implicit description of air flow splits and flow conditions for openings into the combustor liner, and (2) prediction of pressure losses distribution from the diffuser to the combustor exit. Remaining difficult issues such as generating the computational grid and modelling effusion/impingement cooling systems are also discussed.

A first application of the above approach concerns the PERM Combustor currently under development in the framework of EU research program NEWAC, which is focused on new aero-engine core technologies aimed at reducing CO2 and NOx emissions.

List of Acronyms

CFD	Computational Fluid Dynamics
EU	European Union
NEWAC	NEW Aero engine Core concepts
PERM	Partial Evaporation and Rapid Mixing

V - 2

Coal Combustion Ash as a Raw Mix Component for Portland Cement Manufacture

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The cement industry can give a significant contribution to sustainable development due to its ability to use, as alternative fuels or raw materials, industrial wastes and by-products derived from other activities. The waste utilization as an energy source is favoured by the peculiar characteristics of the processes occurring in the cement kiln, whereas their employment as raw materials for the cement manufacture can occur in two different ways: 1) as constituent of the end product; 2) as component of the kiln raw feed.

This paper is focused on the utilization of pulverised coal fly ash as a raw mix component for portland cement manufacture.

Pulverised coal fly ash often shows an excellent pozzolanic behaviour, but the recent tendency to reduce the combustion temperatures in the traditional coal-fired power plants leads to the generation of fly ash with a lower pozzolanic activity and a higher unburnt carbon content. Therefore, new application fields have to be searched for pulverised coal fly ash.

This laboratory investigation has assessed that pulverised coal fly ash-based raw mixes, able to generate portland clinker and containing 77-78% limestone, 15-16% fly ash and 7% silica sand, can usefully replace traditional raw mixes composed by 73% limestone and 27% clay.

Compared to the clinker obtained from natural materials, waste derived clinkers had almost the same mineralogical composition and burnability.

V - 3

Confined After-Burning of Display Pyrotechnics and Explosives

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The afterburning phenomena in large scale storage container have been largely analyzed for TNT and other high-energy explosives: The energy release of the primary explosion is followed by the energy given by the complete combustion of detonation products, thus producing an added energy which is typically twice to five times the primary explosion energy, finally resulting in more severe hazards than expected.

Besides, less information are given on pyrotechnics in the same conditions. In this work the complete combustion course of TNT, RDX, PETN and black powder of different composition (by varying sulfur and/or carbon content), either in nitrogen or in air atmosphere, have been analyzed. The product species and concentrations for any composition were determined by using the CEA thermo-equilibrium code, which calculates chemical equilibrium product concentrations from any set of reactants and determines thermodynamic and transport properties for the product mixture.

Finally, the curve of maximum pressure with respect to the ratio given by explosive volume to the total room volume are given, for each set of composition and for different explosives and pyrotechnics. This latest plot may be usefully adopted for risk assessment of pyrotechnic storage plant and can be extended to any firework composition.

V - 4

Influence of Diesel Engine Operating Conditions on Properties of Emitted Particles

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Not only quantity but also properties of soot particles from engine combustion are influenced by operating conditions. This study is part of an investigation aimed to understand which engine parameters are crucial. For this purpose injection pressure and rate of exhaust gas recirculation (EGR) were varied using an optically accessed single-cylinder diesel engine. Soot formation was observed by C_2-chemiluminescence and emitted soot particles were studied by electron microscopy and electron energy loss spectroscopy (EELS). Measurements show the influence of injection pressure and EGR rate on soot particle properties.

V - 5

Effect of RME Fuel on Combustion in Optical Engine Operating in HCCI Mode

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In the last thirty years the State systems regulate strictly both the fuel consumption and pollutant emissions from the internal combustion engines. One good and cheap solution proposed by the automotive researchers is the adoption of the homogeneous charge compression ignition (HCCI) in the production engine. In particular, HCCI combustion promises to reduce the PM and NO_x emission from diesel engines without penalize the performances. Another solution proposed is the use of biodiesel fuel in order to improve the pollutants emissions from the engines. The benefits of the biodiesel are well known: higher cetane number, low sulphur content, reduction of HC and CO emission, reduction of PM emission, and reduction of CO_2 net emission on life cycle basis. The goal of the paper was to evaluate the development of the HCCI combustion in an optically accessible diesel engine varying the injection pressure with both diesel and RME fuels. The chemical species involved were determined by means of chemiluminescence measurements and UV-visible digital imaging. The pollutants formation and their emission in the exhaust were analyzed and correlated to OH radical that is the dominant species in the combustion chamber. The positive effect in the use of RME fuel for the reduction of pollutant emission was observed. In particular, the use of RME fuel decreases further the PM and NO_x concentrations both in chamber and exhaust with respect to those of REF fuel. The OH behaviour in chamber was strictly correlated to formation-oxidation of PM-NO_x.

V - 6

Resolution Enhancement of 2D Images of Fuel Jets in a Diesel Engine by Pan Sharpening Algorithms

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Collection of two-dimensional images of the chamber of reciprocating engines is a powerful mean for the investigation of the combustion process. Images can be, in some cases, species–specific, basing on the knowledge of the spectral characteristics. However, a trade–off issue arises between spectral selectivity and spatial–temporal resolution. Sometimes the information contained in the low–resolution, spectrally–resolved image is correlated with an available full intensity (Panchromatic), full resolution image. If this is the case, resolution information from the Panchromatic image can be used to improve the resolution of the spectrally selected image. Image fusion techniques allow integration of different information sources by merging complementary spatial and spectral resolution characteristics. This study presents a first attempt to apply image fusion techniques to data obtained from optically accessible internal combustion engines, with the focus on the enhancement of spatial resolution of multispectral image data. Image fusion based on the RGB to HIS transformation of the high resolution gray image with low resolution RGB image obtained in an optically accessible Diesel engine is performed. The results obtained confirm that the technique can be successfully applied to the enhancement of the spatial resolution of multispectral data.

V - 7

Some Issues of a Coal Demineralization Process

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Ground samples of two coals were leached in series with distilled water, ammonium acetate, 1-M hydrochloric acid, 10-M hydrochloric acid, 40 wt% hydrofluoric acid to evaluate the effectiveness of the treatments and the feasibility of the coal demineralisation process. A parallel treatment with the sole 10-M hydrochloric acid was also performed. The solution obtained after each treatment was analysed for the content of metal ions by plasma atomic emission spectrophotometry (ICP-AES). Solid residue was checked for reactivity by air flow TGA. The ammonium acetate treatment leached alkaline and earth-alkaline metals bonded to the organic matrix. Oxides and carbonates were removed by dilute HCl solutions and silicates by concentrate HF solutions. The whole extraction chain gave rise to samples with 0.3 and 0.4 wt% residue after air flow TGA in front of 15.6 and 14.4wt% of the respective untreated samples. In contrast, the treatment with the sole 10-M HCl resulted in a poor sample demineralisation. The complete demineralisation gave rise for both coals to a marked loss of reactivity while the treatment with only HCl 10-M to an huge reactivity increase.

V - 8

Investigation of Agglomeration Phenomena During Fluidized Bed Combustion of Biomass in a 1 MWth Shallow Bed Boiler

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The fluidized bed (FB) combustion of a two biomass fuels – B quality wood and miscanthus pellets – was investigated in a small commercial scale (1 MW_{th}) boiler with shallow bed. As a consequence of the very high content of alkali metals in the ash of miscanthus pellets (especially potassium), extensive bed agglomeration problems were expected.

The focus of the study was a general insight into agglomeration phenomena during biomass combustion on such a scale, as well as an investigation of the effect of the diameter of bed particles on the time to defluidization. Results indicate that sand size can have a significant influence on the agglomeration phenomenon.

Additionally, samples of the bed material discharged from the boiler after test were examined by means of SEM and SEM/EDX analysis. Results confirm that the agglomeration and subsequent defluidization of the bed is a consequence of the fraction of the potassium enrichment on the particles' surface. On the contrary, alkaline earth elements, such as calcium or magnesium, present in high amounts in the wood ash, can prevent bed agglomeration by forming high melting-point compounds.

V - 9

Agglomeration and Fragmentation Phenomena of Bed Materials and Fuel Particles During Gasification of Coal-Biomass Pellets

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The paper reports on a current research on fluidised bed gasification of biomass and coals. The focus is on the bed material agglomeration and fragmentation phenomena that are well known to affect the reliability and the efficiency of fluidized bed combustion processes. Preliminary results of dedicated tests at high temperature are reported and discussed in the paper. On the whole, agglomeration phenomena appear to be less relevant under gasification conditions than during combustion.

Extensive fragmentation has been experienced for a bed of fresh or calcined dolomite, whereas other materials having catalytic properties (sintered dolomite, ?-alumina) are more suitable under this aspect. Attrition tests also confirm the lower mechanical resistance of the calcined dolomite.

V - 10

Validation of Droplets Behavior Model by Means of PIV Measurements in a Cross-flow Atomizing System

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This paper deals with the further development and validation of a numerical model aimed to describe the behavior of a liquid jet, as it issues from a plain nozzle into a square channel and is suddenly exposed to a crossing airflow. An analytical model, validated by confronting it with a large database of experimental data, has been used to describe the trajectory of a liquid jet injected in a cross-flow and. Liquid jet model has been implemented in an in house developed CFD code to evaluate the mutual interaction of the liquid and gaseous phases. A recursive scheme with a grid adapting technique has been used and a lagrangian description of droplet size and trajectory has been set up. Secondary breakup, evaporation and wall impingement of the droplets have been implemented in the droplet tracking algorithm by means of suitable sub-models. Finally, the results of the numerical simulation were compared with the results obtained using a PIV technique. This comparison required the elaboration of an “ad hoc” post processing procedure. The agreement of the numerical and experimental data is quite good in the first two considered cases while it is less good in the case of higher airflow velocity.

V - 11

An Innovative Combustor for Residues and Wastes: Development of a Design Methodology

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This work illustrates the methodology used for designing an innovative combustor conceived by NSE-Industry for burning alternative fuels, e.g. biomass residues and wastes. The use of these materials for energy production couples the valorization of wastes and the renewable nature of the sources. The combustor is a 6 MW compact system based on a patented combustion technology and can be inserted in industrial processes as an end-cycle component. It is well suited for paper and wood industry, hospital districts, ecological islands, platforms for waste and sewage sludge treatment.

The procedure described here helped in the development of an advanced design, by using a multiplicity of mathematical/computational tools, opportunely integrated, to verifying some technological solutions and solving specific criticisms appeared in the preliminary design.

In this paper the methodological approach is discussed, the developments of process and Computational Fluid Dynamic models are described and some valuable results are shown remarking the interactions among the different investigations. The findings of this analysis will be used for specific studies as for instance the structural evaluation and pollutant control strategies, in order to define the executive design of the combustor.

V - 12

Study of Emission of Odorous Substances from Industrial Flares

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Flaring is a high-temperature oxidation process used to burn combustible components, mostly hydrocarbons, of waste gases from industrial operations. Gases flared from refineries, petroleum production and chemical industries are composed largely of low molecular weight hydrocarbons with high heating value and some sulfur-containing material such as hydrogen sulfide and mercaptans. The presence of these sulfur-containing species in the waste gases causes the emission of odorous substances such as H_2S and SO_2 in addition to the typical products of incomplete combustion such as CO, unburned hydrocarbons and soot, which are usually formed when high volumes of waste gases are flared in very short times.

In this work, a modelling study of product of incomplete combustion and odorous substance formation in industrial flares is presented. Flaring is modeled as a turbulent flame by using a detailed kinetic mechanism of oxidation and pyrolysis of hydrocarbons and of sulfur-containing species coupled, through a flamelet approach, to a k-ε based fluid dynamic code. A simplified model based on the prediction of aromatic precursors by the detailed chemistry mechanism and acetylene addition is used to predict soot.

Different flaring scenarios and flare configurations are considered. Predicted emission data are compared with experimental concentrations of pollutants detected by remote imaging and infrared gas quantification. Model results are in reasonable good agreement with flame visualization and gas concentration of CO and SO_2.

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Sorbent Inventory and Particle Size Distribution in Circulating Fluidized Bed Combustors: the Influence of Particle Attrition

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Substantial changes in the particle size distribution of limestone-based SO_2 sorbents can be brought about by particle attrition/fragmentation in Fluidized Bed Combustors (FBC). It has been shown that particle attrition/fragmentation may be related to different and concurrent phenomena: ***Primary fragmentation*** (occurring immediately after the injection of sorbent particles in the hot bed as a consequence of thermal stresses and internal overpressures due to release of gas); ***Attrition by abrasion*** (related to the occurrence of surface wear in the emulsion phase of the FB); ***Secondary fragmentation*** (due to high-velocity impacts against bed material and reactor walls/internals). The mutual interference between chemical reactions (calcination/dehydration, sulphation) and attrition/fragmentation of limestone has also been recognized.

In this work, a population balance model is presented, which aims at predicting the particle size distribution of sorbent particles establishing at steady state in the bed of an air-blown Circulating FBC and the fractional mass of sorbent reporting to the bottom vs fly ash. The influence of attrition and fragmentation on mass fluxes, particle size distributions and related variables is assessed.

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Minimizing Nox Emissions from Reheating Furnaces

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This paper presents an overview of the main results of the work carried out with a financial grant from the Research Fund for Coal and Steel (RFCS) of the European Community in the frame of project "Minimizing NOx emissions from reheating furnaces" or NOXRF. Results obtained in NOXRF give a clear indication of the lowest level of NOx that can be reached with the present state of art for primary reduction technologies.

In particular the combination of staged and separated jets injection of fuel and comburent for oxyfuel and the flameless regime for pre-heated air combustion system have shown a reduction of about 80% of NOx emissions respect to conventional flame burners.

Comparison with secondary NOx removal techniques, such as high temperature reduction (HTR), shows that presently the installation of new generation of burners is the best method for obtaining a significant reduction in NOx, with low operating costs. The set of data produced in the project can be used by steel mills to select the NOx reduction for greenfield projects and the revamping of reheating furnaces, and by burner suppliers to benchmark their own products.

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Investigations on Heat Transfer Between a Bubbling Fluidized Bed and Immersed Tubes for Heat Recovery and Power Generation

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The present research deals with the heat transfer between a bubbling fluidized bed and a single tube exchanger. Theoretical estimates of the heat transfer coefficient have been obtained by adopting a computation procedure from the literature. Experimental data have been produced with a dedicated test facility. The results confirm the high heat transfer coefficient that establishes in a bubbling fluidized bed (up to 200 Wm-2K-1) and, thus, the suitability for a simple coupling between a fluidized bed and external devices for power generation.

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Emission of New Technology Euro 4 Vehicles

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Due to the growing number of vehicles circulating in urban areas, vehicle exhaust emissions remain the main source of organic pollution in urban atmosphere, despite the recent technological improvements in engine, fuel and after treatment emission devices. An experimental activity was carried out to evaluate gaseous and particulate emissions of some new technology Euro 4 vehicles: a Diesel van equipped with a passive particulate trap (DPF), a hybrid car and a bi-fuel SI car. Hot emission factors and the effect of cold start have been also estimated. The results have been compared with those obtained with conventional vehicles belonging to the same class.

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Increasing the Robustness of the Ash Management System in Utility Boilers

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In Italy the coal power generation park is primarily established on pulverized coal-fired power plants. The option to apply wastes/biomass co-combustion with coal can be advantageous by far for environmental and energy aims, but it imposes a thorough control of the co-fuel size distribution fed to the boiler. In a co-combustion condition, indeed, inaccurate control of the feed size often results in significant amounts of unburnt carbon extracted together with coal bottom ash.

Technicians of MAGALDI Ricerche e Brevetti in their past experience registered the existence of significant ash post combustion on the dry ash belt conveyor MAC (Magaldi ash cooler). Within an existing and proactive collaboration, MAGALDI Ricerche e Brevetti, the Chemical Engineering Department of "Università di Napoli Federico II" and I.R.C.-C.N.R. are investigating the upgrade of Magaldi Ash Cooler (MAC) into Magaldi Ash Postcombustor (MAP), in other words into a device that extracts bottom ashes in a "dry" way and at the same time promotes oxidation of the unburnt carbon in ash. Such device, integrated with the boiler, could enhance the robustness of the whole system with regard to the co-fuel characteristics and boiler load fluctuations. Within this framewok a mathematical model has been developed to describe the faith of ashes and the postcombustion of carbon in ash along MAP's belt conveyor. Preliminary results are presented in this paper.

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Thermo-kinetic Parameters of Pulverised Coal-Dust Explosion

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The inconveniences arising from the handling of pulverized coal are essentially related to coal–dust explosions. Indeed, several scientific works have been addressed the reduction of dust explosion hazards in coal mines and related activities. Besides, coal dust explosions are becoming progressively more important issues also in the industrial areas in which pulverized coal is used as the source of energy, both for power plants or other purposes as in cement furnaces.

This paper focuses on the analysis of thermo-kinetic parameters of explosions of pulverized coal, and more specifically on the definition of maximum pressure (P_{max}) and dust deflagration index K_{St}, i.e. the maximum rate of pressure rise, as measured in closed spherical vessel, in order to produce useful data for the design of protection and mitigation systems.

To this aim, a numerical tool for the evaluation of the thermo-kinetic parameters of dust explosion has been first developed. According to Hertzberg et al. (1986) which have formulated a three stages model for the coal-dust flame propagation: i) heating and pyrolysis/devolatilization; ii) mixing of volatiles with air; iii) gas phase combustion, the model starts from the assumption that the first step is very fast and then gas phase combustion controls dust explosion.

The data obtained by the numerical tool for pulverized coal have been successfully compared with the correspondent experimental results obtained in the classical spherical Siwek bomb, as function of dust concentration.

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