Université di Corsica
Pasquale Paoli

UMR SPE 6134

Sixth Mediterranean Combustion Symposium

June 7-11,2009

ABSTRACTS




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COLLOQUIA and COLLOQUIUM CO-CHAIRS

Plenary Lectures

3D-MODELING OF COMBUSTION PROCESSES INSIDE INDUSTRIAL CIRCULATING FLUIDIZED BED BOILERS

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Abstract
Circulating fluidized bed (CFB) combustion of solid fuels is a technology which is rapidly spreading all over the world. Starting with the first prototypes in the early 80's of the last century, today over 900 CFB steam generators are in operation or under construction for the capacity range from 50 up to over 400 MWe. Particularly in China, CFB combustion technology is increasingly applied. The trend of development is going for larger unit sizes. At present 600 MWe CFB combustors are under discussion. From the chemical engineering standpoint these are huge reactors. For example, the combustion chamber of the 235 MWe boiler no. 3 of Elektrownia Turow in Poland has a cross-sectional area of 100 m^2 at the distributor level and 200 m^2 in its upper part with a total height of 45 m. The resulting reaction volume of about 7000 m3 is impressive.
The operation of such big reactors and, even more, the scale-up to even larger sizes, pose serious questions to the engineer which are difficult to answer: how far is the secondary air penetrating into the combustion chamber with a given design or how must the secondary air injection system be designed in order to achieve an even air distribution over the crosssectional area of the combustion chamber? How many fuel feed ports have to be located on the circumference on order to achieve an even distribution of the fuel over the whole width of the combustion chamber?
Answer to these questions may be obtained with the help of sufficiently accurate models with a sound physical and chemical basis. In the present work an overview is given on the development of a complex combustor model which combines descriptions of fluid dynamics, gas-solid contacting and combustion of char and volatiles. The latter includes the drying and devolatilization and primary fragmentation of fresh fuel particles. All submodels are linked by the mass balances of the species involved and by the enthalpy balance. The fluid dynamics part consists of a semi-empirical model.
The combustor model has been applied to two large industrial boilers, namely the 252 MWth cogeneration plant of the Lurgi type of Stadtwerke Duisburg AG, Germany and the 263 MWe boiler no. 3 of the Foster Wheeler design of Elektrownia Turow in Bogatynia, Poland. The simulations were compared with and supported by local measurements of solid volume concentrations, velocities, gas concentrations and temperatures. The suggested model is shown to give new insights into the behavior of large industrial furnaces with strong 3D distributions of gas concentrations and temperatures and opens the possibility of supporting the further scale up of CFB boilers.

MODELLING COAL CONVERSION FOR NEXT-GENERATION COMBUSTION/GASIFICATION SYSTEMS: SOME RESEARCH NEEDS AND PRIORITIES

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Abstract
Exploitation of coal as a primary energy source, favoured by the relative inexpensiveness, security and reliability of supplies as compared with other primary sources, must cope with increasingly compelling environmental constraints, mostly related to emission of greenhouse gases. The development and deployment of the next generation CCS-ready coal conversion technologies pose novel and largely unexplored issues which call for a revision of classical design concepts and emphasize the lack of basic understanding of many fundamental processes underlying coal conversion. These are mostly related to the establishment of "extreme" conversion environments (high temperatures, high pressures, unusual gas compositions and radiative properties, establishment of slagging conditions). Research is urged to provide better understanding of coal conversion under extreme conditions to support the development of more reliable "model-based" design and scale up tool, to shorten the "learning" process, to improve process availability.
The lecture will address some of the issues that are receiving renewed interest by the scientific community, related to single particle coal conversion in CCS-ready combustors/gasifier. The focus will be on conditions establishing in suspension firing entrained flow reactors (combustors/gasifiers). Aspects that will be specifically addressed are: the role of pressure on coal devolatilization, char formation and burn-out; the development and validation of semiglobal kinetic models of carbon combustion and gasification to replace the usual "lumped" kinetic approach; the relevance to combustion/gasification of thermodeactivation phenomena induced by the exposure of carbon particles to high temperatures; the relevance of wall-burning to the late conversion of coal and char particles in slagging PF combustors and gasifiers.

NO_X, N_2O, SO_X, HCL, ALKALI, PARTICULATES AND HEAVY METALS FORMATION AND INTERACTION IN FLUIDIZED BED COMBUSTORS

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The fuels utilized in fluidized bed combustors range from anthracite, medium and low rank coals to peat, wood residues, biomass waste, sewage sludge and other sludges to plastics and municipal solid waste. Because of this wide range pollutants such as heavy metals, particulates, alkali, NO, NO_2, N_2O, SO_2, SO_3 and HCl may be formed during the fuel conversion process depending on the fuel and operating conditions.

These pollutants may lead to difficulties in operation of the fluidized bed combustor e.g. because of slagging and fouling the heat transfer may decrease or the efficiency of the SCR catalyst. High concentrations in the flue gas may lead to health problems and pollution of the environment.

This work investigates the conversion routes of the pollutants from the fuel to the final flue gas. It is discussing the different chemistry of the pollutants and their possible interactions inside the combustor. Primary measures to avoid pollutant formation and reduction paths are demonstrated. Areas for further research are recommended.

ELECTRIC FIELDS EFFECT ON JET FLAME STABILIZATION AND INSTABILITY

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Electric field or plasma assisted combustion has been studied extensively with regard to flame speed, flame stabilization, and pollutant emission. In case of electric field assisted combustion, lower power consumption and less flow disturbance could be expected as compared to plasma-assisted combustion. One of the limiting factors in applying electric fields is that two electrodes are generally conceived to be required. In such a case, the electrodes are exposed to hot combustion products. Recently, the single-electrode configuration has been proposed, where the fuel nozzle can serve as the high voltage electrode and the other electrode is connected to building ground. Ions and electrons existed in a reaction zone could interact with the high voltage electrode in much the similar fashion as a lightening rod and clouds.

Electric fields could affect flame behavior in various ways by the acceleration of charged particles existed in a reaction zone by the Lorentz force. Numerous studies have been performed, however, the characterization of respective contributions from the mobility, ionic wind, and chemical reaction are yet to be identified. It is still required to obtain extensive experimental data. In this regard, several experimental results performed in our group, which are relevant to the effect of electric fields on the stabilization of jet flames, will be presented and discussed.

The stabilization of jet flames is one of the key issues in designing a burner. For the purpose of improving the stabilization characteristics of jet flames, the effects of AC and DC electric fields on the stabilization of jet flames have been investigated, including the influences on liftoff, blowout, blowoff, and reattachment for nonpremixed laminar jet flames, on the propagation speed of tribrachial (or triple) flames, and on the liftoff of nonpremixed turbulent jet flames. The results showed that that the stabilization of these jet flames in terms of liftoff velocity, propagation speed, and reattachment velocity could be improved appreciably by applying electric fields. This implies that the burner capacity when operated in the nozzle-attached flame mode can be increased with relatively low power consumption in the order of 1 W. Additionally, oscillation behavior of a diffusion flame in a counterflow burner as a response to applied AC electric fields will be discussed to identify the effect of AC electric fields on flame behavior through the ionic wind effect. Finally, the effects of applied voltage and frequency on these various effects in jet flames will be summarized.

TOWARDS INEXPENSIVE THIN-FILM SOLAR CELLS: HOW COMBUSTION SCIENCE CAN HELP?

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Abstract

Transforming solar energy from a niche energy resource into a competitive technology is an exciting yet incremental science. Major obstacles towards solar energy utilization include the high costs associated with cell fabrication and installation. While thin-film solar cells can potentially reduce the installation costs, their fabrication remains prohibitively expansive for a broad range of utilization. This talk will argue for a combustion-science based approach to fabricating critical components of thin-film solar cells at low costs, with examples given for Graetzel's dye-sensitized solar cells (DSSCs).

In a dye-sensitized solar cell, a polycrystalline, mesoporous TiO2 film is used as the photoanode. The film acts as an electron-diffusion media. Upon photo-excitation of a chemical dye immobilized on TiO2 surfaces, the electron injects into the conduction band of TiO2 and diffuses into the anode. Anatase with crystal sizes around 10 nm is the preferred over larger, rutile particles. Traditionally, the fabrication of mesoporous TiO2 films require particle synthesis, collection and film preparation in separate steps. We introduce a new method to fabricate these films. The method uses the laminar, premixed, stagnation flame approach, combining particle synthesis and film deposition in a single step. A rotating disc serves as a combination of substrate holder and stagnation surface that stabilizes the flame. Disc rotation repetitively passes the substrates over a thin-sheet, fuel-lean flame doped with an organometalic titanium precursor. Convective cooling of the disc keeps the substrate well below the flame temperature, allowing thermophoretic forces to deposit a uniform film of particles that are nucleated and grown via the flame stabilized just above the surface. Analysis shows that knowledge of the particle thermophoretic velocity is critical to controlled film deposition. For this reason and because the particles of interest approach the molecular size, a fundamental theory of thermophoresis beyond Waldmann's was developed from a gas-kinetic theory analysis. The theory predicts that the thermophoretic velocity becomes sensitive to the particle diameter below ~3 nm only. Above this size, the insensitivity of particle size to thermophoretic velocity ensures narrowly distributed particle sizes in the film prepared. Tests show that the resulting film is capable of producing >9 % photoconversion efficiency in a DSSC, close to its record at 11%.

KINETICS OF SOOT FORMATION AT COMBUSTION ENGINES CONDITIONS

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Atmospheric pollution became, since the last decade, one of the major concerns of the modern countries. A special attention is given to particulate emissions since their bad effects on human health have been proven as well as their role in the depletion of the ozone layer. A tremendous effort is performed in order to reduce pollutant emissions such as COV, NOx and soot particles and one of the major pathways is to increase the engines efficiency. This is achieved by increasing the pressure in engines and gas turbines which in turn has a direct effect on the soot yield. In order to be able to predict the impact of the change in the engine pressure, a better understanding of soot formation is necessary in order to validate soot models. Indeed, decreasing the amount of pollutants generated by engines needs the simultaneous optimization of both fuel formulation and engine design. This goal can only be achieved with a detailed soot model that incorporates a detailed chemical kinetic mechanism for both gas and particle phases with a detailed description of the particles' properties.

In order to better understand the soot formation, in view to reduce emissions, acquisition of fundamental data concerning their inception, growth and oxidation, in well defined laboratory reactors, are needed. Moreover, real fuels are constituted of hundreds or even thousands different compounds which have different tendency regarding soot formation and oxidation. Indeed, the soot amount as well as the size of the soot particulates and their soluble fraction depends strongly not only on the thermodynamic conditions of their inception but also on the fuel type. Despite the effort devoted by the scientific community, the soot inception and growth is not fully understood.

The aim of the present paper is to give an overview of the soot formation process. Soot structure and morphology will be presented. The different laboratory reactors for soot studies and the kinetic parameters that can be deduced from them will also de addressed. Finally, the paper will focus on the importance of shock tube studies in understanding the early soot formation at high pressure will be presented.

USE OF VISUAL ANALYSIS FOR THE WORLD TRADE CENTER INVESTIGATION

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The attack on the World Trade Center (WTC) in New York City on September 11, 2001 by terrorists flying hijacked commercial aircraft into the two 110-story towers (WTC 1 and WTC 2) was one of the worst building disasters in the United States. In response, the United States Congress authorized the National Institute of Standards and Technology (NIST) to investigate the disaster to better understand what happened and the implications for building safety.

The aircraft impacts ignited fires in both towers. WTC 1 collapsed one hour and 42 minutes after being struck, and WTC 2 collapsed 56 minutes after being struck. In addition to the towers, the WTC consisted of five additional shorter buildings, all of which were destroyed. One of these, known as WTC 7, was a 47-story high rise located across the street from the primary WTC site. WTC 7 was moderately damaged by falling steel from WTC 1. Fires developed and spread within WTC 7 over a period of several hours, and the building totally collapsed 6 hours and 53 minutes after WTC 1. The collapses of WTC 1, WTC 2, and WTC 7 were unprecedented, and one of the primary objectives of the Investigation was "to determine why and how WTC 1 and WTC 2 collapsed following the initial impacts of the aircraft and why and how WTC 7 collapsed." The final reports concerning WTC 1 and WTC 2 was released in September, 2005, and those for WTC 7 in November 2008.

Since all three buildings collapsed, little physical evidence was available to guide the NIST WTC Investigation. As a result, models for the aircraft impact, fire behavior, heat transfer to structural elements, and building performance proved crucial for determining the causes. Primary sources of information for estimating initial conditions and for guiding and validating the results of the models were analyses of structural steel, review and analysis of available imagery, and eyewitness accounts. This presentation focuses on the collection, organization, analysis, and use of visual imagery during the NIST WTC Investigation.

The World Trade Center was located on Manhattan Island in New York City in a camera-rich environment. Since the towers were visible from long distances and it was a clear day, the WTC disaster became the most completely visually documented disaster in history. NIST ultimately collected over 300 hours of video and 10,000 photographs. The approaches used for collecting, storing, cataloguing, timing and analyzing this vast amount of material will be discussed along with a general description of the collection.

The timed visual records were analyzed to provide detailed information concerning the initial damage and response of the towers to the aircraft impacts, subsequent fire development and spread within the towers (detailed time lines were developed), building responses to the fires and damage, and collapse behavior. Highlights of the findings and their use by the NIST WTC Investigation team will be provided. The imagery available for WTC 7 was considerably less complete than for the towers due to conditions following the collapses of the towers and the fact that most of the initial damage and fire development occurred near the ground at locations shielded from view by nearby buildings. Nonetheless, analysis of the available imagery was sufficient to provide good estimates for the initial damage to the building caused by collapse debris from WTC 1, the locations and spread of fires that subsequently developed, and important details concerning the collapse behavior. Important findings and observations concerning WTC 7 will be summarized.

THE SCIENCE AND TECHNOLOGY OF DIESEL PARTICULATE FILTERS

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Abstract

Advanced fuel injection technology in conjunction with an inherent high thermal efficiency have lead to increased market share of diesel powered vehicles especially in Europe, and the trend is expected to continue if the diesel engine is able to meet ever more stringent emission limits in the future. This is dependent on the deployment of cost efficient, advanced emission control systems for particulate and NOx emissions. Particulate emission control entails measures to reduce both the solid (soot) particle emissions and liquid particle (droplet) emissions formed due to condensation of the exhaust as it cools down. The latter can be are readily reduced by regulating their precursors (reducing the fuel sulfur level and installing advanced diesel oxidation catalysts to oxidize the complete spectrum of hydrocarbon (HC) emissions). The solid soot emissions however remain intimately connected with the nature of the diesel combustion process and their reduction can be achieved either by in-cylinder measures improving the combustion process itself, or by deploying emission control systems such as Diesel Particulate Filters (DPFs) in both light duty/passenger car and heavy duty/commercial vehicle applications. DPFs represent an important and highly complex type of multifunctional chemical reactors combining, multiphase, separation, chemical reactions and material transformations over many disparate temporal and spatial scales. DPFs have therefore become possibly the most important and complex Diesel Emission Control device. The present work provides an update on the science and technology of Diesel Particulate Emission Control. Both fundamental as well as applications-oriented approaches are presented to study the physicochemical characterisitcs of diesel soot particles and soot deposits formed in DPFs, which are viewed as multifunctional separators/reactors. Theroretical and experimental aspects of filtration efficiency, pressure drop, ash accumulation and soot reactivity (with emphasis on catalyst-assisted soot oxidation) are addressed employing systems ranging from small scale filter samples to full scale devices installed in the exhaust of diesel engines. The current state of knowledge, experimental methods and simulation approaches, properly combined provides a rational and systematic route for enhancing the design and reliability of future Diesel Particulate Emission Control systems.

MEASUREMENTS AND ANALYSIS OF PREMIXED AND STRATIFIED FLAME SCALAR DISSIPATION

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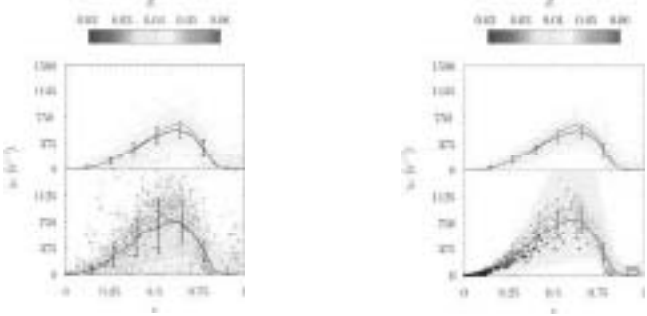
Stratified flames occur in many practical combustion applications, including gas turbines and internal combustion engines. The use of a lean global flow with a rich pilot can reduce pollutant emissions by decreasing mean temperatures without incurring the loss of stability typical of lean combustion. While the benefits of a stratified regime are known in terms of gross characteristics in practical applications, there is currently incomplete understanding of such phenomena at the fundamental level. In particular, the question of whether the flame structure is affected by local mixture fraction gradients commensurate with flame or turbulence structures must be investigated. In this talk, we consider previous and new data and analysis for model development and validation, by measuring conditional statistics of geometric flame structure and scalar dissipation in a stratified and premixed turbulent flame.

The burner is a simple turbulent slot burner with low turbulence (u'/S_L ~1.3), in which the mixing layer between two streams at different equivalence ratios is made to intersect the flame brush. The burner is operated in an overall lean equivalence ratio (ϕ = 0.73), in either premixed (*fs1*) or stratified mode. In the highest stratification case (*fs6)*, the equivalence ratios for the two streams are 3.0 and 0.37, the latter below the flammability limit (0.55) for the fuel used, methane. Instantaneous species data was obtained for along a line via Raman, Rayleigh and two-photon laser induced fluorescence (LIF) of CO. The data was combined with two-plane crossed PLIF of OH to define a flame direction and curvature, so that realistic 3D gradients of progress of reaction c and be calculated. In this study, c is defined as $c = (T - T_u) / (T_b(Z) - T_u)$, where the subscripts u and b refer to unburnt and burnt gases respectively. The temperature in the burnt products, T_b, is conditioned on the locally measured mixture fraction Z in order to give a sensible measure of c in the stratified cases.

The gradients are projected from the original direction from the normal with the flame. By filtering only the cases for which the correction angle is small (with a correction cosine greater than 0.90), it is possible to obtain the flame surface density function $|\nabla c|$ and the scalar dissipation rate $\chi_c = D_c \nabla c \cdot \nabla c$ for each measurement instance. The results are shown in Figure 1 as a function of the instantaneous, local progress of reaction c. Clearly, the presence of stratification leads to an extension of the flammable limit, an increase of the leaner and decrease of the richer dissipation rate. Further work is currently extending the analysis to include the role of ∇Z.



(a) (b)

Figure 1. Measured scalar dissipation rate for premixed (*fs1,top*) and stratified (*fs6,bottom*) turbulent flames, for all points (a) and angles with $\cos\theta$ <0.90 (b). Averages are indicated by the black line, calculated unstrained laminar premixed flames by the pink line. The shaded gray curve in (b) represents the limits 0.034<*Z*<*0.060*. Dark points represent *Z* outside the flammable limit.

ORAL PRESENTATIONS

THEORY AND MODELLING OF FLAME ACCELERATION IN OBSTRUCTED CHANNELS

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We report the theory and direct numerical simulations of ultra-fast flame acceleration in obstructed channels used in modern experiments on detonation triggering. The theory shows that the physical mechanism of the flame acceleration in obstructed channels is qualitatively different from the classical Shelkin scenario of flame acceleration in smooth tubes. It is demonstrated that delayed burning between the obstacles creates a powerful jet-flow, driving the acceleration. Flame acceleration in obstructed channels is much stronger than the Shelkin mechanism; the mechanism under study is independent of the Reynolds number. The flame front accelerates exponentially; the analytical formula for the growth rate is obtained. The theory is validated by extensive direct numerical simulations and comparison to previous experiments. The simulations demonstrate that accelerating flames trigger explosion and detonation.

APPLICATION OF THE REDIM APPROACH IN JOINT SCALAR PDF SIMULATIONS OF BLUFF-BODY STABILISED FLAMES

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Transported joint scalar probability density function (PDF) results are presented for 'Sydney Flames HM1 and HM3', jet type turbulent flames with strong turbulence – chemistry interaction, stabilized behind a bluff body. Chemistry is modelled by means of the novel Reaction-Diffusion Manifold (REDIM) technique, by which a detailed chemistry mechanism is reduced, including diffusion effects. Only N_2 and CO_2 mass fractions are used as reduced coordinates. A second-moment closure RANS turbulence model is applied. As micro-mixing model, the modified Curl's coalescence/dispersion (CD) and the Euclidean Minimum Spanning Tree (EMST) models are used. In physical space, agreement between experimental data and simulation results is good up to the neck zone, for the unconditional mean values of velocity, mixture fraction, major and some minor chemical species. Conditional mean profiles in mixture fraction space are also in reasonable agreement with experiments up to the neck zone, though conditional fluctuations are under-predicted. CD generally yields better predictions for the level of fluctuations in mixture fraction space than EMST, but this is partly due to unrealistic particle evolution in composition space. In general, simulations using the REDIM approach for reduction of detailed C_2-chemistry confirm earlier findings for micro-mixing model behaviour, obtained with C_1-chemistry.

DEVELOPMENT OF STRAIN-RATE RELATIONSHIPS FOR LES SUBGRID MODELS USING TEMPORALLY RESOLVED MEASUREMENTS

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The straining of a premixed flame surface during turbulence-flame interactions was measured using Cinema-Stereoscopic Particle Image Velocimetry (CS-PIV). These measurements allowed the strain-rate model that is commonly used in Large Eddy Simulations (LES) to be evaluated. It was found that the model did not accurately predict the effects of real turbulence-flame interactions for two reasons: the simple interaction geometry used to develop the model was insufficient and the strength of the turbulence was improperly characterized. A new model therefore was proposed that allows the geometry of real interactions to be accounted for and characterizes the turbulence based on the strength of the fluid dynamic strain-rate field. The model effectively transfers the fluid dynamic strain-rate into strain-rate on the flame and is referred to as the Strain-Rate Transfer (SRT) model. The SRT model can be implemented in LES to provide a more physically realistic description of the strain-rate exerted by turbulence.

SIMULATIONS OF SCALAR TRANSPORT IN DEVELOPING TURBULENT FLAMES SOLVING A CONDITIONED BALANCE EQUATION

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A balance equation for the difference in the conditioned velocities $\overline{u}_b$ and $\overline{u}_u$, derived and validated recently, is numerically solved in a statistically planar, one-dimensional case in order (i) to highlight the influence of premixed turbulent flame development on the direction of the mean scalar flux and (ii) to assess the equation by comparing computed trends with available experimental and DNS data. Numerical results show that; (I) The flux $\overline{\rho u'' c''}$ is gradient during an early stage of flame development followed by transition to countergradient scalar transport (i.e. $\overline{\rho u'' c''} \cdot \nabla \overline{c} > 0$) at certain instant t_{tr}. (II) The transition time t_{tr} is increased by the rms turbulent velocity and decreases when the density ratio or the laminar flame speed increases. (III) Transition from gradient to countergradient scalar transport weakly affects the growth of the mean flame brush thickness, because the mean rate of product creation (i) overwhelms the transport term in the combustion progress variable balance equation and (ii) serves not only to control the turbulent burning velocity, but also to cause the growth of the thickness.

SPHERICAL TURBULENT EXPANDING FLAME CHARACTERISTICS AND DAMKÖHLER'S NUMBER EFFECT

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This study aims to simulate one dimensional turbulent premixed flames in an open medium. The turbulence is supposed to be homogeneous and isotropic. The mixture is formed by propane as fuel and air as oxidizer in the atmospheric pressure. The focus of this work lies on a consistent description using Monte Carlo Model. we attempt to calculate respectively, the flame radius R_F, the flame propagation velocity S_t and the flame-brush thickness δ_t. During our study, one varies the equivalence ratio ϕ, the turbulence intensity u' and the Damköhler's number D_a and the ratio u'/S_L. results show that the equivalence ratio enhances the flame propagation from lean to stoechiometric flames. Also, the turbulence intensity yields a notable growth for the three flame characteristics mentioned above. Moreover, the main result concerns the effect of Damköhler's number on the flame brush thickness. Indeed, we find that the dimensionless flame-brush thickness δ_t/L_t increases with the dimensionless time t/τ_t up to a "bending effect". However, δ_t/L_t decreases versus D_a. Also, we notice that the effect of the ratio u'/S_L on δ_t/L_t is much more important than the effect of D_a.

LES STUDY OF INFLUENCE OF OBSTACLES ON TURBULENT PREMIXED FLAMES IN A SMALL SCALE VENTED CHAMBERS

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The LES study reported in this paper presents the influence of number and position of the obstacles on turbulent premixed flames. LES simulations have been carried out for a stagnant, stoichiometric propane/air mixture, ignited from rest in a small laboratory scale, vented chamber, capable of rearranging into various configurations based on number and position of baffle plates. The novelty of the present study is two folded. First is the application of novel dynamic flame surface density (DFSD) model to account the sub-grid scale (SGS) chemical reaction rate in LES. Second is the arrangement of these configurations into four families, which facilitate a qualitative comparison with available experimental measurements. The concept of families also offers to understand the flame-flow interactions and the impact of number and position of the baffles with respect to ignition origin.

A GENERALIZED TFC PREMIXED COMBUSTION MODEL INTENDED FOR THE ANSYS PACKAGES

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We present equations of the generalized TFC turbulent premixed combustion model developed for implementation in the Fluent code in the context of the Agreement with Ansys. The basic TFC model, which has been implemented in Fluent and CFX codes, describes the premixed flame that in simple situations (the Bunsen and V-flames) has increasing width and nearly constant flame speed.). The generalized TFC model describes additionally to this transient flame, which takes during the limited time interval $t_1 < t < t_2$, also initial stage of the flame with fast increasing of the speed at $0 < t < t_1$ (this stage is important in the SI engines) and the final stage at $t > t_2$ when takes formation of the steady state flame (this stage is important for ultra-lean flames). It predicts also They predict also the counter-gradient transport scalar flux and anisotropy of the velocity fluctuations in the flame that is modelled in the context of the gasdynamic (non-turbulent) mechanism of the phenomena. The invariant Favre average equations of the generalized model are consistent with the equations of the "$k-\varepsilon$" turbulence model and have the standard form suitable to the commercial solvers.

MODELING THE EFFECTS OF THERMAL EXPANSION IN TURBULENT PREMIXED FLAMES

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The thermal expansion induced by the chemical reactions taking place in a turbulent reactive flow affects the velocity field so strongly that velocity fluctuations and velocity gradients can be governed by reactions rather than by turbulence. Moreover, thermal expansion is well known to be responsible for counter-gradient turbulent diffusion and flame generated turbulence phenomena. In the present paper, a specific description of the velocity field is used, that allows to separate the influence of thermal expansion from the effects related only to the turbulent motion. Using this description, all the usual turbulent quantities are expressed in term of two contributions: (i) one due to thermal expansion, and (ii) one due to turbulence. The theoretical analysis shows that only the contributions due to turbulence should be resolved by transport equations in which unclosed terms do not depend on thermal expansion. Deduced from this analysis a relatively simple closure model is proposed and successfully validated through comparison with DNS data. Results show the ability of this model to represent the counter-gradient diffusion region of the flame as well as the region controlled by gradient transport, crucial to the propagation mechanism of the flame brush.

APPLICATION OF AN INHOMOGENEOUS TURBULENT MIXING MODEL IN CONDITIONAL MOMENT CLOSURE FOR AUTOIGNITION

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In Conditional Moment Closure (CMC) methods, the conditional scalar dissipation rate is an important quantity that needs to be accurately modelled. The present paper is focused on a new strategy for calculating the conditional scalar dissipation rate that is implemented in a finite-volume code and applied to the autoignition of high pressure methane jets in a shock tube. The conditional scalar dissipation rate is determined from the integration of the probability density function transport equation and in contrast to commonly used models, the assumption of homogeneous turbulence is not invoked. The present results of ignition delay and location are compared with those previously obtained using a homogeneous-turbulence-based mixing model, Amplitude Mapping Closure (AMC). Significant differences are observed in the shape and magnitude of the conditional scalar dissipation rate in mixture fraction space compared to AMC. The ignition delays predicted using the inhomogeneous model are higher than those from the AMC model, ranging from 27% higher for the highest air temperature, to 6% higher for the lowest air temperature. The ignition locations are not much affected by the new model.

GRADIENT AND COUNTER-GRADIENT MODELLING IN PREMIXED FLAMES: THEORETICAL STUDY AND APPLICATION TO THE LES OF A LEAN PREMIXED TURBULENT SWIRL-BURNER

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This paper concerns the modelling of unresolved turbulent fluxes in premixed flames. Classically closed with a gradient assumption, this term may also contain a counter-gradient part as detailed in other works. In a first section, the bibliographical resources giving details about the closure of the unresolved turbulent fluxes are investigated and confronted thanks to time-averaged DNS databases. LES are then performed to underline the possibility to integrate the counter-gradient transport in an industrial-like computation where the mesh may not be thin enough to capture all the turbulent transport at a resolved scale. Results given by the considered closures are compared with experimental points and analyzed.

ESTIMATION OF TURBULENT FLUXES BY SIMULTANEOUS TWO-DIMENSIONAL LIF AND PIV

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In a turbulent flow Reynolds-fluxes and –stresses are important quantities because they reflect the enhanced fluxes of a turbulent compared to a laminar one. Therefore, the knowledge of Reynolds-fluxes and –stresses are of fundamental concern for the development and validation of turbulence- and mixing-models. These quantities are obtained experimentally in a Jet-in-Crossflow arrangement by measuring the scalar concentration fields and the velocity fields simultaneously using two-dimensional Laser-Induced Fluorescence (2d-LIF) in combination with Particle Imaging Velocimetry (PIV), respectively.
For PIV-measurements, droplets are added to both, the crossflow and the jet as well. Additionally, a molecular tracer is added to the jet. The concentration maps of this tracer are detected in the interaction zone of the jet with the crossflow by 2d-LIF. NO_2 is chosen as the molecular tracer, because it absorbs the wavelength of the PIV-laser. The Stokes-shifted broadband fluorescence signal induced by one of both Nd:YAG-double laser pulses is detected by an intensified CCD-camera. The LIF- and the Mie-scattered light-signals are detected perpendicular to the propagation direction of the laser beam through an additional window in the measuring section. Both signals are separated from each other by a 45° dichroic mirror which transmits the fluorescence-signal whereas the Mie-scattered light is reflected perpendicular with respect to the first. The Mie-scattered light from both laser-pulses is detected by the CCD-camera of the PIV-system.

ON THE SENSITIVITY TO SUBGRID TURBULENCE CHEMISTRY INTERACTION MODELS IN LARGE EDDY SIMULATION OF SELF-IGNITION IN VITIATED HOT CONFINED SUPERSONIC AIR FLOW

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In this study we aim at investigating the sensitivity of Large Eddy Simulation (LES) predictions to the finite rate subgrid turbulence chemistry interaction modeling of self-ignition in vitiated hot confined supersonic air flow relevant to scramjet conditions. LES, in which the large-scale flow is resolved on the grid, leaving only the small-scale flow to be modeled, provides a natural framework for scramjet simulation as the transient nature of the flow is reasonably well resolved both in space and time. In most situations, however, the regions of chemical activity, often consisting of thin wrinkled, torn and stretched fronts or interacting pockets, are poorly resolved on the LES grid, and subgrid modeling is required to handle not only the subgrid transport but also the turbulence-chemistry interaction. Based on a previous investigation where we examined the influence of the reaction mechanism, by comparing LES predictions of 1-, 2-, and 7-step mechanisms for NAL's supersonic combustor, equipped with the two-stage strut injector connected to ONERA's vitiation air heater, we here perform similar LES using the 7-step mechanism but with four different subgrid turbulence chemistry interaction models. The models investigated are the Partially Stirred Reactor (PaSR) model, the Eddy Dissipation Concept (EDC) model, the Extended Vulis Model (EVM) and the Thickened Flame Model (TFM). Although all models give acceptable results when compared to the experimental data, best qualitative results are obtained with the PaSR model.

HYBRID RANS/PDF CALCULATIONS OF A SWIRLING BLUFF BODY FLAME (SYDNEY 'SM1')

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In this work, we perform steady 2D axisymmetric RANS and hybrid RANS/PDF calculations to predict the turbulent flow and mixing fields of a swirling bluff body flame (Syndey SM1). The case studied, SM1, is a bluff body stabilized flame, studied experimentally at Sydney University and Sandia National Laboratories. Turbulence is modeled with a non-linear k-ε type model, taking into account effects of rotation and streamline curvature on the turbulence. Flow field predictions are in reasonable agreement with experimental data. However, the agreement for mean mixture fraction and mixture fraction variance with experimental results is less satisfactory. Yet, the mean temperature field is quite well reproduced. We first compare presumed and transported scalar PDF simulation results, with the same laminar flamelet model for chemistry. The influence of the micro-mixing model is small in this case. The mixing model constant C_ϕ has a stronger influence, through the mixture fraction variance. Finite rate chemistry effects are studied in transported scalar PDF calculations using REDIM. For $C_\phi = 2$, a steady solution is obtained with EMST, but with CD the flame extinguishes. The combination REDIM/EMST is not able to predict the local extinction seen in the experiments. Therefore, a final calculation with the CD model with $C_\phi = 3$ is performed and a steady solution is found. With CD, there is more scatter than with EMST, resulting in lower values for temperature and $Y(CO_2)$. Still, this combination REDIM/CD is not able to predict the correct level of local extinction, though.

COMBUSTION MODEL BASED ON JOINT STATISTICS OF PROGRESS VARIABLE, MIXTURE FRACTION AND SCALAR DISSIPATION RATE

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We use a probability density function (PDF) method, where a transport equation for the joint PDF of velocity, turbulent frequency, progress variable, mixture fraction and enthalpy is solved. Based on precomputed flame tables, this information is used to obtain the joint statistics of the compositions. Extinction and re-ignition of fluid particles is controlled by a particle progress variable and its scalar dissipation rate. The precomputed flame tables are only applied for particles in the flammable mixture fraction range. Outside of this range, the particle enthalpy is evolved by a mixing model (like the mixture fraction). Numerical test cases of lifted diffusion flames with a considerable amount of extinction show the ability of the model to account for the major physical effects and comparisons with experimental data show good agreement.

INFLUENCE OF FLOW FIELD SCALING ON FLASHBACK OF SWIRL FLAMES

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The effect of geometrical scaling on the onset of flashback of a swirl flame has been investigated. The study discriminates between two different flashback modes, which occur either at low swirl caused by combustion induced vortex breakdown (CIVB) or at high swirl caused by turbulent burning on the vortex axis (TBVA). Flashback caused by TBVA (FTBVA) is taken as a reference case to identify the role of turbulent flame quenching and of vortex breakdown (VB) aerodynamics in flashback caused by CIVB (FCIVB).
The isothermal and reacting flow fields were examined experimentally by planar particle imaging velocimetry (PIV) and simultaneous recording of the flame luminescence. In order to study the effects of geometrical scaling, flow fields and flashback were studied for two geometrically scaled burners at equal Reynolds numbers. This allows the comparison of the flashback phenomena in similar flow fields but with different turbulent scales affecting the combustion process.
From the investigations it is shown that geometrical scaling of the burner shifts the limits at which flashback occurs and that this shift is different for the two types of flashback. A basic analysis of the governing equations of fluid dynamics and a model for turbulent combustion gives a first explanation of how FCIVB and FTBVA are affected by geometrical scaling at constant Reynolds number which is in good agreement with the experimental observations.

LARGE-EDDY SIMULATION AND EXPERIMENTAL OBSERVATION OF COMBUSTION INDUCED VORTEX BREAKDOWN

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The behaviour of a model gas turbine combustor with respect to flame flashback due to combustion induced vortex breakdown (CIVB) has been investigated, which is a very complex mechanism of interaction between the swirling flow and the flame. The phenomenon has been observed both experimentally and numerically. The experimental rig allows observation of the flame using simultaneously PIV and LIF of the flashback. Since the CIVB is a highly unsteady process Large-Eddy-Simulation was applied to achieve a very detailed view at the flow field during the flashback. The combustion of a perfectly premixed methane-air mixture was modeled using an analytic expression for the flame surface density. Stability limits have been determined with simulations and experiments for a large operating range of the burner. Furthermore the detailed data allow a very close look at the flashback process in all of its stages.

TURBULENT COMBUSTION OF HYDROGEN – CO MIXTURES

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Laminar and turbulent burning velocities were measured in a closed-volume fan-stirred vessel for $H2-CO$ mixtures using two independent methods of flame definition. It has been shown that the unsteady flame development is an important factor and it needs to be taken into account for comparison of the burning rates obtained in different experiments. For the atmospheric pressure flames, the mixtures with faster laminar flame velocities burnt faster in turbulent flow despite the fact that the lean flames exhibit cellular structures. However, even a modest increase of the initial pressure promotes strongly cellularity and causes a significant acceleration of a lean laminar flame. The same lean flame burns faster in turbulent flow as well and this increase in the rate of combustion is greater that can be deduced from variation of the molecular heat diffusivity and laminar flame speed.

DYNAMICS OF LEAN-PREMIXED TURBULENT COMBUSTION AT HIGH TURBULENCE INTENSITIES

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Turbulent premixed flames of propane/air and methane/air stabilized on a Bunsen type burner were studied to investigate the interactions between turbulence and the structure of the flame front in the thin reaction zones regime. The fuel-air equivalence ratio was varied from 0.7 to stoichiometric for propane flames, and from 0.6 to stoichiometric for methane flames. The non-dimensional turbulence intensity, u'/S_L, covered the range from 2.7 to 24.1. The flame front data were obtained using planar Rayleigh scattering technique; while particle image velocimetry was used to measure the instantaneous velocity field of the flames. Thermal structure of the flame front was observed to change with increasing non-dimensional turbulence intensity u'/S_L. The reaction zone and preheat zone thicknesses increased modestly with non-dimensional turbulence intensity in both propane and methane flames. Flame front curvature statistics displayed a Gaussian-like distribution which centered about zero for all the flame conditions studied during the investigation. Flame surface densities evaluated from flame front images showed almost no dependence on the non-dimensional turbulence intensity. Flame surface densities integrated over the flame brush volume also did not show any sensitivity to the non-dimensional turbulence rms velocity.

REACTION-DIFFUSION EFFECTS ON SPECIES MIXING RATES IN TURBULENT PREMIXEDMETHANE-AIR COMBUSTION

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The scalar mixing time scale, a key quantity in many turbulent combustion models, is investigated for reactive scalars in premixed combustion. Direct numerical simulations of three-dimensional, turbulent Bunsen flames with reduced methane-air chemistry have been analyzed in the thin reaction zones regime. Previous conclusions from single step chemistry studies are confirmed regarding the role of dilatation and turbulence-chemistry interactions on the progress variable dissipation rate. Compared to the progress variable, the mixing rates of intermediate species can be several times greater. The variation of species mixing rates are explained with reference to the structure of one-dimensional flamelets. According to this analysis, mixing rates are governed by the strong gradients which are imposed by flamelet structures at high Damköhler numbers. This suggests a modeling approach to estimate the mixing rate of individual species which can be applied, for example, in transported probability density function simulations. Flame turbulence interactions which modify the flamelet based representation are analyzed.

TURBULENT SPRAY FLAMES OF ACETONE AND ETHANOL FUELS APPROACHING EXTINCTION

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This paper presents measurements of mean temperature, axial velocity, turbulence and droplets fields in pilot-stabilized jet flames of dilute sprays where acetone or ethanol is used as liquid fuel. Laser induced fluorescence (LIF) is employed to image hydroxyl radical OH which marks the existence of hot regions or reaction zones. Depending on the fuel used, droplets within the flow are delineated by imaging LIF from acetone or Mie scattering. As the jet velocity is increased, the flames gradually approach blow-off in a region further downstream from the stabilizing pilot. Three jet velocities are investigated for each fuel.
It is found that the mean velocity, turbulence and droplet fields are somewhat similar for both ethanol and acetone flames and these do not change much with increasing jet velocity particularly when normalized with the relevant parameters. However, the temperature and reactive fields are varying and undergo departure indicative of non-premixed to premixed flame behavior depending on the vapor pressure of the fuel and proximity to blow-off. Broad regions of OH as well as breaks in the OH profile marking possible local extinction are observed in the ethanol flames.

HIGH-SPEED MICROSCOPIC OBSERVATION AND MODELING OF THE MULTIPHASE PROCESS IN A MICRO SPHERICAL PET PARTICLE UNDER ABRUPT HEATING

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High-speed expanded and direct observations of the multi-phase process within a micro particle of polyethylene terephthalate resin (abbreviated to PET in the following) under abrupt heating are made along with stereoscopic imaging of solid residuals. High-speed reflection images and stereoscopic images give the conclusive evidence of occurrences of violent multiple micro bubbling within the PET droplet, which is triggered by thermal decomposition of PET resin and flash vaporization of the decomposed products. Multiple and irregular explosions of micro bubbles follow just after the internal bubbling and cause irregular and random micro jets, resulting in randomly fluctuating micro diffusion flames downstream of the micro jets. It is concluded that the key factor to such high burning rate constants of PET particles as exceed those of well-known volatile liquid fuels can be attributed to the multiphase process due to the multiple and internal flash vaporization of thermally decomposed products, being particular to plastic resin combustion. Based on these considerations, a qualitative modelling of the multi-phase process in the micro plastic particle is constructed.

NUMERICAL SIMULATIONS OF PYROLYSIS OF CHARRING AND NON-CHARRING MATERIALS USING AN ENTHALPY-BASED MODEL

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The present work focuses on the application of a pyrolysis model, with enthalpy as basic variable, in numerical simulations of pyrolysis of dry and wet charring materials, as well as non-charring materials. In case of wet charring materials, the moisture first flows out after evaporation, leaving dry virgin solid material. This material then further heats up and finally generates a mass flow rate of combustible volatiles during the pyrolysis process. Evaporation and pyrolysis, possibly occurring at the same time, are assumed to take place in infinitely thin fronts. Pyrolysis is thus modelled as an infinitely fast, irreversible endothermic process at the 'pyrolysis temperature' (T_{pyr}) and as such, all kinetics are ignored. The cases considered are one-dimensional in nature, in order to focus on the principal model performance. The temperature distribution inside the material, along with the evaporation and pyrolysis front positions, are related to the distribution of enthalpy. A piecewise linear temperature field representation is adopted. Pyrolysis of non-charring materials is modelled with the same enthalpy based model.

POROUS CARBON PARTICLE GASIFICATION IN CARBON DIOXIDE

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The model of porous carbon particle gasification in carbon dioxide is developed. The model considers the processes of heat and mass transfer both inside the porous particle and in the gas outside the particle above it. Heterogeneous chemical reaction of carbon interaction with carbon dioxide inside the porous particle is considered as well. Analysis of the model shows that heat and mass transfer play significant role in the process of particle gasification in carbon dioxide. Gasification of carbon particle in carbon dioxide is impossible if particle temperature is lower about than 1000 K because concentration of carbon dioxide at the particle surface becomes lower than equilibrium concentration. The rate of the carbon particle gasification is determined as a function of the porous particle internal surface for different pressures and furnace temperatures.

NUMERICAL SIMULATION OF PEAT LAYER COMBUSTION

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Peat fires is a serious economic and ecological problem of Belarus and other countries that possess big amounts of drain peatbogs. Reliable numerical simulation of peat fires was not realized until recently, mainly because of complexity of the problem and insufficient computer powers.
In order to estimate the critical parameters of a peat ignition an appropriate physical and mathematical model should be constructed. Such a model should describe heat and mass transfer processes in peat layer, peat pyrolysis and organic component oxidation. A specific difficulty which was not resolved in previous works is simulation of self-consistent onset of convection at the peats- air boarder. In this work this specific difficulty was resolved by formulation of self-consistent non-steady problem. Several important qualitative and quantitative characteristics of the peat fires are determined.

CHARACTERISTICS OF ASH DEPOSITION BEHAVIORS OF UPGRADED BROWN COAL (UBC) AND BITUMINOUS COAL

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The molten ash causes slagging and fouling problems in pulverized coal combustion boilers. The ash deposition on the heat exchanger tubes makes the overall heat transfer coefficient reduce. The ash compositions in coal as well as the operational conditions in the boilers strongly affect the ash deposition behaviors. This study focuses on the relationship between ash deposition characteristics and ash melting characteristics. Upgraded brown coal (UBC) and two types of bituminous coal with the different melting temperatures and ash compositions are used as the sample coals. The deposition tests are conducted using a refractory furnace. A water cooled tube is inserted into the furnace to make the ash adhere. The molten slag fraction in ash is estimated by means of chemical equilibrium calculation. As a result, the ash deposition characteristics have a close relationship with the ash melting characteristics. The UBC tested in this study shows relatively high ash deposition. The molten slag fraction in ash obtained by the chemical equilibrium calculation correlates with the deposition fraction of ash obtained by the experiments even under the coal blending conditions. Therefore, the molten slag fraction in ash obtained by the chemical equilibrium calculations is one of the useful indices for the proper coal blending with the UBC to reduce the ash deposition.

3D MICROSCALE SIMULATION OF SMOLDERING

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A 3d microscale numerical tool for the simulation of smoldering in fixed beds of solid fuels is presented. The description is based on the local equations and fully preserves the coupling of the transport and reaction mechanisms. A set of simulations demonstrates the ability of the model to handle a variety of situations, with non trivial chemical scheme, and to provide detailed local information. A phenomenological chart is established, depending on a few dimensionless numbers, which exhibit very different regimes and provides guidelines for the practical operation of a reactor and for a macroscopic homogenized description.

EFFECTS OF ADDITIVES ON THE REDUCTION OF FINE PARTICLES DURING PULVERIZED COAL COMBUSTION

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This paper aims to evaluate the possibility of chemical additives on the reduction of fine ash particles during pulverized coal combustion. Three kinds of chemical additives (Ca-based, Mg-based and Fe-based) were mixed with coals A and B. Coals and the mixtures were burnt in a lab-scale drop tube furnace, respectively. The impact of the added additives on the transformations of coal minerals, as well as on the emissions of fine particles with an aerodynamic diameter smaller than 2.5 μm ($PM_{2.5}$) was investigated. The generated ash particles were collected using a cyclone combined with a low-pressure impactor and their physical and chemical properties were analyzed. The results indicate that the addition of chemical additives can affect the mineral transformation process, and thus, control the emissions of $PM_{2.5}$ and PM_1 during combustion. In particular, added additives have a visible impact on the particle size distributions and chemical compositions of PM, wherein, it improves the degree of coalescence of sub-micron and fine mineral particles, which reduces $PM_{2.5}$ emissions. The effects of added additive on the reduction of $PM_{2.5}$ emissions depend on coal type and combustion temperature.

NUMERICAL SIMULATION OF COMBUSTION INSIDE THE ENTRAINED FLOW GASIFIER

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Gasification is making a strong comeback as a sustainable energy source in clean energy systems such as IGCC, and as a renewable source utilizing millions of tons of waste dumped in the landfill, and avoiding risking our ecological system as a result of ground water leaching, and CO_2 & CH_4 emissions. In this paper, reviews of the physical characteristics and conditions of the feedstock, and gasification technologies are first performed. Systematic gasification analyses for different feedstocks, including coal, biomass-coal blend, and industrial waste are presented. Species concentration and product/feedstock ratios that define the gasifier metrics including cold gas efficiency, conversion rate, and steam and Oxygen requirements are computed. A baseline gasifier geometry is selected and discretized to carry out detailed CFD. Mesh resolution study of the incompressible, turbulent flow is carried out. Two-phase flow representing the continuous and the discrete (particle) feedstock is analyzed while maintaining two-way coupling. The velocity field is compared with that of a single phase and results on the effect of the particle size and injection velocity is presented. A coupled thermochemical analysis is then carried out while incorporating the species transport for both the homogeneous (gas/gas phase) and heterogeneous (gas/solid phase) interaction. Species distributions, including, CO, H_2, CO_2, H_2O, and O_2 and other flow variables including temperature and velocity are computed and presented.

IGNITION AND SUPPRESSION OF SMOULDERING COAL FIRES IN SMALL-SCALE EXPERIMENTS

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Subsurface smouldering fires are a global phenomenon which until recently have received little study. These fires occur in natural subsurface deposits of peat and coal and are the longest continuously burning fires on Earth. In this paper, experiments are conducted for the first time to study the combustion and extinguishing behaviour of smouldering coal fires. Small-scale experiments are carried out using samples of 100□100□100 mm^3 in the laboratory and three suppression methods were compared: an injection pipe, a shower and a spray. The results show that particle size has little effect on the maximum smouldering temperature for particles over 15 mm in diameter but does have an enhancing effect on the burning rate. The amount of water required to extinguish a smouldering fire was found to be a weak function of the particle size with approximately 1 to 2 l/kg^{-1} of water being required per unit mass of burning coal. The experiments highlighted the importance of the method of water delivery and application. The spray was found to offer the most effective extinguishing as the low flow rate allowed a wider penetration into the coal bed. The other two methods resulted in significant water run-off which channelled through the sample reaching a smaller fraction of the coal bed. These experiments aim to provide a first step into the understanding of subsurface fires and the best method to extinguish them.

COMPARATIVE RESULTS CONCERNING CO-FIRING OF BIOMASS RESIDUES WITH BROWN COAL IN A PILOT PLANT

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This study assesses the near-term technical potential for biomass co-firing with coal in existing coal-fired infrastructure in the EU27 Member States, with special relevance to Romania. Fluidized bed technology (FBC) is developed for the combustion of mixtures of different coals and biomass based waste to operate in an environmentally friendly way. Biomass waste has combustion characteristics which improve the combustion behavior of coals, due to high volatile content and low sulphur, nitrogen and ash contents. In this work, the objective is to improve co-combustion of coal and wood-based biomass waste in fluidized bed, by pilot plant experiments. The paper focuses on a pilot plant equipped with a stationary fluidized-bed furnace for solid fuels co-firing. The pilot plant is fitted with latest measuring instrumentations and retention equipments of main gaseous and solid pollutants from flue gases. In steady stable operation, measurements regarding temperatures behavior and pollutants' concentration were conducted. The used biomass is a mixture from different sorts of local sawdust with hard coal. The experimental results are presented comparative with and without the biomass blending of the basic fossil fuel, using mixing ratio of 15 % and 30 % by mass with brown coal. The ultimate goal is to develop complete burnout (i.e. no unburnt pollutants), which needs temperature, time, and turbulence. The experiments conclude that the technology is cleaner in comparison to using singular fossil fuel, has as main advantage the possibility to reduce the SO_2, in a certain amount of NO_x as well, simultaneously with the decrease of fossil generated CO_2 and particulate exhaust from flue gases, in comparison to stand alone fossil fuel combustion. The results have been based on many representative and repeated experiments.

UTILIZATION OF COAL COMBUSTION ASHES FOR THE SYNTHESIS OF ORDINARY AND SPECIAL CEMENTS

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Raw mixes containing pulverised coal fly ash (with limestone and silica sand) or fluidised bed coal combustion ash (fly and bottom, with added limestone, anodization mud and, when necessary, flue gas desulfurization gypsum), aimed at generating Portland or calcium sulfoaluminate clinkers, respectively, were heated in a laboratory electric oven at temperature ranging from 1150° to 1500°C and submitted to X-ray diffraction analysis. The former had the same qualitative phase composition as that of a reference mixture, composed by limestone and clay; furthermore, they exhibited an excellent burnability, on the basis of the residual free lime contents, measured after heating at 1350°, 1400°, 1450° and 1500°C. The latter showed very good results in terms of conversion of reactants and selectivity degree towards the main mineralogical constituent, calcium sulfoaluminate ($4CaO \cdot 3Al_2O_3 \cdot SO_3$), even if the behaviour of a reference mixture consisting of limestone, bauxite and natural gypsum was slightly better. The introduction of a fluidised bed coal combustion ash in the raw mix generating calcium sulfoaluminate clinker implies a saving of bauxite and natural gypsum which can be fully replaced through the addition of anodization mud and flue gas desulfurisation gypsum, respectively.

COMPARISON OF SPONTANEOUS COMBUSTION NUMERICAL MODEL PREDICTIONS WITH BULK COAL LABORATORY TESTING RESULTS

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A spontaneous combustion numerical model has been used to study the hot spot development in a high volatile bituminous coal from the Spring Creek Mine in New Zealand. Important kinetic parameters required by the model were obtained from adiabatic oven tests so that the reaction rate is specific to the coal. In addition, bulk coal laboratory testing was performed using a 2-metre column enabling comparisons to be made with the model results. The hot spot development pattern is the same for both the model and laboratory results. Initially a hot spot is developed approximately 1.4m from the air inlet and then begins to migrate upwind at successively higher temperatures. These initial results for Spring Creek coal are encouraging and provide an opportunity for future benchmarking of coals from other mines.

THE INFLUENCE OF TEMPERATURE ON LIMESTONE SULFATION AND ATTRITION UNDER FLUIDIZED BED COMBUSTION CONDITIONS

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The influence of temperature on attrition of two limestones during desulfurization in a fluidized bed reactor was investigated. Differences in the microstructure of the two limestones were reflected by a different thickness of the sulfate shell formed upon sulfation and by a different value of the ultimate calcium conversion degree. Particle attrition and fragmentation were fairly small under moderately bubbling fluidization conditions for both limestones. An increase of temperature from 850°C to 900°C led to an increase of the attrition rate, most likely because of a particle weakening effect caused by a faster CO_2 evolution during calcination. This weakening effect, however, was not sufficiently strong to enhance particle fragmentation in the bed. The progress of sulfation, associated to the build-up of a hard sulfate shell around the particles, led in any case to a decrease of the extent of attrition. Sulfation at 900°C was less effective than at 850°C, and this was shown to be related to the porosimetric features of the different samples.

EXPERIMENTAL AND NUMERICAL STUDIES ON THE BURNING OF ALUMINUM MICRO AND NANOPARTICLE CLOUDS IN AIR

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An experimental study has been conducted to determine flame propagation velocities in clouds of micro- (4.8 μm) and nano- (187 nm) aluminum particles in air at various concentrations. The experimental results show faster flame propagation in nanoparticle cloud with respect to the case of microparticles. Maximum flame temperature has been measured using a high-resolution spectrometer operating in the visible range. Analysis of combustion residual shows that nanoparticles combustion is realized via the gas-phase mechanism. A 3-stage particle combustion model has been proposed based on these observations. Model parameters have been fitted to match the experimental results on the flame velocity and maximum temperature. Particle burning time is estimated from the flame simulations.

MATHEMATICAL MODELLING OF A BUBBLING FBC CO-FIRED WITH LIGNITE AND BIOMASS

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A comprehensive system model of fluidized bed combustor, previously developed and tested for prediction of combustion behaviour of fluidized bed combustors fired with lignite was extended for modelling of co-firing of lignite with biomass by incorporating volatile release, char combustion and population balance for biomass. The model predictions were validated against measurements taken on METU 0.3 MW_t AFBC fired with lignite only, lignite with limestone addition and about 50/50 lignite/olive residue mixture with limestone addition. Predicted and measured temperatures and concentrations of gaseous species along the combustor were found to be in good agreement. Introduction of biomass to lignite was found to decrease SO_2 emissions but did not affect NO emissions significantly. The system model proposed in this study proves to be a useful tool in qualitatively and quantitatively simulating the processes taking place in a bubbling fluidized bed combustor burning lignite with biomass.

DESIGN ASSESSMENT OF A 150kWt CFBC TEST UNIT

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For clean and efficient energy generation from coal, the most suitable technology known to date is 'Fluidized Bed Combustion' technology. Applications of circulating fluidized bed (CFB) combustion technology have been steadily increasing in both capacity and number over the past decade. Designs of these units have been based on the combustion tests carried out in pilot scale facilities to determine the combustion and desulfurization characteristics of coal and limestone reserves in CFB conditions. Similarly, utilization of Turkish lignites in CFB boilers necessitates adaptation of CFB combustion technology to these resources. However, the design of these test units are not based on firing coals with high ash, volatile matter and sulfur contents like Turkish lignites. For this purpose, a 150 kWt CFB Combustor Test Unit is designed and constructed in Chemical Engineering Department of Middle East Technical University, based on the extensive experience acquired at the existing 0.3 MWt Bubbling Atmospheric Fluidized Bed Combustor (AFBC) Test Rig. Following the commissioning tests, a combustion test is carried out for investigation of combustion characteristics of Çan lignite in CFB conditions and for assessment of the design of test unit. Comparison of the design outputs with experimental results reveals that most of the predictions and assumptions have acceptable agreement with the operating conditions. In conclusion, the performance of 150 kWt CFBC Test Unit is found to be satisfactory to be utilized for the long term research studies on combustion and desulfurization characteristics of indigenous lignite reserves in circulating fluidized bed combustors.

DUAL BED REACTOR FOR THE STUDY OF CATALYTIC BIOMASS TARS CONVERSION

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A dual fixed bed laboratory scale set up has been used to compare the activity of a novel $Rh/LaCoO_3/Al_2O_3$ catalyst to that of dolomite, olivine and Ni/Al_2O_3, typical catalysts used in fluidized bed biomass gasification, to convert tars produced during biomass devolatilization stage. The experimental apparatus allows to operate the catalyst under controlled conditions of temperature and with a real gas mixture obtained by the pyrolysis of the biomass carried out in a separate fixed bed reactor operated under a selected and controlled heating up rate.
The proposed catalyst exhibits much better performances than conventional catalysts tested. It is able to completely convert tars and also to strongly decrease coke formation due to its good redox properties.

SIMULATION OF GASLESS COMBUSTION OF SOLID POWDER MIXTURES

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The direct 3D method of numerical simulation of gasless combustion of solid powder mixtures is developed. The method under consideration falls into three stages. On the first stage, a simulation of mixture structure is performed. An analysis of the structure obtained in simulations is carried out. On the second stage, the thermal conductivity of solid powder mixture is calculated. On the third stage of simulation, the ignition and combustion of each particle of the mixture is considered with taking into account of heat exchange between contacting particles. The results of numerical simulations are represented dynamically and compared with the experimental data, obtained by high-speed digital recording of mechanically activated SHS systems combustion.

SET UP OF AN EXPERIMENTAL APPARATUS FOR THE STUDY OF FRAGMENTATION OF SOLID FUELS UPON SEVERE HEATING

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An experimental apparatus has been developed in order to perform tests of primary fragmentation of solid fuels under severe heating conditions. The devise is a modified heated strip reactor, capable to reach 2000°C in less than 0.2s. Particles are laid on the strip and pyrolysed under inert or moderately oxidizing conditions. The char particles and their fragments, generated upon pyrolysis, can be recovered and analysed to assess the fragmentation propensity of the fuel.
Some preliminary experiments have been carried out on two biomass samples in order to assess the temperature time history of particles in the experimental apparatus. In particular biomass particles of approximately 2-3 mm have been used. The temperature of the heated strip reactor in such preliminary tests was varied between 1000 and 1600°C, while the strip nominal heating rate was kept at 10^4°C/s and the holding time was set at the value of 10s. A near infrared fast camera (38000 frames/sec) has been used to measure the temperature of the heated strip and of the particles during the tests. A heat up model was developed and validated against experimental results. The model was then used to estimate the temperature gradients across particles of biomass and of coal as well.
Results show that the strip of the reactor reaches the set temperature in less than 0.2s. When particles are laid on the strip, their bottom surface, which is in physical contact with the strip, immediately reaches the set temperature value. For 1mm coal particles the upper surface can be considered at the same temperature as well. Under the most severe conditions tested (strip temperature of 1600°C , biomass particles of 2mm thickness) the temperature difference between the bottom and the upper face is 200°C after 3s and drops to 100°C after 10 s. On the whole the experimental apparatus simulates uniform heating of the particles with reasonable approximation. In the next future the apparatus will be further upgraded to operate at pressures up to 20 bar.

DEVOLATILIZATION AND ASH COMMINUTION OF TWO DIFFERENT SEWAGE SULDGES UNDER FLUIDIZED BED COMBUSTION CONDITIONS

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Two different wet sewage sludges have been characterized under fluidized bed combustion conditions with reference to their devolatilization behavior and ash comminution with the aid of different and complementary experimental protocols. Analysis of the devolatilization process allowed to determine the size of fuel particle able to achieve effective lateral spreading of the volatile matter across the cross-section of medium-scale combustors. Primary fragmentation and primary ash particle characterization pointed out the formation of a significant amount of relatively large fragments. The mechanical properties of these fragments have been characterized by means of elutriation/abrasion tests using both quartz and sludge ash beds.

FLUIDIZED BED GASIFICATION OF NATURAL AND WASTE BIOMASS

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Three commercially-available biomass fuels, made of natural and waste wood, were fed in a pilot plant bubbling fluidized bed gasifier, having an internal diameter of 0.381m and a maximum feeding capacity of 100kg/h. The experimental runs were carried out at about 850°C and under values of the equivalence ratio between 0.20 and 0.30. The fluidized bed was generally made of natural olivine even though some runs utilized beds of dolomite or quartz sand. Measurements taken during each run include the gas composition (at three levels along the gasifier, at the reactor exit and downstream of the scrubber unit), the content of tar in the syngas, the mass flow rate and composition of entrained fines collected at the cyclone and the characterization of bed material. To this end, different on-line and off-line apparatus were used, such as on-line analyzers for CO, H_2, CO_2, O_2, CH_4, together with a gas-cromatograph and an innovative quasi-continuous on-line analyzer for tar.
The results indicate that the air gasification process is technically feasible with all the biomass tested. The flexibility of the fluidized bed gasification was confirmed as remarkable, making it the preferred technology for the gasification of biomass as well as post-consumer packaging and processed waste in general, especially in multi-fuel installations.

NUMERICAL CHARACTERISATION OF THE MECHANISMS OF NO_X FORMATION DURING MSW INCINERATION

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A numerical model has been developed (Chemkin) to study combustion processes in a fixed bed reactor. The test section is divided into several successive Perfect Stirred Reactor (PSR). At the entry, the thermal degradation species of the solid are used as input and at the exit the exhaust gases are recovered. Comparison of previously experimental results and the current model output has been compared with good agreement. The study demonstrates that the NO formation and reduction is controlled by the combustion regime so are mainly dependant of the primary excess air of combustion. The model has been used to establish the reaction pathways of formation and reduction of the NOx at different locations in the reactor as a function of this parameter. This has allowed defining what is occurring at each specific location of the reactor. The reaction pathways and sensitivity study has shown that the production of NO is controlled mostly by local oxygen concentration, thus the location of the NO production region depends mostly on the primary air injection. From this description of the principal reacting zones and of the intermediate species it is possible to develop and to optimize primary technique of NOx reduction.

EXPERIMENTAL AND NUMERICAL STUDY OF THE ACCURACY OF FLAME SPEED MEASUREMENTS IN A BUNSEN BURNER

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Despite their importance for turbulent combustion, premixed laminar flame speeds are still a weak part of CFD models: they remain difficult to measure and multiple techniques are still being tested and developed to measure them accurately. This paper studies sources of uncertainties in the measurement of laminar flame speeds using the Bunsen burner technique. To evaluate these uncertainties a two-dimensional slot burner is operated both experimentally and numerically. Sources of potential mismatch between the flame speed measured in the Bunsen setup using the classical flame surface method and the true laminar flame unstretched flame speed are studied and quantified. Curvature at the flame tip, strain on the flame sides and local quenching at the flame base can modify the local flame speed and require corrections: they are studied using a two-dimensional DNS code and shown to be small (of the order of 1 percent). DNS also provides strain, curvature, stretch, displacement and consumption flame speed along the flame front, confirming that stretch remains small and that the local consumption speed remains very close to the unstretched premixed flame speed, thereby validating the principle of the method. A second correction is required by the finite aspect ratio of the slot used to inject the premixed gases (10 in this case) which induces a flow acceleration in the measurement region. This correction can be evaluated from velocity measurement in the slot section and found to be of the order of 5 percent. Corrections are then applied to a methane - air flame Bunsen burner and results are compared to experimental results found in the literature and to a one-dimensional premixed flame code (COSILAB) using the GRIMECH 3 scheme.

LARGE-EDDY SIMULATION OF SINGLE-SPECIES FLOWS UNDER SUPERCRITICAL THERMODYNAMIC CONDITIONS

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The thermodynamic and transport properties of fluids above their critical point is far from that of a perfect gas. Strong non-linearities in the equation of state and transport properties may modify the structure of turbulence but also require additional terms in turbulence models. The present work addresses the influence of a real-gas equation of state (Peng-Robinson) on turbulence properties and turbulence models. The numerical simulation of two single-species flows is conducted with the intent of validating the Large-Eddy Simulation (LES) methodology for flows under supercritical thermodynamic conditions. First, the set of equations for LES is presented, with appropriate approximations and assumptions, in particular those relevant to the non-linear thermodynamic properties of real-gases. A homogeneous isotropic turbulence case is considered to study the influence of equation-of-state effects on the properties of turbulence. It is shown that the peculiar thermodynamic properties of single-species supercritical fluids do not affect the spectral content of the flow, which is promising for LES. Then, the case of a dense jet at supercritical pressure is computed with the LES methodology. This jet corresponds to an actual experimental setup, which allows for comparison with Raman measurements of density profiles.

IMPACT OF ETHYLENE AND NO ADDITION ON FUEL OXIDATION UNDER SIMULATED HCCI CONDITIONS

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New combustion modes, such as HCCI in internal combustion engines, are going to be industrially developed due to their savings in terms of NOx and particulate matter emissions. However, in order to achieve a quasi homogeneous air/fuel mixture in a Diesel engine, high rates of EGR are needed in order to dilute the air/fuel mixture and to control ignition delay. Moreover, it has been recently shown that EGR gases influence also combustion via a chemical effect (due to the presence of NO, CO, HC, ...) in addition to their thermodynamic and dilution effects. The goal of this study is to better understand how the EGR compounds influence the fuel combustion.

First, the effects of NO and ethylene addition were performed in an HCCI engine with different concentrations of NO (50, 100, and 200 ppmv) and C_2H_4 (200, 400, and 2000 ppmv). These compounds were chosen due to the known high reactivity of NO and the high content in C_2H_4 in the EGR gases. Since the impact of EGR compounds on engine control is difficult to understand in an engine itself, some experiments were also performed in a Jet-Stirred Reactor (JSR) where conditions are well-controlled. In accordance with the literature, a complex impact of NO and few influence of C_2H_4 on oxidation kinetics were observed. However, a synergistic effect on the oxidation of n-heptane/toluene blend was observed here by coupling between NO and ethylene, leading to a considerable inhibition of fuel oxidation at low temperatures, and a significant promotion of fuel oxidation in higher temperatures. These results tend to demonstrate the importance of taking into account the complexity of EGR composition.

FLUID DYNAMICS AND DETAILED KINETIC MODELING OF POLLUTANT EMISSIONS FROM LEAN COMBUSTION SYSTEMS

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A methodology for computing steady turbulent reacting flows in combustors is presented. A 3-D computational fluid dynamics (CFD) proprietary code and a kinetic post-processor (KPP) have been coupled and applied to calculate the gas temperature and pollutant emissions. A first application of the above calculation methodology has been carried out on Lean-Burn innovative injection system (PERM), designed and developed in the frame of the EU program for NEW Aero engine Core concepts NEWAC. This injection system was studied experimentally in a tubular combustor in order to perform the first assessment in terms pollutant emissions at the outlet at different operating conditions.
Measurements and the corresponding model results refer to the tubular combustor operating at medium pressure (8 bar) and different AFRs. The model predictions are compared with experimental results and globally the agreement is satisfactory, especially for NO emissions. The observed deviation between measurements and prediction is discussed for both CO and NO_2 and further investigations are underway to explain the observed behavior. The analysis of data provides useful information for further improvements in modeling and experimental activities. A validation activity in a wider range of operating conditions, both in terms of inlet air pressure and temperature, is planned to further validate the modeling approach and to provide new experimental data aimed at addressing the mechanisms of CO and NOx emissions from lean combustion systems.

DETONATION AND DEFLAGRATION TO DETONATION TRANSITION IN STOECHIOMETRIC H_2/CH_4 - AIR MIXTURES

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To improve detonation data in connection to safety in the development of H_2 fuel technology stoechiometric binary fuel H_2/CH_4 with Air mixtures are studied. The detonation characteristics, pressure P, velocity D and cell size λ, and deflagration to detonation transition (DDT) run up distance L_{TDD}, are measured as function of molar fraction x of H_2 in H_2/CH_4 fuel. x is ranging from 0.5 to 1. For detonation data, λ decreases strongly as x increases. The ratio $k = \lambda/L_i$ is found to be equal to 30 - 50, L_i being the ZND reaction zone length. For DDT data, L_{TDD} not exceed 1.5m and a correlation $L_{TDD} \approx 30\,\lambda$ is suggested. In general way, adding Hydrogen in Natural Gas promotes the detonability of the mixtures and for $x \geq 0.7$ these mixtures become more detonable than common heavy Alkane/Air mixtures.

EFFECTS OF EQUIVALENCE RATIO VARIATION ON LEAN, STRATIFIEDMETHANE-AIR LAMINAR COUNTERFLOW FLAMES

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Flame propagation and structure in stratified combustion, a key technology for advanced low emission combustors, has been investigated using lean methane-air laminar counterflow flames. Configurations with steady spatial equivalence ratio gradients and with unsteady, time varying equivalence ratio profiles were examined in order to isolate the effects of equivalence ratio gradient from unsteady history effects. Stratified flames were compared with perfectly premixed flames where the equivalence ratio was matched at the location of peak heat release. Back supported flames (where the products were closer to stoichiometric than the reactants) propagated significantly faster and with reduced thickness compared to perfectly premixed flames which, in turn, were faster and thinner than the corresponding front supported flames. This observation, which corroborates the findings of previous studies, holds in both the steady and unsteady configurations. In order to understand the underlying processes, the composition and species flux were analyzed through the reaction zone in the steady cases. At the location of peak heat release, back supported flames exhibit temperatures and levels of major species which are similar to premixed flames, while radical species concentrations, including OH, as well as the heat release rate are enhanced. The increased (reduced) levels and fluxes of OH in back (front) supported flames were attributed to the shifting equilibrium of the CO-H_2 recombination reactions due to the stratification induced temperature gradient. The stratified flames were found to respond to equivalence ratio variations following a delay on the order of the characteristic flame time-scale. The unsteadiness adds to the effects of the instantaneous flame normal equivalence ratio gradient observed in the steady flames. When the equivalence ratio oscillates with a period similar to, or less than, the flame time scale the flame response is attenuated. The presence of equivalence ratio variation through the flame implies that flame speed, flame thickness or reaction rate can not be modeled accurately as functions of only the progress variable and equivalence ratio. Models accounting for temporal and spatial equivalence ratio variation may be advantageous.

RECONSTRUCTION OF TRANSIENT EMISSIONS FROM LIGHT-DUTY VEHICLES

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The need for accurate emissions measurements has conducted researchers into trying to reconstruct the true transient emissions signals from raw measured data. In this study, a reconstruction methodology was applied to obtain time-resolved emissions from a light-duty vehicle. The methodology uses the cross-correlation technique and the differential coefficients method to account for the pure time delay and for the dispersion of the each emission signal, respectively. The pure time delays for O_2, CO_2, CO, NO_x and HC were determined by applying the cross-correlation technique to several step transient tests from a light-duty vehicle. For the characterization of the analyzers dynamics, tests with zero and span gases have been performed and the coefficients of the differential coefficients method evaluated. Reconstruction of the transient emissions measurements for both a imposed step and real cases has been examined. The results demonstrated that the signal reconstruction using only one coefficient (the time constant) results in signals with higher quality than those obtained using two coefficients. It has been shown that the cross-correlation technique, when coupled with reconstruction techniques such as the differential coefficients method, can be a powerful tool in the phasing of raw experimental data from light duty-vehicles.

MODELING DIESEL SPRAY FLAME LIFT-OFF USING DETAILED CHEMISTRY AND A NEW PRIMARY BREAKUP MODEL

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Combustion in direct-injection diesel engines occurs in a lifted, turbulent diffusion flame mode. Numerous studies indicate that the combustion and emission characteristics in such engines are strongly influenced by the lifted flame behavior, which in turn is determined by fuel and air mixing in the region upstream of the lifted flame, and consequently by the liquid breakup and spray development processes. Thus primary jet breakup plays a key role in engine processes, and is induced by cavitation and turbulence inside the injector nozzle, and aerodynamic (Kelvin-Helmholtz) instability outside. In the present study, we examine the effects of these three primary breakup processes in the flame liftoff behavior. A new primary breakup model incorporating the inner nozzle flow (cavitation and turbulence) and aerodynamic effects is developed and evaluated for predicting the flame liftoff characteristics. The effects of various ambient and injection characteristics on flame lift-off are simulated using a detailed chemistry, and validated against data from Sandia National Laboratory. In general, very good agreement is observed under all measured conditions. The effect of nozzle orifice geometry on flame lift-off is also characterized.

SPRAY COMBUSTION DYNAMICS UNDER THERMOACOUSTIC OSCILLATIONS

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Thermoacoustic instabilities in combustors have remained a topic of investigation for over two decades due to the challenges it posses to the operation of low emission gas turbines. For combustors burning liquid fuel, understanding of the cause-and-effect relationship between spray combustion dynamics and thermoacoustic oscillations is imperative before the successful development of any control methodology for its mitigation. Some very unique operating characteristics of a kerosene-fueled test combustor under limit-cycle oscillations are reported.

STRUCTURES AND STABILIZATION OF LOW CALORIFIC VALUE GAS TURBULENT PARTIALLY PREMIXED FLAMES IN A CONICAL BURNER

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Experiments were carried out on partially premixed turbulent flames stabilized in a conical burner. The investigated gaseous fuels are a mixture of CH_4, CO, CO_2, H_2 and N_2, simulating typical products from gasification of biomass. The fuel and air were partially mixed in a concentric tube. Flame stabilization behavior with and without the cone was investigated and significantly different stabilization characteristics were observed between flames with and without the cone. Planar Laser induced fluorescence (LIF) imaging of a fuel-tracer species, acetone, and OH radicals was carried out to characterize the flame structures. The data show that the flames with the cone are more stable than those without the cone. Without the cone the burner is a typical jet; the critical jet velocities for blowoff and liftoff of biomass derived gases are found to be much higher than that for methane/nitrogen mixture with the same heating values. With the cone, it was shown the stability of flames is not sensitive to the compositions of the fuels. From the PLIF images it was shown that in the conical burner, the flame is stabilized by the cone at nearly the same position for different fuels. The flame is believed to be controlled by the recirculation flows inside cone, which depends on the cone angle and flow speed, and less sensitive to the fuel compositions.

DIFFUSIVE-THERMAL INSTABILITIES OF TUBULAR FLAMES

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Diffusive-thermal instabilities of tubular premixed flames are studied in the frame of the diffusive-thermal approximation. The problem becomes amenable to a complete analysis when a simplified flow field and the flame-sheet combustion model are applied. The dispersion relation determining the growth rate of instabilities is obtained in an analytical form which therefore is analyzed numerically. Stability diagrams showing stable and unstable states, in particular those manifesting the cellular behavior, are presented.

ZERO-DIMENSIONAL MODEL OF PREMIXED COMBUSTION IN DIESEL ENGINES

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This paper presents a new 0D phenomenological approach to predict the combustion process in Diesel engines operated under various operating conditions. The aim of this work is to develop a physical approach in order to improve the prediction of cylinder pressure and heat release. This study focuses on the modeling of the premixed part of the Diesel combustion.
In phenomenological Diesel combustion models the premixed combustion phase is usually modeled by the propagation of a turbulent flame front. However, experimental studies showed that this phase of Diesel combustion is actually a rapid combustion of part of the fuel injected and mixed with the surrounding gas. This mixture burns quasi instantaneously when favorable thermodynamic conditions are locally reached. A chemical process then controls this combustion.
In the present model, the rate of heat release by combustion is related to the mean reaction rate of fuel. The latter is evaluated by an approach based on the determination of the Probability Density Function (PDF) of the mixture fraction (Z), in order to take into consideration the local variations of the fuel-air ratio. The shape of the PDF is presumed with a standardized β-function. Mixture fraction fluctuations are described by using of a transport equation for the variance of Z. The standard mixture fraction concept established in the case of diffusion flames is here adapted to premixed combustion to describe the inhomogeneity of the fuel-air ratio in the control volume.
Premixed zone volume and total entrained ambient gas mass flow rate are calculated using a detailed spray model. The developed premixed combustion model is one sub-model of a thermodynamic model based on the mathematical formulation of the conventional two-zone approach. This zero-dimensional model incorporates several sub-models describing turbulence, vaporization, fuel introduction rate and mixing-controlled combustion. The purpose of this approach is to directly relate physical model parameters to operating conditions and engine parameters.
Numerical results from simulations are compared with experimental measurements carried out on a 2 liter Renault Diesel engine. For all investigated operating conditions, simulated cylinder pressure and heat release rate traces show a good agreement with experimental measurements.

SIMPLIFIED KINETIC MECHANISM OF ETHYL ACETATE OXIDATION FOR HCCI ENGINES

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Homogeneous Charge Compression Ignition (HCCI) is a combustion mode which virtually allows any kind of combustible liquids to be used in internal combustion engines. The production of biofuel could take advantage of this characteristic by driving the processes towards less refined fuels and so less energy-consumming operations. In particular, the products of the acidogenic fermentation will be discussed here. This process produces organic volatile acids which can be combined partly with ethanol (produced in the first step of the acidogenesis) and partly with glycerol (by-product of the biodiesel industry) to obtain a large range of esters. In this work, we have developed a kinetic mechanism for ethyl acetate (simplest fuel obtained in this route) in HCCI conditions. This paper describes the method used to simplify the mechanism and then compares the simulated results with those obtained for the iso-octane and the ethanol. The kinetic mechanism includes 45 chemical species and 215 elementary reactions. CFD simulations show that ethyl acetate is very similar to iso-octane and ethanol. However, ethyl acetate shows a small difference in the low temperature chemistry.

PARTIALLY PREMIXED PREVAPORIZED KEROSENE SPRAY COMBUSTION IN TURBULENT FLOW

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A detailed numerical simulation of kerosene spray combustion has been carried out on a partially premixed Prevaporized three dimensional configuration. The investigations were focused on the flame temperature profile dependency with respect to the length variation of the pre-vaporization zone. The results have been analyzed and compared to the experimental data. A fundamental study has been performed by changing the droplet diameter, the kerosene flammability limits, a combustion model parameter and the location of the combustion initialization to observe the temperature variation and flame flashback. The investigations were performed for atmospheric pressure, inlet air temperature of 90°C and a global equivalence ratio of 0.7. The simulations were carried out using the Eulerian Lagrangian procedure under a fully two way coupling. For the combustion, the Bray-Moss-Libby model has been adjusted to account for the partially premixed combustion.

BEHAVIOR OF PREMIXED HYDROGEN-AIR-STEAM FLAMES NEAR FLAMMABILITY LIMITS

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The behavior of premixed hydrogen-air-steam flames has been investigated near the flammability limits versus initial temperature between 25°C and 150°C at 1 and 2.5 bars of initial pressure. The experiments have been carried out in a 60 L spherical chamber using both electric spark and laser ignition sources. The experiments reported in this paper describe the flames structure for lean and rich mixtures and the data are collected in flammability diagrams where are distinguished the partial and total combustion limits in a closed vessel. The values generally confirm the data of previous investigators and clarify the phenomena associated with selective diffusion and cellular flames formation. The diagram of hydrogen-air-steam flammability limits is given at 1 bar and 100°C and discussed in regards of the previous studies at higher temperature.

HCCI COMBUSTION MODEL BY ONE STEP REACTION FUNCTION: IN VIEW OF ASSISTING THE ENGINE MANAGEMENT OPTIMIZATION

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To reduce the number of tests during engine tuning phases, a model with a very short computational time to simulate Diesel homogeneous combustion (Homogeneous Charge Compression Ignition HCCI) is needed. Therefore, the goal of this study is to provide the engine manufacturers with a simple physical combustion model to assist engine tuning and engine management system optimization, with the aim of predicting in-cylinder pressure evolutions and mean effective pressure (IMEP).
A reduced model driven by to two state variables: the temperature and the mass fraction of burning fuel in the combustion chamber, is described in this paper. The chemistry is modeled by a global degradation reaction where the reaction rate coefficient, usually modeled through the Arrhenius law is driven in this approach by a global function $\Omega(T)$. This global function takes into account the slow dynamic of the cool flame and the fast dynamic of the main ignition and the transition between the two stages. A drawback of the global approach is the introduction of some new parameters which need to be correlated to give reliable results; this has required an important and large parametric study to calibrate the reaction rate coefficient. The proposed model is then autonomous, meaning that the model parameters are function of the engine operating conditions only.
The results show that this type of model can be useful to describe the ignition delay time of HCCI combustion and the rate of heat release, with very short computational times around two seconds. The model has been compared to the model including reduced n-heptane mechanism developed previously and to Renault engine experimental data. This comparison shows that the model gives reasonable accuracy in terms of in-cylinder pressure and IMEP with very short computation time.

HCCI ENGINE COMBUSTION ON-SET CONTROL UTILIZING PROTO-TYPE IN-CYLINDER FUEL REFORMATION CHAMBER

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In this study, a new in-cylinder fuel reformation strategy has been implemented into a HCCI engine to control the on-set of combustion or Start of Combustion (SOC). The in-cylinder reformation methodology utilizing a pre-chamber, demonstrated in this work, provides control over the mixing of the reformation products with fresh charge and does not affect the volumetric efficiency of the engine as in the case of Negative Valve Overlap (NVO) technology. The two benefits from the new reformation strategy are; firstly, it temporarily changes the engine's nominal compression ratio thus providing additional control over HCCI SOC. Secondly, the strategy utilizes in-cylinder fuel reformation to generate hydrogen enriched gas (which includes other intermediate species), which is then used to alter the subsequent HCCI cycle combustion on-set. The experimental engine used for the study is a four-stroke, three cylinder In-Direct Injection (IDI) type compression ignition engine which was converted to single cylinder operation for HCCI combustion. The HCCI engine was fuelled with lean ethanol/air mixtures. A proto-type reformation chamber has been designed and fabricated with direct injection capabilities to examine the benefits of the proposed strategy. The engine performance was evaluated based on cycle-resolved in-cylinder pressure measurements and regulated engine-out emissions. This work also includes a computational component which involves HCCI cycle calculations with fuel reformation using a single-zone model. The computational portion was used to analyze the advantages of proposed in-cylinder reformation strategy on HCCI combustion before experimental trials. The experimental and simulation results demonstrate that the proposed in-cylinder reformation strategy is an effective method for controlling HCCI SOC. The temporary change in the compression ratio that arises from utilizing the proposed methodology has also a strong influence on HCCI SOC. The experimental and simulation results also indicate that there is an optimal in-cylinder reformation fuelling percentage which will have a positive impact on regular HCCI combustion at some operating conditions.

A RESONANT RESPONSE OF SELF-PULSATING SPRAY-FLAME SUBMITTED TO ACOUSTIC WAVE

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Recently, experiments and theoretical investigations have shown that spray-flame can exhibit oscillatory regimes for standard set of parameters. Theoretical and numerical investigations on flame propagation in two-phase pre-mixtures have put forward an intrinsic (and robust) mechanism based on the interaction between the locus where droplets vaporize and the reaction zone. This mechanism does not invoke neither droplet inertia (very small droplets are studied) nor differential diffusive effects (pulsations take place for unity Lewis number, too). Self-oscillations of spray-flame occur as in a supercritical Hopf bifurcation, controlled by Zeldovich number (*Ze*, the reduced activation energy), the onset threshold being on the order of $(Ze)_c \approx 10$. The issue addressed in this contribution is whether acoustic wave and self-pulsating spray-flame can interact. This study has been carried out in the open loop context: a spray-flame is submitted to small amplitude fluctuations of pressure; the gain towards acoustics has been found as depending on Zeldovich number, since energy transfer is found magnified in the case of a close frequency fit between acoustic resonator and natural spray-flame oscillations. Moreover, energy transfer is found as of resonant type.

ON NITROGEN OXIDE FORMATION IN SPRAY-GUIDED SPARK-IGNITED GASOLINE ENGINES

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Spark-ignited turbulent combustion in a constant volume propane/air homogeneous charge (ϕ = 0.84) cylindrical vessel and in a spray-guided (SG-SIDI) gasoline engine is investigated using the recently developed non-spherical flame kernel model *SparkCIMM* together with the G-equation flamelet approach. The formation of nitrogen oxides is modeled using the extended Zeldovich mechanism. Concentrations of involved intermediate species are approximated using a chemical equilibrium assumption. Motivated by a numerical analysis of NO_X formation rate conditioned mixture fraction variances which are induced by the late and direct spray-injection in SG engines, turbulent mixture property fluctuations are incorporated into the NO_X prediction model.

An analysis of the enthalpy equation revealed that peak gas temperatures result from, besides combustion heat release, the effect of a pressure increase on burnt gas. This temperature increase induced by a pressure rise can not be converted into mechanical energy but intensifies, however, the formation of thermal NO and must therefore be considered as an unwanted enthalpy rise.

The simulation of turbulent combustion in the constant volume vessel shows, even though homogeneously charged, a strong radial temperature stratification which is assigned to this pressure induced temperature increase. It is shown that this effect also substantially contributes to peak gas temperatures in SG-SIDI engines.

Therefore, a further optimization of mixture preparation in spark-ignited engines with regards to minimize the combined effects of combustion heat release and pressure induced temperature increase seems to be capable to reduce engine-out nitrogen oxide emissions without loss of engine power or fuel economy.

MEASUREMENTS OF ULTRAFINE PARTICLES FROM A GAS-TURBINE BURNING BIOFUELS

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Measurements of ultrafine particles have been performed at the exhaust of a low-emission microturbine for power generation burning, under different loads, liquid fuels, including a commercial diesel oil, a mixture of the diesel oil with a biodiesel and kerosene. Primarily attention has been focused on the measurements of the size distribution functions of the particles emitted from the system by means of particle differential mobility analysis. A bimodal size distribution function of the particle emitted has been found in all the examined conditions. Burning diesel oil and its mixture with the biodiesel, the first mode of the size distribution function of the combustion-formed particles is centered at around 2-3nm, whereas the second mode is centered at about 20-30nm. The increase of the turbine load and the addition of 50% of biodiesel do not cause changes in the size distribution of the particles but even slightly decreases the amount of particle formed. By using kerosene the amount of emitted particles increases of more than one order of magnitude. Also the shape of the size distribution function changes with the first mode shifted towards larger particles of the order of 8-10nm but with a lower emission of larger 20-30nm particles. Overall the mass concentration of kerosene burning conditions is increased respect to the diesel oil operation. Particle sizes measured with the diesel oil have been compared with the results on a diesel engine operated in the same power conditions and with the same fuel. Measurements have showed that the sizes of the formed particles do not change in the two combustion systems but diesel engine emits a number concentration of particles more than two orders of magnitude higher in the same conditions of load and fuel. By running the engine in more premixed-like conditions the size distribution function of the particles approaches that measured by burning kerosene in the microturbine indicating that turbine combustion behaviors affects the distribution function of the sizes of the emitted particles.

OPTICAL INVESTIGATION OF THE COMBUSTION BEHAVIOUR INSIDE THE ENGINE OPERATING IN HCCI MODE AND USING ALTERNATIVE DIESEL FUEL

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HCCI combustion is analyzed in an optically accessible diesel engine. The effect of fuel and injection strategy is studied by means of UV-visible imaging spectroscopy. Soot, OH, CH, and HCO* concentration evolution are evaluated with high spatial and temporal resolution using chemiluminescence measurements. Multi-pulse early injections are employed to modulate the homogeneity history of the cylinder charge. RME and diesel commercial fuel are tested. The positive effect in the use of RME fuel using HCCI strategy is observed for the further reduction of pollutant emission. In particular, the use of RME fuel decreases further the PM and NOx concentrations both in chamber and exhaust with respect to those of REF fuel. The OH behaviour in chamber is strictly correlated to formation-oxidation of PM-NOx. The HCO light emission detected in the combustion chamber are well correlated with the CO emission measured at the exhaust.

RESULTS CONCERNING THE CO-COMBUSTION OF FOSSIL AND BIO-FUELS IN A COGENERATION PLANT, USING INTERNAL COMBUSTION DIESEL ENGINES

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The major problem of the existing Power Plants focuses on the price of the final product – energy - and the level and quantity of emissions causing harmful conservancy upon the environment. Actual limits imposed by the European Union represent a great "danger" for the existing power plants. At this moment for several states in the EU the traditional, fossil fired plants represents a vast energy resource that the states relay on, and it is not expandable. The paper presents an experimental study from the environmental impact point of view of pilot plant working in cogeneration, using an internal combustion engine, working with fossil and blended fuels with a specific biofuel ratio. The reference values were established by using as primary fuel in the pilot plant only pure diesel. In the following tests, the primary fuel was replaced by butanol, with a concentration by volume of 2, 5, 7, 10 % butanol in diesel. The pollutant emissions levels for the main species can be kept in normal limits, without being significantly affected by the mixture with butanol. The emission level for the NO_x species is slightly affected by the mixture of butanol in diesel. The study was made on pilot plant mounted in the multifunctional Lab of renewable energy resources at the University "POLITECHNICA", from Timisoara.

INVESTIGATION OF FINE-SCALE STRUCTURE OF TURBULENT AND MOLECULAR DIFFUSION IN COAXIAL JETS OF HE/CO_2 IN AIR BY LDA AND RAYLEIGH SCATTERING

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This paper revisits the important issue of differential diffusion and provides new experimental results and subsequent analysis that attempts to quantify the relationship between molecular diffusion, turbulent diffusion and their mutual interference in non-reacting axisymmetric coaxial jets of variable Reynolds number. The reported investigation has been focused on the analysis of molecular diffusion of a He/CO_2 mixture in air by combining line imaging of Rayleigh scattering and laser Doppler anemometry (LDA) to determine length scales associated with differential diffusion and turbulent transport. Line imaging Rayleigh scattering was performed applying the index-matching method with a mixture of two gaseous species having scattering cross-sections respectively lower and higher of that of air and the cross section of the mixture identical to that of the co-flowing air. Any measured variation in scattering intensity is therefore due to differential diffusion between the two species. Instantaneous and ensemble averaged line profiles of Rayleigh scattering intensity are presented and a characteristic length scale associated with differential diffusion is deduced. Autocorrelation analysis is applied to obtain the characteristic scale of differential diffusion fluctuations and the integral length scales of velocity fluctuations, as measured by LDA. Theoretical information from the literature is used in relating these scales to the molecular and turbulent diffusion coefficients, assuming homogeneous and isotropic turbulence, and then the ratio of molecular to turbulent diffusivity is estimated as a function of the Reynolds number. The results confirm that the average contribution of molecular diffusion to the effective diffusivity into the air stream progressively reduces when the turbulence level increases. They also suggest that, at higher Re, the differential diffusion remains significant down to the scalar dissipation length scale, and could influence mixing at the molecular level and thus chemical reactions.

ACCOUNT FOR RATIOS OF H_2O TO CO_2 IN THE CALCULATION OF THERMAL RADIATION OF GASES WITH THE WEIGHTED-SUM-OF-GREY-GASES MODEL

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The standard formulation of the weighted-sum-of-grey-gases (WSGG) model uses parameters that are fitted to a range of temperatures but only for specific ratios of H_2O to CO_2. As such, the model is limited to specific fuels with the proper composition of hydrogen and carbon unless several setups of parameters are used. Here, the WSGG model is modified to account for various ratios of H_2O to CO_2. To test the model, predictions of the radiative source term and wall fluxes in a gaseous domain between two infinite plates are compared with predictions by a statistical narrow-band model. Included in the comparison are also two grey approximations, which is a common approach to account for gaseous radiation in comprehensive combustion models. Results show that the modified WSGG model significantly improves the estimation of the radiative source term compared to the grey models, although the accuracy of the wall fluxes is of the same magnitude.

COMPARISON OF ELECTRICAL AND LASER SPARK EMISSION SPECTROSCOPY FOR FUEL CONCENTRATION MEASUREMENTS

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Emission spectra from electrical and laser sparks in flowing methane-air mixtures of various compositions have been collected and analysed. The differences and similarities between the electrical and laser sparks in the context of their emission are discussed. The emission spectra from the laser spark were characterized by a weak continuum, onto which several strong atomic lines and some molecular bands were superimposed, in contrast to the spectra of electrical spark where a strong continuum, few atomic lines and several strong molecular bands were evident, making thus the laser spark spectroscopy a more accurate technique to measure hydrocarbon concentration. For both types of spark, the total intensity of the CN chemiluminescence around 388 nm was found to correlate almost linearly with fuel concentration in methane-air mixtures.

REACTION ZONE STRUCTURE IN A LABORATORY DUAL-MODE SCRAMJET COMBUSTOR FROM SIMULTANEOUS OH/CH_2O - PLIF

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Planar laser-induced fluorescence (PLIF) imaging of hydroxl (OH) and formaldehyde (CH_2O) was performed simultaneously in a laboratory dual-mode scramjet combustor in order to determine the structure of the reaction zone. The combustor consisted of a single, sonic, transverse fuel jet upstream of a wall cavity pilot flame. A mixture of 50% ethylene and 50% hydrogen by volume was used for fuel. Ramjet mode (thermally choked) combustion was studied at air stagnation temperatures of 1270 K and 1470 K, which lead to two different reaction zone structures (cavity stabilized and fuel-jet-wake stabilized). Cavity stabilized combustion was found to have a relatively thin and continuous high OH gradient structure indicative of a premixed flame. Jet-wake stabilized combustion had OH in discontinuous pockets starting upstream of the cavity. For both cases, the formaldehyde images show the initial fuel breakdown occurs well upstream of most the reaction zone. The base of the reaction zone exists in an intermediate flame / auto-ignition regime. Upstream finite rate chemistry reactions cause a buildup of combustion precursors which serve to increase the propagation speed of the flame where the main heat release occurs.

IR IMAGING FOR STABILITY ANALYSIS OF INDUSTRIAL BURNER

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In this paper, a new diagnostic tool is presented to spatially characterize combustion fluctuations. This tool based on FAst IR Imaging of flames was applied on two different types of gas turbine burners and on two traditional industrial burners varying the fluid dynamic conditions. Both GT burners evidenced oscillation at low frequencies around 25 Hz, 100 Hz and at higher frequencies up to several kHz. Typical frequencies bias toward combustion were identified. The investigations also evidenced that the typical frequencies shift up while increasing AFR. The FAIRI technique allowed to identify higher frequencies (up to several kHz) in the 2D dimensions. The extension of the technique to a practical Lean Premixed gas turbine gave good results either for frequency analysis of fluctuations, either for the location of the phenomenon of humming. Regarding industrial boiler combustion the FAIRI technique allowed to identify on both gas and coal combustion the proper location of the flame root and its better performance in stability. Further information have to be collected on air/fuel mixing and local flame temperature. The technique came out as an interesting tool for further development and investigations.

STATISTICAL ANALYSIS PROCEDURES FOR MORPHOLOGICAL INVESTIGATION OF JET IN CROSSFLOW IMAGES

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A methodology of image statistical analysis to investigate spray shadowgrams is presented. The developed procedures aim to point out quantitative information embedded in shadowgrams. Due to the peculiar morphology of the jet in crossflow images a purposely-defined criterion for proper selection of the threshold had to be proposed. Such methodology is applied to an extensive set of sprays shadowgrams, obtained by crossflow injection. Jet leading edge and centerline could be easily determined using the proposed procedure. Thus the progressive divergence of the two curves, representing the spray aperture angle, can be measured. Results indicate that the ruling parameter for liquid placement and dispersion is the momentum flux ratio. Further weaker dependences on injection diameter and surface tension were pointed out.

VALIDATION OF A NOVEL SOOT MODEL IN LAMINAR DIFFUSION FLAMES: FUEL, FLOW RATE AND THERMOPHORETIC EFFECTS

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The paper addresses a validation study on a soot model for fires developed from laminar smoke point measurements. The work presented here is complementary to a previous study and looks mainly at several aspects of soot distribution in laminar axisymmetric non-premixed flames: thermophoretic, flow rate (and transition from non-smoking to smoking) and fuel effects. The numerical results, obtained by implementing the soot model into Fire Dynamics Simulator (FDS, version 4.07) and using its Direct Numerical Simulation (DNS) mode, show a good agreement with the experimental data for the studied flames, underlying therefore the ability of the model to capture the several effects and features cited above.

COMBINED CONTROLLED CO, CO_2 IN DIESEL ENGINE EXHAUST TO THE ENVIRONMENTAL POLLUTION

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When looking at the effects of diesel engine exhaust on the environment, it is important to first look at the composition of the exhaust gases. Over 99.5% of the exhaust gases are a combination of nitrogen, oxygen, carbon dioxide, and water. With the exception of carbon dioxide, which contributes about 5% of the total volume, the diesel engine exhaust consists of elements which are part of the natural atmosphere and are not harmful to the environment. Carbon dioxide emissions are directly related to the efficiency of the combustion unit. The higher the efficiency, the lower the CO2 emissions. The diesel engine has a relatively high efficiency and, therefore, the carbon dioxide emissions are lower as compared to other less efficient prime movers.The investigation was conducted on a direct injection diesel engine and was concerned with the effects of exhaust gas recirculation (EGR) on diesel engine combustion and emissions. In particular, the effects of carbon dioxide (CO_2), water (H_2O), carbon monoxide (CO), some different constituents of EGR, on combustion and emissions were analysed and quantified numerically. The second parameter influent directly on rate of oxides carbon is the bowl shape. The Mexican hat and spherical piston geometry are analyzed in this work. A modified version of the computational fluid dynamics (CFD) Code KIVA-3V has been used for modeling combustion process and engine emission in particular carbon oxides emission and his control. Simulation was carried out by using a two-stroke single-cylinder direct injection diesel engine.

NO REMOVAL BY GAS REBURNING AND SELECTIVE NON-CATALYTIC REDUCTION USING AMMONIA IN A PILOT-SCALE REACTOR

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An experimental investigation has been performed to study the efficiency of NO reduction by three technological approaches: Reburning by methane, Selective Non-Catalytic Reduction (SNCR) by ammonia and a hybrid approach by coupling Reburning and SNCR. Experiments were performed on a semi-industrial pilot equipped with a Mc Kenna flat flame burner able to generate the flue gas with well known features. The desired levels of initial NO were achieved by seeding the flame with known amounts of nitric oxide. Experiments were performed throughout the temperature range of interest, i.e. from 973 to 1213 K to investigate the effects of main working parameters on the performance of the NO reduction process. As a result, very high efficiencies of NO reduction have been obtained by using respectively methane (up to 90%) and ammonia (up to 75%) as reducing agent. By coupling these two processes in a Reburn/SNCR hybrid technique, higher efficiencies in NO reduction have been obtained by comparison with the classical SNCR technique. The Computational Fluid Dynamic (CFD) modeling has been also investigated to characterize the fluid dynamics in the reactor notably the gas homogeneity. Furthermore the modeling results obtained with the commercial CFD code FLUENT 6.3 showed a good agreement with measurements.

HOT GAS DESULFURIZATION BY MOLTEN ALKALI CARBONATES

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When the coals with high sulfur content are gasified in coal gasification technology, H_2S and COS are contained in the gasified gas. If the gasified gas is used as the fuel for fuel cells or synthesis gas for chemical materials, H_2S and COS in the gasified gas should be removed almost completely. The development of reliable methods to remove gaseous sulfur in the gasified gases at high temperatures, instead of a practical wet scrubbing technique, is one of the important technological advances. Therefore, this study proposes a novel technology on hot gas desulfurization by using molten alkali carbonates (MACs), consisting of $43Na_2CO_3$ and $57K_2CO_3$ as a solvent. As a result, H_2S and COS were completely removed by the molten alkali carbonates at high temperature. The sulfur balance analysis of used MACs proved that the MACs completely capture H_2S and COS.

YIELD OF TOXIC SPECIES IN CONE CALORIMETER TESTS DURING POLYETHER POLYURETHANE FOAM FIRE

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This paper present the calculation of yield of toxic species released by a Polyether Polyurethane Foam (PPUF) during test in cone calorimeter (CC). Around twenty chemical species are analyzed in real time with a Fourier Transform Infrared gas analyzer (FTIR) and Flame Ionization Detector (FID). In CC ventilation conditions, only five chemical species were found above their limit of quantification: CO_2, CO, H_2O, NO and Total hydrocarbons. Yields of gaseous compounds as well as the classic CC measurements Heat Release Rate (HRR) and Mass-Loss Rate (MLR) are performed at five irradiance levels 10, 20, 30, 40, 50 $kW \cdot m^{-2}$. The mechanism of thermal decomposition of PPUF is studied according to release of gaseous products in relation to time. PPUF thermally decomposed in two stages during heating up, first, PPUF molecules break down and isocyanate is oxidized, latterly, polyol is burned. This process is controlled by thermal balance in the decomposition front and is not modified by heat loses in the rear face of the sample. An analysis of elements is performed and the raw matter formula is determined.

DEVELOPMENT AND IMPLEMENTATION OF OXIDATION-DRIVEN SOOT AGGREGATE FRAGMENTATION MODELS INTO A LAMINAR COFLOW DIFFUSION FLAME

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The oxidation-driven soot aggregate fragmentation phenomenon has been reported from soot experimental studies in flames. However, it has not been considered in soot modeling studies in a laminar coflow diffusion flame which encompasses the soot oxidation region. Its effect on soot aggregate structure remains to be investigated. In this study, three different oxidation-driven soot aggregate fragmentation models with the 1:1, 2:1, and 10:1 fragmentation patterns are developed and implemented into a laminar coflow ethylene/air diffusion flame, together with a pyrene-based soot model and a sectional aerosol dynamics model. It is found that the average degree of particle aggregation (n_p) in the soot oxidation region is not correctly predicted if oxidation-driven aggregate fragmentation is neglected; whereas, the incorporation of aggregate fragmentation significantly improves the n_p prediction in the soot oxidation region. Similar results are obtained using the 1:1 fragmentation pattern and the 2:1 fragmentation pattern. However, as the pattern ratio increases to 10:1, appreciable difference in the predicted n_p is observed. In fact, as the ratio becomes larger, the fragmentation effect diminishes and the predicted n_p approaches that of the original model neglecting fragmentation. Also, as the pattern ratio increases, the fragmentation model becomes more difficult to implement as it involves breaking an aggregate and assign the fragments to more sections.

INFLUENCE OF BURNER DIAMETER AND FUEL TYPE ON EINO$_x$ OF DIFFUSION FLAME

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This paper presents emission index of nitrogen oxide (EINO$_x$) obtained from a small diameter burner fed with methane and syngas. The EINO$_x$ results when expressed as function of the jet Froude number exhibit two different trends that can be linked to the buoyancy controlled or the momentum controlled regime of the flame. To further examine this trend, experimental data reported in the literature are examined and plotted for different fuels and different burner diameters. It is observed that the EINO$_x$ is dependent on the burner size and fuel type. Furthermore, the behavior of the EINO$_x$ for small size burners differs markedly from the behavior of the bigger ones. From our experimental results, the leveling-off of the EINO$_x$ once a Froude number of 10^4 is reached might be explained by two experimental observations: 1) the CO emissions started raising which indicates incomplete oxidation of the fuel; 2) the flame height stops increasing once *Fr* reaches 10^4 which in addition to the increase of the presence of incomplete combustion by-products resulted in a constant emission of NO$_x$ until flame blow-off.

GAS PHASE MERCURY CONVERSION IN H_2, O_2, CHLORO AND BROMO C_1-HYDROCARBON AND NOX COMBUSTION EFFLUENT FROM USE OF AN ELEMENTARY KINETIC MECHANISM

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Emissions of gaseous mercury from combustion sources are one of the major environmental concerns facing power generators. The removal of mercury by conversion to mercury halides is evaluated by use of an elementary reaction mechanism that is developed from fundamental principles of thermodynamics and statistical mechanics. Thermochemical properties have been calculated for needed species using CBS-QB3 and density functional methods, and an elementary reaction mechanism have been constructed. Comparisons of mercury loss versus halogen, halocarbon, H_2, H_2O, O_2, CH_4, and NOx presence in a typical combustion effluent stream are performed. Results illustrate dramatic effects of H_2 on the formation of $HgCl_2$, HgClBr, $HgBr_2$, and the competing effects of NOx species with Hg for the halides.

THERMODYNAMIC MODELING OF A PISTONS ENGINE: CALCULATION OF THE NOX EMISSIONS

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The internal combustion engines, are under development remarkable these last decades, but they represent, currently, a very important source of polluting gas emissions. The nitrogen oxides (NOx) form part of these polluting emissions, and have a harmful effect on human health, as well as the environment.
Considering the complexity of the process of formation of the latter, many numerical simulations were developed, to work out a model of calculation close to the reality, which is so complex to describe by the theory. Within this framework, our work, allows the calculation of the nitrogen oxide rate (NO) in exhaust gases, starting from the developed equations of the chemical kinetics, while being based on the thermal mechanism of Zeldovich, which requires to know the concentrations of the various species chemical constituting exhaust fumes (CO_2, H_2O, CO, O_2, H_2, N_2, O, H, N, OH, NO) by supposing that system C-H-O is in chemical balance. To carry out this calculation, a simulation of the thermodynamic cycle was necessary, for the rate of NO is strongly dependent on the temperature.
A model of combustion at two zones (burned and unburned) was adopted and the application of the equations, mass, energy and state, to each zone, makes it possible to determine the variation in the instantaneous temperature and pressure in the cylinder. Simulation, is carried out for a spark-ignition-engine (gasoline), and the results obtained, were compared with other simulations as well as with results of measurement from the literature.

MASS SPECTROMETRIC ADVANCES IN THE ANALYSIS OF LARGE AROMATIC FRACTIONS OF HEAVY FUEL OILS AND CARBON PARTICULATES

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Advanced mass spectrometric apparatus have been tested for the analysis of heavy fractions of fuel oils and combustion-formed particulate in terms of mass range detection and resolution. The analysis of these complex aromatic samples is not amenable to conventional chromatographic/mass spectrometric techniques due to their low volatility and degradability. In this paper, the advantages and the shortcomings of different ionization methods (electron impact, photoionization, laser ionization) and different mass analyzers (quadrupole, ion trap, time of flight) have been carefully investigated. The optimization of operative parameters has shown to be crucial for the extension of mass detection range.
The Atmospheric Pressure Photoionization-Mass Spectrometry techniques showed the best performances in terms of low fragmentation of the parent ion and sensitivity for the analysis of asphaltenes. By contrast, Laser Desorption Ionisation-Mass Spectrometry showed to be the best technique for the analysis of aromatic tarry combustion-formed species.

SIZE DISTRIBUTION FUNCTIONS AND HYDROGEN CONTENT OF COMBUSTION-FORMED PARTICLES: A MODELLING APPROACH

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In order to go deep inside the nature and chemistry of combustion-produced particles a kinetic modeling approach is proposed. It is based on modeling of gas-to-particle transition through sections in which 125 lumped species are used having a C number ranging from 24 to $4x10^8$ and H/C ratio ranging from 0 to 1. This gives the possibility to numerically follow not only the mass evolution of particles but also their hydrogen content. The model is tested in a premixed flat flame of ethylene/oxygen with C/O=0.8. Comparison of modeled results with experimental data is satisfying both in terms of concentration of species and in terms of H/C ratio.

SIZE DISTRIBUTION FUNCTIONS OF ULTRAFINE ASHES FROM PULVERIZED COAL COMBUSTION

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Coal fired boilers are widely used for electric utilities and power plants because of the low cost and the abundance of this fuel. The major drawbacks of coal combustion are connected with the large emission of particulate matter. This paper deals with the experimental investigation of ultrafine (D<100nm) and nano (D<10nm) ashes formed during conventional high temperature pulverized coal combustion on a laboratory scale reactor. The reactor consists of an atmospheric pressure laminar premixed flame homogeneously doped with pulverized coal particles, monodisperse in size. It allows the investigation of the early stage of ashes formation. Generated aerosols, sampled using high dilution probes, are conveyed into high resolution Differential Mobility Analyzers (DMA) to perform on-line measurements of the size distribution function of ultrafine ashes. Two DMA systems are used: the first one is equipped with a Faraday cup electrometer detector and identifies particles as small as 1nm; the second one is equipped with a condensation nucleus counter and exhibits 3nm lower detection limit. Measurements have been performed at several dilution ratios to understand nature and behavior of detected particles. Results indicate that nanosized coal ashes are formed during pulverized coal combustion. They are the most abundant in number and also a not negligible fraction of ultrafine ashes mass implying they should be detected at the exhaust of pulverized coal furnaces.

SPECTRAL SIGNATURES OF CARBON PARTICULATE EVOLUTION IN METHANE FLAMES

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UV-visible spectra of the particulate matter caught on quartz plates were measured in sooting methane/oxygen premixed flames with the same C/O ratio (0.6) and different flame temperature. Optical parameters as the Energy Band Gap and the position of the maximum absorbance were used to characterize the carbon particulate matter and its evolution along the carbon formation region. The Energy Band Gap (E_g), using the Tauc optical band gap model, allowed the identification of classes of chromophores having different aromatic sizes. The E_g showed to be correlated with the measured values of the H/C ratio of the particulate matter sampled along the flame. Some changes of the maximum absorbance position at 210-240 nm were detected along the flame indicating changes in the carbon internal structure in terms of sp^3/sp^2 carbon hybridization. The internal structure in terms of both E_g and the maximum absorbance position also showed to be affected by the flame temperature.

FLAME RESTRUCTURING DUE TO FORMATION OF PREHEATED ZONE AS MECHANISM OF DEFLAGRATION-TO DETONATION TRANSITION IN GASEOUS COMBUSTIBLE MIXTURES

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The deflagration-to-detonation transition (DDT) in tubes with smooth and moderately rough walls is studied to gain better insight of how a reactivity gradient ripe for the onset of detonation originated and how it is involved in the DDT. We show that the DDT process consists of three separate stages stipulated by dynamics of the flame acceleration. During the first stage, the flame accelerates producing weak shock wave ahead. During the second stage, the flame slows down and creates conditions ripe for creation of the preheated zone ahead of the flame front. The third stage is restructuring of the steep temperature profile inherent to a deflagration, formation of a reactivity gradient and the actual onset of the detonation wave itself. Theoretical analysis, numerical simulations and experiments provide solid evidence that dynamics of the flame in tubes with no-slip walls results in the creation of background conditions for the preheated zone formation. We carried out well-resolved numerical computations to determine evolution of the flame structure caused by the presence of the preheated zone. The shallow temperature gradient formed due to the flame restructuring triggers detonation through the Zel'dovich-SWACER gradient mechanism. The extensive experimental studies of DDT in hydrogen-oxygen and ethylene-oxygen mixtures focused on the key characteristics of DDT with the purpose to validate the developed theoretical model show that the theory is well consistent with the experimental observations.

FIRE SCENARIO WHIRLING FLAMES – STABILITY ANALYSIS AND EXPERIMENTAL STUDIES

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This paper describes the formation, development and sustainment of fire scenario whirling flames phenomena. The focus is on stability – instability transition, and main results of a modelling study are reported to clarify such phenomenon. Critical dimensions that are dividing stability and instability zone are reported. The main results of a heptane pool fire experimental activity are then described to explain some conditions permitting the stable development of whirling flame.
Such results are mainly oriented to obtain indications about the conditions favoring the stable development of fire scenario whirling flames in order to permit actions for their prevention and mitigation.

A NEW CORRELATION FOR THE GAS TEMPERATURE INSIDE A BURNING ENCLOSURE

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A new correlation for predicting enclosure gas temperature is presented in this paper based on the energy balance for adiabatic conditions, an estimate of the heat flux imposed on the walls and the transient thermal response of the wall. This correlation has been verified being able to predict enclosure gas temperature in both well and under-ventilated fires by comparing with the existing experimental results. It is also compared with the well known and widely used MQH (McCaffrey, Quintiere & Harkleroad) correlation.

CFD MODELLING OF UNDER-VENTILATED FIRE IN A FULL-SCALE ENCLOSURE

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Ejected flame by incorporating transient fire growth and progressive vitiation of the ambient medium in full-scale enclosure is investigated. Large-Eddy-Simulation (LES) incorporates a two-step reaction scheme together with an eddy-dissipation concept to formulate interaction between combustion and turbulence. The numerical model solves three dimensional, time-dependent Navier-Stokes equations, coupled with sub-models for soot formation and thermal radiation transfer. The computed, time-averaged velocity/temperature profiles and CO production are compared with experimental data, and a relatively good agreement is attained. The critical value of the global equivalence ratio close to 2 is identified for the onset and development of a flashover or a backdraft fire inside a full-scale enclosure.

VLES OF LEAN HYDROGEN-AIR DEFLAGRATIONS IN A CLOSED VESSEL 5.7 M HIGH

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The very large eddy simulation (VLES) model previously applied for prediction of large scale unconfined stoichiometric hydrogen-air deflagrations, and 20-30% hydrogen-air deflagrations in a 78.5 m long tunnel, is developed further to reproduce dynamics of lean uniform and non-uniform (gradient) hydrogen-air premixed combustion in a 5.7 m height and 1.5 m diameter cylindrical vessel. Flame propagation is simulated by the progress variable equation with the gradient method as a source term. Chemical kinetics enters the governing equations only through its influence on the laminar burning velocity, which dependence on pressure, temperature, and concentration of hydrogen. Similar to previous studies the turbulent burning velocity comprises three mechanisms affecting the flame surface density at unresolved sub-grid-scale (SGS) level: flow turbulence, which is computed by Yakhot's formula for premixed turbulent combustion, derived from the renormalization group theory; evolution of a turbulence generated by a flame front itself with a maximum value calculated based on the Karlovitz's theory; and increase of a total flamelets area proportional to an integral flame scale (outer cut-off) and reciprocal to the flame front thickness (inner cut-off) according to the fractal theory. In this study of lean hydrogen-air premixed combustion an additional mechanism based on the leading point concept as formulated by Kuznetsov and Sabel'nikov and implemented by Zimont and Lipatnikov is introduced into the VLES model. The results of numerical simulations reproduced experimental data on flame propagation in uniform 12.8, 14, 16 and 20% by volume hydrogen-air mixtures in the large-scale vessel. The model is further applied to simulate non-uniform hydrogen-air deflagration: a mixture with concentration gradient (27% by volume of hydrogen at the top of the vessel and 2.5% at the bottom, average concentration 12.6%). Good agreement is achieved between simulations and experimental data for dynamics of both pressure and flame propagation.

FIRE INDUCED WALL VENT FLOWS

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A formula for fire induced flow rate through a wall vent of a room fire has been developed based upon a theoretical derivation and a mathematical fit to data. The formula accounts for any fire configuration burning on the floor of a room, and its development as indicated by the increase in room temperature. The formula is shown to be within 15% accuracy for a wide range of fire conditions. The formula only requires information about the average room smoke temperature and the vent geometry. A factor related to fuel entrainment characteristics allows more precision in representing the fuel configuration. The use of the formula is demonstrated to show the effect on flow rate of window geometry, sill height, entrainment, and smoke temperature.

EXTINGUISHING OF FIRES USING THE AEROSOL OF AQUEOUS SOLUTIONS OF SALTS

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Search for novel effective and ecologically friendly fire suppressants is the important task for fire fighting science. In this connection, the extinguishing of model fire source (*n*-heptane) by fine aerosol of flame suppressants with diameter of 1 μm was studied. The optimal effective concentrations (OEC) for flame inhibitors were determined. The aqueous solutions of organic and inorganic salts of alkali metals were studied as flame inhibitors. Basing on data obtained, the field experiments on extinguishing of two types of model fire sources using mobile aerosol generator with adjustable dispersity of particles and salts solution were carried out. In the first set of experiments it was shown that exposure of aerosol inhibitor cloud with particles size about 1 μm and with close to OEC mass concentration of the inhibitor on flame front of ground forest fire resulted in its extinguishing. By means of thermal imaging it was established that during the moment of extinguishing the temperature at the flame front lowered from 1000 to 500 °C. In the second set of experiments it was shown that exposure of aerosol cloud of flame inhibitor with average particle diameter of 15 μm on the model fire source of category "A" (burning wood) led to its extinguishment. Results of the experiments revealed an opportunity of suppression both flame and smoldering modes of combustion using aerosol technology. At this minimal mass flow rate of inhibitor solution it was found to be 16 times less than that of pure water.

URANS APPROACH FOR BUOYANCY DOMINATED TURBULENT DIFFUSION FLAMES

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This study deals with the modelling of a buoyancy-dominated turbulent diffusion flame, characteristic of pool-fire through an URANS approach with *Code_Saturne* EDF's CFD freeware. The aim is to test the degree of physics that could be captured by this mean resolution for fire simulation. The numerical models are validated through the experimental data from a turbulent diffusion flame stabilized on a porous burner. Despite underestimation of the vertical velocities and overestimation of both the temperature and air entrainment, the flame extent prediction is good and the part of unsteady behaviour due to shear-stress is correctly captured. Ongoing work on soot effect and finite one-step reaction should further improve the prediction of buoyancy controlled fire.

RADIANT HEAT FROM PROPANE JET FIRES

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Sonic propane jet fire experiments were carried out in absence of wind, with visible flame length ranging between 2.2 and 8.1 m. The thermal radiation intensity increased with the mass flow rate and the flame length. The net heat released was also computed and a correlation for the flame length as a function of Q is proposed. The surface emissive power and the fraction of heat irradiated were estimated by applying the solid flame model, assuming the flame to be a cylinder. The variation of the emissive power as a function of flame length was found to follow a linear equation. This equation was compared with those provided by other authors. The fraction of heat irradiated η was obtained from the value of the total radiative power. The average value of η for sonic propane flames was 0.07. Finally, the flame temperature was analysed.

FIRE TESTS AND NUMERICAL MODELLING OF FLAME AND PLUME TEMPERATURES

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The objective of the study was to analyse the behaviour of pool fire plumes, and more particularly the evolution of temperatures along the plume centreline, depending of the height above the fire source. In order to achieve a characterization of pool fires, several fire tests were conducted. Then, tests results (temperatures, mass loss rate, heat release rate, etc.) were compared to theoretical models (Zukoski, Heskestad, McCaffrey and Thomas) and Computational Fluid Dynamics (CFD) tools. Current CFD capabilities were illustrated using the Fire Dynamics Simulator (FDS, Version 5), developed by the National Institute of Standards and Technology, USA. Comparisons between theoretical results, computational fire models results and fire tests results allowed to verify the accuracy of theoretical and computational models and to analyze the influence of different parameters in the results.
Theoretical models essentially differed as we get closer to the burner but the characterization of the temperatures evolution in the fire plume had more sense in the region near the source. Zukoski and Heskestad models got the best fit both experimental data (thermocouples, infrared camera, load cells, etc.) and computational model results. McCaffrey overpredicted the temperature values.
FDS results were close to the tests, with and without roof. The exception was the last one because other fuel was used, with a different HRR curve.

DEFINING THE EFFECTS OF AMBIENT CONDITIONS IN LARGE-SCALE FIRE TESTS

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The paper documents the results of an analysis of the effects of ambient conditions, temperature and relative humidity, on the development of large-scale fires during their initial growth. While the study has focused on the behavior of hygroscopic cartoned commodities, because their burning behavior is greatly affected by propensity to absorb ambient moisture, non-hygroscopic materials and their reduced sensitivity to ambient humidity could also be considered. The analysis introduces the heat release rate at the time of first sprinkler activation as a meaningful measure to represent the impact of ambient conditions on the development of a free-burning fire. The next step of estimating the behavior under extinguishment conditions is not possible at this time, though general considerations on expected trends are offered on the basis of the results obtained from another research program. The practical output of the work is in the form of the identification of the desirable range of operating conditions for ambient temperature and relative humidity in large-scale fire testing.

UNDERVENTILATED ENCLOSED FIRES: A FULL SCALE TEST WITH WOOD PALLET FIRE

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Underventilated enclosed fires are recognised to be important scenarios, owing to their potential risks. They occur with ventilation, natural or mechanic, providing too small amount of oxygen or over production of combustible gazes in the fire zone. A full scale test has been performed using wood pallet fire. The test rig is built with marine containers. It allows fire growth in a room and smoke spread in other connected rooms. The experimental set up provides source mass loss rate, temperatures close to the fire and in the smoke flows. Fire growth and smoke spread will be detailed and analysed. It will be shown that, after a short ignition period, oxygen depletion is strong in the fire room and underventilated combustion occurs, and the temperatures begin to increase continuously everywhere in the rooms and in the smoke plume at the exit. Observed temperatures in the different rooms will be presented and analysed. CFD modelisation of the fire growth has been performed. Comparisons between calculated and observed temperature values highlight the difficulties to determine the correct Heat Realease Rate (HRR) inside the fire room. Discussions on HHR values are provided.

FLAMES SPREAD MODELLING OVER A POLYURETHANE MATTRESS

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In France, numerical models are used in the fire safety engineering for structural fire behaviour and smoke control studies. Simulations are performed in order to define buildings structures and smoke control strategy. When fire engineering studies are applied to sleeping rooms they have to consider furniture present within the room, which is often involved at the beginning of a fire; polyurethane foam mattresses for instance. A relevant model of fire spread on mattress, especially its temporal evolution, is important as it provides information about fire conditions and time available for evacuation. Thus, this work is intended to provide a fire spread assessment from FDS calculations. In the first step an enclosed mattress fire test has been carried out in a simple environment (a maritime container) to measure flame spread velocity on the mattress surface after the fire started from the upper part of the mattress. The observations are used for validation purposes of the pyrolysis model in FDS. First simulations revealed that fire spread velocity is highly influenced by ignition temperature defined in the pyrolysis model. Heat of combustion and ignition temperature have been measured previously with a cone calorimeter in order to be used as the input data. Then sensibility analysis has been performed and the ignition temperature has been changed so that FDS gives closest predictions of fire spread velocities as in fire experiments. In a second step a fire in more elaborated environments is studied (geometry and ventilation). In this case the polyurethane mattress is located in a corner of a room given access to corridors provided with smoke control. Experimental results are compared with results obtained with FDS, using pyrolysis parameter values as previously determined. The conclusion is that after few minutes following ignition, when the fire is well ventilated, the flame spread velocity is quite properly reproduced. However after the ventilation condition changes the combustion of mattress is poorly predicted by FDS.

INFLUENCE OF VENTILATION ON IGNITION RISK OF UNBURNT GASES IN THE EXTRACTION DUCT OF AN UNDERVENTILATED COMPARTMENT FIRE

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Ignition risk of unburnt gases in the extraction duct of an underventilated compartment fire is studied from 8-cubic-metre room-fire at the Laboratoire de Combustion et de Détonique (LCD), in France. A study of factors that have an influence on the ignition risk at the extraction is made. Two main factors appear: heat release rate and ventilation flow. These factors are studied by changing ventilation flow for different diameters of fire source. Fire tests are also made in order to understand the impact of closing the inlet vent on the production of unburnt gases. Criteria of heat release rate and ventilation flow are determined in order to predict conditions that lead to an ignition risk.

THE INFLUENCE OF OXYGEN CONCENTRATION ON THE COMBUSTION OF A FUEL/OXIDIZER MIXTURE

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The aim of the present study is to investigate the influence of the O_2 concentration on the combustion behaviour of a fuel/oxidizer mixture. The material tested is a ternary mixture of lactose, starch and potassium nitrate, which has already been used in an attempt of estimating the heat release rate using the FM-Global Fire Propagation Apparatus. It provides a well-controlled combustion section to study the evolution of the combustion products when varying the O_2 concentration, from air to low oxidizer conditions. Different chemical behaviours have been exhibited. When the O_2 concentration was reduced beyond 18%, large variations were observed regarding CO_2 and CO concentrations. This critical O_2 concentration seems to set the distinction where the material only uses its own oxidizer to react. On the other hand, mass loss did not highlight the change in chemical reactions and remained similar whatever the test conditions. This presumes that the oxidation of CO into CO_2 are due to reactions occurring in the gas phase especially for large O_2 concentrations. This actual behaviour can be verified using a simplified model of flammability limit adapted for the current work. Finally, a sensitivity analysis has been carried out to underline the influence of CO concentration in the evaluation of heat release rate using typical calorimetric methods. The results of this study provide critical basis for the investigation of the combustion of a fuel/oxidizer mixture and for the validation of future numerical models.

A THEORY FOR ESTIMATING MAXIMUM HEAT RELEASE RATE FOR VENTILATION-CONTROLLED ROOM FIRES

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The execution of fire computer codes requires data making it possible to lead to thermodynamic aggressions of the equipment and structures of the building. It should be noted that the Heat Release Rate (*HRR*), depending particularly on the nature of fuel and ventilation, is the most important and difficult data to obtain.
The standard ISO 178173 recommends the use of the maximum *HRR* to determine the thermodynamic aggressions reasonably conservative. However, the standard does not give any indication making it possible to define it precisely. Moreover, if the curve ISO 834 can be used to represent the temperature of hot gases generated by fire in certain rooms of buildings, it is not directly adapted to the rooms ventilated naturally at two levels: lower and upper natural ventilation.
The phenomenon of combustion of solid combustibles inside a closed room is not easy to predict, more especially as it is rarely reproducible in fire experiments. Therefore, this paper suggests a simple theoretical formula, corresponding to the natural ventilation controlled fire, to predict the maximum *HRR* in the case of fire inside a closed room. The formula can also be used to represent the electric/electronic cabinet fire with lower and upper natural ventilation installed in a room.
The suggested formula is intended to be used in the field of engineering. It can also be used to assess fire safety in nuclear facilities, especially the fire Probabilistic Risk Assessment.
Its implementation is very easy and requires a minimum of data which are the fire growth coefficient, the surfaces of lower and upper ventilation and the distance in heights between the centres of the two vents.

FIRE PROPAGATION IN BUILDINGS. A MODEL OF THERMAL CELLS

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The thermal model for simulation of fire propagation in buildings and constructions is considered. The model allows simulating a fire progress and assessing a fire risk in the buildings.

THE INFLUENCE OF THERMAL INSTABILITIES ON THE INITIAL CONDITIONS OF THE BACKDRAFT PHENOMENON

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The objective of this study is to describe experimentally the mechanisms of thermal instabilities likely to cause the formation and the propagation of a gravity wave in a hot enclosure. In fire conditions, this phenomenon appears when dense fresh air enters an enclosure rich in hot combustible products. At the interface between the hot and cold flows, a potentially ignitable premixed zone is created. If ignition occurs, a devastative flame propagates in and outside the enclosure. This phenomenon is called a *Backdraft*.
In order to gain a better understanding of the formation conditions of this gravity wave and the resulting mixing according to chosen test parameters, a specific device and an experimental procedure were developed. In this work, the phases of ignition and flame propagation in and out of the enclosure are not apprehended.
The objective of this work is thus to initially observe and then to quantify the development and the progression of this wave, to evaluate the mass transfers involved and to understand the mechanisms of mixture between inflow and outflow. The information collected will allow predicting the zones where the flow is likely to present equivalence ratios (combustible /oxidant ratio) able to initiate a combustion that will first propagate in, then out of the compartment. Finally, the characteristic time separating the air intake and the formation of the combustible mixture is evaluated.
Fast laser tomography is used for the observation of the different phenomena involved, and PIV (Particle Image Velocimetry) is used to measure the inflow and outflow rates. Finally, the displacement of the wave is recorded by RT-PIV (Time resolved PIV). The time order of magnitude of the displacement (length: 0.8 meters) is 4 seconds. The system used allows the treatment of a 15x15 cm^2 area, which is smaller than the total zone of interest, therefore a displacement system of the PIV camera was conceived in order to follow the wave during its propagation in the enclosure. This technique allowed not only a good temporal resolution of the formation and the propagation of the gravity wave (periodicity of passage of the vortices), but also a precise determination of its characteristics (size, shape, …), which cannot be determined using a traditional PIV, which usually has a 4 Hz maximum acquisition frequency.
The results show a strongly unsteady flow, with formation in a pulsative mode of large scale Kelvin-Helmholtz structures. Understanding these mechanisms is essential for the determination of the parameters and assumptions to be set-up in a numerical code that is being developed in the mean time. The obtained experimental results are essential for the calibration and validation of the sub-grid turbulence model used by the numerical model.

A NOVEL METHODOLOGY FOR DETERMINING DESIGN FIRES FOR STRUCTURAL FIRE ANALYSIS

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A novel methodology has been developed to determine design fires for structural fire analysis of modern buildings that are outside the range of applicability of traditional methods. It has been applied to determine a family of fires for a floor in the Mumbai C70 building. The family of fires was generated by considering different burning areas that travelled on the floor plate. The methodology calculated both the near and far field temperatures to characterise the thermal environment for structural analysis. Future work will develop the tool used to determine the temperature fields, examine the effect of the path of fire travel, as well as determine the impact of this family of fires on the structure.

OXIDATION OF ETHYLENE AND PROPENE IN PRESENCE OF CO_2 AND H_2O: EXPERIMENTAL AND DETAILED KINETIC MODELING STUDY

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Ethylene and propene are major products of the thermal cracking of heavy oil. Under flameless combustion, these hydrocarbons are oxidized in presence of large amounts of carbon dioxide and water vapor which may affect their kinetics of oxidation. In this study, we present new experimental results for the kinetic of oxidation of ethylene and propene in presence of carbon dioxide and water in a fused silica jet-stirred reactor (JSR). The reactor was operated at atmospheric pressure, over the temperature range 950-1450 K, from fuel-lean to fuel-rich conditions. Sonic probe sampling followed by on-line FTIR analyses and off-line GC-TCD/FID analyses allowed the measurement of concentration profiles for the reactants, stable intermediaries, and final products. A chemical kinetic reaction mechanism recently proposed for modeling the oxidation of hydrogen, carbon monoxide, methane, methanol, formaldehyde, and natural gas over a wide range of conditions including JSR, flame, shock tube, and plug flow reactor was used to model the experiments. An overall reasonable agreement between the present data and the modeling was observed. Reaction paths analyses were used to delineate the important reactions influencing the kinetic of oxidation of the fuel mixtures studied here. The presence of water tends to inhibit the combustion of the fuels whereas carbon dioxide has a small accelerating effect upon the oxidation of ethylene in fuel-rich conditions.

LEAN AND RICH PREMIXED DIMETHOXYMETHANE/OXYGEN/ARGON FLAMES: EXPERIMENTAL AND MODELING

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Experimental structures of two methylal/oxygen/argon flames at equivalence ratios of ϕ = 0.24 and 1.72 have been determined by using the molecular beam sampling coupled with mass spectrometry (M.B.M.S). Mole fraction profiles of stable and unstable species have been gathered from an appropriate calibration of the measured corresponding signal intensities profiles. The detected species throughout the flame thickness were: H_2, CH_3, CH_4, H_2O, C_2H_2, CO, CH_2O, CH_3O, O_2, Ar, CO_2, $C_2H_4O_2$ and $C_3H_8O_2$.
The aim of this work is to extend an original model for ethylene combustion by building a sub-mechanism taking into account the formation and the consumption of oxygenated species involved in dimethoxymethane oxidation. By using kinetic data from the literature, we were able to elaborate a new mechanism containing 480 elementary reactions involving 90 chemical species in order to simulate these neat methylal flames.
The new mechanism provides numerical results which are in good agreement with experimental data for all species detected in both flames. Whatever the equivalence ratio of the flame, the two main degradation pathways of methylal ($CH_3OCH_2OCH_3$) are the same:
1) $CH_3OCH_2OCH_3 \rightarrow CH_3OCH_2OCH_2 \rightarrow CH_3OCH_2 \rightarrow CH_2O$
2) $CH_3OCH_2OCH_3 \rightarrow CH_3OCHOCH_3 \rightarrow CH_3OCHO \rightarrow CH_3OCO \rightarrow CH_3O \rightarrow CH_2O$
with the first one being the fastest.

PHOTOLYTICALLY AND THERMALLY INITIATED REACTIONS OF NH_3 WITH NO_X (X=1,2)

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The kinetics and mechanisms of the $NH_3 + NO_x$ (x =1, 2) reactions have been systematically studied by pulsed laser photolysis/mass spectrometry (PLP/MS) and pyrolysis/FTIR spectrometry (P/FTIRS). In the PLP/MS experiment, the total rate constants and product branching ratios of the $NH_2 + NO_x$ (x =1, 2) reactions have been tested by measuring the time-resolved concentrations of H_2O, N_2O and NO_2 in the laser-initiated reaction of NH_3 with NO in the presence of varying amounts of NO_2 in the temperature range of 300 - 725 K. The measured concentrations can be quantitatively accounted for by our comprehensive mechanism for the H/N/O-system recently established for the ammonium dinitramide decomposition reactions, confirming our reported product branching ratio for $NH_2 + NO_2 \rightarrow N_2O + H_2O$ (0.19 ± 0.02) over the temperature range investigated. In the thermally initiated reaction of NH_3 with NO_x investigated by the P/FTIRS technique in the temperature range 575 - 710 K, the measured kinetic data for the disappearance of the reactants and the formation of products have been modeled with the same mechanism applied to the PLP/MS study. Agreement between the kinetically modeled concentrations and the experimentally measured values is quite satisfactory for both the reactants (NH_3 and NO_x) and the products (NO and N_2O). Sensitivity analyses show that the reaction of NO_x with NH_3 is most sensitive to the $NH_2 + NO_x$ reactions, with a slightly lower sensitivity to subsequent reactions involving HONO. Our comprehensive mechanism also accounts reasonably for the concentration profiles of NH_3, NO_2 and N_2O reported by Glarborg and coworkers (ref. 57) in their study of the isothermal reaction of NH_3 with NO_2.

SUPEREQUILIBRIUM INCREASE OF A CHEMICAL REACTION RATE IN THE FRONT AND OTHER EFFECTS OF DETONATION WHICH WAS SIMULATED IN THE TUBE BY INSTANTANEOUS HEATING OF ONE ITS FLAT END

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The Monte Carlo non-stationary method of statistical simulation (MCNMSS) (another name DSMC) was used in calculations. Non-stationary case of forming a detonation wave in the tube by instantaneous heating of one its flat end was considered. It was supposed that chemical reaction $A+M \rightarrow B+M$ ($M=A$ and B) took place. The molecular masses of gases A and B were equal to each other. Different thresholds of the reaction were considered. For the case of low reaction thresholds, velocity of detonation wave was higher then Chapman-Jouguet velocity. A region with unchangeable values of parameters in the flow inside product beside front took place. Increase of the reaction threshold led to disappearance of the quasi-stationary region and a rise of something like to an expansion wave with peaks of parameters of flow at the leading part of the detonation wave. The meanings of these parameters remain constant with time. Velocity of detonation wave became appreciably lower then Chapman-Jouguet velocity. Farther increase of the reaction threshold led to disappearance of detonation and rise of combustion. The reaction $A+B \rightarrow B+B$ was very important for initiation of detonation.

EFFECTS OF HYDROGEN ADDITION AND NITROGEN DILUTION ON THE LAMINAR FLAME CHARACTERISTICS OF PREMIXED METHANE-AIR FLAMES

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The effect of hydrogen addition and nitrogen dilution on the laminar flame characteristics was investigated. The spherical expanding flames technique, in a constant volume bomb, was used to extract laminar flame characteristics. The mole fraction of hydrogen in the methane-hydrogen mixture was varied from 0 to 1 and the mole fraction of nitrogen in the total mixture (methane-hydrogen-air-diluent) from 0 to 0.35. Measurements were performed at an initial pressure of 0.1 MPa and an initial temperature of 300 K. Investigated mixtures were with stoichiometric conditions. A new correlation for calculating the laminar flame speed of methane-hydrogen-air-nitrogen mixtures is proposed. The laminar flame speed was found to increase linearly with hydrogen mass fraction for all dilution ratios while the burned gas Markstein length decreases with the increase of hydrogen amount in the mixture except for high hydrogen mole fractions (>0.6). The nitrogen dilution has a nonlinear reducing effect on the laminar burning speed and an increasing effect on the burned gas Markstein length. Experimental results and the proposed correlation were found in good agreement with data found in literature.

EXPERIMENTAL AND KINETIC MODELING STUDY OF RICH BENZENE AND TOLUENE LOW PRESSURE FLAMES

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Structures of laminar, premixed and one-dimensional benzene-oxygen-argon (11.6 mol % C_6H_6, 43.6 mol % O_2 and 44.8 mol % Ar) and toluene-oxygen-argon (9.9 mol % C_7H_8, 44.5 mol % O_2 and 45.6 mol % Ar) flames, both with equivalence ratio of 2 and burning at 36 Torr were analyzed by Gas Chromatography. Mole fraction profiles of 23 chemical species including permanent gases of combustion and first Polycyclic Aromatic Hydrocarbons as naphthalene, methylnaphthalene isomers and biphenyl have been measured. A kinetic model based on recent literature has been constructed to predict measurements performed in benzene and toluene flames. An experimental flame structures comparison and an extensive analysis of kinetic modeling results have allowed us to highlight main chemical pathways involved in benzene and toluene consumption and first PAH formation.

EXPERIMENTAL INVESTIGATION AND NUMERICAL SIMULATION OF THE STRUCTURE OF CH3CHO/O2/AR FLAMES AT DIFFERENT EQUIVALENCE RATIOS

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The main objectives of this research consist in achieving both experimental and numerical studies of the combustion of several flames using acetaldehyde as a fuel. Experimental mole fraction profiles of chemical species (stable, radical and intermediates) have been measured in three $CH_3CHO/O_2/Ar$ flat premixed flames stabilized at low pressure (50 mbar) and with equivalence ratios equal to 0.75, 1 and 1.25, respectively. The experimental setup used to determine the structure of one-dimensional laminar premixed flames consists of a molecular beam mass spectrometer system (MBMS) combined with electron impact ionization (EI). The reaction mechanisms proposed by Yasunaga et al. and by Marinov are tested by comparison of model predictions with experimental results. The results show that modelling predicts reasonably well reactants and products mole fraction profiles but significant differences for many intermediate species remain. In order to improve the predictions for these intermediate species, several improvements on the Marinov's mechanism are suggested. They ensure a reasonably good modelling of the acetaldehyde flame structures.

STRUCTURES OF COUNTERFLOWING LAMINAR METHANE/NITROGEN/OXYGEN, METHANE/OXYGEN AND METHANE/LIQUID OXYGEN COUNTERFLOW FLAMES FOR CRYOGENIC CONDITIONS AND ELEVATED PRESSURES

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The understanding of physical and chemical processes occurring in many applications in sciences and engineering is important to ensure stability and efficiency of their performance. Examples are the combustion process in direct-injection engines, gas turbine combustors, and liquid rocket propulsion systems. The objective of this paper is the numerical investigation of laminar methane/air and methane/oxygen flames where different mixtures of nitrogen and oxygen in the oxidizer stream are studied. Moreover, liquid oxygen (LOX) spray flames with carrier gas methane against a methane stream are investigated in the counterflow configuration. These structures may be used in (spray) flamelet library or flamelet generated manifolds computations of turbulent combustion. The mathematical model is based on two-dimensional equations which are transformed into one-dimensional equations using a similarity transformation. The numerical simulation concerns the axisymmetric configuration with an adaptive numerical grid for the gas phase. Detailed models of all relevant processes are employed; in particular, a detailed chemical reaction mechanism is used which comprises 35 species involving 294 elementary reactions. The thermodynamic data for CH_4 and O_2 below 300K are implemented for normal and elevated pressures. For the CH_4/air and an oxygenated flame, the present results are compared with results from literature. The CH_4/O_2 flame is studied for elevated pressures up to 2MPa. Both extinction strain rates and the scalar dissipation rate at stoichiometric conditions is evaluated for use in turbulent flamelet computations. It is shown that oxygen dilution, pressure, and strain rate have a pronounced effect on flame structures. The use of liquid compared to gaseous oxygen has a pronounced effect on flame structure.

STUDY OF HYDROGEN NON-PREMIXED AUTO-IGNITION IN MIXTURE FRACTION SPACE USING DETAILED MECHANISMS

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This work concerns numerical simulations of auto-ignition of hydrogen, diluted with nitrogen, in a co-flow of heated air, with conditions as in the experiment of Markides and Mastorakos. Numerical simulations are performed with the Conditional Moment Closure model. Combustion is at atmospheric pressure. In studies of auto-ignition phenomena, the use of detailed chemical mechanisms is important. We focus on the low temperature non-premixed auto-ignition behaviour of five different chemical mechanisms: Yetter et al., Mueller et al., Li et al., O'Conaire et al. and Konnov. The temperature of the air stream (945K-1100K) is higher than the temperature of the fuel stream (650-930K). The effect of the coflow temperature, the fuel temperature, the conditional scalar dissipation rate and the resolution in mixture fraction space is investigated. With respect to the conditional scalar dissipation rate, we discuss the Amplitude Mapping Closure (AMC) model. We compare to results when a constant scalar dissipation rate is applied over the entire mixture fraction range.

A SIMPLE METHOD FOR INITIAL CONDENSED PHASE COMBUSTION REACTIONS PREDICTIONS

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Combustion modeling of energetic materials has undergone a tremendous amount of development in recent years. Gas phase combustion properties predictions are possible and have been shown to agree with experimental results. For solid energetic materials, the gasification reaction products must be determined if gas phase models are to be applied. The majority of actual models still involve a guessing step for gasification products due to the lack of knowledge in the condensed phase. Quantum dynamical calculations are presently the only way to predict initial condensed phase reactions but require tremendous computing power, thus limiting their application. In this work, an empirical method that uses spectroscopic measurements of energetic molecules as the source for the complete modal molecular picture is presented. The method enables a qualitative prediction of the first combustion reaction in the condensed phase. The application of the methods with nitrocellulose and nitroguanidine shows that it predicts initial reactions matching the current ideas used in modeling.

H ATOM ATTACK ON PROPENE: COMPARISON WITH PROPYNE

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The reaction of propene ($CH_3CH=CH_2$) with hydrogen atoms has been investigated in a heated single-pulsed shock tube at temperature of 919-1078K and pressures of 2-3 bar. Stable products from various reaction channels (H atom addition and by inference H abstraction) have been identified and quantified by gas chromatography and mass spectrometry. The reaction for the H addition channel involving methyl displacement from propene has been determined relative to the methyl displacement from 1,3,5-trimethylbenzene (1,3,5-TMB), with k (1,3,5-TMB + H → m-Xylene + CH_3) = 6.7×10^{13} exp(-3255/T) cm^3/mol s,
k (Propene + H → $H_2C=CH_2$ + CH_3) = 3.0×10^{13} exp(-1709/T) cm^3/mole sec; (925-1078K)
The rate constant for the abstraction of the allylic hydrogen atom is determined to be,
k (Propene + H → $CH_2CH=CH_2$ + H_2) = 4.2×10^{13} exp(-2940/T) cm^3/mol s, (1037-1149K)
The reaction of Propene + H has also been studied relative to the reaction of Propyne + H,

$$\log\frac{k(propyne + H \rightarrow acetylene + CH_3)}{k(propene + H \rightarrow ethylene + CH_3)} = (441.23 \pm 36)\frac{1}{T} + (0.5266 \pm 0.036); (919 - 1058K)$$

The results showed that the rate constant for the methyl displacement reaction with propyne is a factor of 1.2 ± 0.1 larger than that for propene.
The present is compared with relevant previous results on aromatics and olefins.

VIBRATIONAL NONEQUILIBRIUM OF HO_2 RADICAL IN HYDROGEN-OXYGEN REACTION

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Suggested is a theoretical model of chemical and vibrational kinetics of hydrogen oxidation based on consistent account for the vibrational nonequilibrium of HO_2 radical. The chain branching $H+O_2 \rightarrow O+OH$ and inhibiting $H+O_2+M \leftrightarrow HO_2+M$ is interpreted as a general multichannel process which involves forming the vibrationally excited HO_2 intermediate, its evolution and decay. According to this model, the chemical and vibrational kinetics in a reacting complex gas mixture is described by equations for the concentrations of the individual components and the average energies of the vibrational modes. The results of calculations for conditions of shock tube experiments at $1000 < T < 1200$ K, $0.9 < p < 2.0$ atm are presented and compared with experimental data for strongly diluted H_2-O_2 mixtures. It is shown that the H_2+O_2 reaction proceeds in the absence of vibrational equilibrium; for considered conditions, the nature of this reaction is especially nonequilibrium, and the vibrational nonequilibrium of HO_2 radical is the essence of the process; the apparent rate constant of the $H+O_2 \rightarrow O+OH$ overall reaction depends on experimental conditions. The suggested approach seems rather promising for elucidating a physically adequate mechanism for high-temperature oxidation of hydrogen. It is such a mechanism that has to solve the problem of theoretical model agreement with the available experimental data obtained by different authors in different conditions and for various compositions.

THE OXIDATION REACTION OF $C_6H_5C\bullet(=O)$ RADICAL

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Alkyl substituted aromatics are a major component of both gasoline jet and other engine fuels. The major reaction pathways to oxidation of this class of molecules, is through loss of a benzyl hydrogen atom on the alkyl group via abstraction reactions in the radical pool. One of the major intermediates in the combustion and atmospheric oxidation of the benzyl radicals is benzaldehyde, which rapidly loses the weakly bound aldehydic hydrogen to form benzoyl radical ($C_6H_5C\bullet=O$). A detailed study of the thermochemistry of intermediates and the oxidation reaction paths of the benzoyl radical is initiated in this study. Structures and enthalpies of formation for important stable species and intermediate radicals resulting from the benzoyl radical + O_2 association reaction are reported with reaction paths and transition state barriers. The enthalpies, $\Delta_f H^0_{298}$, are calculated using ab initio (G3MP2B3), Density Functional (at B3LYP/6-311g(d,p) calculations, and literature data. Bond energies on the benzoyl and benzoyl-peroxy systems are also reported. The reaction of benzoyl with $^3O_2$ is shown to result in a number of reaction channels that are not currently included in combustion or atmospheric chemistry models. The reaction paths include several important, highly exothermic, chain branching reactions and a number of unsaturated oxygenated hydrocarbon intermediates along with formation of CO_2. The initial reaction of the $C_6H_5C\bullet=O$ radical is shown to have a well depth of 38 kcal mol^{-1} with three channels that have barriers below the entrance channel.

A SHOCK TUBE AND CHEMICAL KINETICS MODELING STUDY OF METHYL ETHYL KETONE (MEK) OXIDATION

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Shock tube ignition delay times for MEK (or 2-butanone) have been measured at a reflected shock pressure of 1 atm (± 2%), in the temperature range 1250-1850 K, at equivalence ratios of 0.5-2.0 for dilute mixtures in argon with fuel concentrations of 1.0, 1.5 and 2.0%. Rate constants for unimolecular fuel decomposition reactions have been treated for fall-off in pressure and temperature, with nine-parameter fits in the Troe formulism. A detailed chemical kinetic sub-mechanism has been developed and coupled to an existing C_4 mechanism comprising 234 species and 1369 reversible reactions. Model simulations show generally good agreement when compared to the available experimental data. MEK may be used as a fuel tracer, and thus further ignition delay time measurements have been carried out by adding MEK to n-heptane in order to test the effect on ignition delay timing of blending these fuels together. It was found that auto-ignition characteristics of n-heptane remained unaffected by the presence of MEK fuel tracer.

KINETIC MODELING OF THE OXIDATION OF ETHANOL AND GASOLINE SURROGATE MIXTURES

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The kinetic characterization of the oxidation of ethanol/gasoline mixtures is of interest due mainly to its role in sustainable combustion processes. The aim of this paper is to revise and validate a kinetic mechanism of ethanol combustion inside a general scheme able to describe the pyrolysis and oxidation of hydrocarbons. Model predictions and experimental measurements are discussed and successfully compared across a wide range of operating conditions.

This study moves from the detailed analysis of species profiles of pure ethanol oxidation in jet-stirred, flow reactors and laminar flames to global combustion properties (ignition delay times and laminar flame speeds) by referring to a large set of literature data; the analysis is then extended to the effect of ethanol on the combustion of ethanol/gasoline mixtures. The large experimental dataset discussed in this paper includes very recent measurements and covers a wide range of operating conditions in terms of pressure, equivalence ratio and fuel mixture composition. The chemical effect of ethanol on the combustion properties of ethanol/gasoline mixtures is also highlighted.

A COMPREHENSIVE KINETIC MODELING OF IGNITION OF SYNGAS/AIR MIXTURES AT LOW TEMPERATURES AND HIGH PRESSURES

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Syngas has reached increasing attention due to the possibility to be produced by coal and biomass. In order to develop more efficient process suitable for different combustion conditions a study of the kinetics of ignition delay has been carried out. Several models present in the literature have been compared with experimental data. Different conditions have been investigated, varying parameters such as temperature, pressure and composition. Due to mismatching of model results in comparison with experimental data, a sensitivity analysis has been conducted. $H_2O_2+M=OH+OH+M$ and $H+H_2O_2=HO_2+H_2$ have been found to be determinant in the prediction of ignition time. Enhancements have been carried out by splitting the reactions in forward and backward reactions, and adjusting values of rate constants in the range of confidence of their evaluation. The new model is able to correctly predict the behavior of syngas in all condition examined, in particular in gas turbine-like conditions. Moreover the influence of pressure and of CO concentration has been investigated with the new enhanced model.

PIV, 2D-LIF AND 1D-RAMAN MEASUREMENTS OF FLOW FIELD, COMPOSITION AND TEMPERATURE IN PREMIXED GAS TURBINE FLAMES

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Several laser diagnostic measurement techniques have been applied to study the lean premixed natural gas/air flames of an industrial swirl burner. This was made possible by equipping the burner with an optical combustion chamber that was installed in the high pressure test rig facility at the DLR Institute of Combustion Technology in Stuttgart. The burner was operated with preheated air at various operating conditions with pressures up to $p = 6$ bar and a maximum thermal power of $P \approx 1$ MW.
The instantaneous planar flow field inside the combustor was studied with particle image velocimetry (PIV). Planar laser induced fluorescence (PLIF) of OH radicals on a single-shot basis was used to determine the shape and the location of the flame front as well as the spatial distribution of reaction products. 1D laser Raman spectroscopy was successfully applied for the measurement of the temperature and the concentration of major species under realistic gas turbine conditions.
Results of the flow field analysis show the shape and the size of the main flow regimes: the inflow region, the inner and the outer recirculation zone. The highly turbulent flow field of the inner shear layer is found to be dominated by small and medium sized vortices. High RMS fluctuations of the flow velocity in the exhaust gas indicate the existence of a rotating exhaust gas swirl. From the PLIF images it is seen that the primary reactions happened in the shear layers between inflow and the recirculation zones and that the appearance of the reaction zones changed with flame parameters. The results of the multiscalar Raman measurements show a strong variation of the local mixture fraction allowing conclusions to be drawn about the premix quality. Furthermore, mixing effects of unburnt fuel and air with fully reacted combustion products are studied giving insights into the processes of the turbulence-chemistry interaction.

A JOINT PDF APPROACH TO MODEL TURBULENCE MODIFICATION IN TURBULENT SPRAYS

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Turbulent sprays find their application in many combustion devices ranging from internal combustion engines to gas turbines. It is known that dispersed phase (e.g. droplets) volume fractions as low as 2.5 □ 10^{-6} modify the carrier fluid (e.g. gas) turbulence, which in turn affects the mass and momentum transfer rates. In order to accurately predict the evolution of both continuous and dispersed phases, a probability density function (PDF) approach accounting for continuous phase turbulence modification due to the dispersed phase turbulence is employed. In the present study, a stochastic model based on dispersed and continuous phase turbulence length scales has been proposed. For validation, quantitative comparisons with experimental data have been performed. The results are in good agreement with the experiments for varying dispersed phase volume fractions. Numerical experiments have been performed to study the impact of the model and other factors on the decay of continuous phase Reynolds stresses.

INFLUENCE OF ACOUSTIC EXCITATION UPON THE ENTRAINMENT PHENOMENON IN COMBUSTION APPLICATIONS

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This paper presents the results of an experimental investigation performed about the entrainment phenomenon induced by an axisymmetric jet, which can be used for premixed combustion appliances or in the field of free diffusion flames. Particularly, the main goal of the research activity was a systematic analysis of the influence of an acoustic excitation upon the jet development and entrainment of the surrounding stagnant air. The analised jet presents a quite low Reynolds number ($Re_D \cong 3600$), constituting a test case non yet thoroughly studied in literature, but peculiar of some technical appliances, for instance in the field of premixed gas burners. At first, the flow field generated by the stationary free jet has been characterised both through laser Doppler velocimetry, to estimate the global and local entrainment coefficient, and hot wire anemometry, to attain the natural frequency (Strouhal number) of the jet. Subsequently, the jet has been acoustically excited through an active loudspeaker placed in a stagnation chamber upstream the jet outflow, operating at a frequency corresponding to the natural one of the stationary jet (210 Hz). The flow field induced by the excited jet has been analised through laser Doppler velocimetry, comparing the jet development (mean axial velocity and turbulence intensity profile) and the entrainment phenomenon with respect to the stationary (i.e.: not-excited) jet. The results put into evidence that the excited jet presents, especially in the initial region, higher turbulence levels and a larger radial expansion, contributing to a noticeable reduction of the potential core length (backwarding of the jet virtual origin). Moreover, this induces an increase of the entrainment phenomenon with respect to the stationary jet (up to 25% of the entrained flow rate from the surrounding stagnant air).

DEVELOPMENT OF AN HYBRID CATALYTIC GAS BURNER FOR CONDENSING BOILERS

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A novel hybrid catalytic radiant gas burner suitable for EU condensing boilers (4-25 kW) based on the concept of rich-catalytic homogeneous combustion with interstage heat removal was developed. Operation of the hybrid burner was completely characterised with special focus on the catalytic stage which also acts as radiant element. Methane combustion tests were conducted in direct comparison with two low-NO_x forced air commercial systems: a fully premixed gas burner stabilized with a knitted metal wire cover, and a blue-flame turbulent diffusive burner with multiple swirled fuel nozzles and high speed air injection. The novel burner shows improved performance with regards to efficiency, emissions, stability, and safety of operation.

NUMERICAL SIMULATION OF THE COMBUSTION IN POROUS MEDIA: RELATIVE IMPORTANCE OF THE DIFFERENT TRANSPORT MECHANISMS FOR THE FLAME STABILIZATION

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The present work aims to investigate relative importance of the different transport mechanisms for the flame stabilization using one-dimensional model of the combustion in porous inert media (PIM). With this purpose three models including different transport mechanisms have been investigated and their ability to predict burning velocity in a porous burner containing a SiSiC reticulated structure was validated by corresponding experimental investigations. The already developed models of the combustion in sponge-like structures predict successfully the temperature maxima and the NOx formation in a porous burner. However the experimentally validated numerical predictions regarding the large enhancement of the burning velocity detected experimentally are scarce. The inaccuracy of the numerical models in predicting the burning velocities in a porous burner could be caused by neglecting of the influence of the hydrodynamic dispersion on the species and temperatures profiles in the flame front. The results of the present study reveal that burning velocities as high as experimentally detected in PIM can be predicted using one-dimensional numerical simulation only by taking into account all of the considered transport phenomena: solid conduction, solid-to-solid radiation and flow dispersion.

RICH N-HEPTANE AND DIESEL COMBUSTION IN POROUS MEDIA

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Rich n-heptane and diesel flames in two-layer porous media are experimentally investigated in the context of syngas production. The stable operating points of n-heptane reforming have been determined and the H_2, CO, CO_2 and light hydrocarbon content in the exhaust gas were analysed at an equivalence ratio of 2 for different thermal input values. The reformer performance has been assessed also from the point of view of the heat losses and the mixture homogeneity. The range of flow rates for stable flames decreased with increasing equivalence ratio. Overall, the pre-vapourizer produces a uniform vapour-air mixture upstream of the flame front. Heat losses were about 10% of the thermal input at high firing rates. 77.2% of the H_2 at equilibrium was achieved at a flame speed of 0.82 m/s and at the equivalence ratio of 2. The same reactor with a different porous matrix for the reforming process demonstrates diesel reforming in syngas with a conversion efficiency of 77.3% for a flame speed of 0.65 m/s at ϕ=2. Higher equivalence ratios give higher H_2 and CO concentrations together with a lower dilution in N_2 and CO_2, but richer flames also display a larger presence of light hydrocarbons, a lower conversion efficiency and particulate emission.

LARGE EDDY SIMULATION BASED MIXING PROCESS ANALYSIS IN MICRO-COMBUSTOR FUELLED WITH LIQUID: PRELIMINARY RESULTS

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Future small-scale devices such as laptop computers, mobile phones, etc. shall be supplied by miniature energy sources. The best adapted seem to be mini gasturbines. However, designing of suitable gasturbine combustion chambers measuring a few cubic millimeters requires a best understanding of ongoing processes, like flow, mixing and subsequent combustion in typical geometries under given micro-manufacturing and thermal environments. In both cases of gaseous and liquid flows with chemical reactions, scalar mixing governs the combustion process and is a rate determining step in the most of chemical engineering applications. In the present work, a CFD model is designed and applied to analyze the mixing process in a micro-scale combustor fuelled with non- premixed liquid streams using large eddy simulations (LES). In particular, a newly developed subgrid-scale (SGS) model for the filtered scalar flux vector is applied and assessed. As first step, small-scale combustor representing a confined reacting impinging jet in which a pair of second-order parallel reactions are used to evaluate the extent of mixing. This configuration is simulated using the in house FASTEST-3D CFD code. LES simulations are performed with the dynamic Smagorinsky SGS model for the flow field. The SGS scalar flux has been modeled by the recently developed model. For evaluation of the predictive ability of the designed model, comparisons with experimental data and with results using existing SGS scalar flux models are provided and discussed. It turns out that the CFD model predicts accurately all mixing properties and will be in the next applied to more complex combustion micro-devices.

CHARACTERISTICS OF METHANE INVERSE DIFFUSION FLAMES WITH CO-FLOWING AIR AND COMBUSTION PRODUCTS

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Non-premixed flames of methane in co-flowing air and co-flowing combustion products from a lean, premixed, burner-stabilized, methane-air flame are studied with an additional central air flow, creating a double-flame structure. Measured CH* chemiluminescence emission is compared to numerical simulations using a two-dimensional laminar flame code with detailed chemical kinetics, thermal radiation transfer and a simple soot formation model. Particular attention is paid to the effects of the co-flow on the hysteresis of the inner partially-premixed flame, which transitions to an inverse diffusion flame as the central air velocity is increased. A relationship is found between the height of the normal diffusion flame, without central air flow, and the height of the partially-premixed inner flame prior to transition to an inverse diffusion flame. With co-flowing combustion products, the region of inverse diffusion flame stability is found to be larger, and the height of the partially-premixed inner flame prior to transition is found to be a smaller fraction of the corresponding normal diffusion flame height.

EXPERIMENTAL INVESTIGATION OF DYNAMICS OF PREMIXED ACETYLENE-AIR FLAMES IN A MICRO-COMBUSTOR

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This paper describes a detailed experimental study performed to investigate the flame propagation behaviour of premixed flames in micro-channels. A novel, modular, stackable micro-combustor was developed for this purpose. For a chosen planar channel geometry, the flow condition and the mixture equivalence ratio of premixed acetylene-air were varied to investigate various modes of operation. Three different modes of operation were observed; they were i) stable periodic operation- consisting of ignition, flame propagation, flame extinction and re-ignition ii) a-periodic operation and iii) anchored flame condition. The present work also aims to provide quantitative information on the dynamics of premixed acetylene-air flames propagating inside micro-channels. A novel measurement approach based on OH* chemiluminescence measurements employing a single photomultiplier unit was developed for this purpose. The data recorded was post processed using an in-house developed MATLAB code to evaluate the mean flame propagation speed measured between three different spatial locations. The results from the flame propagation speed measurements performed during 'periodic' mode of operation indicated that the flame traveled at higher propagation speed in the mid-length region of the channel compared to that at the initial entry point, suggesting flame acceleration. This flame acceleration could be attributed to a situation where the flame experienced different local equivalence ratios at different upstream locations. The results suggest that after completion of one cycle of operation consisting of ignition, flame propagation and flame extinction, the fresh mixture that filled the channel was diluted with the exhaust gas from the previous cycle. This pocket of diluted mixture convected downstream with time, thus enabling the spatial variation in local equivalence ratio along the micro-channel.

EXPERIMENTAL INVESTIGATION ON METHANE/AIR DIFFUSION FLAME SUBMITTED TO THE INFLUENCE OF MAGNETIC GRADIENT FIELDS

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We propose here to investigate, by the means of an experimental study, the influence of two magnetic gradients -positive and negative- on the structure of a laminar diffusion flame developed in ambient air and issuing from a coaxial burner with a central methane jet and an annular air jet. At fixed methane flow rate, the experimental results show a modification of the flame behaviour when the air flow rate increases and which is not modified by the variation of the burner position compared to the magnetic gradients locations. From the analysis of geometrical data such as the position of the flame compared to the burner and the length of the flame, we show that the presence of the magnetic gradients influences these sizes due to the magnetic force acting on the paramagnetic substances and to thermomagnetic convection phenomena.

EXPERIMENTAL AND NUMERICAL INVESTIGATION OF NON-STATIONARY COMBUSTION IN HIGHLY POROUS MEDIA

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Detailed numerical simulation and experimental study of the flame dynamics in closed 2D vessel with highly porous media was performed. Comparison demonstrates qualitative adequacy of the simulation. It is shown that quasi-steady regime of the flame propagation is possible in the case of sufficiently high aspect ratio of the system L/D>9 and specific area of the porous media $S_{sp} \geq 10^{-4}, [1/m]$. The new regime of combustion in highly porous inert media (weak thermal coupling between gas and solid) was investigated qualitatively, the corresponding physical model was proposed. The regime is characterized with three phases: intensive acceleration, deceleration and specific "leapfrog" stage of combustion with the speed of the front propagation $S_f / S_n = 2 \div 3$. The characteristic parameters of the "leapfrog" regime are described by using Landau theory of the plain flame hydrodynamic instability. The results may be applied to design of flame arresters and explosion safe vessels.

REACTOR TEMPERATURE PROFILE ON Rh/Al_2O_3 CATALYST DURING PARTIAL OXIDATION OF METHANE IN A REVERSE FLOW REACTOR

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Catalytic Partial Oxidation of methane was investigated in a reverse flow reactor with commercial Rh/Al_2O_3 catalyst in pellets. The process is carried out in a catalytic fixed bed reactor and switching of feed flow direction is obtained through four electrovalves synchronized in pairs. Temperature profile along the catalyst bed was measured by fast IR thermography and product composition was measured with a continuous gas analyzer.
The effect of water addition to Catalytic Partial Oxidation mixture on reactor performance and on catalyst thermal stress is presented both in reverse flow and in steady state operation.
Feed direction switching time and water to methane ratio were investigated as process operating parameters.
Comparison of dynamic heat integration with external feed preheating in terms of product composition and catalyst temperature profile is also presented.

EXPERIMENTAL STUDY OF LEAN FLAMMABILITY LIMIT IN METHANE/HYDROGEN/AIR MIXTURES IN TUBES OF DIFFERENT DIAMETERS

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Lean limit flames in methane/hydrogen/air mixtures with in tubes of different internal diameters, in the range of 8.9-50.2 mm. have been experimentally studied. The flames propagated upward from the open bottom end of a tube to the closed upper end. The content of the hydrogen in the fuel has been varied in the range of 0-40 mol%. Lean flammability limit has been determined; flame shapes recorded and visible speed of flame propagation measured. At hydrogen content in the fuel gas 20% or more all lean limit flame had (hypothetically) enclosed front and had relatively small size compared to the tube diameter in all tubes used in experiments. "Regular" open-front lean limit flames were observed only for smallest diameter (8.9 mm) and largest diameters (35.0 and 50.2 ID) tubes for methane/air and (90%CH_4 + 10%H_2)/air mixtures. In all experiments, except for the lean limit flames in methane/air and (90%CH_4 + 10%H_2)/air mixtures in the 8.9 mm ID tube, visible flame speeds very weakly depended on the hydrogen content in the fuel gas and were close to- or below the theoretical estimate of the speed of a rising hot bubble. This observation suggests that the buoyancy is the major factor which determines the visible flame speed for these limit flames. A decrease of the lean flammability limit value with the decrease of the tube diameter was observed for methane/air and (90%CH_4 + 10%H_2)/air mixtures for tubes having internal diameters in the range of 18.4-50 mm. This effect has been attributed to the stronger combined effect of the preferential diffusion an flame stretch in narrower tubes.

REGENERATION OF SPENT CATALYSTS IN OXY-COMBUSTION ATMOSPHERE

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The feasibility of adopting an oxy-combustion stage to regenerate a spent catalyst proposed for methane thermo-catalytic decomposition has been investigated in a laboratory scale bubbling fluidized bed reactor operated at 800°C and different inlet oxygen concentrations. The efficiency of carbon oxy-combustion regeneration strategy has been evaluated on the basis of the efficiency of carbon removed from the catalyst and the performance of regenerated catalyst. The effect of multiple cycles of decomposition and regeneration steps has been also quantified. Experimental activity confirmed the possibility of producing a CO_2 stream that can be finalized to a sequestration unit but also indicated the requirement of a good temperature control of catalytic particles.

ON THE USE OF STEREOVISION TO DEVELOP A NOVEL INSTRUMENTATION SYSTEM TO EXTRACT GEOMETRIC FIRE FRONTS CHARACTERISTICS

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This paper presents a novel instrumentation system, based on stereovision, for the visualization and quantitative characterization of fire fronts in outdoor conditions. The system consists of a visible pre-calibrated stereo camera, and a computer with dedicated software. Images of the scene are captured simultaneously and processed using specialized algorithms. These algorithms were developed in order to model three-dimensional fire fronts and to extract geometric characteristics like volume, surface area, heading direction and length. Experiments were conducted in outdoor conditions and the results show that the system can successfully measure three-dimensional geometric parameters of fire fronts over a range of combustible and environmental conditions.

SHOCK-WAVE EFFECT ON THE FOREST FIRE FRONT

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Possibilities for an increase in intensity of generated shock waves by application of the shock tubes with conic confuser nozzles were studied experimentally and theoretically. Dynamics of the shock waves, generated by gunpowder cartridges in cylindrical channels with confusers, was studied. The effect of conic confusers on the shock wave intensity was analyzed. The optimal geometrical characteristics of the channel, providing maximal amplification of the pressure in the shock wave front, were found out. The mathematical model of the studied process was developed and numerical simulations were carried out. The scale-down experiments on fire front extinguishing by the shock waves were carried out.

ON THE EMISSION OF RADIATION BY FLAMES AND CORRESPONDING ABSORPTION BY VEGETATION IN FOREST FIRES

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Experimentations have been carried out in the infrared using Fourier Transform Infrared spectrometers. The obtained data characterize the emission of radiation by flames using vegetation as fuel. In a study conducted in parallel, the absorption of radiation by the vegetation has been investigated for several species. Usual assumptions of an emission equivalent to the one of a high temperature blackbody on the one hand, or of absorption close to the one of a black surface on the other hand, are discussed. Indeed, the emission by flames is strongly governed by hot gases produced by the combustion and the corresponding spectral emission is far from the one of a blackbody. In parallel, the spectral absorption of the vegetation varies with the wavelength, indicating a non gray behavior. Fine descriptions should therefore involve a spectral modeling of radiation propagation, which is known to require huge computational costs. For simpler models aimed at producing approximate results but with a reduced computational effort, average values of absorptivities are suggested for two species (*Quercus coccifera* and *pinus halepensis*) on the basis of the present results.

NUMERICAL INVESTIGATION OF RADIATION EXTINCTION COEFFICIENT USING FRACTAL GEOMETRY FOR VEGETATION MODELLING

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As radiative transfer plays a key role in the forest fire propagation process, an accurate knowledge for the radiative properties of the vegetation has to be defined. Indeed, the radiative transfer is mainly depending on the extinction coefficient value. This coefficient for every kind of vegetation is usually evaluated using the well-known De Mestre correlation. This relation does not take into account the leaf orientation and position.
In order to evaluate the role of the leaf orientation and position on the extinction coefficient, a realistic vegetal structure is numerically created using Leaf Area Index data from measurements on real trees, De Wit's model to represent the leaf orientation and fractal geometry to compute the tree structure.
A ray-tracing method is used to simulate the radiative transfer inside the numerical tree. Then, the extinction coefficient is computed as the inverse of the mean free path between two extinction events. A sensitivity study is conducted on the extinction coefficient according to the radiation propagation direction.
The paper will present the discrepancies between the De Mestre correlation and the numerical results in order to evaluate the role of the leaf orientation and position in the extinction coefficient determination.

A 3D PHYSICAL MODEL OF SURFACE FIRES UNDER CRITICAL CONDITIONS AT LABORATORY SCALE

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The physical model we developed in a previous work predicts fire behaviour with a computational time faster than real time, but it has the inconvenient of introducing an empirical law which provides flame height according to heat release rate. The present study introduces two improvements of this model: the triangular flame hypothesis and a modification taking into account the air cooling on the rear fire front. To test this variant of our simplified model, it has been compared with important experimental results. The experiments were performed in homogeneous and plane fuel beds made with dead needles of Pinus pinaster under high values of wind and slope. In spite of high values of wind and slope this physical model provides a good approximation of the fire front perimeter.

FIRE INTENSITY REDUCTION IN STRAW FUEL BEDS TREATED WITH A LONG-TERM RETARDANT

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The present paper reports fire intensity reduction factors in partially retardant-treated straw fuel beds with a bulk density of 7.5 kg m^{-3}. The main results concerning fuel moisture content and slope and wind effects on fire behavior are also described. For a retardant concentration of 0.2 kg of dry retardant product per kg of fuel, it has been statistically inferred that fire intensity reduction factors are constant regardless of the fire intensity of the flame front at the untreated area of the fuel bed. A mean fire intensity reduction factor of 0.80 has been computed.

COMPUTING AERIAL SUPPRESSION EFFECTIVENESS BY IR MONITORING

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This paper describes the methodology developed to analyse the IR images obtained during the aerial suppression experiments that were conducted in Ngarkat Conservation Park, South Australia, on 3-5 March 2008. This methodology has been specifically developed in order to be able to extract the maximum information from the IR images taken from an observing helicopter, in those tests were chemical suppressants are applied directly on the fire, although it could eventually be applied to other similar situations. The information obtained after applying this methodology allows quantifying the aerial suppression effectiveness.

EFFECT OF WIND AND SLOPE WHEN SCALING THE FOREST FIRES RATE OF SPREAD OF LABORATORY EXPERIMENTS

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This paper uses the scaling laws obtained from a *Froude Modeling* perspective to analyze the variations experienced in the rate of spread of wind-aided and up-slope laboratory fires when changing the size of a scale model. The results have shown that the rate of spread scaling law is no longer verified when working at laboratory scale in steep slopes and high wind speed conditions. The paper also provides a framework for scaling and scale issues in forest fire research.

MEASUREMENT OF COMBUSTION LIMITS OF MOIST PINE NEEDLE BEDS

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We measured the extent of fire propagation on moist *Pinus radiata* needle beds under different wind speeds. The experimental apparatus follows Frandsen's study of fire propagation in organic soils. Since pine needle beds are porous, which significantly affect the way it burns, we used a sample holder with permeable walls. Wind speed varied from 0 to 8.5 m/s. The relevant variable measured was the percent of the initial sample mass burned to ashes. We defined the combustion limit moisture content for each wind speed as the highest moisture that allowed full consumption of the fuel. This limit moisture ranged from 25% to 42% for 0 and 8.5 m/s wind speed, respectively, following a linear correlation. After a simplified analysis, we conclude that enhanced heat feed back from combustion zone seems to explain the linear dependence of limit moisture on wind speed.

SCALING THE TRANSPORT OF FIREBRANDS BY WIND BLOWN PLUMES

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The possibility of using reduced-scale model based on Froude-scaling technique to study the transport of spherical, cylindrical and disk-shaped firebrands by windblown plume is investigated theoretically. The cases of hot particles produced by arcing copper power lines and burning sparks produced by arcing aluminum power lines are also considered. In each case, scaling relationships are derived for mass, momentum, angular momentum and energy transport equations of the firebrands using well-established models. The analysis shows that, in the case of cylindrical firebrands, incompatible conditions on brand diameter are obtained to scale both the momentum equation and mass and energy equations. It shows also that all physical processes scale properly for hot copper particles and spherical and disk-shaped burning embers with the exception of the conservation of angular momentum in the case of disks. Despite this drawback, numerical results, obtained using an integral model to model the wind blown plume, show that the mass and spatial distributions for disk-shaped firebrands can be satisfactorily reproduced up to a 1:10 reduced scale.

PILOTED IGNITION OF WILDLAND FUELS

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Piloted ignition of wildland fuel litters was experimentally studied using the FM Global Fire Propagation Apparatus (FPA) with an applied external radiant heat flux up to 30kW/m^2. Fuel types (i.e. Maritime Pine needles and Kermes Oak leaves) and loadings are representative of Mediterranean ecosystems. For the fuel beds considered the inverse of the ignition time was found to be linearly dependent on the imposed heat flux, as observed for thermally-thin solids. A systematic study was carried out to determine the critical (minimum) heat flux for piloted ignition. On the other hand, a dimensionless analysis of the energy equation for the homogeneous equivalent medium was carried out based on the assumptions that the solid and gas phases are in thermal equilibrium and that piloted ignition occurs when the average equivalent medium temperature over the radiation penetration depth reaches a critical value. Using experimental data, a correlation was found between dimensionless ignition time and imposed heat flux.

DETERMINATIONS OF THE MAIN PARAMETERS INFLUENCING FOREST FUEL COMBUSTION DYNAMICS

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This work aims to characterize pine needles as a fuel for a better understanding of the behaviour of forest fuels in wildland fires. The attempts are of two kinds: classify vegetation as a fuel for forest fires and understand the role of transport in fuel beds. For that purpose, physical and chemical characteristics of each fuel are taken into account. Three species of pine needles were studied: *Pinus halepensis*, *Pinus pinaster* and *Pinus laricio*. These were chosen because they are representative of the Mediterranean ecosystem and present different characteristics such as surface-to-volume ratio and chemical compounds.
The experiments were performed using the FM Global Fire Propagation Apparatus and a Fournier Transform Infrared gas analyser to determine the pyrolysis gases released by the three species. The Heat Release Rate (HRR) estimation was done using oxygen consumption calorimetry. Dedicated sample holders were used, with holes and different percentages of basket openings, to allow different air flow rates to pass through the fuel sample. Forced flows, of different magnitudes, were also imposed through the sample in some cases.
In this study, the focus has been made upon the influence of the two main experimental parameters, i.e. flow conditions through the fuel bed (varying with basket opening and forced flow conditions) and fuel species particularities, on the time dependent variable HRR. Discrete variables such as time to ignition, duration of flames and mean HRR during the flame were also analysed.
Flow conditions appear to be an important parameter when analysing the combustion dynamics of a porous fuel. Fuel species also have an influence on the Heat Release Rate. The role of these parameters and their interaction prove to be more complex than anticipated. Surface-to-volume ratio and fuel packing ratios do not drive alone the burning dynamics even for closely related species as pine needles. Chemical properties proved to have an influence too when the oxygen supply in the combustion zone is high.

FIRE INTENSITY ACCUMULATION IN UNSTEADY FIRELINE MODELLING

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Eruptive wildfires and any other form of unsteady fire-spread involve a process of dynamical interaction between spread rate R and fireline intensity I. If, for example, spread rate changes abruptly, the intensity is then adjusted more slowly as the amount of vegetation that is actively pyrolysing varies through the initiation of aming in new vegetation and the burning out of previously ignited vegetation.

Using a fairly simple model description for the movement of a narrow zone of pyrolysis through such a vegetation layer, which thus generalises an earlier approach, the unsteady dynamical behaviour of a fireline is examined. In its simplest expression, the intensity can be determined as a weighted integral of previous rates of spread from a burnout time into the past up to the present moment. The weighting arises because different parts of a stratified vegetation layer can contribute differently to the overall intensity of an evolving fireline. The problem is closed, dynamically, if the rate of spread is then expressed as a function of the intensity.

By examining a power-law expression for a rate-of-spread law, of the form $R \propto I^{\nu}$, it is found that fires have stable rates of spread in all sublinear cases (having $0 < \nu < 1$). This is the usual nature of fire-spread that is found in the field. But eruptive fire growth is also sometimes observed in the field and this is found to be reproduced by the model in linear cases ($\nu = 1$) or superlinear cases ($\nu > 1$) provided only that a dimensionless ratio (here called the "Byram number") exceeds unity in value. These features arise for any realistic form of weighting in the integral that is used to determine the intensity, modified only through relatively modest differences of detail.

DETERMINANT-PROBABILITY SYSTEM OF FORECASTING A FOREST FIRE DANGER

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The work suggests more accurate (physical and mathematical) models of forecasting a forest and steppe fire danger within the framework of which all known reasons of initiation of natural fires are taken into account. The retrospective analysis of ignitions has been carried out in view of particular meteorological conditions and anthropogenous load on forests of Timiryazevskiy forestry of Tomsk district of the Russian Federation within the period of 2000-2004, and it is shown that the new technique of forecasting a forest fire danger specifies the date of forest fire initiation more exactly than GOST P 22.1.09-99 nowadays in Russia.

CHARACTERIZATION OF IGNITION BY DIRECT RADIATION FROM FLAMES FOR URBAN/WILDLAND APPLICATIONS

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Fires within the wildland/urban interface are becoming increasingly relevant. Therefore, the need to accurately model the impact of a fire on a structure has never been so pertinent. However, the present state of knowledge added to limitations in available computational power make necessary a multitude of simplifications when modelling fires. The use of simplifications is most relevant in the case of forest fire modelling, due to the occurrence of physical and chemical processes at widely ranging scales, which is particularly important when modelling the interaction of forest fires with buildings. The present study focuses on ignition of solid fuels within the context of the wildland/urban interface with the objective of providing a mechanism to assess the potential for ignition while not adding an excessive computational burden to CFD models. When a solid fuel is subject to a constant heat flux, the ignition delay time can be represented by $\left(\int_0^t \dot{q}_e'' dt\right)^2$. However a more realistic heating regime for a wildland fire corresponds to a linearly increasing heat flux (ramping heat flux). Novel experiments were performed using the Fire Propagation Apparatus (FPA). Samples of PA6 and PMMA were subjected to a ramping heat flux, with in-depth temperature recordings taken within the PA6 only. Results show that for a ramping heat flux, time can be scaled by $\left(\int_0^t \dot{q}_e'' dt\right)^2$, thus surface temperature and ignition delay time can be presented as a function of the integral of the heat insult as a single curve that can be used to completely decouple the solid and gas phase in the numerical modelling of the ignition process.

DETERMINATION OF THE FIRE FRONT CHARACTERISTICS BY MEANS OF A FLAME MODEL AND INVERSE METHOD

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The aim of this paper is to propose a methodology for the identification of the flame spread characteristics for experiments in fire tunnel. This methodology is based on the use of a simplified flame model derived from the radiative transfer equation and takes into account the curved shapes of the fire fronts due to wind effect. The inverse method which consists to minimize an objective function between the theoretical and the experimental heat fluxes given by a specific wireless thermal sensor is used in this application. The proposed method gives promising results and shown that this methodology can help fire fighters to optimize the distribution of fighting in forest fires.

PREDICTION MODEL OF OCCURRENCE OF FOREST FIRE ON THE COMMUNITY OF CANTABRIA (NORTHERN SPAIN)

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Forest fires are a plague that affects every year to the Iberian Peninsula to produce dramatic environmental consequences such as deforestation and forest soil degradation, as well as consume significant financial resources for prevention and extinction of forest fires.
This communication provides a mechanism to help combat forest fires raging in Spain and the region of Cantabria in particular. We have created a prediction model with three days in advance to determine the fire danger in each 10x10 Km^2 grid of the 81 which divides the territory. Besides the weather conditions, our index for fire risk in Cantabria uses the evolution of the forest fires for the last 12 years as well.
Once the prediction model is calculated, this is presented in a G.I.S. for its display on a map grid with 4 levels of risk: low, middle, high, extreme, which will validate the results achieved by the model in the years 2003 to 2006 and state that our model only has an average error of 9.75% in the cases studied.

POSTERS

CHOICE OF PRESUMED PDF MODELS FOR PREMIXED TURBULENT FLAME SIMULATION USING FPI CHEMISTRY

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Abstract

In this work, the turbulent premixed flame experiments of Chen et al. [Combustion and Flame **107** (1996) pp.223-244] are simulated using a RANS approach for turbulence and a flamelet model for turbulence-chemistry interactions. In the flamelet model, the mean reaction rates are approximated using a progress variable approach and Flamelet Prolongation of ILDM (FPI) for chemistry reduction. This method requires presumption of the shape of the probability density function of reaction progress variable. Two shapes have been examined: the widely used β-function and the modified laminar famelet PDF of Jin et al. [Flow, Turbulence and Combustion **81** (2008) pp.563-582]. Radial distribution of the calculated temperature field, axial velocity and chemical species mass fraction are compared with experimental data. This comparison shows that the modified laminar PDF is a better choice for the statistical description of the reaction progress variable than the β-PDF.

Keywords: Premixed fames, modeling and FPI chemistry

ATOMIZATION OF WATER IN OIL EMULSIONS: EFFECT OF WATER DROPLETS GRANULOMETRY

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Context: Emulsified fuels derived from biomass are quite promising alternative fuels for engines and boilers due to their simultaneous reduction of nitric oxide and particulate emissions [1,2]. When water in oil (W/O) emulsion is heated in a flame, the internal droplets of water vaporize and form steam nucleus that lead to a vigorous expansion. The energy released in this stage breaks the molecular bonds of the surrounding oil, resulting in a fragmentation into numerous and smaller droplets. This physical phenomenon is called *micro-explosion*. The size reduction of the oil droplets leads to more effective vaporization and resulting in more complete combustion [3-4]. Emulsions are generally classified by a number of host characteristics such as droplet size, surfactant used, method of preparation etc. The most powerful and well known tool to find the average size of the droplet dispersed in a fluid is to estimate the Sauter Mean Diameter (*D32).* In W/O emulsions, the sauter mean diameter depends mainly on the proportion of the components (oil/water/surfactant) present as well as the mechanical power spent to make the emulsion.
Objective: The main objective of this work is to study the droplet size of the oil water emulsions and its effects on micro explosion using high speed photographs.
Experimental system and Experiments: Emulsions were prepared by using sunflower oil, water and a surfactant (span83). The characterization of the W/O emulsions on droplet size was made by using a microscope with the optical magnification capacity of the image of *500* times. The effects of the micro-explosion phenomenon were studied by using a high speed camera which can be able to take images with a frequency of *24 kHz*, coupled with a *6W* continuous laser light. Accurate images have been taken to study the micro explosion of emulsion droplet quantitatively. The photographic view of the microscopic structure of oil-water emulsions can be seen in Fig.1. The photographic view of the emulsion droplet (using Leidenfrost burning effect) before micro explosion can be seen in Fig.2 and the occurrence of micro explosion can be seen in Fig.3 and Fig.4.

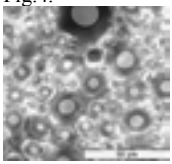
Fig.1. Microscopic view of emulsion


Fig.2. Emulsion Droplet Before microexplosion

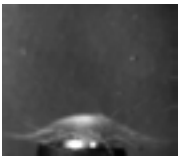
Fig.3. Starting of microexplosion

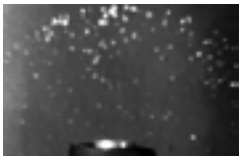
Fig.3. Droplet fragmentation after microexplosion

Expected Results: Results are awaiting for the complete analysis of the *droplets* size (*D32*) of different (micro and macro) emulsions. Complete study will be carried on the water droplet size distribution and its consequences on micro - explosion. Best emulsion will be identified and tested in the future in a conventional boiler to study the performance and emission characteristics.

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NUMERICAL STUDY OF PARTIAL OXIDATION STEP IN ORDER TO IMPROVE TAR CRACKING IN GASIFICATION PROCESS

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The most portion of energy under consumption in the world has a fossils combustibles origin coming from limited sources. The need for sustainable energy production has prompted new research into the possibility of gasification as a key source of energy production.

Gasification is a thermal process converting biomass feedstock into a mixture of gases that can be used in internal combustion engines, fuel cell, oven and gas turbine. It is an environment friendly process as it releases few amount of toxin and NO. However, an important problem preventing the breakthrough of biomass gasification systems is the inevitable production of tars during biomass gasification. Tars form a nasty byproduct that can cause fouling, plugging and breakdown of after-treatment or end-use equipment **[1]**. In gasification with separated steps, partial oxidation is one of several methods for tar removal produced during a pyrolysis step, which the raw product gas is partially combusted at a low air-excess ratio. Partial oxidation is a technique for tar reduction that based on tar cracking.

This paper presents a tool for validating burner of two-stage downdraft gasifier design. In this type of installation, temperature field in the partial oxidation zone is crucial. Indeed gas produced during pyrolysis must pass through a hot uniform zone to crack satisfactorily tar, the main issue of gasifier. As a result reactor diameter and throat shape have to be well designed in order to ensure an optimum process **[2]**.

Numerical 3D model is used to simulate the complex phenomena occurring in the partial oxidation zone. It includes detailed chemical mechanism, heat transfer, turbulence and swirl effect. Results are then confronted with the experimental data get from the Houben et al **[3]**. In particular this tool permits also to determine temperature and flow patterns in the most important part of the gasifier. Thus the burner design is going to be optimised regarding tar cracking efficiency. The first results obtained were interesting. For example the figure (1) shows the temperature profile at the burner outlet compared to the result of Houben et al. **[3]** showing in figure (2).

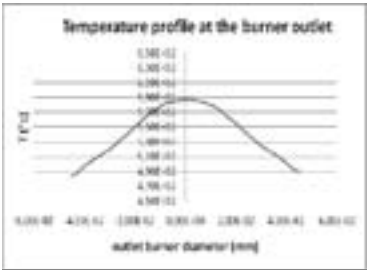

Figure 1 : Numerical result

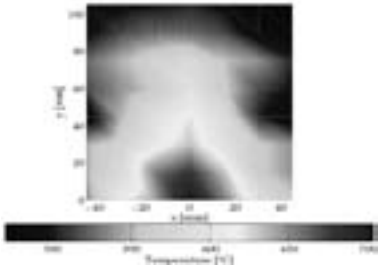

Figure 2 : Houben and al. [3] result

References:
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THERMOGRAVIMETRIC AND REACTION KINETIC ANALYSIS OF OLIVE MILL WASTEWATER/SAWDUST BLENDS

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The demand of olive oil, mainly produced in the Mediterranean region, is increasing rapidly worldwide. Therefore, environmental pollution from olive oil mill wastewaters (OMWW) is becoming a growing problem. In fact, the olive oil producer countries will face serious challenges to find environmentally and economically solutions in handling and disposal of OMWW. The composition of OMWW is variable, depending on parameters as olive variety, ripeness of the fruit and extraction process. With very high Chemical Oxygen Demand (COD up to 200 kg. m-3), high content in phenol-like substances and acidity, OMWW is one of the most polluting agro-industrial effluents. It could not effectively be treated by classical biological treatment because of its phytotoxicity and antimicrobial properties. On the other hand, it holds high heating values (up to 20 MJ/kg, dry basis) for energy recovery.

Although different treatment options for OMWW have been described and evaluated, a new combined process which implies the absorption on natural biopolymers followed by oxidative pyrolysis was evaluated. Sawdust was found to be an effective, low cost absorbent of OMWW. The high surface area of sawdust allows an efficient evaporation of the water content under normal atmospheric conditions and consequently removes smells associated with the OMW. After evaporation of the water, the thermal behaviour of different OMWW/Sawdust blends was studied under inert and oxidative atmosphere at 5°C. min-1 of heating rate from room temperature to 900°C by thermogravimetric analysis (TGA). Gaseous emissions as CO2, CO and volatile organic compounds (VOC) were measured under oxidative conditions. Kinetic parameters were obtained and compared for the different mixtures of OMWW and sawdust.
Pyrolysis of OMW/Sawdust under inert atmosphere proceeds in three distinct stages of weight loss. The first stage (water loss) ranged from 25 to 125°C, the second stage designed as active pyrolysis (rapid weight loss) from 125°C to 310°C and the third stage designed as passive pyrolysis zone (continuous and slow weight loss) from 310°C to 900°C. During the active pyrolysis zone, activation energy was approximately 40 kJ.mol-1 and the reaction order was 0.5. This value confirms the high reactivity of OMWW/Sawdust comparing to other biomass (Wood, Corn stover,.). During the passive zone, the order of the reaction was 0.04-0.07, which suggested that it was a zero-order reaction.

Oxidative pyrolysis of OMWW/Sawdust under air proceeds in five stages. The two first steps are similar to those in inert atmosphere. The three following stages corresponding to oxidative processes are ranged from 340-480°C, 490-560°C and 600-780°C respectively. The oxidation steps ranging from 340°C to 560°C were significantly affected by the percentage of OMWW in the mixture.

Regards to emissions, oxidative pyrolysis of OMWW/Sawdust blends proceeds via complete reactions compared to sawdust in the same conditions. Hence, oxidative pyrolysis of mixtures generates higher amount of CO2 and lower amounts of CO and tar than for sawdust only. Therefore, presence of OMWW enhances the thermal degradation of sawdust. Hence OMWW/sawdust blends may be an environmentally friendly process for the disposal of OMWW.

REAL GAS EFFECTS IN MIXING-LIMITED SPRAY MODELS

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The influence of real gas effects in existing mixing-limited spray models was investigated. In these mixing-limited spray models it is assumed that the mixing of fuel with air is the limiting factor in fuel evaporation. Because of their good accuracy at high density and temperature they are widely used to describe the so-called "liquid length" of evaporating fuel sprays. Critical evaluation of two mixing-limited spray models, by Siebers [1] and by Versaevel et al. [2], reveals that in these models real gas effects are implemented in a wrong way and neglected, respectively. The influences of these effects on both models are studied using Matlab.

In this work, air is modeled as a one component gas and its properties are determined using van der Waals mixing rules. This leads to a more simplistic model with only binary calculations (fuel and air). In the original model [1] real gas effects are included by using a real gas equation of state to determine the compressibility ratio of both fuel and air, which leads to a decoupling of the densities of both components. The molecules of the fuel and air in the mixture interact, however, so a better way to include real gas effects is by using the enhancement factor, which is a direct measure of the deviation from ideal gas behavior of the mixture. In order to calculate it, the equilibrium mole fraction of fuel in the vapor phase is determined, by extending the original Siebers model with a flash calculation based on the Peng-Robinson equation of state.

Comparing the results of the original and the extended Siebers model with experimentally obtained data for different fuels shows that the liquid length is calculated more accurately using the enhancement factor. More specifically, at relatively low temperatures and high pressures (700 K and 100 bar, i.e. conditions where real gas effects are important), the extended model leads to a reduction of 10-15% in the calculated liquid length (depending on which fuel is used).

A second subject for discussion is the enthalpy of fuel and air that appear in the energy balance. In the original models, the enthalpy at the liquid length is calculated by adding the ideal gas enthalpies of each component. Hence the enthalpy is, like the densities, also decoupled. To improve the model the energy balance is rewritten using the enthalpy of the mixture at the liquid length and departure functions based on the PR equation are used to include real gas effects. The influence of this adaptation on the liquid length will also be presented at the conference.

The Versaevel model [2] is based on the Siebers model [1] but is more detailed since it also predicts the vapor phase void fraction upstream of the liquid length. We have also adapted this model to include real gas effects using the enhancement factor. The influence on the model results is still under investigation but is expected to be presented at the conference.

Based on the results obtained so far it can already be concluded that inclusion of real gas effects in mixing-limited evaporation models leads to improved predictions of the liquid length, especially at low temperatures and high pressures where real gas effects are most relevant.

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JATROPHA OIL AND BIOGAS IN A DUAL FUEL CI ENGINE FOR RURAL ELECTRIFICATION

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The technical feasibility was investigated of using jatropha oil and biogas (CH_4 and CO_2) in a diesel generator set. This so-called dual fuel technology can be used for electricity generation in rural areas in developing countries, making optimal use of jatropha seeds. It adds to a sustainable electricity production and could therefore help in economic development and poverty reduction. To investigate the technical feasibility, a parameter study was performed and experiments were carried out. Three performance parameters are studied: overall fuel efficiency, volumetric efficiency (which affects power output) and air-excess ratio (which affects particulate emissions and unburnt hydrocarbons).

Experiments were carried out on a 12 kW diesel generator set. Pure jatropha oil was used.

Artificial, bottled, biogas of different quality (CH_4/CO_2 ratio ranging from 0.4 to 1) was added using a venturi. Its design limited the gas flow to a maximum heat release fraction of methane of about 80% for pure methane and to 25-55% for biogas (depending on load and biogas quality). Tests were performed at different loads above 6 kW; below that, efficiency was found to suffer too much and the engine was running irregularly.

For pure jatropha oil (i.e. without biogas addition), the engine showed the same thermal efficiency characteristic as for standard diesel, with about 32% full load thermal efficiency. In dual fuel operation, for the higher loads thermal efficiency was hardly affected. For lower loads, biogas addition leads to a decrease in thermal efficiency, down to 22% at the highest biogas heat release. This can probably be attributed to a later combustion phasing. Remarkably, use of lower quality biogas (more CO_2) appeared to increase the engine's tolerance to methane addition.

The experimental efficiency data were cast in a curve fit, which was used in the parameter study to predict volumetric efficiency and air-excess ratio. The predicted decrease in both corresponds reasonably well to experimental results, determined from inlet mass flows (volumetric efficiency) and from either mass flows or exhaust oxygen concentration (air excess ratio). The latter did not decrease dramatically, which suggests, together with the significant replacement of oil by methane, that soot emissions have not increased.

Although the amount of carbon dioxide in the biogas does not dramatically influence efficiency, its effect on volumetric efficiency is greater. This results in a maximum of about 30% of methane heat release at the lowest biogas quality (60% carbon dioxide). For each biogas quality, irregularities are observed above a certain methane heat release fraction, probably attributable to light end-gas knock. A different engine design (i.e. different compression ratio) might be able to operate without problems with more biogas in the fuel mixture.

For a better understanding of the combustion process, more research is still required. Heat release rates should be determined from in-cylinder pressure measurements, and smoke emission should be measured. This would give a better insight into the observed changes in thermal efficiency and (smoke and knock) operating limits.

In conclusion, it is possible to use a CI engine to generate electricity with jatropha oil and biogas as fuels, removing the need for expensive diesel imports. The technology is fairly low-tech and locally available. Therefore it is considered to be appropriate for use in rural areas in developing countries, although the problem of deposit formation should be taken care of.

EFFECT OF HYDROGEN ADDITION ON COMBUSTION DURATION AND INITIAL FLAME VELOCITY IN A SPARK IGNITION ENGINE COMBUSTION FUELLED WITH CH4/H2

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FRANCE

Abstract

An experimental study was performed in the combustion chamber of a spark ignition engine fuelled with various CH4/H2 mixtures and for different equivalence ratios in order to quantify the effect of hydrogen on combustion duration and on the initial flame velocity. With an optical fibbers spark plug, the behaviour of the flame front during the first part of the mixture combustion is studied in the engine combustion chamber. Four fuel CNG/H2 mixtures have studied with up to 3% mass fraction of H2 in the fuel.
The evolution of pressure signal has been studied for various equivalence ratio from 1.0 to 0.5. A spark plug equipped with optical fibers allows us to determine the flame arrival delay and then to compute a flame front propagation velocity.
Regarding to the coefficient of variation (COV) of indicate mean effective pressure (IMEP), addition of hydrogen reduces it significantly as mentioned in the literature.
Different combustion durations (CA 5, CA 10, CA 50 and CA 90) determined from in-cylinder pressure signal, and for various amount of hydrogen in the fuel show that the reduction of combustion duration is more important at low equivalence ratio (less than 0.7) than higher where the effect is less significant. As mentioned in the literature, addition of H2 allows a more stable combustion (less cycle to cycle variations) even a very low equivalence ratio. When adding various amount of H2 in the fuel, there is no effect on the DAF for equivalence ratio higher than 0.7. The same conclusions can be drawn when studying combustion duration. From the determination of flame arrival delay (DAF) in the vicinity of the spark plug electrodes, it is also possible to calculate the laminar flame velocity during the beginning of flame kernel growth. To validate these determinations, we also compare these experimental measurements with flame velocity calculations using two chemical kinetic mechanisms to describe methane combustion (GRI 3.0 and GRI 2.11) and a freely propagating flame model (Cantera code). A good agreement is found between measurements and calculations for equivalence ratio between 0.6 and 1 with up to 3% mass fraction of H2 in the fuel.
The results showed that :

-the effect of hydrogen addition on initial laminar flame velocity is well described by the two chemical kinetic combustion models even in the beginning of flame kernel growing.

-this effect is important even just at the beginning of combustion in the first few percent of burnt mass fraction, certainly due to lower ignition energy, shorter ignition lag of hydrogen.

Comparison with determination of laminar flame velocity in a high pressure chamber in the same physical conditions would be performed in the next future.

MODELING IGNITION IN ENGINE APPLICATIONS

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Combustion in Diesel engines is essentially an instationary process, involving injection of fuel, followed by auto-ignition and the establishment of a more or less stationary diffusion flame. To cope with this in most CFD packages some kind of hybrid approach is implemented. An ignition model is provided, either based on few-step global kinetic models (e.g. Hardenberg and Hase, Halstead, Kirsch and Quinn[1]) or full detailed models, in combination with a Livengood-Wu integral or generalizations thereof. Typically a progress variable is solved for, viz.

$$\rho\frac{\partial R}{\partial t}+\rho\vec{v}\cdot\vec{\nabla}R-\vec{\nabla}\cdot\left(\rho D\vec{\nabla}R\right)=S_R \tag{1.1}$$

where $S_R=\rho\tau^{-1}(\varphi,p)$ and $\tau(\varphi,p)$, the ignition delay determined by the chemical model employed. After this 'progress variable' reaches a set value (typically 1) the conventional (stationary) combustion model is switched on for the remainder of the combustion process. Now, especially in view of emerging new combustion concepts like (H/P)CCI, MK and LTC, and possible developments in future fuel quality (i.e. bio-fuels, Dieseline) accurate models for auto-ignition will become even more important and need to be re-evaluated.

Recently we have extended the FGM [2] approach to model an igniting Diesel spray in a high-pressure/high temperature pressure cell. To do so the conventional database, based on stationary flame solutions is expanded to incorporate the ignition process. The benefit of this approach is that both ignition and the stationary phase of the Diesel combustion process are computed by one consistent approach. Still, several conceptual ways exist to extend the database as illustrated in the figure 1.

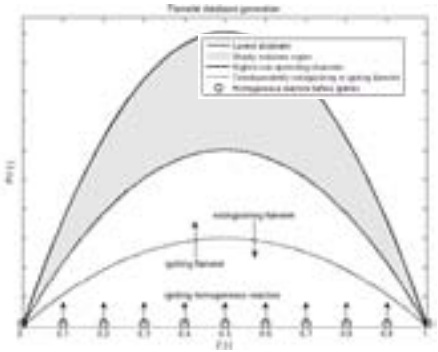

Figure 1: Illustration of the possible extension of the stationary database.

In this study two ways to extend the database are presented, the homogeneous reactor and igniting flamelets. To rule out effects of the averaging procedure, which is unavoidable in the case of an igniting Diesel spray, the effect of the implemented extension is studied in basic, 0D and 1D, laminar cases. The analogy between the FGM and Livengood-Wu approach will be highlighted and a new hybrid approach is presented.

[1] The Shell ignition model
[2] Flamelet Generated Manifold, a hybrid flamelet/manifold method.

CHARACTERIZATION OF PREMIXED LAMINAR SYNGAS FLAMES USING PIV AND RAYLEIGH SCATTERING DIAGNOSTICS: EFFECT OF STRETCH AND PRESSURE ON THE FUNDAMENTAL FLAME VELOCITY AND THE FLAME THICKNESS.

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It is recognized that addition of hydrogen into a gas mixture extends its flammability limits. Addition of hydrogen into natural gas or the presence of hydrogen in syngas composition is of particular interest for gas turbines or internal combustion engines because this allows operating at lean conditions which is a way to reduce pollutant emissions. Thus, by burning at low equivalence ratio, both the quantity of unburnt gas and thermal NOx decrease.
It is generally assumed that, in most practical applications, turbulent premixed combustion takes place in the laminar flamelet regime, hypothesis which is largely used in combustion modelling. Flames at very low equivalence ratio and high turbulence intensities, which correspond to gas turbine operating conditions, are characterised by a Karlovitz number (Ka) much greater than unity. In the Klimov-Williams criterion sense, combustion does not take place in the flamelet regime anymore. Nevertheless, as it can be seen in the work of Poinsot et al. [1] and Peters [2], flamelet regime can be extended beyond the limit defined by Ka=1. In this case, the smallest eddies are able to penetrate and enlarge the preheat zone but not the reaction zone which remains laminar-like. Therefore, the knowledge of laminar flame properties such as fundamental flame speed and flame thickness is essential to understand turbulent combustion phenomenon.
To characterize premixed syngas flame properties in laminar conditions, a counter-flow flame experiment has been combined with a high pressure chamber allowing to control stretch rate and pressure for parametric study. Fundamental flame velocity measurements using Particle Image Velocimetry diagnostic and flame thickness determination using twodimensional Rayleigh scattering diagnostic are performed on a wide range of mixture composition and pressure conditions.
We will present the experimental set-up, the implementation of the two diagnostics with the experimental precautions taken and the validations performed. Finally, we will present the first results obtained at atmospheric pressure.

1. T. Poinsot, D. Veynante, S. Candel, *J. Fluid Mech.* 228 (1991) 562-606
2. N. Peters, *J. Fluid Mech.* 384 (1999) 107-132

A LABORATORY STUDY OF THE RELEASE OF SELECTED TRACE METALS DURING COMBUSTION OF COAL

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Recently, the trace elements have drawn more and more interest from scientists mainly because of the great concern for their toxicological and environmental effects. The heavy metal species, such as mercury, arsenic, lead, cadmium etc., can be found in most fuels (like coals, biomass, and heavy oils, industrial and municipal wastes) in at least trace amounts. The amounts of the heavy metals present in solid fuels vary very widely depend on origin. The occurrences of trace metals in fuels are described. Transformations of metal species during combustion and post-combustion processes are briefly depicted. Several important aspects, like heavy metals partitioning in emission streams, enrichment in submicron particles, vaporization and emission in flue gas, are summarized.

The objective of the presented work was to evaluate the dynamics of selected trace metals release from coal during combustion and pyrolysis processes. According to their toxic effect, the trace elements selected were As, Cd, Co, Cr, Cu, Hg, Mn, Ni, Pb, Se, V and Zn.

Tests were performed using a coal designated to small combustion boilers which are very popular in Polish municipal sector. Coal was crushed and sieved to a maximum particle size of 1 mm. The tests were carried out in a laboratory using Netzsch STA 409 PC apparatus in thermogravimetric mode. The coal samples were heated up to the temperature from a range of 400 to 1450°C in the atmosphere of nitrogen/oxygen mixture. When the reactor temperature reached the desired value, process was continued to get the constant mass of the residue. Dynamics of the trace metals release was measured by comparing their concentrations in a coal sample and in solid residues obtained after heating.

The concentrations of trace metals in coal and residues samples were determined in certified laboratory using inductively coupled plasma-atomic emission spectrometry (ICPAES) technique. ICP-AES technique enables simultaneous multielement analysis of trace metals in char, ash, or fuel samples, which can be especially useful in industrial tests.

The release of the elements tested proceeds with different dynamics and to different extents. Trace metals studied may be classified, according to their volatile behavior expected during coal combustion/pyrolysis, into three groups. The trace elements in the first group would include those that may be mainly present in gas phase in most conditions (Hg, Se, Cd, Pb). On the other hand elements like cobalt, copper, chromium and vanadium volatilize only in small extent (partitioning factor >70%). It can be expected that these elements during combustion will be distributed more or less equally over bottom ashes and fly ashes. The rest of elements studied would form an intermediate group (As, Mn, Ni, Zn).

Further investigation of the behaviour of heavy metals during coal and biomass cocombustion is planned. The influence of the fuel properties and the selected combustion parameters on the fate of heavy metals during coal combustion, co-combustion and pyrolysis will be examined.

A SIMULATION EXERCISE FOR CFD AND ZONE MODELS IN THE CASE OF AN UNDER-VENTILATED FIRE

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Modelling is now often used to improved fire safety, mainly in public or tall buildings. One key is the availability of verified and validated fire models that can correctly predict the consequences of fires. So a modelling exercise has been organised on behalf of the French CNRS research group "GdR Incendie". The main aim of this work has been to look at the accuracy of several models in the case of an under-ventilated fire and by means of comparison to experimental results. Seventeen research laboratories or institutes have participated.

The full scale test will be described and it corresponds to fire growth in a room and smoke spread in other connected rooms. The experimental set-up will be also presented. It has allowed observations of the weight loss of the fire source, temperature field (230 thermocouples) inside rooms, and gas concentration (O2- Nox) in the exit smoke flow.

The round robin exercise has been planned in two blind steps. First, calculations had to be performed knowing only the dimensions and wall properties of rooms and also the dimensions and the initial weight of the two sources (wooden pallets). Then in the second step, the heat release rate was known and it had to be used as an input data for the calculations. The first step is to highlight the influence of the model user choices. The assumptions which are made, in particular for the heat release rate calculations, and the collection of data for the input are crucial parts of fire safety engineering applications. The second step is to reflect more the mathematical model's inherent capabilities. It is to highlight differences between models as for example those existing in calculations of radiation, wall heat flux, smoke production or with different mesh sizes. These differences could have been hidden in the previous blind test, due to the predominant influence of the HHR calculations on the results.

Results for the two steps will be presented and discussed.

Acknowledgments: The fire test has been performed and financed by the PROMESIS* consortium in September 2008 using the SERAFIN research station (located at Roanne, France). P.R.O.M.E.S.I.S is an initiative of GIMAEX and 'Commissariat à l'Energie Atomique' and it get closer 18 partners on a research program dedicated to the comparative study of the means and the methods for the fire extinguishing systems.

ROLE OF CONDENSATION ENERGY IN DETONATION OF C_3O_2 AND C_2H_2

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The processes of combustion and detonation of most gaseous hydrocarbon fuels are accompanied by the formation of condensed carbon particles and the process of condensation, just as the oxidation reactions, is characterized by the essential heat release. Therefore the important question is - what is a role of the processes of condensation in formation and maintenance of a detonation wave?

In the recent paper [1] the process of carbon cluster formation in deflagration and detonation waves in acetylene-air and acetylene-oxygen mixtures has been studied. Results of this work stated that at high acetylene concentrations the energy of carbon condensation plays an extremely important role in steady-state propagation of the detonation wave. This inference confirms the observations of older works [2,3], where the formation of condensed carbon during the detonation of undiluted acetylene was studied. However an extraction of quantitative input of condensation energy to the detonation wave is hampered by the complex intermediate reactions of various hydrocarbons formation during acetylene decomposition.

Much more bright demonstration of detonation, driven exclusively by the energy of condensation, was lately presented in [4], where the formation of detonation wave driven by the condensation of supersaturated carbon vapor, formed at the thermal decay of carbon suboxide C_3O_2 behind a shock wave, has been observed. Carbon suboxide is rather unstable volatile compound and under heating up to 1400 – 1600 K its molecules immediately decompose to carbon atom and two CO molecules. An important property of the process of C_3O_2 decomposition and consequent carbon condensation is the total absence of secondary gaseous reactions (in the system remains only CO, which is chemically stable at $T < 4000K$).

In this work the further experiments of detonation wave formation in the mixtures of C_3O_2+Ar and C_2H_2+Ar have been carried out. Based on these data the current analysis of interconnection of cluster growth and heat release behind the shock and detonation waves is presented.

Present work is supported by DFG, Goettingen Academy of Sciences, Russian Academy of Sciences (Program P-09) and RFBR.

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MEASUREMENTS OF LOW HEAT RELEASE RATES IN THE CONE CALORIMETER

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Recently, several developments have been made to allow the testing of materials with very low heat release rate (HRR) using standardized equipment like bench scale calorimeters, and particularly the ISO-5660-1 Cone Calorimeter in a new standardized procedure: ISO-5660-4. This becomes useful when it comes to test so-called "non-combustible" materials, whose peak HRR is expected to be very low. It is worth noting that HRR criteria have been suggested as an alternative to "old fashioned" non-combustibility tests.

In the cone calorimeter, the heat release rate is classically determined via oxygen consumption (OC) method, i.e. measuring the oxygen depletion in the exhaust gases. The oxygen consumption may be directly related to the HRR of a fire, assuming the molecular composition of the fuel is known, or using an average value.

However, when the HRR becomes very small, so does the oxygen depletion and thus the relative error made on the measurement may become significant. Using a high-performance oxygen analyzer together with other adjustments (better laboratory practices, reducing air flow to increase the oxygen depletion, or increasing sample size & heat flux, as recommended in ISO-5660-4) may lead to a reduction of this error. However, such equipment is not available on all calorimeters, and the modifications of testing conditions have their own limitations.

Alternative techniques exist for determining the HRR, for example based on the production of carbon oxides (known as CDG, for carbon dioxide generation). The later is generally used in equipments like the Fire Propagation Apparatus (FPA, also known as the "Tewarson Calorimeter"), and may be transposed with very little adjustments on a cone calorimeter fitted with a CO/CO_2 analyzer.

Some preliminary experiments were conducted with acetone in the cone calorimeter. Acetone was selected for these bench scale experiments since its combustion can be assumed as complete (generations of CO, THC and soot measured in these fire tests were negligible). Different cylindrical sample holders made of glass were used in order to obtain low and very low heat release rates. The diameter of the pans ranged from 88 to 44 mm. The actual HRR was calculated from the fuel mass loss rate and the heat of complete combustion. As expected, for oxygen concentration in the exhaust duct lower than 20.75%, oxygen consumption and carbon oxide generation methods give similar HRR results with relatively small error levels.

However, for extremely low HRR (for oxygen depletion lower than 0.20 %), carbon dioxide generation seems to provide a smaller relative error, and thus a better precision on the determination of the heat release rate measurements.

THE USE OF FIRE DYNAMIC SIMULATOR FOR FIRE SCENE INVESTIGATION

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ABSTRACT

Fire scene reconstruction helps investigators to assess the fire behaviour in a building. Fire scene simulation may bring evidences for fire investigation. Simulation procedure may reproduce the fire scene and reconstruct fire processes. It explains fire expansion and smoke movement using the fire source, the design of the building, the effects of ventilation and occupant behaviour. From the comparison of different scenario simulations with investigation reports, more data toward the fire and smoke development may be obtained. A field model (Fire Dynamic Simulator, FDS) was used in this investigation to simulate an arson fire in an accommodation unit for older person in France. The obtained results were compared with the real situation in the fire scene in order to guide the investigation direction to the thermal conditions that may have occurred during the fire. The inputs of the model were provided from 3 sources : Laboratoire Central de la Préfécture de Police (LCPP), Centre Scientifique et Technique du Bâtiment (CSTB), Département Sécurité Structure et Feu staff and FDS database. These inputs allowed getting a representation of the actual building geometry, material thermal properties and fire behaviour.

In order to reconstruct the fire scene, a scenario established by the reconstruction Committee was considered and 6 fire conditions were simulated. Since, it was difficult to estimate the fire design, we used for fire development $Y= \alpha t^2$ (MW) fire growth to stable heat release rate (HRR) (Y_{max} = 0.5 MW, 1.5 MW and 3 MW) after 5 minutes. Moreover, the climatic conditions were unknown during the arson fire. Hence, we used 2 wind speed values were tested (0 and 5 km h^{-1}).

The FDS calculations which allowed reproducing the reported fire conditions indicated that a 3MW High Release Rate was reached in the arsonist room reached in 5 min after ignition. Moreover, computational results showed that a wind speed of 5 km h^{-1} was impacting the window with North East direction. Similar investigations on the reconstruction of an arson fire in a psychiatric hospital room performed by SP Swedish National Testing and Research Institute found a HRR of 2.4 MW reached in 9 min.

The results obtained with 3MW HRR and 5 km h^{-1} have demonstrated good prediction of fire development and smoke movement. In particular the upper layer variations for temperature and height as well as the temperature reached in some damaged objects were in agreement with the combustion evidence of the scene description.

SAFETY ISSUES OF HYDROGEN-METHANE UNINTENDED RELEASES AND IGNITION

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This research work is focused on safety aspects connected with use of hydrogen as a fuel and it represents a significant starting point towards an hydrogen economy, safe and ready to be regulated by standards and codes.
In this study methane-hydrogen blends jet flames were analyzed with the aim to characterize their dimensional properties and their interactions with warm surfaces.
Tests of ignition and stability of the flame to several flow rates and different diameters of nozzles were carried out to simulate accidental losses of the system varying operating pressures. In this way pressure drops and discharge coefficients have been characterized.
Different conditions of blends ignition according to the temperature of warm surfaces with different heights as a function of the leakage of the gas from the nozzle were determined.
Images of flames in the visible, infrared and UV regions were acquired and were afterwards computed in order to estimate the length, the width and the morphologic characteristics of flames.
This work only describes the preliminary step of this research in which the visible flame morphology and the conditions of ignitions have been investigated.
The data will supply a technological base for the determination of the entity of the risk connected to unintentional releases in storage and distribution areas of hydrogen eventually mixed to methane or natural gas.

FIRE SCENARIO WHIRLING FLAMES – STABILITY ANALYSIS AND EXPERIMENTAL STUDIES

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Abstract
In the fires, the development of whirling flames (identified also like fire whirls or fire tornadoes, in high intensity cases) is a rare and potentially catastrophic event. In the past, some large dimension fire tornadoes were observed during Chicago Fire (1871), great Kanto earthquake (1923), town fire bombings (Hamburg – 1943, Dresden - 1945) and Peshtigo fire (Wisconsin, USA – 1871) where a fire tornado with diameter and highness values up to hundreds of meters was observed, an area of 6000 km^2 was destroyed, and 1200 ÷ 2500 fatalities occurred. Also recently, a little fire tornado was seen in California (Camp Pendleton - San Diego county, Oct. 2007).
Whirling flames can be developed both outdoor and indoor, and they are caused mainly by great values of HRR (Heat Release Rate) and some ventilation conditions. In such cases, the enhancement of HRR, the large sizes, especially those vertical, and the strong winds in the surrounding areas, are causing significant damages.
In the first part of paper, the physics – mathematical analysis and modelling results are described, while in the second part, the results of experimental testing activities are presented.
The causes of whirling flames formation, development and sustainment, a modelling of some type of whirling flame and a dynamical stability analysis are exposed, with the focus on the link between whirling flame transversal dimensions and fluid motion stability. The role of whirling flames primary mechanisms (a vorticity source; a mechanism capable to amplify this motion; some conditions improving flame rotational motion stability) has been explained, as well as the importance of ventilation conditions to improve motion stability.
The influence of whirling flame shape and transversal dimensions on the rotational motion stability has also been studied by using of dynamical analysis algorithms. Mainly, it is evident that the inverted cone type whirling flames can be frequently stable, and that upright cone type whirling flames are stable only with transversal dimensions smaller than a critical value r^* that is a growing - increasing function of kinematic viscosity υ and angular velocity absolute value $|v_\theta|$ (stabilizing factors), and a decreasing function of radial velocity absolute value $|v_r|$ (unstabilizing factor). Therefore, the fires with high values of HRR and/or angular velocity are more likely to develop whirling flames than other type of fires.
In the second part of paper, the essential results of an experimental activity related to a heptane pool fire inside a natural ventilation room are reported. Such activity was focused on the identification of some ventilation conditions imposing the whirling flame stabilization.
Finally, because of the great uncertainty that characterizes such phenomena, we think that the physics – mathematics analysis and the modelling must be complemented, mainly, by experimental activities and, secondarily, by numerical tool (CFD) analysis, to be really effective to perform good predictive and interpretative analysis (our CFD studies, that are only in a first stage, are encouraging, because FDS code calculation results are reasonably in agreement with the experimental ones, mainly as regards the stable motion of inverted cone type whirling flame).

AN EXPLICIT REDUCED MECHANISM FOR H_2-AIR AUTOIGNITION AND PARTIALLY PREMIXED COMBUSTION

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Abstract

This study aims at developing a single reduced chemical-kinetic mechanism able to describe with sufficient accuracy auto-ignition and partially premixed combustion in hydrogen-air systems at atmospheric pressure.

The so-called San Diego mechanism [1] of 21 reversible reactions is used as a starting point in the chemistry-reduction development. To guide and test the different simplifications introduced, numerical integrations of homogeneous auto-ignition processes, non-premixed auto-ignition processes, adiabatic planar deflagrations and counter-flow diffusion flames are employed. The detailed mechanism is first simplified by noting that 9 elementary reactions, only four of which are reversible, suffice to describe accurately the solution in all of the configurations tested. Further simplifications arise from assuming steady-state assumptions for O, OH and HO_2, leading to a reduced description consisting of two overall reactions. Different truncated expressions are investigated for the steady-state radicals, which, in their simplest form, enable the global rates of the two overall reactions to be written in explicit form in terms of the concentrations of O_2, H_2, H_2O, H, and the temperature.

[1] Available at: http://maemail.ucsd.edu/combustion/cermech.

THE EFFECT OF FUEL STRUCTURE ON THE BURNING VELOCITY OF NAPHTENIC COMPOUNDS

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In order to predict the performances and emissions of modern diesel and HCCI engines, manufacturers couple CFD codes with detailed kinetic models. Therefore, a good knowledge of the kinetics of the fuel oxidation under high pressure is required. To do so, experimental data are needed to constrain these kinetic models. Aromatics compounds are widely found in fuels such as gasoline and gasoil. In the literature, numerous studies dealing with the high temperature oxidation of benzene, toluene, xylenes or light alkyl-benzenes can be found. Nevertheless, it is to be noticed that, very few studies [1-3] are currently available for α-methylnaphthalene which is a reference for determining the cetane number of a gasoil. In this study, the oxidation of α-methylnaphthalene was studied using both the shock tube and the spherical bomb techniques. The ignition delay times at 10 bars were determined in the temperature range 1 200-1 800 K based on OH* radicals chemiluminescence. The effect of equivalence ratio ($0.3 \leq \phi \leq 1$) was tested by both increasing the concentration of oxygen and decreasing the concentration of hydrocarbons in mixtures highly diluted in argon. The results show that the ignition delay times decreases with decreasing equivalence ratios for both constant hydrocarbon concentration and constant oxygen concentration mixtures. Using the spherical bomb method, the laminar flame speeds of α-methylnaphthalene-air mixtures were determined at atmospheric pressure and 403 K over the equivalence ratio range $0.65 \leq \phi \leq 1.30$. The flame propagation was monitored using high speed (4000 i/s) Schlieren visualization. A stretch correction was applied to the data in order to obtain the unstretched laminar flame speed which is an intrinsic property of a fuel. The results show that the maximum burning velocity (50.67 $cm.s^{-1}$) is observed just above stoichiometry ($\phi \approx 1.03$) and then drops sharply as the equivalence ratio increases or decreases. This is in good agreement with what is usually observed for hydrocarbons [4].

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LAMINAR COMBUSTION PROPERTIES OF HYDROGEN / METHANE / AIR MIXTURES

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A cleaner environment and a more efficient use of the energy supply are mandatory in order to meet the more stringent regulations. A more effective use of fossil fuels as well as the development of alternative ones are the road map of the last decade. Among the alternative fuels, hydrogen is one of the most promising energy carrier especially if it is produced from renewable energy. However, in order to make it available to the general public, the safety of distribution as well as combustion must be addressed. The safe use of hydrogen includes a period of transition during which it is distributed as a mixture with natural gas. From an economic point of view, the distribution through the already-used natural gas network of pipelines would reduce the cost and make the transition smooth and fast. However, the natural gas network was designed based on the explosive properties of natural gas, ad from this point of view is very different of hydrogen. So, the effect of adding hydrogen to natural gas on the safety issues has to be studied.

The aim of the present study is to provide experimental data on the combustion properties of hydrogen / methane / air mixtures with a ratio of H_2/CH_4 between 0.5 and 1. The laminar properties of these mixtures have been determined using the constant-volume spherical bomb. The laminar flame speed and the Markstein length have been extracted from the evolution of the radius of the flame as a function of time. The flame was recorded using a Schlieren imaging coupled with a high speed digital camera. The experiments were performed at ambient temperature and pressure for an equivalence ratio ranging between 0.6 and 1.7. Several models from the literature have been used in order to compare the calculated laminar flame velocities to the experimental one. Based on this confrontation, a model was chosen and used in order to derive an activation energy from the variation of the laminar flame velocity with the adiabatic flame temperature. The knowledge of this activation energy is necessary in order to derive the Zeldovich number.

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HIGH-TEMPERATURE DECOMPOSITION OF NITROMETHANE IN THE SHOCK WAVES

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Nitromethane (NM) is the elementary aliphatic nitro compound, and its decomposition represents a great interest for studying of combustion processes and the theory of elementary chemical reactions, since until recently remain some uncertainty in definition of NM decomposition rate constant dependence on temperature and pressure and even in interpretation of a initial stage of the nitromethane decomposition. This stage used to be represented as isomerization of NM in methyl-nitrite with its subsequent decomposition on CH_3O and NO [1].

Our experiments were carried out in a stainless-steel shock tube of 75 mm inner diameter in incident and reflected shock waves. We used the direct absorption spectroscopic technique, described in [2], for monitoring of NM consumption at $\lambda = 230$ nm and yield of NO_2 at $\lambda = 405$ nm. As a light source the powerful pulse xenon lamp of a continuous spectrum was used. In this work observed rate constants at initial stage of the nitromethane decomposition (k_1^{obs}) were measured at T = 1050—1600 K and p = 0.1—40 atm. For minimization of secondary reactions effect on the kinetics of NM decomposition we used the mixes strongly diluted with inert gas and containing 30–5000 ppм of NM. It was found that values of k_1^{obs} obtained by measures of NM consumption or by measures of NO_2 yield, were identical each other both on the preexponential factor and on the activation energy. It proves that decomposition of nitromethane proceeds by detachment of C-N bond, with formation as a primary product of this decomposition a molecule of NO_2. It means that the isomerization of NM in methyl-nitrite as an initial stage of the nitromethane decomposition should be excluded from consideration, so:

$$CH_3NO_2\ (+M) \rightarrow CH_3 + NO_2\ (+M) \qquad (1)$$

The results of computational modeling of our experiments confirms correctness of use this mechanism of NM decomposition and allows to draw a conclusion that observed (k_1^{obs}) constants measured in our experimental investigations of NM decomposition should to be elementary. Besides, obtained in our work six Arrhenius dependences of observed (k_1^{obs}) constants of NM decomposition illustrates that with increasing of pressure values of k_1^{obs} increases on the preexponential factor and on the activation energy from 38 to 53 kkal/mol, that is they are in the pressure falloff region near its lower limit [3, 4]. The ratios of NM decomposition rate constants at low pressure region for various diluent gases was determinate: $k_{1o}(Ar):k_{1o}(He):k_{1o}(N_2):k_{1o}(CO_2):k_{1o}(CF_4) = 1:2:2:3:3$.

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STUDY OF HIGH PRESSURE COUNTER-FLOW METHANE FLAMES

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The optimisation of practical combustion devices requires a detailed knowledge of the combustion kinetics. Moreover, most practical combustion systems operate at pressures well above 1 bar (gas turbines: 15 bars, aeronautic turbines: 40 bars, rocket engines: up to 100 bars), the construction and validation of detailed kinetic models must therefore take into account the influence of pressure. Most combustion kinetic mechanisms have been validated in well-defined laboratory conditions (shock tubes, flow and homogeneous reactors, premixed flames) and are suited for atmospheric or sub atmospheric pressures. However, they can not generally be directly extrapolated towards high pressure, due to the lack of experimental data or uncertainties in the rate constants of elementary reactions. Then, it is necessary to complete the experimental database and to extend the validation domain of combustion mechanisms at high pressure.

Experiments were carried out in a counter-flow burner (two twin burners in an opposed flow configuration) located in a high pressure chamber (pressure range: 1-10 bars) equipped with optical accesses for laser technique (LIF, Absorption, CRDS…) applications. This facility was set-up recently at ICARE-CNRS and it allows the stabilisation of flat (1D) twin-premixed flames and then the investigation of large ranges of equivalence ratios, temperatures and pressures. The main difference with the so-called water-cooled flat flame stands in flames stabilisation by aerodynamic stretch rather than by heat losses to the burner, so that nearly adiabatic premixed flames can be obtained. The second advantage of this configuration is that it allows the resolution of species concentration profiles even for moderately high pressures, which is impossible with a standard flat flame burner because the flame front sits extremely close to the burner surface at high pressure. Furthermore, the two nozzles were defined as aerodynamically converging, by using an empirical equation, so that a uniform velocity profile is obtained at the burner exit and the flame stability is enhanced. This facility will allow the study of different kinds of gaseous mixtures (methane, biogas, syngas…).

In this work, methane was studied because it is the main component of natural gas, generally used in gas turbines. CH_4/air flames conditions were selected to ensure flames stability, and the influence of pressure, equivalence ratio, total flow rate and distance between the two nozzles was considered. Preliminary OH Laser Induced Fluorescence measurements were performed at atmospheric and high pressure. OH has been chosen as its concentration profile in the flame can mimic the temperature profile and then it allows the localization of the flamefronts. Emission spectroscopy measurements have also been performed to interpret visible red emission appearing in the burnt gases region between the flames at high pressure.

DYNAMICS OF A HITAC FURNACE FIRING NATURAL GAS

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Abstract

A semi-industrial 200 kWth furnace equipped with two pairs of regenerative HiTAC burners firing natural gas has been investigated at the research facilities of KTH. Two different firing configurations (parallel and staggered, Figure 1) are compared based on their emissions (NOx and CO) and efficiency (heat flux to the heat sink). Measurements show that in staggered firing configuration more NOx is produced, at constant CO concentrations, compared to parallel firing mode. Moreover, an increased heat flux to the heat sink has been observed in parallel firing mode, at constant furnace temperature.

Besides the continuous measurements (thermocouples, pressure, flow meters), detailed in-furnace temperature and species (O2, CO2, NOx and CO) data has been acquired using a sampling and a suction pyrometer probe. These measurements will be used for validation of simulations, which are performed with a commercial CFD code (FLUENT 6.3). Using the Eddy Dissipation Concept (EDC) model for turbulence-chemistry interaction in combination with the realizable k− model for turbulence, the infurnace measurements have been reasonably well reproduced in non-transient simulations.

Currently, transient simulations are performed. These simulations can give more insight in the regenerative dynamics of the furnace (burner switching).

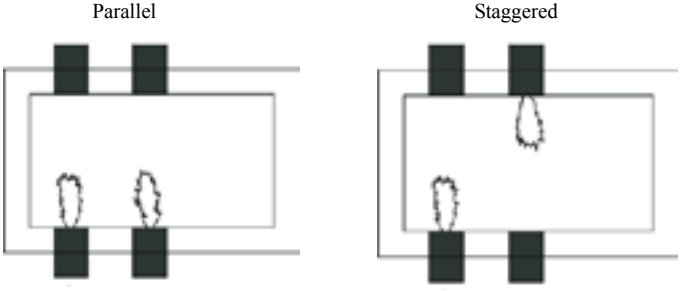

Figure 1: Firing configurations.

Acknowledgement

The European Union is kindly acknowledged for the financial support in the framework of SUSPOWER.

HYDROTHERMAL PROCESS FOR HYDROGEN ENERGY PRODUCTION

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The use of the biomass as a biofuel is a controversial topic because of the competitive use of the same resource as human or animal food. However, organic materials coming from various wastes could be used in place of biomass to avoid various ethical problems. Heterogeneous biomass waste of low calorific value (such as agricultural biomass residues) can be converted using supercritical water (SCW) processing into biofuels and hydrogen for their further application *via* combustion in burners, engines or gas turbines.

The main goal of the project is to optimize the biomass decomposition process in SCW to form hydrogen fuel. Studies of the SCW dissolution, hydrolysis, and oxidation of pure substances in a hydrothermal diamond anvil cell (HDAC) have been completed by Sobhy *et al* [1] and Fang *et al*. [2]. Unique results concerning homogeneous dissolution of naphthalene, cellulose & glucose in SCW were obtained, revealing the possibility of using pure substances as a co-fuel in generating SCW flames. These studies have proved the proposed concept.

The current investigation has been carried out for samples representing real biomass (effluent and winegrape slurry, see Table 1, which are winery residues) rather than pure substances. The variety of molecules composing winery wastes makes it difficult to determine details of the decomposition process. Nevertheless, unique technique applied towards visualization of the process offered initial explanations.

Winery wastes have been decomposed in SCW producing gas and a solid phase residue. The composition of the solid phase depends of the chemical composition of the sample and the level of concentration. Current results indicate that wastes coming from agricultural industries can be converted into fuels (including hydrogen). Thus, the valorization of wastes *via* replacing their disposal by SCW conversion into biofuel/H_2, could become important for selected practical applications.

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Table 1: Sequence of images extracted from the recorded decomposition of a small amount of winegrape slurry.

Visualization of the reaction hole							
Time from the beginning of the heating (s)	0	6	10	15	19	29	33
Medium Temperature (°C)	25	25.5	31	84	130	244	311

							
38	43	46	51	56	73	111	150
350	398	451	475	496	503	479	38

THE CONTROL OF PROPANE COMBUSTION BY PULSED-PERIODIC CO_2-LASER RADIATION

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Development of laser technics and technologies has enabled application of local zones of energy release to control gasdynamics of flows, including reactive ones. Presence of high, up to breakdown, radiation power densities may cause not only change of gasdynamic flow pattern, but also, in certain cases, change of kinetics of burning process.

In this work, the results of investigation of focused pulse-periodic CO_2-laser radiation exposure on formation and development of flame distribution process in a flow of homogeneous propane-air mixtures are presented. Various fuel mixtures and conditions of laser action are considered. It is established that at formation of optical discharge (OD) in a stream the flame propagation velocity increases and stability boundaries on velocity and a mixture composition expand. It is shown that at combustion stabilization by OD there is no change of the flame distribution mechanism what proves to be true by a type of dependence of turbulent flame velocity on the physicochemical properties of mixture and coefficient of turbulent exchange, characteristic for representation of this interrelation. In conditions without optical breakdown of medium, as the analysis results of the experiments have shown, the velocity of a turbulent flame is approximately by 25 % higher as compared to ignition by the optical pulsing discharge.

Influence of pulse-periodic CO_2-laser radiation (without OD) on ignition and combustion processes at the laminar and turbulent flows of homogeneous mixtures of propane with air is experimentally investigated. Experiments were carried out with different ways of flame stabilization: on an edge of a glass tube (a Bunsen burner) with parabolic profile of mix speed and the separation zone formed behind the central body located on the nozzle axis of a burner unit with uniform profile of fuel-air mixture flow rate. For these regimes conditions of ignition and flame blow off, the flame form, normal and turbulent flame propagation velocity, total radiation on lines of reaction intermediates (CH, C_2 and OH) and ignition delays depending on composition, speed and temperature of an initial mixture and parameters of laser radiation are investigated. It is established that total radiation of reaction intermediates does not depend on initial temperature of a mixture and does not change under the action of laser pulse energy. It is shown, that the basic influence on burning rate and deformation of the formed flame front it is related to the thermal effect caused by absorption of a part of energy of laser radiation (LR).

Local absorption of pulse-periodic laser radiation energy by reactive medium leads to a local heating up of a mixture what is defined by efficiency of absorption processes depending on mixture properties and parameters of LR. On the other hand, the mechanism of decrease in an induction period of the ignition occurs, caused by weakening of intramolecular bonds (activation energy decrease) because of transition of a part of fuel molecules into excited mode. The estimation of the thermal effect contribution (from the part of LR energy absorbed by reacting medium) and influence of possible change of kinetic properties of a mixture on formation of the nucleation site for ignition and the flame surface was carried out by comparison of calculated ignition delay periods with the data registered in experiments. On the basis of calorimetric measurements of the power absorbed by a propane-air mixture, estimations of the temperature level in a LR absorption zone are made. For these temperatures calculations of spontaneous ignition of a mixture have been carried out. It is shown that LR ignition is different from thermal spontaneous ignition.

The work was supported financially within the framework of Russian Foundation for Basic Research (grants No. 08-01-00582-a).

EXPERIMENTAL CHEMISTRY AND COMBUSTION SYNTHESIS IN MICROGRAVITY, LUNAR-GRAVITY AND MARS-GRAVITY FLIGHT CONDITIONS

Doct. Eng Carlo Viberti

Experimental chemistry in low-gravity conditions as well as in weightlessness represent a relatively new research area which can largely benefit from low-cost testing on board parabolic flights.

On board the SpaceLand "flying laboratory" science users can drastically accelerate research, analysis, design, development, testing and qualification of equipment, systems, methodologies and processes related to all gravity-dependent chemical-physical phenomena.

In particular, cutting-edge experimentation can be carried out on such flights to address weightless and low-gravity related disciplines on chemical processes such as, for instance:
1) combustion synthesis in microgravity for, e.g., the development of advanced materials such as new metal powders and net-shape articles featuring exceptional thermal-mechanical properties
2) macro-crystal growth for three-dimensionally-perfect macromolecular compounds
3) low-gravity chemical processes for the so-called In-Situ-Resource-Utilization (ISRU) and In-Situ Fabrication and Repair (ISFR) related to on-going and future Moon and Mars exploration programs.

Multiple experimental sessions on such research areas can be carried out on board the SpaceLand flying lab without having to cope with those large investments proper of space research missions, also benefiting from the unique possibility provided by this parabolic-flight-test methodology to rapidly access, reconfigure and reiterate the experimental set-up to optimize the respective test programs.

Since 2005, taking off and landing using the NASA Space Shuttle L.F. at Cape Canaveral, such opportunities provide flexible, quick experiment-turn-around operating modes to enable the science community to carry out experimental tasks in so-called "Moon-gravity" and, respectively, "Mars-gravity" flight conditions as well as, depending on the user requirements, in total weightlessness.

Such experimental missions are possible thanks to the particular parabolic flight profiles flown by an adapted Boeing 727-200 aircraft, authorized by the USA Federal Aviation Administration, used to fly parabolas which can be dynamically smoother than the standard zero-gravity flight pattern, in order to compensate only partially the gravitational force acting on the aircraft such as to generate, for all the experimental hardware installed on board, low-gravity levels reproducing the gravitational fields proper of the mean gravity levels on the surface of the Moon and, respectively, Mars.

This poster shall provide detailed information on the on-going activities in this respect together with a comprehensive outlook on the upcoming research flights which shall be carried out to support cutting-edge experimental work by some of the best experts in the above mentioned chemical fields.

FUEL LOAD PREDICTION IN BURNED AND UNBURNED MEDITERRANEAN MAQUIS

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In several European countries, fuel load estimation is still a relevant issue that needs to be addressed, in order to improve effectiveness of wildland fire prevention and management. Mediterranean maquis is characterized by high complexity and structural heterogeneity. In addition, fuel type and fuel load are strongly affected by both long and intense human impact on vegetation and recurrent occurrence of fire. Therefore, in order to quantify the main characteristics of fuel by collecting field data, the above mentioned factors must be taken in consideration. Design the sampling units needs to capture the field variability of fuel type due to the species composition and the effect of the anthropogenic disturbances (fire, grazing, etc.).

The general aim of this study was to analyze the main structural characteristics of Mediterranean maquis in order to define several non-destructive parameters able to predict fuel load for the different fuel classes.

In the first phase of this study, in several sites located in North-western Sardinia (Italy), the height of vegetation and the cover percentage were measured in burned and unburned plots. All phytomass inside the plots was collected, separated in live and dead fractions, and partitioned into diametric classes according to stem diameter: 0 to 0.6 cm (fine fuels), 0.6 to 2.5 cm (medium branches), and 2.5 to 7.5 cm (thick branches). Subsequently, a correlation matrix between fuel complex properties (shrub's height, cover, and the product of height and cover) and fuel load components (live and dead at 1hr load, total available shrub load, total shrub load) was built and the relationship between these variables were investigated. The analysis was carried out for all the sampling plots, whether recently burned or not. The most significant relationships provided by the correlation matrix were used in order to perform regression analysis and to establish the physical properties of fuel that best explained the variance of the different fuel load components.

Experimental results showed high presence of the fine live component (green leaves and fine woody) in all the burned and unburned sites: overall mean value of about 35% of total fuel load. Fine dead load represented the 10% of the total fuel load. The results from the correlation matrix showed that the parameter "*height multiplying cover*" appeared to be the most strongly correlated with fuel load components, except for dead fine fuel load. The regression analysis confirmed that "*height multiplying cover*" accounted for a significant amount of variance of the load variables, but the values of R^2 were higher in the burned sites than in the unburned sites. The results are in agreement with those published by other authors, and are encouraging for a future development of a non destructive index to quantify fuel load.

EXPERIMENTS USING A COUPLED ATMOSPHERIC-FIRE MODEL

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The proposed approach of wildland fire simulation combines discrete event simulation (Zeigler 2000), front tracking (Glimm et al.1996) and a Meso-scale atmospheric model (MesoNH). Front tracking methods are used to study interface or boundary dynamics. In front tracking, phenomenon behavior is represented by a polygon, which is the discrete view of the continuous front system. Using this schema ensures that there is no « ghosting » effect and a total independence over time steps.

The atmospheric model, Meso-NH is the non-hydrostatic mesoscale atmospheric model of the French research community. The model is intended to be applicable to all scales ranging from large (synoptic) scales to small (large eddy) scales and it is coupled with an on-line atmospheric chemistry module.
The forest fire front tracking model is running as a sub-mesh model in Meso-NH. The coupling is done at each atmospheric time-step. Coupling between the fire spread and atmospheric model is done through wind fields of the first atmospheric level.
Coupling between the atmosphere and the fire model is done through total heat and water vapour flux. A burning raster is generated at every step from the front-tracking propagation model. To generate the heat flux raster input, the same raster is normalized by the local fire heat flux (set at 1500Kw/m² for shrubs).

Simulations have been performed on a 1km by 1km area, with a 25 meters atmospheric resolution and a 1m front resolution. Simulation time is about 2 hour for 1hour of fire propagation on a cluster of 4 processors. Results, in case of a 15% slope and a 100m wide line ignition, show that the fire spread and fire regime is heavily influenced by feedback from the atmosphere, with winds accelerating about an order of magnitude faster than the ambient wind near the front. In terms of rate of spread, the coupled model shows that strong acceleration can occur before a steady rate can been reached. Moreover, simulated fronts show local deformations that are typical of a real wildfire front (swirls near the fire head). Both these local acceleration phases are and local deformations are impossible to simulate using conventional reduced fire spread model because those model prognoses directly a steady rate of spread that is used to force front advance, resulting in typical ellipsoids shapes.

The fire plume is reaching an altitude of 800 meters that is comparable to a large wildfire in case of constant wind and simple topography. Further enhancements are planned to perform simulation with the chemistry module in order to investigate fire smoke and particle transport. Eventually, reanalyses of real fire accidents will be necessary to fully validate the approaches, requiring the use of super computing facilities.

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FLAME STRUCTURE MODELING IN FOREST FIRES

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Abstract

The knowledge of flame structure is a key issue when evaluating forest fire behavior for prevention and suppression management. Flame geometry, thermal and flow characteristics are needed as input variables in many sorts of fire studies; i.e. to compute heat transfer mechanisms, crown fire activity, fuel-breaks efficiency, suppression effectiveness, etc. Also, flame structure has to be very well described to validate the new generation of fire behavior CFD-type prediction models that are being developed. This work in progress presentation wants to summarize the work done in flame modeling applied so far to forest fires and to present the on-going efforts at empirical and physical level that CERTEC is devoting to reach in a near future the goals set in this subject. We are distinguishing here two different approaches depending on whether flame modeling is based on spreading fires or on stationary fires.

Flame modeling of spreading fires has been generally performed through semi-empirically or empirically based approaches, particularly when dealing with flame geometry. This has lead to environment dependent flame models, i.e. models restricted to particular fuel complexes and narrow meteorological conditions. In this sense, an extensive collection of experimental data by which these models have been developed and validated has been gathered. A deep exploratory analysis has been performed to detect gaps in terms of fuel and experimental conditions. Following, the models have been evaluated undertaking the corresponding analysis concerning conceptual validity, sensitivity and predictive validation. The final objective of this study is to integrate pre-existing efforts proposing an empirical flame model system with a global scope, i.e. workable in a wide range of fire situations. Results obtained up to now and future steps are presented.

Regarding stationary fires –i.e. fires that represent for instance static or very slow spreading flame fronts or torching fires in isolated fuel clumps–, they have been studied either using empirical or theoretical approaches. Furthermore, CFD numerical simulations have been already shown its great potential to study this type of fires. Some significant contributions have been already done in terms of flame dimensions and thermal characteristics. Here we briefly present our results already obtained through stationary fires experiments –both at laboratory and field scenarios– and we give some bullet points of the idealization phase of a theoretical model that shall be performed in following stages of this work.

STUDY ON FOAMABILITY AND EXTINGUISHING POWER A NEW COMPOSITION OF WETTING AGENTS FOR FOREST FIRE FIGHTING

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The aim of this work was to formulate and optimize the foaming and extinguishing performance of an alkylpolyglucoside-based wetting agent. The liquid composition was formulated with ingredients of commercial origin: anionic (fatty alcohol C_{12}-C_{15}ethoxy sodium sulphates), nonionic (C_8–C_{10} alkylpolyglucoside, oxyethylenated synthetic fatty alcohol C_{13}-C_{15},). The purpose of this study was to determine the foaming power and fire extinguishing time for commercial wetting agent and mixture of the basic components of the new wetting agents intended to fight with forest fires. Extinguishing fires of forests is a serious problem for fire brigades since vast areas can be involved in a relatively short time.

The wetting agents are the mixtures of numerous components, inclusive of surfactants, which are water-soluble and which lower the surface tension value of aqueous solutions, and hence the wettability of solutions on hydrophobic surfaces is improved. When added to water, those compounds improve its fire extinguishing properties, and thus improve efficiency of rescue actions. The purpose of tests and search for new agents is certainly development and implementation of the best and most effective arrangements. Efficiency of wetting agent is a function of the concentrations and types of the active ingredients that are delivered into the solution.

The foam achieved by solutions of commercial wetting agent and new surface-active composition, in a concentration 1.0% (v/v), prepared using municipal water were also compared.

Scientific work financially supported from MNiSW funds reserved for science in years 2007-2010, as a research and development project R00-O0046/03.

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Réalisation : Eleven Design - www.eleven-design.fr - 04 95 35 43 39
Imprimé par Exaprint

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