XXXIX

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edited by

Mario Commodo, Wolter Prins, Fabrizio Scala, Antonio Tregrossi

XXXIX

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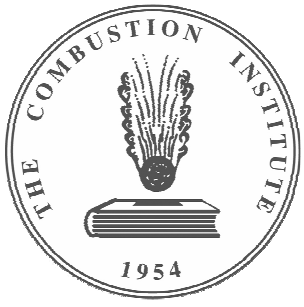
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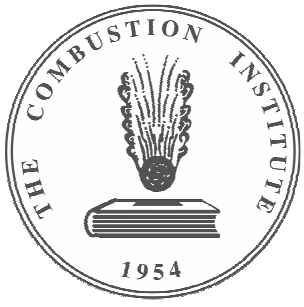
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SESSION I

SOLID FUEL COMBUSTION, PYROLYSIS AND GASIFICATION

GLOBAL KINETICS OF BANANA PEEL COMBUSTION

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Abstract

A comparison is made between the thermogravimetric behavior in air of banana peel and wood, always characterized by devolatilization and combustion. Apart from the wider temperature interval, banana peels exhibit two peaks for both the first zone (instead of a shoulder and a peak) and the second zone (instead of a single peak), which can be described by a four-step mechanism. The two devolatization steps require low activation energies (82 and 86kJ/mol), consequent to the presence of a large number of chemical components (starch, sugars, pectin, lipids and proteins, in addition to cellulose, hemicelluloses and lignin). The first and chief combustion step is also described by a low activation energy (112kJ/mol) whereas the second one requires an activation energy (180kJ/mol) coincident with that typically estimated for lignocellulosic chars.

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DEVELOPMENT OF A FRONT-BASED MODEL FOR THE GLOWING COMBUSTION OF WOOD

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Abstract
Simulation results are presented about the glowing combustion of thick moist wood samples exposed to fire-level heat fluxes, using a front model comprehensive of all the relevant heat and mass transfer phenomena and based on thermally controlled drying, finite-rate kinetics pyrolysis and mixed kinetic-diffusive controlled combustion. The solution shows that, apart from short initial and final transients, an ablation regime is established given high external heat fluxes and/or high moisture contents. Drying, pyrolysis, and combustion take place simultaneously along a constant-thickness layer that propagates at a constant rate (the same for the three fronts) towards the cold sample side. Good quantitative agreement is obtained between model predictions and measurements.

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EFFECT OF CO2 ON COAL PYROLYSIS AT HIGH AND LOW HEATING RATES ON CHAR REACTIVITY

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Abstract
In oxy-fuel combustion, coal particles undergo pyrolysis in CO_2 rich atmospheres. The composition of the gaseous atmosphere under which pyrolysis takes place may have important effects also on the formation of pyrolysis products.
In the present work, pyrolysis experiments have been carried out with a medium rank high volatile bituminous coal substituting N_2 with CO_2. Experiments have been carried out in a laminar drop tube reactor as well as in a fixed bed reactor.
CO_2 chars prepared in the drop tube reactor turned out to be less reactive towards combustion than the corresponding N_2 chars. Differently chars prepared at low heating rates and temperature have similar combustion reactivity regardless of the N_2 vs CO_2 pyrolysis atmosphere.

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EFFECT OF CO2 ON CHARS PRODUCED FROM COAL AND BIOMASS AT HIGH HEATING RATES

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Abstract

Several papers showed that substitution of N_2 with carbon dioxide has non-trivial effects on char combustion. Previous work showed that the reactivity and properties of chars can be affected by the peculiar conditions under which pyrolysis occurs in oxy-combustion systems.

In the present work, pyrolysis experiments have been carried out in a laminar drop tube reactor on a high volatile bituminous Colombian coal and walnut shells in N_2 and CO_2 at a temperature of 1300 °C with high heating rates of approx. $3 \cdot 10^4$ °C/s.

The reactivity of the resulting chars has been analyzed by TGA. Results are compared and discussed to highlight the effect of CO_2 on char properties in relation to the different parent fuel.

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Separation and characterization of size-segregated fractions (soot and char) of carbonaceous particulate produced from coal pyrolysis.

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Abstract

The aim of the present work is the structural characterization of the solid carbon produced during the early stages of coal pyrolysis in a drop tube furnace operated at 1300°C in different environment gases, namely N_2 and CO_2. Electron microscopy has shown that the carbonaceous particulate is a mixture of char particles and submicronic particles/aggregates, here named soot. An ad hoc method based on the sedimentation of ethanol suspensions was used for separating these two fractions suitable for further structural characterization. The properties of soot and char have been investigated by applying several techniques as electron microscopy, laser granulometry, Raman and FT-IR spectroscopy. Results showed that these two fractions do not differ only in particle size: the fine carbon particulate is less reactive and is mostly ash-free, suggesting that its formation occurs in the gas phase, while the coarse (char) fraction mainly derives from coal pyrolysis as it presents inorganic matter from the parent coal.

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HETEROGENEOUS KINETICS FROM CFD DIAGNOSTICS IN AN ENTRAINED FLOW REACTOR

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Abstract
A Computational Fluid Dynamics model of a pilot-scale entrained flow reactor is developed with the aim to shed light into the cloud of solid fuel particles. An iterative procedure is suggested to derive devolatilization kinetics: particle average residence times and heating rates are estimated from the numerical model, and a linear dependence of the particle temperature with residence time is assumed. In this manner the volatile release equation can be integrated analytically and subsequently kinetic parameters can be obtained from experimental conversion data. The procedure is shown for a Sebuku type coal in oxy-fuel conditions.

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NEAR-WALL PHENOMENA IN ENTRAINED-FLOW SLAGGING GASIFIERS

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Abstract

This paper deals with near-wall particle segregation phenomena in entrained-flow slagging coal gasifiers. The recent literature has addressed the fate of char particles by assessing the relative importance of coal conversion associated with the entrained-flow of carbon particles in a lean-dispersed phase and the segregated flow of char particles in a near-wall dense-dispersed phase. Different micromechanical char–slag interaction patterns may establish, depending on the stickiness of the wall layer and of the impinging char particle. The main objective of this study is to use the tool of the physical modelling, to give a contribution in the development of a phenomenological scenario of the fate of coal/ash particles in entrained-flow slagging coal gasifiers, which considers the establishment of a particle segregated phase in the near-wall region of the gasifier. Different scales of investigation were pursued, relevant to study the fluid dynamic conditions which lead to near-wall particle segregation, as well as the particle–wall micromechanical interactions. Montan wax was used to mimic, at atmospheric conditions, particle–wall interactions relevant in entrained-flow gasifiers. As a matter of fact, this wax had rheological/mechanical properties resembling those of a typical coal slag (under molten state) and those of char particles (under solid state).

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MASS AND ENERGY BALANCES FOR A STAND-ALONE TOMATO PEELS TORREFACTION PLANT

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Abstract

Torrefaction is an emerging thermal pretreatment of biomass, which produces a solid biofuel having superior handling, milling, storage and co-firing properties compared to raw biomass. During the process a combustible gas ('torgas') consisting of different organic compound is also produced in addition to the torrefied solid product. In a properly designed and operated torrefaction system the torgas may be combusted to generate heat for the drying and torrefaction steps, thus increasing the overall process efficiency. In this paper, a simple process simulation of a stand-alone torrefaction plant with internal heat integration was performed to assess whether autothermal operation is conceivable for high moisture tomato peel residues (TPs). Results show that for typical torrefaction conditions where about 20-30% of the dry mass is removed in the form of volatile gases (i.e., 285 °C and 30 min for TPs), the process cannot be autothermal and, consequently, an additional utility fuel is required. Under these conditions, in fact, the total thermal energy potentially available in the torgas was approximately 72% lower than the overall energy required for torrefying raw tomato peels, which have 80.5% initial moisture content. The net thermal efficiency of the whole conversion process was estimated to be approximately 70%, whereas the energy yield of the torrefaction unit was 85%. This suggests that for high moisture content agro-industrial residues the integration of torrefaction unit with another plant providing waste heat may be a better option compared to stand-alone plant with internal heat integration in order to save the overall energy efficiency.

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SESSION II

LAMINAR AND TURBULENT FLAMES

Darrieus-Landau induced regime of propagation of turbulent premixed flames in Bunsen configurations

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Abstract
Hydrodynamic or Darriues-Landau (DL) instabilities in weakly turbulent Bunsen flames are numerically investigated under low-Mach number assumptions and a simplified deficient reactant thermochemistry. The DL instabilities are responsible for the formation of sharp folds and cusps in the flame front. Varying the ratio between the flame thickness and the Bunsen diameter the cut-off wavelength is modified and the instabilities induced. It is shown that stability criteria developed in the framework of asymptotic theory for planar flames can adequately predict the behavior of turbulent premixed flames in Bunsen configurations. A statistical characterization of flame morphology in the presence/absence of hydrodynamic instability is given in terms of flame curvature. Similar flame conformations were obtained in a recent experimental work. The statistical analysis highlight that the skewness of the flame curvature probability density function is a consistent marker of the instability presence and two different turbulent modes of flame propagation are identified.

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NO_x formation in a spatially developing turbulent premixed Bunsen flame

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Abstract
A Direct Numerical Simulation of a three-dimensional lean methane/air flame in a spatially developing turbulent slot Bunsen burner is performed. This configuration is of interest as it retains selected characteristics of real devices, such as turbulent production by mean shear.
The jet consist of a methane/air mixture with equivalence ratio $\phi = 0.7$ and temperature of 800 K. The simulation is performed at 4 atm. The coflow is composed of Argon at the temperature of the combustion products.
The flame is in the thin-reaction zone regimes and the Reynolds number based on the jet width and velocity is 5600. The grid has a resolution of 20 μm resulting in a total of 350 million points. A supporting simulation is performed to generate the inflow conditions for the jet.
Chemistry is treated with a new skeletal chemical mechanism developed specifically for the DNS with 33 species.
The macroscopic and microscopic characteristics of the flame are analyzed. Due to the inert coflow, the flame develops from a location few millimeters above the nozzle. The flame structure is found to be similar to the one of one-dimensional premixed flame. Heat release rate and NO rate of formation are analyzed taking into account four paths of decomposition on N_2 as initiation steps for NO formation: NNH, Thermal, Prompt and N_2O.

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From G-Equation to Michelson-Sivashinsky Equation in Turbulent Premixed Combustion Modelling

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Abstract
It is well known that the Michelson-Sivashinky equation describes hydrodynamic instabilities in turbulent premixed combustion. Here a formulation of the flame front propagation based on the G-equation and on stochastic fluctuations imposed to the average flame position is considered to derive the Michelson-Sivashinky equation from a modelling point of view. The same approach was shown to reproduce the G-equation along the motion of the mean flame position, when the stochastic fluctuations are removed, as well ast the Zimont & Lipatnikov model, when a plane front is assumed. The new results here presented support this promising approach as a novel and general stochastic formulation for modelling turbulent premixed combustion.

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SESSION III

SOOT, NANOPARTICLES, PAH AND OTHER LARGE MOLECULES

EFFECT OF C9 ALKYLBENZENES ON PARTICLE FORMATION IN DIFFUSION FLAMES: AN EXPERIMENTAL STUDY

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Abstract
In this work we have extended to C_9H_{12} isomers the study about the tendency of light alkylbenzenes to emit particulate matter. N-propylbenzene, iso-propylbenzene and mesitylene have been studied in atmospheric pressure, counter-flow diffusion flames of ethylene, whose fuel stream was doped with 10%, 20% and 30% of C_9H_{12} isomers. The detection of different types of combustion-formed nanoparticles has been performed with in-situ spectroscopy, namely laser UV-induced emission, by changing the detection wavelength from the UV to the visible. Laser induced incandescence has been also measured to detect soot particles. Experimental results have been compared to those obtained in an ethylene/toluene flame operated in the same operating conditions to understand the effect of the alkyl chain length and branching on particulate formation.
The experimental results showed that a branched alkyl chain in the fuel molecular structure enhances particles formation. In particular, in the pyrolytic zone of the flame, the additives with a single chain produced particulate in larger amount with respect to the oxidant side. Instead the presence of three single methyl groups attached to the aromatic ring stabilizes radicals during pyrolysis, making harder the pyrolytic degradation of the compounds. At the same time, radical stabilization allows these compounds to be more exposed to oxygenated radical attacks in the oxidative flame region, subtracting species to particulate formation, and slowing-down the soot formation pathways.

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Molecular Dynamics Simulations for Structural Analysis of Combustion-Generated Particles

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Abstract
Combustion-generated particle nucleation remains the least understood process of particle formation. Stacking of polycyclic aromatic hydrocarbons (PAHs) has been recognized as key step of particle inception, but uncertainties remain on the PAHs involved in the process and on their interaction mechanism that determine the characteristic soot structure. In this paper, a study of the evolution of PAHs and analysis on the structure of particles obtained has been made using a molecular dynamics (MD) approach. Simulations of evolution of homomolecular systems at 500K have been performed using a MD code (GROMACS). Two different types of PAH molecules have been analysed in order to understand if they exhibit a different coagulation efficiency: coronene ($C_{24}H_{12}$) representative of pericondensed aromatic hydrocarbons (PCAHs), and dicoronene ($C_{48}H_{22}$) representative of aromatic aliphatic linked hydrocarbons (AALHs). A significative dependence of the coagulation efficiency has been found whether PCAHs or AALHs are considered. Successively, particle morphology has been systematically studied analysing the distribution function of the distances between the centres of mass of the coagulated aromatics. A different size and morphology of the nascent particles has been found. Looking at this indicator of internal disposition of molecules in the clusters, coronene clusters show mainly an ordered arrangement of stacked molecules whereas, an enhancement of disorder in the structure has been observed for clusters of dicoronene molecules.

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SOOT FORMATION IN LAMINAR PARTIALLY PREMIXED COFLOW FLAMES BY THERMOPHORETIC PARTICLE DENSITOMETRY

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Abstract
The formation of soot particles in combustion depends on several factors that include: pressure, temperature, fuel chemical structure and extent of premixing. An improved version of the thermophoretic particle densitometry (TPD) method, has been used in this study for quantitative and qualitative characterization of soot particles generated in laminar partially-premixed co-flow flames having different equivalence ratios. To this aim, the dependence of thermocouple temperature response on particle concentration and properties of collected material has been exploited. A variety of thermal emissivity values are measured for flame-formed carbonaceous particles, ranging from $\varepsilon \approx 0.4 - 0.5$ for freshly nucleated particles up to the value of $\varepsilon = 0.95$, typical of a mature soot particle. The correct determination of ε is necessary to accurately evaluate the particle volume fraction at the early stage of the soot formation, where particle concentration measurement is indeed particularly challenging. Data also evidence that oxidation has a severe role in affecting both soot emissivity and soot concentration determination by TPD. However, an attempt to include soot oxidation in the TPD volume fraction procedure is also illustrated resulting in a good agreement of the data obtained with other techniques. Moreover, a modeling analysis based on a sectional approach has been performed in order to corroborate the experimental findings.

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THERMAL ANNEALING METHODS FOR THE RESTRUCTURING OF DISORDERED CARBON MATERIALS

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Abstract
The structural analysis of carbons formed by thermally-induced annealing of an anisotropic carbon as naphthalene pitch is presented in this work. Naphthalene pitch has been heated in a furnace in mild conditions (low pressure and temperature ≤ 1000 °C). The carbonization/ graphitization process has been found to occur at a different extent in dependence of the experimental conditions employed for the annealing.

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SOOT EVOLUTION IN A LAMINAR FLAME PERTURBED WITH A PLANAR VORTEX

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Abstract
The goal of this work is to numerically investigate the role of curvature, strain rate, and unsteadiness on the evolution of soot production in a laminar diffusion flame. A planar flame, fed with a mixture of C_2H_2/N_2 and air, is numerically modeled using a detailed kinetic mechanism based on the Discrete Sectional Method (DSM). The flame is wrapped up by a line vortex, injected from the fuel side, and a Lagrangian analysis is carried out to better understand the production and evolution of soot, localizing nucleation, growth, and aggregation regions, as well as their dependence on local flame stretch.

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TiO_2 NANOSTRUCTURED COATING OBTAINED VIA TERMOPHORETICAL DEPOSITION OF FLAME SYNTHETIZED NANOPARTICLES

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Abstract
A one-step method to produce coatings of TiO_2 nanoparticles on metallic substrates is presented. TiO_2 nanoparticles have been synthesized by Aerosol Flame Synthesis (AFS) and deposited through the mechanism of thermophoresis onto aluminum alloy substrates. The deposition system is constituted by a rotating disc, in order to increase the heat exchange and to promote a uniform distribution of the nanoparticles on the substrates. A fuel-lean flame is used as flame reactor. The average dimension of the nanoparticles is about 5 nm. Three different coatings have been obtained by varying the time of exposure of the substrates into the flame. A full experimental campaign, including SEM observation, thickness detection obtained via confocal microscopy and Electrochemical Impedance Spectroscopy (EIS) has been conducted, in order to characterize the surface and the electrochemical behavior of the coatings. Results show an improvement of the electrochemical behavior, since the deposition is uniform and the coating does not present agglomerates on the aluminum alloy substrates.

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SESSION IV

FORMATION AND CONTROL OF POLLUTANTS AND GREENHOUSE GASES

NANOSTRUCTURED MnO_X CATALYSTS FOR LOW-TEMPERATURE NO_x SCR

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Abstract
Manganese oxides in different structures and morphology have been investigated as catalysts for low temperature SCR by preparing a series of samples by both SCS (Solution Combustion Synthesis) and co-precipitation methods. The samples have been characterized and their catalytic activity tested for NO_x removal in the range of temperature of interest. The different preparation procedures allowed to obtain MnO_x systems with variable average oxidation state that can be put in correlation with the porosity and the morphology and the resulting catalytic performances in the SCR. The presence of Mn_3O_4 in the resulting material with low degree of crystallinity seemed to be the key factor to get the best catalyst among those prepared, being this phase not only active, but very selective towards the production of N_2.

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CERIA-BASED NANOCATALYSTS FOR CO OXIDATION AND SOOT COMBUSTION

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Abstract
We synthesized novel ceria nanocubes doped with zirconium and praseodymium via the hydrothermal procedure (namely pure CeO_2, $CeZrO_2$, $CePrO_2$, and $CePrZrO_2$) For comparison, a set of similar ceria catalysts was prepared by the solution combustion synthesis (SCS). The catalysts were tested for the CO and soot oxidation. These materials showed different surface reducibility, as measured by H_2-TPR, CO-TPR and Soot-TPR, despite their comparable compositions (Zr = Pr = 10 at.%). Soot-TPR appears a suitable characterization technique for soot oxidation catalysts, whereas CO-TPR technique allows to better discriminate among the CO oxidation activities. Praseodymium contributes positively towards the soot oxidation activity. On the other hand, it has an adverse effect on the CO oxidation over the same catalysts, as compared to pure ceria. The incorporation of zirconium into the ceria lattice does not have a direct beneficial effect on the soot oxidation activity, although it increases the catalyst performances for the CO oxidation.

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NEW FOUR-WAY SILVER- AND RUTHENIUM-BASED CATALYSTS FOR NO_X AND SOOT REMOVAL. PART I

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Abstract

The paper is focused on the main achievements accomplished during the SOLYST project. The project aimed at developing a radically new generation of catalytic converters for pollutants emissions. This fundamental research has been achieved by four groups lead by young researchers with complementary expertise: Politecnico di Torino, Università di Udine, Politecnico di Milano and IRC-CNR di Napoli. The University of Udine Research Unit was involved in the development of innovative catalytic materials for storage-reduction NO_x applications (LNT) and for simultaneous removal of NO_x and soot ($DeNO_x$ - DeSoot). The Unit, during the entire project, has been supported by a strong collaboration with the other units, mainly Politecnico di Milano Research Unit. The interaction and the constant exchange of feedback among the Units allowed to improve progressively the formulations and to identify the materials with the best catalytic activity. Herein, the best formulations obtained during the project are reported. The work has been conducted by a strong synergy with Politecnico di Milano Research Unit, for this reason in this first part we will presented the preparation and characterization of the best formulations, while in the second part, Politecnico di Milano will showed the catalytic activity for simultaneous removal of NO_x and soot ($DeNO_x$ - DeSoot).

Silver- and ruthenium-based materials have been synthetized and have been extensively characterized by means of BET, XRD and HRTEM experiments. The formulations has been investigated for the simultaneous removal of particulate matter (soot) and NO_x and their behavior is compared with that of a model DPNR catalysts. Both the Ag- and Ru-based formulations result active in the soot oxidation, more than the traditional Pt-containing DPNR catalyst. Besides, the Ru-based samples show remarkable performances in the $DeNO_x$ - DeSoot activity, although their activity in the reduction step of the stored NO_x still needs further improvements.

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NEW FOUR-WAY SILVER- AND RUTHENIUM-BASED CATALYSTS FOR NO_X AND SOOT REMOVAL. PART II

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Abstract
The paper presents the main results achieved during the three years-SOLYST project. The objective of this project was to develop a new generation of catalytic converters for pollutants emissions from vehicles, through the fundamental understanding of the multiphase particulate-gas-catalyst interactions. Four research groups have been involved in the project: Politecnico di Torino, Università di Udine, Politecnico di Milano and IRC-CNR di Napoli. The Politecnico di Milano Research Unit was mainly involved in the testing of the innovative catalytic materials for storage-reduction NO_x applications (LNT) and for simultaneous removal of NO_x and soot ($DeNO_x$ - DeSoot). Silver- and ruthenium-based catalysts have been prepared and fully characterized by the Università di Udine Research Unit (see abstract part I). Here, they are investigated for the simultaneous removal of particulate matter (soot) and NO_x and their behavior is compared with that of model DPNR catalysts. The catalytic activity for diesel soot combustion, in loose contact conditions, has been studied by means of TPO experiments while NO_x removal is investigated through NO_x storage-reduction cycles. Both the Ag- and Ru-based formulations result active in the soot oxidation, more than the traditional Pt-containing DPNR catalyst. Besides, the Ru-based samples show remarkable performances in the $DeNO_x$ - DeSoot activity, although their activity in the reduction step of the stored NO_x still needs further improvements.

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EFFECT OF THE SOOT CAKE THICKNESS ON THE REGENERATION PERFORMANCE OF A CATALYTIC DIESEL PARTICULATE FILTER

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Abstract
In this work, the effect of the soot-catalyst contact on the regeneration performance of a diesel particulate filter (DPF) wash-coated with nanometric ceria particles was investigated. The catalyst was highly dispersed inside the filter walls. Furthermore, its load was suitably chosen to avoid major changes in pore size distribution of the bare filter. Different amounts of soot were loaded into the filter, thus varying the conditions of soot-catalyst contact.
At the lowest soot load explored, the deep penetration of soot particles into the macro-pores of the filter walls and the consequent good contact with the catalyst particles result in a large fraction of soot burned via catalytic path at low temperatures. At the highest soot load explored, in addition to the soot particles trapped inside the macro-pores, a rather thick soot cake layer accumulates on top of the catalytic walls of the filter. The soot cake is oxidized via thermal path at high temperatures, being substantially segregated from the catalyst.

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ZnO–CuO nanoparticles supported on activated carbon for biogas purification from H_2S at room temperature

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Abstract

Novel sorbents for reactive adsorption of H_2S from biogas at room temperature were prepared by dispersing Zn and Cu oxides nanoparticles onto a commercial activated carbon at fixed total metal loading (10%wt.) and Cu:Zn atomic ratios ranging from 0:1 to 1:1. The functionalized sorbents showed a significantly larger adsorption capacity with respect to the raw activated carbon, and a high utilization factor of the active phase increasing with Cu loading. This was associated to the high dispersion of the metal oxides and the positive interaction with the support. Temperature Programmed Desorption (TPD) of H_2S and SO_2 from saturated sorbents showed that H_2S adsorption was coupled with oxidation phenomena, leading to the formation of metal sulphates apart from metal sulphides and/or elemental sulphur.

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Pt-Fecralloy foams for methanol catalytic combustion

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Abstract

Pt-Fecralloy structured foam catalysts were prepared by an electrodepositon method and tested for methanol catalytic combustion under lean conditions. Noble metal loading was easily controlled through the Pt deposition charge. Characterization of catalysts as prepared, after a thermal pre-treatment and after combustion tests was performed by SEM, XRD and cyclic voltammetry. Methanol deep oxidation could be ignited at as low as 80 °C, reaching complete conversion to CO_2 at temperatures that decreased progressively for increasing Pt loadings.

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MULTI-FUEL COMBUSTION ON PARTIALLY CATALYST-COATED HONEYCOMBS

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Abstract
In this work, we investigated the use of partially coated monoliths as catalytic combustors for syngas/methane mixtures in the presence of significant CO_2 partial pressure. In particular, the effects of CO_2 content and partial coating degree were studied on perovskite-based monoliths. Results have shown that syngas substitution to methane is effective in improving the resistance to the inhibiting effect of carbon dioxide. It has been found that the operative window of the reactor is dependent on both, catalyst-coating degree and CO_2 partial pressure.

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WET ELECTROSTATIC SCRUBBER FOR GAS POLLUTANTS EMISSION CONTROL

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Abstract
In this study, we investigated the remove of combustion particles by means of wet electrostatic scrubbers. In particular, the role of droplet charging on particle capture was investigated. To this end, the experiments were performed to estimate the Droplet Charge to Mass Ratio (D-CMR) for two hollow cone spray nozzles. The experiments revealed that the D-CMR increased linearly with the potential with a slope β until to an optimum potential named V_{opt}. At different potential, the removal efficiency was estimated. It increased more than linearly with the voltage, reaching values higher than 80% for particles in the investigated size range.

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ALUMINA-SUPPORTED [EMIM][GLY] IONIC LIQUID FOR CO_2 CAPTURE FROM MODEL FLUE-GAS

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Abstract
In this paper, we report on CO_2 capture results under model flue-gas conditions for a commercial γ-Al_2O_3 functionalized with [Emim][Gly] ionic liquid (IL) at 5 and 9% wt. loadings. N_2 pore size analysis for the selected sorbents demonstrated that the adopted impregnation protocol was effective in producing a uniform distribution of the IL into the substrate pores. CO_2 dynamic adsorption runs at 303 and 353 K revealed that an increase in the operating temperature determines longer breakpoint times and slower saturation kinetics for the functionalized sorbents. Both functionalized sorbents displayed an enhanced CO_2 capture capacity with respect to the parent sorbent, mainly at 353 K and at larger IL loading (up to a threefold increase in the best case), likely for a greater availability of reactive centers deriving from a reduction of the active phase viscosity at higher temperature.

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Assessment of fine sorbents performances for CO_2 capture in a sound assisted fluidized bed

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Abstract
The aim of the present work is to compare the adsorption performances of different materials (two activated carbons, four zeolites and a metal organic framework) under sound-assisted fluidization conditions (140 dB–80 Hz) in order to maximize the gas–solid contact efficiency and, in turn, minimize the limitations to the intrinsic adsorption capacity of the sorbents. All the tests were performed at ambient temperature and pressure with values of CO_2 concentration typical of flue gases (5–10 vol.%). The different behaviors exhibited by the materials were explained on the basis of their textural properties. In particular, the microporosity falling in the range of 8.3–12 Å strongly affects the CO_2 adsorption performances under the investigated operating conditions.

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CALCIUM LOOPING FOR POST-COMBUSTION CO_2 CAPTURE – EFFECT OF WATER VAPOUR

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Abstract

This study reports on a preliminary investigation concerning the role of water vapour in calcium looping cycles, and is based on results of an experimental campaign performed in a lab-scale fluidized bed reactor under operating conditions that are representative of a realistic calcium looping process. Tests have been designed so as to characterize the effect of steam in either the calcination or the carbonation stages, or in both. A reference limestone has been used as sorbent. Uptake of CO_2 by the Ca-based sorbent with and without exposure to steam during the calcination and carbonation stages has been correlated with results of porosimetric characterization of the samples. Results indicate that exposure to steam is beneficial as it improves in any case the ultimate CO_2 uptake. Exposure to steam during the calcination stage favours the development of accessible porosity, inducing incremental CO_2 uptake in the order of 10% with respect to a reference no-steam case. Exposure to steam during the carbonation stage is also favourable, due to the positive role of steam as a "catalyst" for CO_2 diffusion through the sorbent $CaCO_3$-based product layer. Synergistic effects were observed when steam was added during both the calcination and carbonation stages, resulting in a very pronounced increase of sorbent CO_2 capture capacity as compared with the no-steam case.

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CHARACTERIZATION OF CALCIUM LOOPING SORBENTS WITH AN INNOVATIVE LAB-SCALE APPARATUS

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Abstract
The loss of sorbent CO_2 capture capacity and the extent of particle attrition over iterated cycles are relevant to the design of Calcium Looping processes. Thermogravimetric analyzers or single batch fluidized bed reactors are typically used at the lab-scale to evaluate the sorbent performance. One drawback of these devices is that they do not reproduce the thermal history that is actually experienced by sorbent particles in real looping cycles. In this study, a novel experimental device is proposed to overcome this limitation. The test reactor has been used to assess the effect of the thermal history of the limestone on its CO_2 capture capacity and attrition tendency. The results were compared to those previously obtained with the same limestone under comparable operating conditions in a single bed apparatus. The comparison reveals that the thermal history experienced by the limestone has a non-negligible effect on its performance.

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Primary fragmentation of Biomass-Cement-CaO pellets for Calcium Looping

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Abstract

This work explores the effect of biomass templating on fragmentation of calcium-aluminate based pellets. Three different types of pellets have been tested: one with calcium aluminate cement (LC), another with flour (LF) and one with both cement and flour (LCF). Fragmentation has been investigated by two different techniques, namely with a pressurized heated strip reactor (PHSR) and a bubbling fluidized bed (BFB), under different conditions. Both sets of experiments showed that that the addition of biomass enhances the propensity to undergo fragmentation. The addition of cement partially counteracts this effect.

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SESSION V

GAS TURBINE COMBUSTION SPRAY, DROPLET AND SUPERCRITICAL COMBUSTION

ON SPECIFIC ASPECTS OF SPRAY-FLAME DYNAMICS

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Abstract
Recent experiments in Wilson chambers have shown that spray flames are much more sensitive to wrinkles or corrugations than the single-phase flame propagating in a gaseous mixture of the same equivalence ratio. This leads to spray-flame propagation faster than that of single-phase flame [1-3]. These observations, often carried out in microgravity [2], have motivated our recent numerical works on the spray-flame dynamics [4-6]. In the numerical approach, the spray is schematized by alkane droplets, located at the nodes of a centered 2D-lattice and surrounded by a gaseous mixture composed of alkane and air.

The compositional parameters of these studies are φ_G, the equivalence ratio of the gaseous surrounding mixture, φ_L, the liquid loading and φ_T, the overall spray equivalence ratio ($\varphi_T = \varphi_G + \varphi_L$). The geometrical parameters are s, the lattice spacing, L_X [resp. L_Y], the size of the computational domain parallel to propagation [resp. transverse to propagation]. All geometrical parameters are reduced by δ_L^*, the flame thickness of the stoichiometric single-phase flame.

The numerical results indicate that droplets can play an important role with respect to Darrieus-Landau instability (DL instability). On the one hand, the presence of droplets brings a perturbation, the level of which is enough to trigger the DL instability. On the other hand, when the DL instability is developed in the non-linear domain, the droplets induce additional wrinkles at smaller scales, which increase the effective surface and promote the spray-flame velocity.

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Assessment of a numerical procedure for scale resolved simulations of turbulent spray flames

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Abstract
The present paper consists in a collection of CFD simulations with increasing geometrical complexity aimed to investigate phenomena occurring in turbulent spray flames and to develop a reliable numerical procedure useful in the design of aero-engine combustors. Scale Resolved Simulations (SRSs) were performed using Flamelet Generated Manifold (FGM) and Eddy Dissipation Model (EDM) for combustion modelling and an Eulerian-Lagrangian approach for droplet evolution. Results highlight outstanding enhancements in the prediction of spray flame behavior using SRSs in place of classical RANS approaches.

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Burning behaviour of selected biogas and syngas mixtures

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Abstract
Experimental evaluation of the combustion characteristics of carbon-neutral, biomass-derived fuels has been carried out. Since these fuels are meant as likely replacement for CH_4, a comparison was drawn with methane in the same operating conditions. Tests were performed in the high-pressure, constant-volume DHARMA reactor at Istituto Motori - CNR. The laminar burning parameters were evaluated analyzing spherical expanding flames. The flame growth was recorded by means of high-speed, high-resolution shadowgraph; image processing and stretch analysis allowed to infer the laminar burning velocity and the Markstein length for each test case. Results are presented for the combustion in air of CH_4-CO_2 (55-45 % vol.), H_2-CO (5-95 % vol.) and a wood gasification product. All the tests were performed at 0.6 MPa and 301 K. The equivalence ratio ranged between 1.0 and the lower flammable limit. The unstretched laminar burning velocity and the Markstein length are reported for each fuel as a function of the equivalence ratio.

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SESSION VI

REACTION KINETICS
COMBUSTION DIAGNOSTICS

Simplified chemical kinetic mechanisms for hybrid rocket propulsion

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Abstract

A set of simplified chemical kinetic mechanisms for hybrid rockets applications using gaseous oxygen (GOx) and hydroxyl-terminated polybutadiene (HTPB) is proposed. The starting point is a 94-species, 614-reactions, detailed chemical kinetic mechanism for butadiene combustion, the primary HTPB pyrolysis product. The simplification is carried out systematically by means of a Computational Singular Perturbation (CSP) based algorithm. The simplification algorithm is fed with the steady-solutions of classical flamelet equations, these being representative of the non-premixed nature of the combustion processes characterizing a hybrid rocket combustion chamber. Three simplified chemical mechanisms, each comprising approximately 20 species, are obtained for three different pressure values selected in accordance with an experimental test campaign of lab-scale hybrid rocket static firings. Finally, a comprehensive simplified mechanism containing 27 species is shown to be capable of reproducing the main flame features in the whole pressure range considered.

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GENERALIZED ENTROPY PRODUCTION ANALYSIS FOR MECHANISM REDUCTION

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Abstract
This paper introduces a generalized formulation for the entropy production analysis. The use of relations valid under the hypothesis of validity of the principle of detailed balance, that is violated in the remarkable case of irreversible reactions, is avoided by using more general expressions for the entropy generation due to the chemical reactions. As a result, the new formulation is applicable to generate reduced mechanisms involving both irreversible reactions or ad hoc estimated reverse rates.

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NON-LINEAR REGRESSION OF THE THERMOCHEMICAL STATE-SPACE ONTO A REDUCED NUMBER OF PRINCIPAL COMPONENTS

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Abstract
Large kinetic mechanisms are required in order to model accurately combustion systems. If no parameterization of the thermo-chemical state-space is used, solution of the species transport equations can become computationally prohibitive as the resulting system contains a wide range of time and length scales. Parameterization of the thermo-chemical state-space without an a priori prescription of the dimension of the underlying manifold would lead to a reduced yet accurate description. To this end, the potential offered by Principal Component Analysis (PCA) in identifying low-dimensional manifolds is very appealing. The present work seeks to advance the understanding and application of the PC-transport approach by analyzing the ability to parameterize the thermo-chemical state with the PCA basis using non-linear regression. In order to demonstrate the accuracy of the method within a numerical solver, unsteady perfectly stirred reactor (PSR) calculations are shown using the PC-transport approach. The PSR analysis extends previous investigations by the Authors to more complex fuels (e.g. methane, propane), showing the ability of the approach to deal with relatively large kinetic mechanisms. The ability to achieve highly accurate mapping through Gaussian Process based nonlinear regression is also shown. In addition, a novel method based on local regression of the PC source terms is also investigated.

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EXPERIMENTAL CHARACTERIZATION AND MODELING OF A NON-PREMIXED METHANE/AIR FLAME

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Abstract

Non premixed combustion is the most common combustion mode in practical systems because of its wide operating range, safety and stability. In this work a simple laminar non premixed methane/air flame has been experimentally characterized with different diagnostics: thermocouples, chemiluminescence, laser induced breakdown spectroscopy (LIBS). The experimental data obtained were compared to the results of a detailed chemical kinetic model. These results are discussed in the manuscript.

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IR thermal imaging characterization of a hybrid catalytic radiant gas burner

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Abstract
The novel concept of hybrid catalytic combustion based on Catalytic Partial Oxidation + homogeneous flame combustion was tested for the first time with fuel mixtures of methane and hydrogen. A prototype radiant hybrid burner was characterized by IR thermal imaging while safely operating with up to 80% vol. of H_2 in the fuel and a primary equivalence ratio in the range 2.4 – 4.0. Outstanding NO_x emission levels were attained due to the effective reduction of both thermal and prompt NO_x formation.

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SESSION VII

FUEL PROCESSING AND UPGRADING

THE HELMETH PROJECT: CARBON DIOXIDE METHANATION COUPLED WITH HIGH TEMPERATURE ELECTROLYSIS FOR SYNTHETIC NATURAL GAS PRODUCTION

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Abstract
Hydrogenation of carbon dioxide for synthetic natural gas (SNG) production has been investigated in an integrated process. The attention has been focused on the coupling between high temperature (SOEC-based) electrolysis and a methanation section with two isothermal reactors operating at 300 °C and 15 bar. Such integration is very promising because the vaporization heat required for the high-T electrolysis can be supplied by the exothermal methanation. The experimental activity has been carried out by testing two inlet mixtures (reproducing the two reactors). A commercial catalyst available at pellet size has been used for the activity test. The experimentally obtained high conversion (up to 93% and 83% for the first and the second reactor, respectively) enables the production of a SNG that could be directly injected in the natural gas distribution grid. Through the thermal integration between hot and cold streams an achievable electricity-to-SNG conversion efficiency equal to 84% (on HHV basis) has been calculated.

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CATALYTIC PERFORMANCE OF COMPOSITE OXIDE SUPPORTED Ni-BASED CATALYSTS FOR CO_2 METHANATION

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Abstract
Composite oxide supported Ni-based catalysts were prepared by wet impregnation technique and applied for the methanation of carbon dioxide. The composite oxide supports were prepared by an impregnation-precipitation method using commercial γ-Al_2O_3 powder loaded with different percentages of ZrO_2, TiO_2 and CeO_2 promoters. The as prepared catalysts were characterized by BET specific surface area, AAS, XRD, H_2-TPR and CO chemisorption. Catalytic activity of the synthesized catalysts was investigated towards hydrogenation of CO_2 at atmospheric pressure by varying reaction temperature between 250 and 400 °C. Experimental results revealed that the composite oxide supported Ni-based catalysts showed superior performance than the γ-Al_2O_3 only supported Ni-based catalyst. Among the investigated catalysts, the catalyst with the highest amount of promoter oxides showed the best activity: 81.4% conversion of CO_2 to CH_4 at 300°C. The better performance of the composite oxide supported Ni-based catalysts was achieved due to the improvements in reducibility nature of the catalysts (investigated using H_2-TPR).

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DEVELOPMENT OF A ROBUST AND EFFICIENT BIOGAS PROCESSOR FOR HYDROGEN PRODUCTION IN THE FRAMEWORK OF THE EUROPEAN BIOROBUR PROJECT

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Abstract

The present work deal with the development and testing of a robust and efficient decentralized fuel processor based on the direct autothermal reforming (ATR) of biogas with a nominal production rate of PEM-grade hydrogen of 50 Nm^3/h. The system energy efficiency of biogas conversion into green hydrogen is 65%, for a reference biogas composition of 60%vol CH_4 and 40%vol CO_2.

Modelling and simulation (CFD and FEM) were carried out to select the innovative catalyst support with promising results for the BioRobur fuel processor and furthermore, 2D CFD analysis was also used to examine flow uniformity issues due to soot trap integration close coupled to the ATR. X-Ywt.% Ni-Rh/$MgAl_2O_4$ - SiSiC structured catalyst was selected as a potential catalyst for the conversion of biogas to hydrogen. Homogenous lattice structure composed of cubic rotated cell showed excellent performances, guaranteeing a high reliability of the process. Moreover, $LiFeO_2$ catalyst was selected as the most prominent candidate towards to carbon gasification in a reducing atmosphere. The catalyst was in-situ deposited directly over the wall-flow filter. Tests of the coupled system under realistic conditions at the pilot and demonstration scale have showed satisfactory results in terms of, hydrogen yield and pressure drop in the system, reaching the target with a nominal production rate corresponding to 50 Nm^3/h of hydrogen.

Besides, Aspen simulation and LCA analysis has demonstrated that BioRobur is the most promising process to hydrogen production compared to other types of reforming process. The work is being performed within the SP1-JTI-FCH.2-Collaborative Project 'BIOROBUR'. The partners involved in the Biorobur project bring together a sufficient number of important European actors on the scientific, research and industry level.

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SESSION VIII

INTERNAL COMBUSTION ENGINES

OPTICAL FLOW ESTIMATION OF FLAME VELOCITY IN A SPARK IGNITION ENGINE

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Abstract
The present study reports on the detailed investigation and characterisation of spark-ignited combustion events. In order to provide a statistical analysis of turbulent flame front propagation, a large amount of data was collected, starting from experiments conducted in an optically accessible single spark ignition engine. To extract all needed information, the flame propagation recorded images were pre-processed digitally. Then, the detection of the flame front was obtained by using a new hybrid level-set method. Finally, an optical flow estimation technique, based on the model of Horn and Schunck, was used for the evaluation of velocity.

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CORRELATION BETWEEN SOOT FORMATION AND EMISSIONS IN A SMALL DISPLACEMENT SPARK IGNITION ENGINE OPERATING WITH ETHANOL MIXED AND DUAL FUELED WITH GASOLINE.

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Abstract

This paper deals with the evaluation of the effect of different methods of ethanol fueling on in-cylinder soot formation and exhaust emissions in a small displacement spark ignition engine. The engine was fueled with gasoline and ethanol. In particular, the ethanol was both blended with gasoline (E30) and dual fueled (EDF). In this latter case, ethanol was direct injected and gasoline was injected into the intake duct. For both the injection configurations, the same percentage of ethanol was supplied: 30%v/v ethanol in gasoline. The experimental investigation was carried out in 4-stroke small single cylinder engine. The measurements were carried out at 2000 and 4000 rpm under full load condition. Optical technique based on 2D-digital imaging was used to follow the combustion process. Two-color pyrometry was applied to assess the soot formation. Particle emissions were measured at the exhaust by means of a smoke meter. Particle size distribution function was measured in the range from 5.6 to 560 nm by means of an Engine Exhaust Particle Sizer (EEPS). For E30 the in- cylinder soot formation and emissions are larger than for EDF because of the different contribution of gasoline. In EDF the better evaporation and mixing of gasoline, typical of PFI configuration, coupled with the soot reduction tendency of ethanol lead to a low particle formation and emissions.

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SESSION IX

BIOFUELS, BIOCHEMICALS AND BIOREFINERY NOVEL CONCEPTS, TECHNOLOGIES AND SYSTEMS

COMPARATIVE STUDY OF BIOCHAR FROM SHORT ROTATION COPPICE FOR OPTIMIZATION OF PHYTOEXTRACTION BY-PRODUCTS MANAGEMENT

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Abstract

Phytoremediation technique is of growing interest in the restoration of trace elements contaminated soils. An integrated approach, combining land restoration and biomass post-processing, using a pyrolysis process for material and/or energy recovery, could allow for effective realization of such a process. The dependence of yields, chemical and structural characteristics of char on the biomass feedstock and pyrolysis thermal conditions are important features to be evaluated to explore the possible applications of such a product. In this framework, a comparative study of steam assisted slow pyrolysis of five biomasses has been carried at 873 K. Results demonstrate that for applications requiring high specific surface area *Populus Nigra*. On the contrary, if the goal is the maximization of the energy recovery in the char, *Eucalyptus* represents the best choice.

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Lignin removal for biomass biorefinery: ultrasound-assisted dilute acid pretreatment of coffee silverskin

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Abstract

In the last years the decreasing availability and increasing price of fossil resources, as well as global climate changes, forced scientists to focus the attention on the biorefinery concept. Agriculture food processing wastes (AFWs) are potential feedstock for biorefinery processes. Pretreatment and enzymatic hydrolysis are required to reach an efficient recovery of monomeric fermentable sugars form the biomass feedstock. The first step concerns removal and potential valorization of non-fermentable lignin and is commonly called biomass pretreatment. Current research is focused on the selection of novel processes for biomass pretreatment able to provide extended lignin removal and cost saving with respect to conventional pretreatments (e.g. steam explosion).

This contribution reports on the study of ultrasound-assisted acid pretreatment (USAAP) of the AFW coffee silverskin (CS). The effects of several pretreatment variables, such as time and power of sonication, biomass loading and acid concentration, were studied using Response Surface Methodology (RSM).

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INVESTIGATION OF A CALCIUM LOOPING-CONCENTRATED SOLAR POWER INTEGRATED PROCESS

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Abstract
The integration of a Calcium Looping (CaL) cycle with a Concentrated Solar Power system can represent an important climate-change mitigation technology. In this work, the solar CaL process has been experimentally investigated by the use of a solar Fluidized Bed (FB) reactor. Three short-arc Xe-lamps of 4 kW_{el} each, coupled with elliptical reflectors, were used as solar simulator obtaining a peak flux of nearly 3000 kW m^{-2}. Several calcination-carbonation tests were carried out on a commercial limestone sample, to evaluate the sorbent performances in terms of CO_2 capture capacity increasing the number of cycles. Results show that, for the limestone sorbent at hand, the higher temperatures obtained on the FB surface do not produce a severe worsening of the reactive material properties, thus encouraging the research on the solar-driven CaL process.

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TOWARDS IMPROVEMENTS IN STABILITY, EFFICIENCY AND EMISSIONS REDUCTION OF COMBUSTION PROCESSES BY USING A STRONG CYCLONIC RECIRCULATION

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Abstract
A challenging strategy to stabilize the oxidation process in novel combustion technologies is the exhaust gas recirculation. In such systems the mass and sensible enthalpy ratio of recycled exhausted gas represents a key parameter to promote and stabilize the oxidation process.
The chemical/thermodynamic features of the oxidation process were investigated by means of a numerical analysis. The process was schematized as a CSTR where part of the exhausted gas was recirculated back to the reactor. The stability of the process was investigated as a function of the pre-heating temperature and of the dilution level of propane/oxygen/nitrogen mixtures for a fixed recirculation ratio.
On the other hand experimental tests were realized in a small size burner characterized by a strong internal recirculation ratio, induced by a cyclonic fluid-dynamic pattern obtained with the geometrical configuration of the reactor and of the feeding system.
The experimental results suggest that the cyclonic configuration represents a challenging choice to stabilize the oxidation process in small-size applications, extending the burner operability conditions.

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SESSION X

FIRE AND SAFETY RESEARCH

Preliminary CFD analysis of a ventilated chamber for candles testing

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Abstract
As candles have grown in popularity with consumers over the last few years, so has the potential safety concern with their use in indoor environments. Carbon monoxide, particulate matter and different volatile and semi-volatile species can be found in candles emissions. Currently it is not possible to predict theoretically which emissions will be produced by a specific candle and in order to quantify real emissions is still necessary to proceed with experimental tests. A common way to quantify released pollutants is to burn candles in a well-controlled environment, such as a laboratory-scale test chambers. Obviously, it is required that these chambers are able to reproduce the environmental combustion regime of the candles, so as to guarantee that an equal level of emissions is produced and measured. Another crucial point is related to the measurements themselves: generally, air quality is measured in a single point inside the chamber with the assumption that the air and the exhausts in that point are representative of the whole ambient. This work aims to reproduce one of these chambers by means of a CFD (Computational Fluid Dynamics) model, with the purpose of obtaining an adequate tool to analyze and design more efficient test chambers. A comparison with an ad hoc experiment is performed to validate the CFD model.

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HOW DROUGHT IS AFFECTING WILDFIRE RELATED RISKS FOR NATURAL GAS PIPELINE

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Abstract
Wildfires can be triggered by either natural or human causes. Lightning is the single biggest natural cause of wildfires, but spontaneous ignition due to local heating may also occur. Human causes include deliberate actions (arson), or sparks for machinery as train wheels, barbecues, camp-fires and cigarettes which haven't been extinguished properly, or even electricity pylons falling down in high winds. Whatever the ignition cause, the presence of large amount of dry vegetation is essential for the fire propagation. In the last decades, this option has clearly increased because of the duration and intensity of droughts in some regions of the world, including southern Europe and the Mediterranean region. Eventually, drought has significantly affected the hazard and the severity of wildfires, which can in turn produce adverse impact on human activities and, in particular, with gas pipelines. In this work, a preliminary analysis of the risk of accident due to wildfire on natural gas pipeline systems passing through forests, woods and bush fields is shown, in the framework of the more general analysis of Natech risks.

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A ZONE MODEL FOR ULTRAFINE WATER MIST FIRE EXTINCTION IN COMPARTMENTS

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Abstract
A zone model suitable for a preliminary fast assessment of the required release of Ultra Fine Water Mist (UFWM) for fire extinguishment in compartments is presented. Developed starting from the two zone model, it includes separately the fire plume zone to account for the peculiar behavior of UFWM that vaporize before reaching the burning surface. Evaluation of the effectiveness is based on a-posteriori observation of results. An example of application to an office workstation compartment is reported.

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LARGE EDDY SIMULATION OF POOL FIRE OF A DIATHERMIC OIL

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Abstract
In this work, the flash point (FP) of a diathermic oil used in the circuit of a packaging industry was measured. It has been found that the oil is operated at temperatures (~ 250°C) higher than the FP (~ 210°C). This issue increases the risk of fire. In order to estimate the consequences of a pool fire involving diathermic oil, a CFD model based on Large Eddy Simulation (LES) was developed. Numerical results have shown that, under the simulated conditions, the height of the fire is such to reach the roof of the boiler room.

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POSTER

ELECTRICAL CHARACTERIZATION OF FLAME-SOOT NANOPARTICLE THIN FILMS

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Abstract

Studies focused on soot formation showed that flames can produce a broad variety of carbon nanoparticles, CNPs, with different morphology, chemical, physical, optical and electronic properties. In addition, flames can be optimized to form tailored CNPs for specific applications [Shuiqing Li et al. Prog Energy Combust Sci 2016;55:1-59]. The assembly of nanoparticles into a uniform thin film poses a significant challenge and various techniques have been developed over the years to deposit homogeneous layers of nanoparticles that can lead to novel applications. Thermophoretic sampling is a technique often used to collect on a substrate isolated particles from flames for analytical purpose. This method relies on the thermophoretic forces driving the aerosol particles in the hot gas flame towards a cold surface inserted in the flame.

In this work, carbon nanoparticles were produced in a premixed ethylene-air flame and their potentiality as a medium for electronic applications has been investigated. To this aim, CNPs thin films were prepared by the direct deposition of the flame-synthesized CNPs on multilayer substrates consisting on highly-doped (500 μm thick) Silicon layers, thin (200 nm) SiO_2 insulating barriers and gold electrodes (drain/source contacts) with interdigitated layout. CNPs size has been measured by a Scanning Mobility Particle Sizer, and their physico-chemical properties by UV-visible light absorption and Raman spectroscopy. Current-voltage (IV) measurements recorded for all films showed a linear (ohmic) behavior for applied voltages up to 10V. Moreover, it was found that, as a function of the thickness, the electrical conductivity (σ) of these layers exhibit a distinctive behavior typical of the percolating systems with a threshold localized at about 100 nm and maximum values slightly higher than 10^{-3} S/cm. . Upon the application of a further external voltage signal to the highly-doped Silicon substrate, working as the gate electrode in a field-effect transistor configuration, we were also able to modify reversibly the current flowing in the CNPs channels. In this way, by the basic equations of the Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) theory, we estimated a maximum charge carrier mobility (μ) of about 10^{-4} $cm^2/V*s$.

DETAILED KINETICS MODELING OF SOOT FORMATION

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Abstract
It is well known that soot carbonaceous particles cause adverse effects to health and environment and also reduce the combustion efficiency. The accuracy in predicting particle sizes and number density of soot particles is essential in addition to mass yield prediction. The present work addresses the study of the detailed kinetic modeling of soot formation process, with the aim to compare different number of classes of lumped pseudo-species (BIN). The benchmark premixed ethylene burner-stabilized stagnation (BSS) flame [1] is simulated to compare between the current POLIMI soot sub-mechanism with 20 BINs presented by Saggese et al. [2] and the developed soot sub-mechanism with 25 BINs. Model predictions of mobility particle size distribution functions (PSDFs) of both sub-mechanisms are in qualitative agreement. The developed soot sub-mechanism with 25 BINs is able to predict carbonaceous particle formation from incepted to mature soot particles.

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NUMERICAL MODELING OF SOOT FORMATION AND EVOLUTION IN LAMINAR FLAMES: THE LIMITS OF THE HYBRID METHOD OF MOMENTS

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Abstract
Soot has a negative effect on human health and environment. Therefore, their reduction is one of the major priorities for both transport and process industries. Improving the prediction capability of the numerical simulations of industrial configurations can help to achieve this goal.

The objective of this work is to investigate the abilities of Method of Moments (MOM). In order to identify the best compromise between the accuracy of the results and the computational effort.

The hybrid method of moments (HMOM) [2] represents the state-of-art model for large eddy simulations of soot production in turbulent flames. It is very efficient in terms of computational cost, but it accuracy may be limited [3]. Here, some preliminary tests on the performances of the HMOM will be presented. The discretization error and the role of the model constants will be quantified by comparing the results to some reference data obtained using a Monte-Carlo solver and a Discrete Sectional model [1].

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INVESTIGATION OF THE INDUCED FLOW FIELD AND FLAME ENHANCEMENT BY NON THERMAL PLASMA

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Abstract
The present work investigates the effects of sinusoidal dielectric barrier discharge (DBD) on a lean non premixed methane/air flame in a Bunsen-type burner has been investigated under different actuation conditions and fueling configurations and flow rates.
High speed flame imaging was done by using an intensified CCD camera equipped with different optical filters in order to selectively record signal from the chemiluminescent species OH*, CH*, or CO2* to evaluate the flame behavior in presence of plasma actuation. It was evident that the plasma flame enhancement was significantly influenced by burner operating conditions and DBD configurations. At high plasma power values the increase of the air mass flow rate at lean blowout was up to 30 % for low methane flow rate and up to 10% at high fuel flow rate.

In order to investigate separately the fluid-dynamic effect of the actuator, velocity measurements of the jet were carried out in absence of combustion by using the Laser Doppler Velocimetry technique. Methane flow was replaced by air at the same flow rate, using incense smoke to seed both air/air flows. Temperature profiles were also acquired in correspondence with the measured velocity locations by using an in-house calibrated type K thermocouple. The obtained results showed a similar velocity profile pattern between actuated and non actuated cases, revealing also a high thermal effect, translated into higher velocity values at equal flow rates. The temperature was found also to vary strongly along the radius. For the higher electrical input power tested, 29 W, the temperature of the air flow reached a peak of 154 ºC and a velocity augmentation of around 1 m/s, with an evaluated thermal power of 23 W.

A new approach to biogas fuelled micro gas turbine: experimental setup, CFD simulations and preliminary results

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Abstract
The research activity concerns the utilization of biogas into a commercial micro gas turbine (MGT) Ansaldo Turbec T100P. Through a 3D CFD analysis were explored the limits (in terms of CO_2 percentage in the fuel) of the stock combustor, designed for natural gas feeding. Initial and boundary conditions of the numerical approach were obtained from a validated 0D thermodynamic matching model.
The use of biogas in MGT has been already quite explored in literature. However, conflicting and not yet fully comprehensive results highlight the need for further scientific investigations. Numerically it has been demonstrated by several authors the possibility for using biogas with amount of CO_2 up to 40-50% by volume in commercial MGT. But, they are not yet present experimental evidences of this condition. In fact, the CO_2 concentration limit experimentally validated in literature, prior to which phenomena of detachment and instability of the flame happen, is considerably lower (~12%).
The utilization of biogas in micro gas turbines generally requires structural adaptations, often invasive and expensive, to fuel compression unit and control valves. Not infrequently a partial redesign of the combustor is necessary. It is clear that similar modifications, increasing plant costs, may be antithetical to the concept of a rational and sustainable exploitation of energy resources of lower value as the biogas.
Aim of this activity is to overcome these constraints, by identifying a structurally non-invasive and cost-effective solution to increase the CO_2 concentration in the fuel. Through a synergistic activity between numerical modeling and experimental work it has been evaluated, implemented and tested an innovative management strategy of fuel feeding and combustion. The preliminary results of this novel approach are here discussed.

A HIGH EFFICIENCY TURBOCHARGED ENGINE DESIGNED FOR LHV GASEOUS FUELS

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Abstract
This paper deals with the design and the construction of a small power unit (about 25 kW @ 1500 rpm) based on a widespread automotive internal combustion engine, to be fed with L.H.V. (Low Heating Value) gaseous fuel like syngas. The latter is characterized by a bad behavior in respect of combustion when adopted in an engine, because of its content of CO and H_2. This aspect can lead to unstable working condition and easily lead to knock, this involving mechanical overload and higher emissions (NOx). As consequence, the adoption of these fuels can reduce very much global efficiency as a lower compression ratio is achievable. These issues could be partly resolved through the design of an engine especially conceived to be fed with very reactive fuels. The unit has been obtained transforming a robust Diesel turbocharged engine in a spark-ignition prototype, by means of a new combustion chamber with lowered compression ratio (if compared to the previous value of the compression ignition engine). The original high turbulence swirl arrangement has been kept, in order to reduce the influence of hot spot like exhaust valves (causing local critical temperature), while mixing perfectly fuel with air, in order to get a very homogeneous fresh charge. A dedicated control apparatus, designed for previous microcogeneration prototypes, has been modified in order to manage the stoichiometric setting (through a Lambda probe) while avoiding knock conditions by means of an active waste-gate which can reduce intake pressure when critical conditions are detected (by means of a piezometric sensor). As syngas is normally available at low pressure, an innovative compression system has been conceived, based on a first turbocharger (for gaseous fuel) put on the exhaust line before the main turbocharger (for air), this permitting to keep separate the two streams until their mixing into the intake manifold runners (i.e. the last section) for safety reasons (backfire).

EXPERIMENTAL ASSESSMENT OF DARRIEUS-LANDAU INDUCED REGIME OF PROPAGATION IN TURBULENT BUNSEN FLAMES

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Abstract

Hydrodynamic or Darrieus-Landau (DL) instabilities in turbulent Bunsen flames are experimentally investigated. The DL instabilities are responsible for the formation of sharp folds and cusps in the flame front.
Mie scattering images of particle tracers dispersed into reactants allows for the determination of velocity field by particle image velocimetry (PIV) and the flame front position, educed from particle number density jump between reactants and products.
By varying the equivalence ratio of an air/propane mixture at atmospheric pressure the cut-off wave-length is modified -made lower or larger than the hydrodynamic length scale of the system L- and the DL instability induced or not, respectively prompting the onset of super- or subcritical regimes of flame propagation. We also inhibit DL instability formation by reducing the hydrodynamic length scale L. This is driven by a substantial reduction of bunsen diameter, which can be considered of the order of L. The critical value of L below which DL instability is inhibited can be derived by a linear stability analysis of a planar flame.

In the present work, we aim to gain more insight about the role of DL instabilities upon flames at increasing turbulence level and to which extent the curvature skewness can identify the cusp-like structure of the unstable front. The statistical analysis highlight that the skewness of the flame curvature probability density function is a consistent marker of the instability presence and two different turbulent modes of flame propagation are identified.
It is also shown that as turbulence intensity increases, a less pronounced influence of hydrodynamic instability on the flame front dynamics emerges and, in turn, it is reflected on the behavior of the resulting skewness values.

Direct Numerical Simulation of high pressure turbulent lean premixed CH_4/H_2-Air slot flames

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Abstract
A numerical study on lean turbulent premixed methane/hydrogen-air slot flames at high pressures is conducted through two-dimensional Direct Numerical Simulation (DNS). A single equivalence ratio flame at ☞=0.7 and 50% of hydrogen content is explored for three range of pressure (0.1,1,4 MPa respectively). Due to the decreased kinematic viscosity with increasing pressure, the turbulent Reynolds numbers increase with an associated decrease of smallest turbulence scales.
Finite difference schemes were adopted to solve the compressible Navier-Stokes equations in space (compact sixth-order in staggered formulation) and time (third-order Runge-Kutta). Accurate molecular transport properties were also taken into account and, a detailed skeletal chemical mechanism for methane/hydrogen-air combustion, consisting of 23 transported species and 124 elementary reactions, was used.
A general description of the three flames is provided, evidencing their macroscopic differences by means of turbulent displacement speed, flame surface areas and mean flame brush thickness.
Furthermore, topological features of the flames are explored by analyzing the probability density functions of several quantities: curvature, curvature shape factor, alignment between vorticity and principal strain rate vectors with flame surface normal, displacement speed and its components.

Large eddy simulation of non-premixed combustion with detailed chemistry

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Abstract
The present work in progress aims at investigation of the possibility of exploiting eddy dissipation concept (EDC) model as a SGS combustion model in the large eddy simulation (LES) of reactive flows with detailed chemistry. Introduced in 80s by Magnussen [1], EDC has been used widely in RANS of reactive flows. However, the possibility of extending the model to LES of reactive flows with detailed chemistry has not been systematically investigated. Recently, Lysenko et al. [2] exploited LES/EDC with one step methane chemistry to simulate Sandia D flame and got results with acceptable accuracy.
The governing equations are filtered Navier-Stokes equations plus filtered equations for species transport in low-Mach formulation. The computational tool is edcSMOKE which is composed of OpenFOAM and OpenSMOKE++ [3] numerical libraries. The methodology used here to validate the proposed LES/EDC model is to use the DNS data. Two DNS cases are considered. DNS1, is a lifted hydrogen and Ethylene flame [4] (jet into hot-coflow regime). DNS2 is the temporal evolution of mixing layer of a syngas flame [5]. The flame exhibits strong turbulence-chemistry interaction resulting in local extinction followed by re-ignition. Questions to be answered are how to define fine structures by filtered and SGS LES data and how to treat these fine structures.

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KINETIC MECHANISM OF ACETIC ACID COMBUSTION

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Abstract
Oxygenated species are very abundant in the tar released from biomass pyrolysis. Acetic acid is the major acidic components of bio-oils [1]. Therefore, a proper knowledge about its pyrolysis and combustion behavior is necessary to characterize the combustion of biomass pyrolysis oils. This work is specifically focused on the characterization of the gas-phase kinetics of acetic acid, starting from an existing kinetic mechanism [2] already validated in pyrolysis conditions [3]. In this work, this mechanism is updated and further validated in oxidative conditions, using very recent experimental data [4-6]. Moreover, the updated kinetic model is also compared to the previous pyrolysis measurements of Mackie and Doolan [7]. Since acetic acid can decompose forming CH_4 and CO_2 and also CH_2CO and H_2O, through decarboxylation and dehydration reactions, the kinetic mechanism is also compared to pyrolysis and oxidation experiments of ketene [8,9]. The wide range of conditions studied in this paper allowed to further validate the mechanism and characterize the relative role of molecular, initiation and H abstraction reactions.
This work is supported by the EU Residue2Heat project (G.A. 654650).

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Enhancing the performances toward CO_2 capture of MIL-96: hybridization with graphene-like material

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Abstract
CO_2 is one of the major greenhouse gases responsible for global warming. To face the problems related to the large amount of CO_2 released into the atmosphere, a number of carbon capture and storage (CCS) strategies are formulated [Yang, Environ. Sci., 2008]. Post-combustion capture offers considerable advantages because it prevents the need for substantial modifications of the combustion process and on the technologies usually used [Bhown, Environ. Sci. Technol. 2011]. Metal-organic frameworks (MOFs) are technologically advanced solid sorbents for post-combustion capture strategy [Raganati, CEJ, 2014], combining large surface area, permanent porosity, tunable pore size/functionality, selectivity, ease of handling, renewability for repeated cycles, [Stock, Chem. Rev. 2012]. MOFs are coordination polymers typically synthesized, under mild conditions, by a self-assembly reaction between metal ions (nodes) and organic ligands (linkers).
This work focuses on an aluminum-based MOF known as MIL-96 in which aluminum ions are coordinated with benzene tricarboxylic acid linkers [Loiseau, JACS, 2006]. We performed the synthesis of MIL-96 as pure phase and also in presence of growing amounts of carbonaceous material in form of graphene-like layers [Alfè, App. Surf. Sci. 2015]. The pure MIL-96 phase and four MIL96/GL composites were characterized in terms of elemental composition, thermal behavior and porosity. The ability of those materials to act as CO_2 sorbents was evaluated on the basis of the breakthrough curves performed in a lab-scale fixed bed micro-reactor. The evaluation of CO_2 capture performances indicated that the composites are better CO_2 sorbents compared to the pure MOF. Studies for the comprehension of the effect of the introduction of GL layers on CO_2 adsorption capacity are ongoing.

Magnetite loaded on carbonized rice husk: low cost biomass-derived composites for CO_2 capture

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Abstract

Recent studies of CO_2 sorption on low-cost metal oxides strongly encourage their use as sorbents [Alfè, PROCI, 2015] in CO_2 capture and storage (CCS) strategies. Magnetite (Fe_3O_4, FM) and CO_2 interaction proceeds through acid–base interactions involving unsaturated metal and O sites exposed on FM surface. The FM sorption capacity is lowered by the tendency of magnetite particles to agglomerate causing a decrease of the exposed surface area. The dispersion of magnetic particles on carbon-based solid matrices has been proposed to face this limitation.

Thanks to their low-cost, high surface area and porosity, carbonized biomasses are good candidates for supporting FM phase. Rice husk (RH) is an agricultural residue abundantly available in rice producing countries, obtained during the milling of paddy (22 wt. % of the weight of unmilled rice is received as husk). It presents a high ash content, which is 92 to 95% silica, highly porosity and a high surface area. RH is a green material that has a great potential for technological applications since it can be converted to different types of fuels and chemical feedstocks through a variety of thermochemical conversion processes. Following the same approach presented in our previous works on the CO_2 capture performances of FM supported on a carbon-based reference material (carbon black) [Alfè, PROCI, 2015; Gargiulo, App. Surf. Sci. 2016], the synthesis and characterization of RH/FM composite materials were performed. A set of RH/FM composites were produced by varying the amount of carbonized RH from 20 to 80 wt.% in order to optimize the sorbent properties for CO_2 adsorption applications. Preliminary data about the CO_2 sorption capacity were also obtained.

CO_2 capture by enzyme assisted absorption: theoretical and experimental study of a slurry bubble column

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Abstract

Novel post-combustion Carbon Capture and Storage (CCS) processes include absorption of CO_2 into aqueous solutions assisted by enzyme catalysis. Carbonic anhydrase (CA) catalyzes CO_2 hydration in alkaline solutions and it has been proposed to develop industrial biocatalyst for biomimetic CCS processes. Immobilized CA on fine dispersed solids promotes the heterogeneous biocatalysis close to the gas-liquid interface and the enhancement of CO_2 absorption rate.

This contribution reports on theoretical investigation on staged slurry bubble column and preliminary set up of lab scale units for experimental tests on CA assisted CO_2 absorption. The theoretical model was developed adopting the 'tanks-in-series' model to describe the unit; the two films theory to describe the absorption rate at the gas–liquid inter-face; the pseudo-homogeneous approach and a reversible Michaelis and Menten kinetics to describe CO_2 conversion by the slurry biocatalyst. Theoretical results clarify the performances of both free and immobilized CA biocatalyst on CO_2 absorption rate enhancement.

The preliminary experimental efforts concerned the setup of two lab scale bubble columns (1L and 10L). The smaller one was a glass jacketed column (30 mm ID, 1 m high) equipped with porous stone gas sparger and was developed to allow experimental tests on scale consistent with the poor biocatalyst availability. The second one is a Plexiglas® column (120 mm ID, 1.20 m high) and will be used to perform tests on larger scale according to improved biocatalyst availability and to test the biocatalyst recovery strategy. For both the reactors the mass transfer coefficient, the specific gas-liquid interface and the gas hold-up were assessed as a function of the gas flow rate. The preliminary CO_2 absorption tests in $20\%_w$ K_2CO_3 tests confirmed homogeneous gas bubbling regime in the adopted range of gas flow rates. Future tests will be carried out in the presence of slurry biocatalysts.

Carbonic anhydrase biocatalysts for enhanced CO_2 capture and utilization

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Abstract
Novel post-combustion treatments include biomimetic CCS processes based on CO_2 absorption into aqueous solutions assisted by enzyme catalysis. Carbonic anhydrase has been proposed as biocatalyst for biomimetic carbon capture: it catalyzes CO_2 hydration with a turnover number ranged between 10^4-10^6 s^{-1}, can be produced via fermentation and may be disposed without any detrimental impact on the environment. In order to increase CA stability at the typical process conditions, CA can be covalently immobilized on solid supports or through carrier free techniques. Among the later technique, Cross Linked Enzyme Aggregates (CLEA) are characterized by several economic and environmental benefits. Moreover, immobilization yields close to 90% of the originary enzyme can be obtained. On the other hand, CLEAs show poor mechanical resistance and tend to cluster after the conventional separation operation (centrifugation/filtration).
CLEA were prepared using bovine carbonic anhydrase (bCA) as reference enzyme. The aim of the study was the optimization of the immobilization protocol with respect to the specific activity of the immobilized enzyme. The effects of type of precipitating agent and of enzyme/cross-linker ratio on immobilization yield and CLEA specific activity were studied. To mitigate CLEA clustering, paramagnetic nano-particles (100nm) were included into the bCA CLEA structure and separation was performed with the aid of a magnetic field to avoid the use of the conventional separation techniques. CLEA structure and the effects of magnetic harvesting on it were observed by optical microscopy. Results showed that magnetic field separation limited the extent of CLEA clustering even though it was not sufficient to restore the observed former structure.

EXPERIMENTAL AND KINETIC STUDY ON PYROLYSIS OF WOODY AND NOT WOODY BIOMASSES

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Abstract

Several studies show the relevance of biomass chemical composition, besides the thermal conditions, in determining pyrolysis products distribution and characteristics. Many efforts have been directed to characterize pyrolysis kinetic mechanisms in order to predict weight loss curves in inert atmosphere and in some cases the whole spectrum of product yields and gas composition. Kinetic schemes have been developed where biomass main components react independently so that the global thermal behavior reflects the individual behavior of the components, weighed by the composition. When high extractives and ash content biomass are considered the behavior of these compounds cannot be neglected as well as inorganic-organic matter interactions. In this work five biomasses have been selected and divided in two categories basing on their composition in terms of cellulose, hemicellulose, lignin, extractives and ashes: olive and kiwi branches representing woody biomass, pine bark, wheat straw and rice husks as non-woody biomass. Pyrolysis tests have been carried out up to 973 K at heating rate HR=7 K/min. Product yields and gas composition have been compared with the results of non-interacting model mixtures and numerical predictions. The model mixtures are computed by superimposing the data of isolated biomass components, while numerical predictions are performed by means of a kinetic tool developed in MATLAB using the Bio-PoliMi mechanism and the Cantera reaction kinetics library. The work demonstrates that there is a good agreement on products yield between numerical and experimental data. On the contrary, the model is not able to predict the gas composition.

EXPERIMENTAL AND MODELING ISSUES OF MILD COMBUSTION IN A CYCLONIC BURNER

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Abstract

Reducing pollutant emissions, increasing the fuel flexibility and improving burners efficiency has brought to the development of new combustion concepts. Among these new technologies, the implementation of MILD combustion systems is limited by a lack of fundamental insight into such combustion regime and therefore novel tools are indispensable compared to traditional combustion systems. In this context CFD simulations for the prediction of the burner behaviour and for design and optimization appears essential for a successful introduction of such concept in some industries. Consequently, the simulation tools should include accurate models for describing both turbulent stirring/mixing and chemical reactions. Detailed chemistry has to be included in fluid-dynamics simulations in order to account for the strong turbulence-chemistry interaction in the MILD regime.

An effective strategy to overcome this aspect is represented by tabulated chemistry techniques. In particular the implementation of Flamelet Generated Manifold with IML tabulation seems to be a promising tools for MILD systems and therefore high fidelity and comprehensive experimental data are needed for the assessment of such model. The present study is framed in this context and it investigates the characteristics of MILD Combustion in a Cyclonic lab-scale burner that operates with high level of internal recirculation degrees induced by a cyclonic fluid-dynamic pattern obtained by the geometrical configuration of the reactor and of the feeding system. Experimental tests were realized varying the mixture pre-heating temperatures and the mixture composition. Detailed measurements of local mean temperatures and concentrations of gas species at the stack for several operating conditions were used to validate the FGM model under such unconventional operating conditions. Results suggest that FGM with IML is a promising tool for modeling the complex flame structures of cyclonic MILD burner, with many aspects that need to be further investigated.

BIOHYDROGEN PRODUCTION FROM ORGANIC FRACTION OF MUNICIPAL SOLID WASTE THROUGH MESOPHILIC DARK FERMENTATION

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Abstract

Biohydrogen ($BioH_2$) is considered a promising biofuel being renewable and C neutral, having a high energy content per unit mass (143 kJ/g), being easily converted into electricity by a Fuel Cell systems (FCs) and giving water as the only byproduct the combustion process. Nevertheless, the broad use of $BioH_2$ is still impaired by the necessity to setup a renewable and environmentally friendly process for the large-scale generation of this biofuel.

In this perspective, the Organic Fraction of Municipal Solid Waste (OFMSW) is an interesting substrate for the $BioH_2$ production because of its large supply and because it is made of biodegradable organic matter and nutrients, which are essential for the growth of microorganisms in which drive this biological process.

Nowadays, the Dark Fermentation (DF) process, that allows the conversion of organic substrate to $BioH_2$, is gaining great attention for its efficiency and environmental compatibility.

In this work, DF of OFMSW has been carried out for $BioH_2$ production in mesophilic conditions (37 °C), with semi-dry process in a batch reactor using a pure culture of *Clostridium roseum*. Both the liquid and the gas phase produced have been analyzed during the DF process. The monitoring of the microbial biomass growth, the amount of reducing sugars, the pH, the VFAs (propionic, butyric and acetic), alcohols, the biogas volume and composition were also monitored. The cumulative volume of $BioH_2$ produced was 10 $mL/gVS_{(OFMSW)}$ in 72h of DF, with a maximum percentage of $BioH_2$ in the biogas generated equal to 72 %v/v. As expected, results indicated that the $BioH_2$ production is affected by the thermal pre-treatments and composition of the starting raw biomass, with an increase of the volume of biogas produced by 52% and an enhancement of the rate of sugars degradation in 24h by 65%.

NEW CLASS OF ACID CATALYSTS FOR METHANOL DEHYDRATION TO DME

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Abstract
Dimethyl ether (DME) has attracted much attention because it can be utilized as a fuel in a diesel engine through well-distributed LPG stations. Compared with a diesel fuel, DME can evolve the less amounts of air pollutants such as NO_x, SO_x and particulate matters. It can also be reformed to hydrogen at low temperatures for the fuel cell. Conventionally, DME can be produced through the dehydration of methanol. Other routes such as direct synthesis from CO and H_2 or CH_4 and steam have been sought. In any case, the incorporation of acid catalysts is indispensable for the DME synthesis. Until now, several sold acid catalysts such as Alumina, Silica-alumina, and Zeolites have been examined for this reaction. These materials come with their own sets of problems for the reaction – they are responsible for the formation of unsaturated hydrocarbons and contribute to coking.
This study deals with the use of a new class of acid catalysts for methanol dehydration to DME. Sulfonic acids grafted on inorganic support such as SiO_2 or MCM41 were used and tested in our laboratory. Sulfonic acids are organic compounds that exhibit an acid strength comparable to that of sulfuric and benzenesulfonic acids.
The preliminary results about methanol dehydration carried out in a continuous flow fixed-bed reactor at temperatures between 180 and 320°C and 1 bar will be presented. The prepared systems presents good catalytic activity and selectivity to dimethyl ether and excellent stability in time on stream.

Backdraft in a Large Industrial Building

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Abstract

Backdraft, defined as the sudden combustion of hot flammable products accumulated within an underventilated fire environment, is an event, which may dramatically affect the progression of a compartment fire. Its relevance and its hazardous nature are widely recognized by firemen and by the fire science community. Several experiments, both at laboratory scale and at real scale, have been performed and have been reported in the scientific literature. For example, Gottuk et al. (1999) reported the results of backdraft experiments in ship compartments, including temperature and fuel fractions recorded in test that succeed in triggering strong backdrafts. Experiments and CFD simulations performed at the Lund University and reported by Jimenez et al. (2009) clearly showed that the dynamic of backdraft is strongly influenced by gravity current and exchange flow development during the fresh air inrush phase preceding the combustion flaming and fireball phases. Backdraft events are frequently reported in small to medium sized compartment fires, like apartment or single dwelling fires. In the present work we will report the preliminary analysis of a real world massive backdraft event that developed in a 10000 square meters 6 meter tall industrial building. The fuel load of the building was made by smoldering prone biomass materials and the building was equipped by a forced ventilation system. It was observed that upon fresh air introduction in the hot compartment, several fireballs were emitted by openings of the building and their time sequence is consistent with the characteristic flow velocity of gravity currents reported by Jimenez et al. (2009). The analysis of this large scale backdraft event include the application of lumped modeling, CFD modeling and the application of TGA and DSC method to characterized the combustion behavior of the solid fuel stored within the building. sustain a backdraft.

Fire Safety Engineering CFD Methods for Opera House

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Abstract

The prediction and the analysis of smoke and fire behavior inside complex geometry is the core problem of fire safety engineering. Computational fluid dynamic simulations are suitable tools to address such challenging task and their application is increasing both in fire prevention and in the reconstruction of fire accidents. In this work we report the preliminary results of the application of CFD methods to the fire safety engineering analysis of a generic opera theatre of the XVIII century.
CFD model, in the present case FDS6, enable to calculate the flow of combustion products and the spread of fire within the complex geometry of the stage and of the audience, taking into account the effect of the large volume of the fly loft. Since a significant fuel load characterizes the flow scenery and the grid deck, fire spread to those combustible elements is a key event in fire progression. CFD methods enable to predict and analyze such behavior.
The broader scope of the work is to calculate Available Safe Egress Time respect to a fire scenario represented by an active fire in the stage area. The manual activation of the cut-fire curtain, which divides the stage from the audience/orchestra pit, required by Italian regulations, has been explicitly modeled.
In order to define a credible worst case scenario, CFD simulations of fires with prescribed HRR and predicted HRR curves are being performed. The predicted HRR curve is calculated from combustion properties of the solid materials that forms the flown scenery and the most common furniture usually found on the stage, while the prescribed HRR curve has been developed on the basis of expert judgment and application of the standard t-squared curves. The methods applied in this study are applicable also to other complex geometry cases, with different features and details.

REAL-GAS AND REAL-MIXTURE EFFECTS IN THE EVAPORATION OF MULTICOMPONENT SURROGATE FUELS

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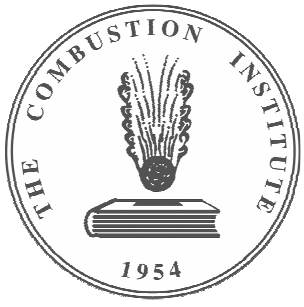
Abstract
When modeling the behavior of real fuels in combustion devices, a major complexity arises from the intricate coupling between the liquid and the gas phase. The presence of a double phase requires the consideration of both physical (density, viscosity, H/C ratio, etc.) and chemical (ignition propensity, flame propagation, pollutants formation) properties to obtain a complete understanding of the global combustion phenomenon. Moreover, the complex composition of fuels derived from fossil sources requires an upstream simplification to allow a more manageable study of combustion dynamics. For this reason, surrogate mixtures are introduced, targeted at mimicking physico-chemical properties of real fuels, and both experimental and numerical studies are carried out on them.
The necessary use of multicomponent surrogates to obtain a more comprehensive description of combustion target properties implies the consideration of multicomponent effects: thus, the related modeling activity needs to take into account for liquid-phase diffusion and non-ideal equilibrium. In addition, the elevated pressures at which combustion technologies often operate require the verification of the ideal-gas assumption, which is one of the common assumptions of the state-of-the-art spray evaporation models.
In this research activity, multicomponent and real-gas effects are investigated by considering the evaporation of spherical droplets in microgravity conditions. In this way, it is possible to isolate the thermophysical processes from combustion dynamics, and the use of a symmetric, 1-dimensional system allows to limit the computational weight of the model. To this purpose, (i) a multicomponent diffusion model, based on a Stefan-Maxwell approach, (ii) an activity model based on UNIFAC methodology, and (iii) the Peng-Robinson equation of state are introduced. The use of different fuel mixtures and operating conditions allowed to identify the critical regions where the introduced models play a key role in the evaporation dynamics.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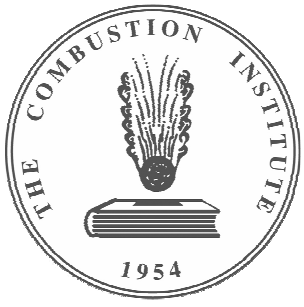
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