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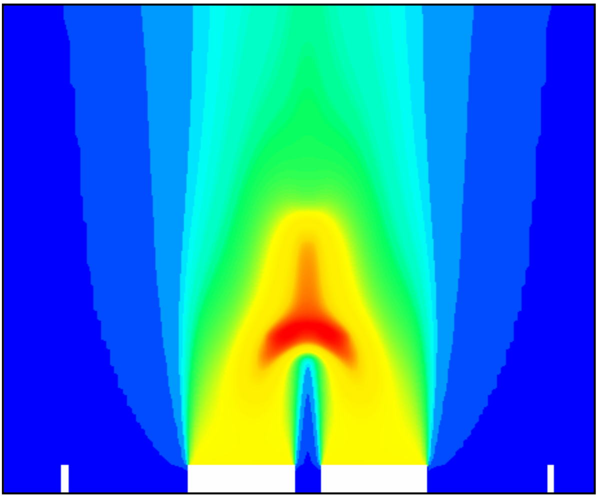

Chemical Kinetics & Diffusion Processes in Reactive Flows

İstanbul Technical University

Organizer : İ. Bedii Özdemir

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CONTENTS

FOREWORD

Attempts to increase the efficiency of combustion processes typically occurring in propulsion and power generation devices, such as internal combustion engines or gas turbines, while complying with the current emission regulations require a detailed examination of the unsteady reactive flow phenomenon. However, numerical simulations of the three dimensional reactive flow processes occurring on the molecular levels and large scales exhibit a challenging task. Even though considerable advancements have been acquired in the field of computer knowledge, it is still difficult to perform simulations of the turbulent flow field for all length and time scales or to get the information about the chemical kinetics by tracking all the elementary reactions and species involved in those reactions. Thus, simulations to understand the finer details of unsteady interactions of different processes are faced up with three major difficulties; need for resolving the turbulent flow field, chemical kinetics and the interaction of both processes. This needs an interdisciplinary research combining chemical, mathematical, computer and mechanical engineering.

The objective of the current workshop is to provide an opportunity for researchers to discuss and exchange the knowledge of integrated models in the areas of chemical kinetics and of turbulent flow simulations. To accomplish this goal, experts from different disciplines working on the development of simplified models are invited into the workshop to deliver lectures on the optimization of new concepts for unsteady reactive flows. In addition, poster contributions are presented.

I acknowledge the financial support from Scientific and Technical Research Council of Turkey (TÜBİTAK), İstanbul Technical University, Mercedes Benz and Zorlu Enerji. Finally, I thank all participants for their valuable scientific contributions.

Prof. Dr. İ. Bedii Özdemir

INVITED SPEAKERS

Prof. Dr. Frank Behrendt
Prof. Dr. John Buckmaster
Prof. Dr. Robert Dibble
Prof. Dr. Sergei Fedotov
Prof. Dr. İskender Gökalp
Prof. Dr. Ömer. L. Gülder
Prof. Dr. R.Peter Lindstedt
Prof. Dr. Ulrich Maas
Prof. Dr. Wolfgang Polifke
Prof. Dr. Uwe Riedel
Prof. Dr. Jürgen Warnatz

LOCATION

Süleyman Demirel Congress Center
ITU Maslak Campus.

Süleyman Demirel Kültür Merkezi
İstanbul Teknik Üniversitesi
Ayazağa Kampüsü
Maslak / 80626 İstanbul

PROGRAM

Monday 07.06.2004

09^{15}-09^{30}	Welcome
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09^{30}-10^{30}	Prof. Dr. Jürgen WARNATZ Detailed Reaction Mechanisms for Hydrocarbon Oxidations and Problems Involved
10^{30}-11^{00}	Coffee Break
11^{00}-12^{00}	Prof. Dr. John BUCKMASTER False Kinetics – Triumphs and Troubles
12^{00}-13^{30}	Lunch Break
13^{30}-16^{00}	Afternoon Sessions Chair: Prof. Dr. Ulrich MAAS
13^{30}-14^{30}	Prof. Dr. R. P. LINDSTEDT The Modelling of Finite Rate Chemistry Effects in Turbulent Flows
14^{30}-15^{00}	Coffee Break
15^{00}-16^{00}	Prof. Dr. Robert DIBBLE Numerical Modelling and Experiments in HCCI Engines
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11^{00}-12^{00}	Prof. Dr. Wolfgang POLIFKE Monte-Carlo Methods for Tabulation of Mean Reaction Rates from Joint Probability Distributions in Turbulent Flow
12^{00}-13^{30}	Lunch Break
13^{30}-16^{00}	Afternoon Sessions Chair: Prof. Dr. John BUCKMASTER
13^{30}-14^{30}	Prof. Dr. Sergei FEDOTOV Stochastic Mixing Model with Power Law Decay of Variance

14^{30}-15^{00}	Coffee Break
15^{00}-16^{00}	Prof. Dr. Ömer L. GÜLDER Hydrogen-enriched Lean-premixed Flames
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Wednesday (09.06.2004)

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11^{00}-12^{00}	Prof. Dr. Uwe RIEDEL Modeling and Simulation of Plasma-Assisted Reactive Flows
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Detailed Reaction Mechanisms for Hydrocarbon Oxidation and Problems Involved

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The knowledge of detailed reaction mechanisms is of extreme importance for the understanding of combustion, e. g., in turbines, engines and furnaces and the design of these devices. In special, reaction kinetics dictate ignition delay times and flame velocities which have to be compared with residence times to guarantee stable combustion. Furthermore, the formation of pollutants (NO_x and soot) cannot be understood without detailed know-how on reaction mechanisms.

Fuels like kerosine are too complex to understand their oxidation, but can be represented by simple two- or three-component mixtures (consisting of aliphatic hydrocarbons like decane and of aromatic hydrocarbons like benzene derivates) which are tuned to have the same flame velocity and ignition behavior and the same soot formation tendency as kerosene has.

Whereas the mechanisms of large aliphatic hydrocarbons can be computer-generated, the reaction mechanism of small aliphatic hydrocarbons is known from direct kinetic studies of the elementary steps involved. Aromatic species are consumed first by oxidation of the side chains, which is similar to the corresponding reactions of aliphatic hydrocarbons, and subsequent slower oxidation of the aromatic core.

Whereas the formation of NO_x is relatively well known, formation and oxidation of soot are very complex and not understood due to the fact that huge reaction mechanisms have to be considered and not only gas-phase, but additionally surface reactions have to be included.

Examples are given for all points considered above, and the problems involved are discussed in detail.

False kinetics – triumphs and troubles

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In recent years there has been a great deal of important work on constructing simplified kinetic schemes via rational strategies, rooted in the fact that some reactions are much faster than others. Prior to this work, the only way to define simple schemes was to use false kinetics, kinetics that is consistent with global requirements – fuel and oxidizer are consumed, heat is generated – but does little or nothing to reflect the behavior of the individual species. This strategy is still of great value, and my talk will examine its role in a number of recent applications. One of the applications reveals a difficulty that may not be widely known.

One of the applications that I shall discuss is that of edge-flames, specifically small Lewis number premixed edge-flames that display cellular instabilities. For this problem, 1-step kinetics for a single deficient component (one therefore that is completely consumed in the reaction zone) can, in the context of a simple counterflow model, properly capture the rich qualitative behavior that occurs experimentally.

The second application is also connected with edge-flames but in the context of smolder – smolder-edge-waves. Early studies of reverse smolder (akin to a deflagration) assume that the structure is always fuel-rich, and a 1-step model for a single reactant (oxygen) suffices. However, this hides important physics – when fuel-lean solutions are constructed (then 2 reactants are accounted for) extinction occurs should the flow of air be large enough, consistent with experiment. Because of this 1-D extinction, interesting edge-wave structures can arise in the neighborhood of the critical blowing velocity, and I shall describe these.

The third application is in the modeling of heterogeneous solid propellant combustion. My colleagues and I at the University of Illinois have constructed a sophisticated unsteady 3-D code for this problem, specifically constructed to examine ammonium perchlorate (AP) in fuel binder propellants. In our earlier work we use 2 1-step kinetics equations for 2 reactants: decomposition of the AP; reaction of these decomposition products with binder gases. Since solutions constructed in this way are not as accurate as we wish, we have recently added a third reaction, one between AP gases (prior to decomposition) and binder gases, which supports what is known in the propellant literature as the primary diffusion flame. In general, better accuracy is achieved in this way, but for certain operating conditions a spurious instability is displayed, and this can have a significant impact on the mean burning rate. It is far from obvious how this difficulty can be circumvented.

The Modelling of Finite Rate Chemistry Effects in Turbulent Flames

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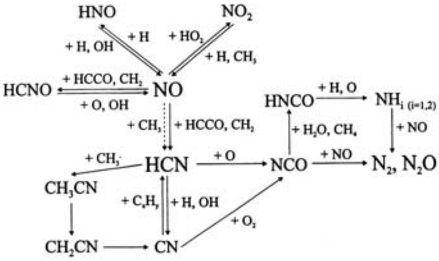
The classical "fast chemistry" analysis by Damköhler remains a common basis for calculation methods aimed at turbulent reacting flows. Perturbation approaches can be used to introduce finite rate chemistry effects, particularly where a distinct chemical time-scale separation is present, though more comprehensive techniques, e.g. based on a transported joint probability density function (JPDF), are typically required. Potential difficulties with the JPDF technique include issues related to the intrinsic structure of turbulent flames, particularly at low Reynolds numbers, and models for molecular mixing. The ability to predict the formation of NO is particularly interesting in this context given the strong sensitivity to chemical kinetic and non-adiabatic effects. The current lecture provides an assessment of uncertainties in the formation chemistry of NO in the context of quantitative measurements, obtained in non-premixed laminar methane/air counterflow flames using ps-LIF, and subsequently explores how these translate to turbulent flames. A consistent systematically reduced (16 independent, 4 dependent and 28 steady state scalars) reaction mechanism is applied to model the turbulent flames of Barlow and co-workers. The highest Re number flame considered permits an investigation into the ability of the transported JPDF technique to deal with emissions of nitric oxide in flames close to global extinction. The work shows that the technique has the potential to reproduce NO levels and conditional PDFs under conditions with significant local extinction/re-ignition to within the uncertainties associated with the principal elementary reaction steps. Further examples of the modeling of extinction and re-ignition will also be given along with an assessment of sensitivities to model parameters.

Results

Recent work on laminar and turbulent flames (Lindstedt et al. 2004) indicates that the rates for the prompt NO formation determined by Dean et al. (1991) and Miller & Walch (1997) bracket current uncertainties when combined with the detailed chemical mechanism of Lindstedt and co-workers (1998). Typical results for laminar flames are shown in Figure 1, which also outlines the dominant reaction channels for nitric oxide formation and destruction in diffusion flames. One objective of the current lecture is to explore how such uncertainties in chemical kinetics translate to computed NO levels in turbulent flames. To this effect, calculations corresponding to the experimental data of Barlow and co-workers (2000) have been performed. The conditional statistics of scalars presented below are defined as the mass-weighted means of any scalar variable Y_ϕ conditioned on f = ψ by $<\rho Y_\phi \mid f = \psi>/<\rho>$, where ψ is the mixture fraction sample space. At a specific axial location, the conditional means are extracted by consideration of all Lagrangian particles that lie in the single strip of cells in the radial direction centered on that location. In the experiment, the conditional means are constructed in a similar fashion from data at all radial locations. A total of 40 bins in mixture fraction space are used for this calculation. Figure 2 shows the evolution of the NO mass fraction in mixture fraction space for Flame D respectively. The overall agreement is very satisfactory and the two rate determinations essentially bracket the experimental data. Arguably, the rate determination of Miller & Walch (1997) results in better agreement with experimental data. However, predictions tend to be a bit on the low side which is consistent with the work in laminar flames. Other thermochemical uncertainties may well influence the current finding and quantitative determinations of CH radical concentrations would be very beneficial. Scatter plots of NO mass fraction versus mixture fraction at x/D = 15, 30 and 45 are presented in Figure 2b for Flame D with the predictions featuring the rate of Miller & Walch (1997). Laminar flamelet data obtained with the same mechanism used in the laminar flame calculations shown above are also shown for two rates of strain $a = 20\ s^{-1}$ and $a = 400\ s^{-1}$. The higher value corresponds to a flame approaching extinction. The laminar flame calculations feature an equal diffusivity approximation and the 25% CH_4/75% air fuel stream of the equivalent turbulent flames. The results suggest that the flames are subject to high rates of strain and that significant departures from the steady-state flamelet approximation are present. Further examples, including conditional PDFs, will be given during the lecture. The lecture concludes that for the turbulent flames under consideration, predictions of oxides of nitrogen are primarily linked to the level of accuracy in the chemical closure rather than other factors (e.g. differential diffusion effects) and that uncertainties in the chemistry arguably translate quantitatively. In particular, the formation rate for the prompt NO channel has been shown to be of paramount importance and results obtained are consistent with those observed in laminar flames.



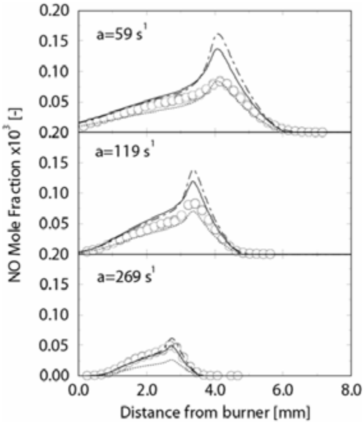


Figure 1. (a) Major NO formation and destruction pathways in laminar diffusion flames featuring methane combustion. (b) Predictions of NO concentrations at 3 rates of strain. The symbols represent experimental data (Barlow and co-workers 2000) and the lines predictions obtained with the rate of Dean et al. (1991) (solid line) and Miller & Walch (1997) (dot-dashed line).

Figure 2**.** The downstream evolution of the NO mass fraction for Flame D. The symbols represent experimental data (Barlow and co-workers 2000) and the lines predictions obtained with the rate of Dean et al. (1991) (solid line) and Miller & Walch (1997) (dot-dashed line). The scatter plot on the right also shows imposed corresponding laminar flamelet solutions for two rates of strain.

Acknowledgement

The contributions of Volker Sick and Sofia Louloudi to the current lecture are gratefully acknowledged.

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Numerical Modelling and Experiments in HCCI Engines

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HCCI is a combustion process that has some advantages with respect to both spark-ignited engines and diesel engines. HCCI combustion has been identified as a global autoignition process. This is significantly different to the flame propagation that occurs in a SI engine, and it is also very different to the stratified combustion of diesel engines. Considering the great differences between these combustion processes, it is natural to expect that the fuels that have been optimized for SI engines and diesel engines may not be optimum for HCCI engines

The paper also includes a ranking of many potential additives. Experiments and analyses have indicated that small amounts (a few parts per million) of secondary fuels (additives) may considerably affect HCCI combustion and may play a significant role in controlling HCCI combustion. Additives are ranked according to their capability to advance HCCI ignition. The best additives are listed and an explanation of their effect on HCCI combustion is included.

Hierarchical Models for Chemically Reacting Flows

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Reactive flows are governed by complex interplay of chemical reaction, flow and molecular transport. They can be described mathematically based on conservation equations for mass, momentum, energy and species masses. These conservation equations form a large system of stiff partial differential equations and, therefore, their solution is a great challenge.

The description of chemically reacting systems leads very often to reaction mechanisms with far above hundred chemical species (and, therefore, to more than a hundred partial differential equations), which possibly react within more than a thousand of elementary reactions. These kinetic processes cover time scales from nanoseconds to seconds. An analogous scaling problem arises for the length scales. The scales of technical systems may be several meters, and on the other hand, typical reaction zones or small turbulent structures have length scales of the order of millimeters. Due to these scaling problems the detailed simulation of three-dimensional turbulent flows in practical systems is beyond the capacity of even today’s super-computers. Using simplified sub-models is a way out of this problem. The question arising in mathematical modeling of reactive flows is then: How detailed, or down to which scale has each process to be resolved (chemical reaction, chemistry-turbulence-interaction, molecular transport processes) in order to allow a reliable description of the entire process. The aim is the development of models, which should be as simple as possible in the sense of an efficient description, and also as detailed as necessary in the sense of reliability. In particular, an oversimplification of the coupling processes between chemical reaction and turbulent flow should be avoided by all means to allow a predictive character.

In the presentation it is shown how hierarchical concepts can be used to solve this problem. Two examples are presented, namely a dimension reduction of the system of conservation equations based on the concept of ILDMs (intrinsic low-dimensional manifolds in composition space) and a hierarchical description of the chemistry-turbulence interaction using a combination of direct numerical simulations and statistical models for the turbulent flow based on the solution of a transport equation for the joint probability density function of velocities and scalars. In these concepts information about processes on the smallest time and length scales enters the global models. Different examples show, that such hierarchical concepts allow a reliable description of reactive flows.

Monte-Carlo Methods for Tabulation of Mean Reaction Rates from joint Probability Distributions in Turbulent Flow

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New methods have been developed to compute and tabulate mean reaction rates by use of probability distributions, taking into account also correlation between the involved properties. Tables can be used to obtain reaction rates for the simulation of turbulent reactive flows within the framework of usual RANS based CFD codes. Further on, this method can be used to model the FDF (Filtered Density Function) in an LES computation.

Determining turbulent mean reaction rates is in general not possible by evaluating only mean quantities, since reaction rates behave strongly non-linear in terms of species mass fractions and temperature. Often PDF (Probability Density Function) approaches are used to compute and tabulate turbulent mean rates:

$$\overline{\dot{\omega}} = \int_{T_{\min}}^{T_{\max}} \int_0^1 \cdots \int_0^1 \dot{\omega}(T, Y_1, \ldots, Y_n) \cdot P(T, Y_1, \ldots, Y_n) \cdot dT dY_1 \ldots dY_n$$

Two PDF methods one can distinguish between, namely transported PDF's and presumed PDF's. For transported PDF's, solving a high dimensional transport equation is necessary, which is not yet practical for industrial applications. More common is the use of presumed shapes for the PDF's, like Gaussian or ☐- distributions. For reactions, which depend only on one quantity, good results can be obtained, but due to a lack of meaningful functions for joint PDF's (PDF's of two and more quantities) joint PDF's have to be split up into several single variable PDF's by neglecting correlations between the flow quantities involved. In 0 it has been shown that neglecting correlations can result in significant errors

. The new proposal does not make use of an analytical form of the PDF. Instead a distribution is generated with a biased random number generator, making it possible to satisfy not only physical constraints of the involved quantities (e.g. for mixture fractions 0 ≤ f ≤ 1 and ☐ fi = 1), but also existing correlations between the quantities. Mean reaction rates can be computed by conventional sample averaging over all particles.

Methods to generate distributions

Several methods have been investigated during the development of this approach. The first method starts from already known distributions, like the multivariate Gauss or Uniform distribution. A random number generator is started to create the basic distribution with given means and (co-)variances of the involved properties. Due to the physical restrictions of the problem, e.g. $0 \leq f \leq 1$ and ☐ fi = 1, some realizations will be invalid and must be corrected. In general, invalid realizations are manipulated and shifted towards the physical boundaries. With this method it is possible to obtain unimodal as well as bimodal distributions. Correction methods are described in more detail in 0 and 0. After generating the distribution, mean reaction rates can be computed with the discretized form of eq. 1.

The second method starts with some ☐-peaks at the physical boundaries of the problem, which are smeared out applying a mixing model like e.g. IEM or Modified Curl 0. First the state field is initialized at some suitable positions with ☐-peaks, whereat the height of the ☐-peaks has to be adapted to the desired mean values of the distribution. This basic distribution represents e.g. the first stage of a mixing process, where largest variances could be observed. After selecting some realizations, their values will be changed by applying a mixing model, which reduces the variances, whereas means retain. A certain covariance between the parameters can be achieved by a suited selection method. Reaction rates are computed after each mixing sequence and stored together with the actual values of the variances for further processing.

Results

Figure 1 shows scatter plots and marginal PDF's of the mixture fraction fFU for distributions generated with the described methods. All distributions have the same means and variances. The marginal PDF is the projection of the jointPDF into direction of fFU. Distributions generated from a basic Gaussian and Uniform distribution look very similar, since many realizations have been corrected. Since the basic uniform distribution is more block shaped the broadness of the marginal PDF obtained with the Gaussian random number generator is slightly smaller. A complete different shape can be obtained with the IEM method. Correlation is not as strong as for the other distributions, showing the need to develop a suited selection method. For comparison, a scatter plot from a LES run is shown, showing a less broad distribution and therefore a strong negative correlation. It has to be mentioned that for very large variances the distributions become even more different.

To investigate the impact of distribution shapes on reaction rates, a simple reaction model for self-ignition has been implemented. Mean rates of an ignition progress variable are computed for each distribution and printed into the scatter plots. Deviations between the Gaussian and the Uniform distribution are within the tolerance and agree well with the rates from the LES distribution. Larger deviations can be observed by comparison with results obtained with the IEM method. CFD computations, performed with the Gaussian and the Uniform method, show very similar results. Computations with the IEM method are outstanding.

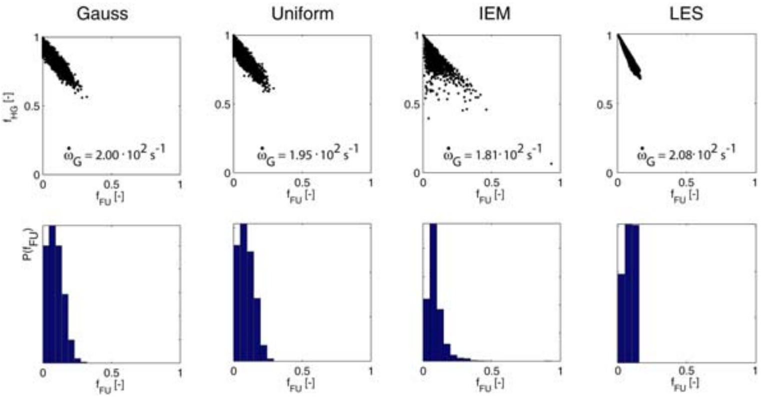

Figure 1: PDF’s of the distributions generated with different methods and from a LES computation.

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Stochastic mixing model with power law decay of variance

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The mixing of a conserved scalar c(t,x) advected by a turbulent flow remains a problem of both fundamental and practical interest. One of the basic characteristics of the mixing process is the rate at which the scalar variance $\sigma 2(t) = <(c- \mu)2>$ decays with time (μ is the mean value, and the angular brackets denote an averaging procedure). There are two different laws governing the decay rate of a passive scalar: (i) the exponential law, $\exp(-t/\tau)$, with the characteristic time τ and (ii) the power law, t-α without any characteristic time scale (Lesieur (1997)). One of the simplest and widely used mixing models is the interaction by exchange with the mean (IEM). Other mixing models are Curl model, mapping closure, Fokker-Planck model, Euclidean minimum spanning trees, Langevin model, etc. Reviews of these can be found in (Peters (2000); Pope (2000)). Most theoretical models introduce a characteristic time scale and assume implicitly or explicitly the exponential decay rate which is only appropriate for stationary turbulence.

The main purpose of this work is to study the mixing process following the power law, $\sigma 2(t) \sim t$-α, which is typical for decaying turbulence. Experimental results show that the decay exponent α strongly depends on the initial ratio of the velocity and scalar length-scales and that there is no universal decay exponent (Durbin (1982)). Here we present a stochastic mixing model based on the law of large numbers (LLN). The reason why LLN is involved in our formulation of the mixing problem is that the random conserved scalar c=c(t,x) appears to behave as a sample mean. It converges to the mean value, while the variance, $\sigma 2(t)$ decays approximately as t-1. Since the variance of the scalar decays faster than a sample mean (typically α is greater than unity), we will introduce some non-linear modifications into the corresponding pdf-equation. Lagrangian mixing process is modelled by a stochastic difference equation, where the mixing frequency and the ambient concentration are random processes. The mixing intensity λ is introduced as a coefficient in the mixing frequency in order to account for initial length-scale ratio and other physical dependencies. Numerical studies of the non-linear integral equation of the probability density function of a conserved scalar are conducted and it is shown that λ has a distinct influence on the decay rate of scalar.

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Hydrogen-enriched lean-premixed flames

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Hydrogen enrichment of lean-premixed combustion of hydrocarbons has significant implications for NOx and CO control as well as flame stability and lean flammability limits. This presentation summarizes the numerical simulation of a hydrogen-enriched lean premixed flame of methane-air, and discusses the extinction limits and NO formation via different routes.The studied flame configuration is an axisymmetric laminar counterflow premixed flame, stabilized near the stagnation plane of two opposed-jets. The fuel used is a mixture of methane and hydrogen. A stretch rate of 30 s-1 was used for all the flames.

The simulations assumed the stagnation point flow approximation. The governing equations can be found elsewhere (Giovangigli & Smooke, 1987). The potential boundary conditions were used. The calculations were carried out with a code revised from that of Kee et al. (1985). Upwind and center difference schemes were respectively used for the convective and diffusion terms in all the governing equations. Adaptive refinement of meshes was done. The arc-length continuation method was employed to obtain the extinction limits. The pressure and the fresh mixture temperature were, respectively, 1 atm and 300 K.

The previous investigation (Guo et. al., 1998) using an improved radiation model, in which the radiation reabsorption was taken into account, showed that the resorption has little influence on the extinction limits and temperatures of lean counterflow CH4/air premixed flames. The optically thin radiation model, employed in Guo et. al. (1997), was used in the present simulation.

The chemical reaction mechanism used is essentially from GRI-Mech 3.0. The thermal and transport properties were obtained by using the database of GRI-Mech 3.0 and the algorithms given in Kee et. al. (1980 &1983) The thermal diffusion velocity of H2 and H was accounted for, while that of other species was ignored.

It has been known that NO can be formed through thermal, N2O intermediate, and prompt routes, based on the initiation reactions by which molecular nitrogen is converted to nitrogen atom or other intermediate species containing nitrogen. The thermal NO formation is comprised of the three reactions: N + NO = N2 + O, N + O2 = NO + O and N + OH = NO +

H, of which the first one is the initiation reaction. The N2O intermediate route is initiated by the reactions: N2O (+M) = N2 + O (+M), N2O + H = N2 + OH, N2O + O = N2 + O2 and N2O + OH = N2 + HO2, and then the formed N2O is partially converted to NO. The prompt NO in hydrocarbon flames is initiated by the rapid reactions of hydrocarbon radicals with molecular nitrogen (Miller & Bowman, 1989). In addition, NO formation can also be initiated by the reactions of molecular nitrogen with other hydrocarbon free radicals, such as H, OH. These reactions include: NH +N = N2 + H, NH + NO = N2 + OH, NNH = N2 + H, NNH + M = N2 + H + M, NNH + O2 = HO2 + N2, NNH + O = OH + N2, NNH + H = H2 + N2, NNH + OH = H2O + N2, and NNH + CH3 = CH4 + N2. Note that although the last reaction is initiated by CH4, we also attribute it to this route due to NNH. This route to form NO is called NNH intermediate route (Rørtveit, et. al. 2002). To identify the relative importance of the four routes to NO formation in current study, four simulations were carried out for each flame.

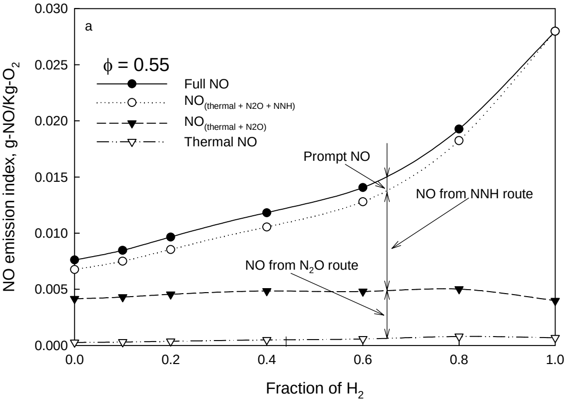

Figure.1. NO emission index in flames with an equivalence ratio of 0.55 at various hydrogen fractions.

The first simulation (SIM1) was conducted by the full chemistry (GRI-Mech 3.0), while the second simulation (SIM2) was carried out by removing the initiation reactions of the prompt routes. In the third simulation (SIM3), the initiation reactions of both the prompt and NNH intermediate routes were removed. All the initiation reactions of the prompt, N2O and NNH intermediate routes were removed in the forth simulation (SIM4). Consequently NO obtained from SIM4 can be attributed to from the thermal mechanism. The difference in NO between SIM1 and SIM2 is attributed to from the prompt route, and the difference between SIM2 and SIM3 is due to the NNH intermediate route. The NO contributed by the N2O intermediate route is the difference between SIM3 and SIM4. Typical results are shown in Fig.1. Further details on NO and N2O emissions, and extinction limits can be found in Guo et. al. (2004).

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Energetic Use of Biomass– An Example for Reactive Multiphase Flows

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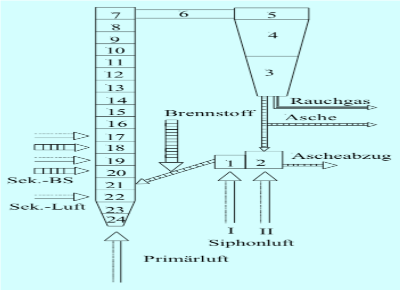
Renewable energy sources are of increasing importance due to two reasons – limited availability of fossil fuels and political restrictions requiring reduced emissions of CO_2 from these sources. Here, significant challenges and chances for future research do exist.

Renewable sources are mainly used thermally (e.g., gasification or combustion) or biochemically (e. g., conversion into biogas consisting mainly of methane). Their low energy density and the strong fluctuation with respect to their availability over the course of the year require significant research efforts aiming to improve the economic viability of the processes involved as well as the integration of renewable energy sources into the existing technical infrastructure.

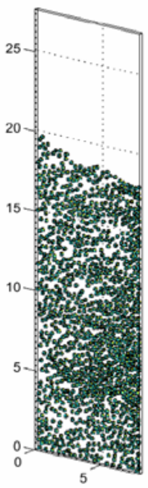
The thermal use of biomass, either in form of combustion or gasification, represents a turbulent two-phase flow. Only closely coupled experimental and numerical efforts will lead to a detailed understanding of the processes involved, and, based on this understanding, will allow to optimize these processes.

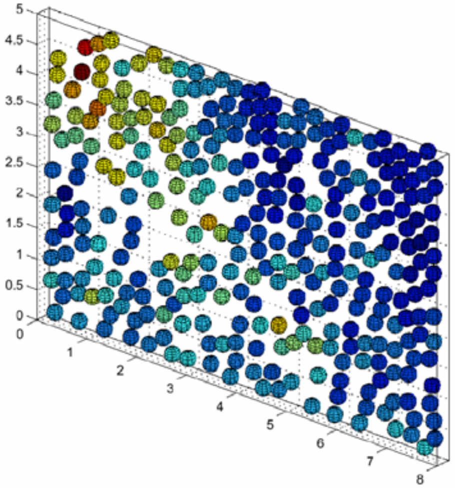
Current approaches applied to the modelling and simulation of particle-loaded reactive flows can roughly be subdived into four categories:



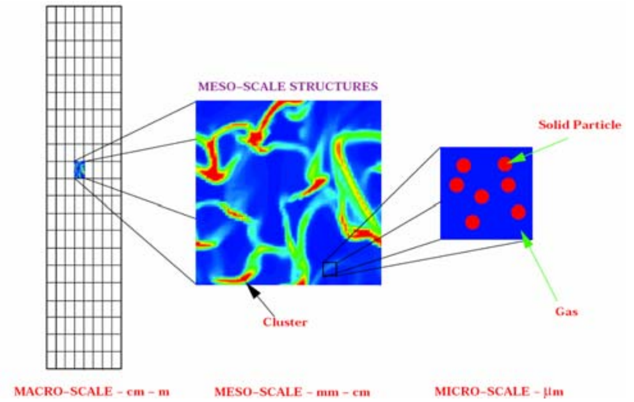
- Cell-based models
- Continuous models (Euler-Euler models)
- Particle models (Euler-Lagrange models)
- Direct numerical simulation.

The main field of application of cell-based models (see left diagram) is the prediction of the dynamic behaviour of complete systems. Due to the spatially one-dimensional approach the compute times are short allowing for extensive parameter studies. Large sets of correlations for the physical processes involved allow predictions for various states of operation of the unit. The advantageous one-dimensionality of this approach offers on the other hand no detailed prediction of the local distribution of flow, temperature, and concentrations.





Direct numerical simulation (DNS, see right diagram, Pan (2002)) represents the other extreme of the modeling approaches. All spatial and temporal scales relevant to the process are resolved avoiding the need to model physical and chemical processes involved. On the downside of this approach are prohibitively high compational costs restricting its application to very small parts of technical systems (dimensions in the order of few mm up to cm).



Current developments in applied research on multi-phase flows focus on continuum and particle models. They both include complex modeling approaches allowing for realistic predictions. Continuum models view the systems as two intermingling phases used mainly for fluids with small particles and strong interactions between both phases. Particle models are preferred for systems with fewer particles showing only a small influence onto the fluid phase.

When simulating a technical unit a resolution of meso or even micro scales normally is not done (see left part of the diagram above, Sundaresan (2004)). Compute time limitations tend to restrict resolution for technical problems to the order of cm. Phenomena on smaller scales like the combustion of a single wood particle (right part of the diagram above) do significantly influence a reactive two-phase flows and have to be dealt with.

Simple modeling approaches like traditional gradient models are not sufficient in all cases.

For the gasification of wood in both fixed or fluidized bed systems an approach similar to the flamelet model for turbulent gas-phase combustion is discussed. The basic building block of this approach, the single particle is exposed to a stagnation-point flow described by a one-dimensional modelling of the flow field allowing for a detailed description of the gas-phase chemistry as well as surface and bulk reactions at and in the particle. The structure of the particle itself changes during the process.

Information based on this detailed modeling and accompanied by experimental results on the gas phase surrounding the single wood particle by both Raman spectroscopy and gas chromatography will be tabulated and used to transfer the detailed chemical knowledge into the modeling of the complex turbulent two-phase flow.

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Modeling and Simulation of Plasma-Assisted Reactive Flows

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Non-thermal process plasmas

Non-thermal process plasmas, as a special category of reactive flows, have a multitude of important applications in various fields of technology, such as dry etching methods for manufacturing semiconductors and the after-treatment of exhaust gases of combustion engines. Focus of this talk is modeling and simulation of such non-thermal process plasmas using detailed physical and chemical models. Concepts to establish a state of modeling for thermal non-equilibrium systems – similar to the one achieved for reactive flows in thermal equilibrium in the last few years – are presented.

Plasma etching of semiconductors

Processes inside a plasma reactor are characterized by the complex interaction of power absorption, chemical reactions in the gas phase and at the reactor surface and flow and transport processes. In a first step, a model of the plasma reactor itself is developed. The main focus is on reaction kinetics in the gas phase, particularly on the electron energy distribution function (EEDF). A new simulation program allows for the calculation of the EEDF fully coupled to the conservation equations of all other species in the system. Models of increasing complexity are compared

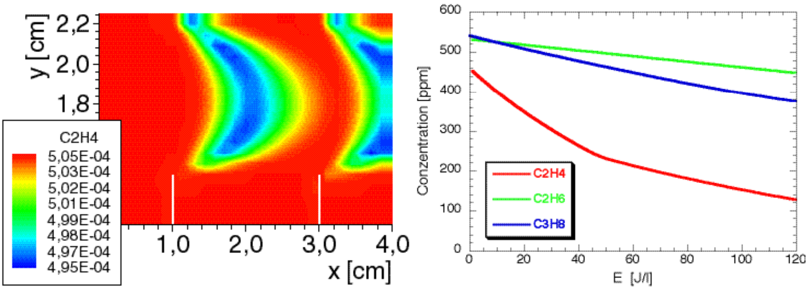

Figure.1 Two-dimensional simulation of the plasma processing of exhaust gases Left: Consumption of C_2H_4, right: Consumption of unburnt hydrocarbons (ethane, propane, and ethene) as a function of the energy input.

to each other. It is shown that only the coupling between reaction kinetics and the EEDF produces sufficiently accurate results. The simplified assumption of a Maxwell-distribution for electrons shows significant deviations.

The two-dimensional description of the etching process is performed using a simulation program specifically developed for these processes to solve the reactive Navier-Stokes equations for two-temperature-models, coupled to a newly developed transport model for ionized flows. In a model reactor species profiles and temperature distribution (electrons and heavy particles) are calculated and the uniformity of the etching process is studied.

Exhaust gas cleaning using plasma sources

Cold start emissions of unburned hydrocarbons (UHCs) are a dominant fraction of the total hydrocarbon emission. To meet future exhaust gas pollution limits, new purification methods of exhaust gases for combustion engines have to be developed. During the cold start phase the non-thermal plasma processing of NO and UHCs will help to reduce emissions. The advantage over other systems for exhaust gas cleaning currently under investigation is their high efficiency right after engine start.

The key for the usage of plasmas as a method for gas purification are the different radicals: they react slowly with the carrier gas and are available for the degradation of the trace components. The overall process of gas purification can be separated into three phases: (a) the discharge phase corresponds to the formation of primary radicals and electronically excited species by electron–molecule interactions; (b) a post-discharge metastable-quenching phase; and (c) a post-discharge radical utilization phase, in which the ‘secondary radicals’ (O3, HO2) are formed and NO and UHC reactions occur.

For typical operating conditions, the discharge phase is in the order of a few nanoseconds, the metastable-quenching phase is in the order of tens of nanoseconds, and the radical utilization phase is in the order of microseconds or longer. The fact that these processes occur on different time scales allows us to treat the radical production and radical utilization as two independent processes. The simulation model is based on detailed reaction mechanisms to describe the reactions initiated by the plasma and solves the Navier-Stokes equations fully coupled to this reaction kinetic model.

The left part of the figure shows a result of a two-dimensional reactor simulation based on a detailed chemistry model (ethane concentration after one discharge pulse). The consumption of pollutants depends specifically on the unburned hydrocarbon. The right part of the figure shows the reduction of unburned hydrocarbons obtained for a model gas consisting of 72% N_2, 18% O_2, 10% H_2O and 440 ppm – 540 ppm unburned hydrocarbon (dependent on the experimental conditions). The consumption of ethane (green), propane (blue) and ethene (red) is shown.

To summarize, these studies on combustion engine exhaust gases after-treatment aim at a detailed modeling of the nitric oxide and hydrocarbon chemistry, which is initiated by radicals formed in plasma-discharges. In addition to volume-averaged models for the discharge and the subsequent reaction phase, spatially two-dimensional simulations of a specific reactor type are developed. The energy input necessary for the degradation of various unburned hydrocarbons is quantified. For exhausts containing additional water the energy input for NO oxidation is also quantified. It is clearly shown that the direct reduction to N_2 is not feasible. Therefore, an application of this technology will be successful only in connection with specific NO_2-catalysts.

Flame front analysis of high-pressure turbulent lean premixed methane-air flames

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An experimental study on lean turbulent premixed methane-air flames at high pressure is conducted by using a turbulent Bunsen flame configuration. A single equivalence ratio flame at $\Phi = 0.6$ is explored for pressures ranging from atmospheric pressure to 0.9 MPa. LDA measurements of the cold flow indicate that turbulence intensities and the integral length scale are not sensitive to pressure. Due to the decreased kinematic viscosity with increasing pressure, the turbulent Reynolds numbers increase and isotropic turbulence scaling relations indicate a large decrease of the smallest turbulence scales. Available experimental results and PREMIX code computations indicate a decrease of the laminar flame propagation velocities with increasing pressure, essentially between the atmospheric pressure and 0.5 MPa. The u'/S_L ratio increases therefore accordingly.

Instantaneous flame images are obtained by Mie scattering tomography. The images and their analysis show that pressure increase generates small scale flame structures. In an attempt to generalise these results, the variance of the flamelet curvatures, the standard deviation of the flamelet orientation angle and the flamelet crossing lengths have been plotted against $Re_t^{1/2}$ which is proportional to the ratio between the integral and Taylor length scales and which increases with pressure.

The results obtained in this study show a significant pressure effect on the topographic characteristics of the instantaneous flame fronts. This effect is mainly related to the large change in the turbulence structure of the reactant flow at high pressures due to the decrease in kinematic viscosity, where smaller scales are generated. As a consequence, the Kolmogrov scale becomes smaller than the Zeldovich thickness at high pressures.

As the integral turbulence scale is not sensitive to pressure, the reduction of small scales implies an increase of the ratio between large and small scales, which is represented by the increase of the turbulent Reynolds numbers. For example, $(Re_t)^{1/2}$ is proportional to the ratio between the integral and Taylor scales and increases as $P^{1/2}$. If the primary effect of pressure is to increase the dynamic range of the turbulence it should therefore be possible to generalise the results presented above by relating them to the increase in the dynamic range of the reactant turbulence structure with pressure. For example, for the variance of the flame front curvature h versus $Re_t^{1/2}$ ($\propto l_t/\lambda$), a linear increase is observed indicating the strong decrease of the radii of curvature with pressure. The variation of the average crossing length with $Re_t^{-1/2}$ shows again a linear decrease with increasing pressure (or decreasing $Re_t^{-1/2}$). Finally, the variation of the standard deviation of the flamelet orientation angle distributions, unconditioned by mean progress variable, versus $Re_t^{-1/2}$ is also linear, indicating the generation of smaller flame wrinkles, almost perpendicular to the average progress variable contours, with increasing pressure. It should be noted that attempts to correlate these data with $Re_t^{-3/4}$ ($\propto\eta\ /l_t$) were not as successful probably because the Kolmogorov scale is too small to wrinkle the flame front significantly.

This synthesis of the pressure effects on the topographic parameters of premixed flames highlights the strong effect of the dynamic range of the turbulence structures as discussed by Soika et al. As this ratio between large and small scales increases with increasing pressure smaller scale flame structures are generated. It is also interesting to note that high pressure turbulent flame experiments allow detailed and systematic experiments on the small scale turbulence effects on turbulent premixed flames to be performed. Indeed, generating significantly different turbulent scales while holding constant the mean flow velocity and the mixture equivalence ratio, for example, was found to be very difficult in previous atmospheric turbulent flame studies.

The increase in the importance of smaller scales have a direct affect on the turbulent burning rate. This affect may be quantified in terms of the flame surface density Σ which increases when the pressure rises as a direct consequence of the generation of smaller scale flame elements with pressure. These data can be used to obtain an estimate for the total burning rate, $\overline{W}$, of the turbulent flame which is also correlated with $Re_t^{1/2}$ ($\propto l_t/\lambda$) and indicates that the burning rate of these flames, which are in the laminar flamelet regime, is primarily determined by the dynamic range of the turbulence

Automatic reduction of detailed kinetic mechanisms

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A method for the automatic reduction of detailed reaction mechanisms is described. The method uses sensitivity analysis, reaction flow analysis and species lifetime analysis in combination. The method is general and can be applied to several different combustion calculation procedures. Here the method is used to create a reduced mechanism for calculations of auto-ignition that precedes knock in spark ignition engines.

The general idea is that a detailed mechanism with a wide range of accurate operating parameters is used as a basis. A more limited range of operating parameters, relevant for the application is selected through a simple simulation. A pre-set level of relative importance is selected, to specify the accuracy as well as size of the created mechanism. The pre-set levels concern relative sensitivity, minimum reaction flow and minimum lifetime of the species.

The method works as follows: The fuel, oxidizer and product species are set as non-redundant and can not be reduced. Sensitivity analysis is performed on the detailed mechanism to identify species with a high impact on the chosen sensitivity parameter (temperature, NO, i.e.). Reaction flow analysis is performed to investigate which reaction pathways are most important regarding the carbon mass flow. If a species has a low sensitivity on the selected sensitivity parameter, and is not involved in reactions with large reaction flows, it is considered redundant, and removed from the mechanism. Thus a skeletal mechanism is created.

The next step uses the quasi steady state assumption (QSSA) on the skeletal mechanism. A measure of the species lifetimes is acquired from the chemical source terms. A species with short lifetime and low concentration is assumed to be in steady state, and reduced from the mechanism. Reactions involving these species remain in the mechanism. The concentrations of the reduced species are assumed constant and calculated using the steady state assumption.

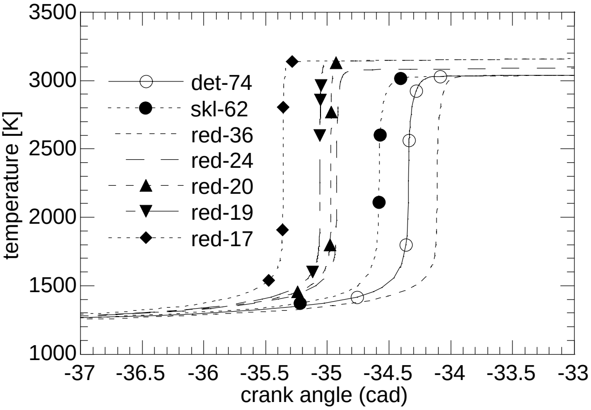

Figure: Calculated temperature profiles, showing auto-ignition in the end-gas of a spark ignition engine. Comparison between the detailed mechanism, the skeletal mechanism and different reduced mechanisms. As shown in the figure, the agreement of the full 74 species mechanism, and the 17 species reduced mechanism is within 1.5 crank angle degrees.

PDF Modelling of a Bluff Body Stabilized Flame

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The probability density function (PDF) method has proven to be among the most promising approaches for accurate modeling of turbulent reacting flows of practical importance(Jenny 2001, Xu 1998). Compared to conventional turbulence models, the PDF method offers the unique advantages of being able to take into account the important processes of convection and non-linear reaction in closed form(Pope 1985). Hence the effects of turbulent fluctuations on chemical reactions are treated exactly, and the gradient diffusion assumption is avoided. Of these advantages, the exact treatment of finite-rate non-linear chemistry makes the PDF method particularly attractive for simulations of complex turbulent reacting flows.

As for any turbulence model, an efficient numerical solution algorithm is of essential importance to apply the PDF method to flow problems of practical interest. Significant progress has been recently made in this direction by the development of the consistent hybrid finite volume (FV)/particle-based Monte Carlo method(Muradoglu 1999, Muradoglu 2001). The hybrid method combines the best features of the FV and particle-based Monte Carlo methods in order to efficiently solve the PDF model equations. The method is completely consistent at the level of governing equations and the full consistency at the numerical solution level is enforced by using efficient correction algorithms(Muradoglu 2001). It has been shown that the consistent hybrid method is computationally more efficient than the best available alternative solution technique by a factor of an order of magnitude or more(Muradoglu 2001, Jenny 2001). The numerical efficiency of the hybrid algorithm is further improved by the recent development of a local time stepping algorithm that has been shown to accelerate the global convergence of the hybrid method as much as by a factor of an order of magnitude depending on grid stretching(Muradoglu 2002). Combined with the local time stepping algorithm, the consistent hybrid method thus makes the PDF methodology a feasible design tool for the practical applications in

engineering or elsewhere.The primary purpose of the present work is to demonstrate the performance of the velocity-turbulent frequency-compositions joint PDF method combined with the hybrid FV/particle solution algorithm in predicting the properties of the bluff-body stabilized turbulent flame studied experimentally first by Dally et al.(Masri) and recently by Kalt and Masrif (Masri). Besides its practical importance, the bluff-body flame studied here provides an excellent but challenging test case for turbulence and chemistry models as well as for numerical solution algorithms for studying turbulence and chemistry interactions in turbulent recirculating flows due to its simple and well defined initial and boundary conditions, and its ability to maintain the flame stabilization for a wide range of inlet flow conditions with a complex recirculation zone.The statistical stationarity is shown and the performance of the PDF method is assessed by comparing the mean fields with the available experimental data. The effects of the model constants Cw1 in the turbulence frequency model and Cø in the mixing model on the numerical solutions are examined and it is found that all the mean fields are very sensitive to the changes in Cw1 while only the mixture fraction variance seems to be very sensitive to the changes in Cø but not the other mean fields. The spatial and bias errors are also examined and it is shown that the hybrid method is second order accurate in space and the bias error is vanishingly small in all the mean fields. The grid size and the number of particles per cell are determined for a 5% error tolerance. The chemistry is described by the simplest possible flamelet/PDF model. Hence the main focus here is on the accurate calculations of the mean flow, turbulence and mixing, which lays the foundation for future work in which the chemistry is described in greater detail.

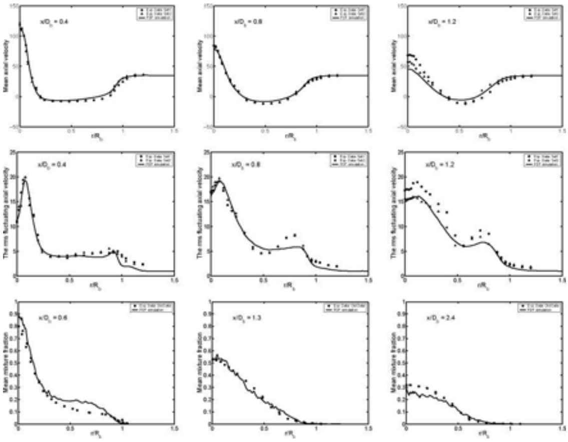

Figure 1: Mean axial velocity $(\widetilde{U})$ (top figures) and the rms fluctuating axial velocity *(u')* (middle figures) profiles at the axial locations $0.4D_b$, $0.8\ D_b$, $1.2\ D_b$, and mean mixture fraction ($\widetilde{\xi}$) (bottom figures) profiles at the axial locations $0.6\ D_b$, $1.3\ D_b$, and $2.4\ D_b$. Symbols denote the experimental data and solid lines denote the PDF simulations. Grid:176 x 136,$iV_{pc} = 50$.

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Method of lines solution of two-dimensional chemically reacting flows

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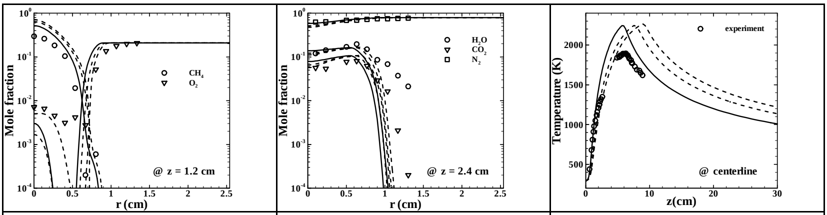
Investigation of three-dimensional, unsteady, turbulent flames is highly important for understanding combustion phenomena including ignition, quenching, and chemistry of pollutant formation. Continuous advances in large scale computers, numerical methods and post-processing environments over the past two decades have led to the application of direct numerical simulation (DNS), which is the most accurate and straightforward technique, to the prediction of turbulent reacting flow fields. However, DNS of turbulent reacting flames including complex chemistry is still beyond the capabilities of current computational resources. Due to the fact that fine space and time resolutions are needed for DNS in the presence of wide range of flow and length scales, both accurate and efficient numerical techniques and high performance computers are required for the simulation in short computation time. The former can be achieved by increasing the order of spatial discretization method, resulting in high accuracy with less grid points, and using not only highly accurate but also a stable numerical algorithm for time integration. The method of lines (MOL), the superiority of which over finite difference method had already been proven (Selcuk 2002), is an alternative approach that meets this requirement for the time dependent problems. The latter requirement is met by either supercomputers or parallel computers which require efficient parallel algorithms. In the MOL approach, the system of partial differential equations (PDEs) is converted into an ordinary differential equation (ODE) initial value problem by discretizing the spatial derivatives together with the boundary conditions using a high order scheme and integrating the resulting ODEs using a sophisticated ODE solver which takes the burden of time discretization and chooses the time steps in such a way that maintains the accuracy and stability of the evolving solution. The most significant advantage of MOL approach is that it has not only the simplicity of the explicit methods but also the superiority of the implicit ones unless a poor numerical method for the solution of the ODEs is employed.

Considering the emphasis on the prediction of transient turbulent reacting flows, a novel CFD code satisfying the above-mentioned requirements was recently developed for the DNS of 2D internal flows in regular and complex geometries. The code uses the MOL approach in conjunction with (i) an intelligent higher-order multidimensional scheme which chooses biased-upwind and biased-downwind discretization in a zone of dependence manner (ii) a parabolic algorithm which removes the necessity of iterative solution for pressure and solution of a Poisson type equation for the pressure and (iii) an elliptic grid generator using body-fitted curvilinear coordinate system for application to complex geometries. The requirement of high performance computing was also met by developing an efficient parallel algorithm for the code. Predictive accuracies and performances of both sequential and parallel codes were assessed on various laminar and turbulent isothermal/non-isothermal flow problems by validating its predictions against either measurements or numerical results available in the literature (Erşahin 2004-Uygur 2004). Favorable comparisons were obtained on these non-reacting flow problems. Comparisons also showed that the flow fields predicted by parallel code agreed well with those of serial code at considerably less execution times.

Encouraging agreements obtained between the predicted flow fields and measurements for non-reacting flows and high performance of the parallel code in the prediction of transient flows have initiated the development of an efficient algorithm based on MOL for direct simulation of unsteady reacting flows. As a first step, chemistry was modeled by the flame-sheet approximation in which a single equation (conserved scalar) is solved for both energy and species equations [Tarhan 2004]. The predictive ability and accuracy of the code was tested by applying it to the prediction of confined methane/air laminar diffusion flame (Mitchell 1975) and comparing its predictions with other numerical results and experimental data available in the literature. Although the flame-sheet model predicts reasonably good flow and species fields, a finite reaction rate model must be employed in order to obtain more detailed and accurate solutions. Therefore, energy and species equations were incorporated into the code and its predictive accuracy was tested on the same flame using three global single-step methane-air reaction mechanisms (M1, M2, M3) (Khalil 1975-Hsu 2003). The radial profiles of the computed mole fractions of the species at two axial positions above the burner inlet and the temperature profile along the centerline for three mechanisms are plotted against the experimental data in Figures 1(a)-(c). As can be seen from Figure 1(a) methane diffuses from the centerline to the reaction zone where it is completely consumed. The oxygen is convected to the reaction zone from the outside of the flame and start to decrease due to combustion. The small increase of oxygen in the fuel side is due to relatively low temperature inside the flame near the burner inlet. This behavior is well captured by all the mechanisms. Figure 1(b) shows that both combustion products and nitrogen are predicted reasonably well with all three mechanisms. In Figure 1(c), it can be seen that along the centerline the temperature increases steeply until it reaches a maximum value at the flame height and then gradually decreases downstream. Temperatures predicted by mechanism M1 shows the best agreement with the experiment.

In order the show the predictive ability of the code for the transient flow field, the time development of the temperature and axial velocity fields for M1 are shown in Figures 2 and 3, respectively. As can be seen from Figure 2, reaction starts as soon as flow is started and high temperature region extends from the boundary of the fuel and oxidizer jets to the symmetry axis. Thereafter, as the flow moves downstream, the temperature field broadens to the walls due to the recirculations. After a distance from the inlet, fuel cannot exist and therefore, temperature starts to decrease downstream. At steady state it takes its final form resulting extremely high temperature gradients in the system. As is demonstrated in Figure 3, the axial velocity increases in the inlet region along the centerline due to increase in temperature, and vortices begin to form near the walls. As time progresses the flame propagates to the exit of the burner with an accelerating velocity and flow starts to separate downstream yielding two large recirculation cells that are established between the hot surface and the cooler shield.



(a) (b) (c)

Figure 1. Radial species at two axial positions (a-b), axial temperature profile at the centerline (c).
Symbols: experimental data [6], ——— M1 [7], - - - - M2 [8], — · · — M3 [9].

1-step mechanism calculations indicate that the code predicts velocity, temperature and species reasonably well in laminar flames. However, for the accurate predictions, incorporation of more detailed chemical reaction model is required. This study constitutes an initial step towards the development of an efficient numerical scheme for direct simulation of unsteady, multi-dimensional combustion with stiff detailed chemistry. To the authors' knowledge, a parallel implemented CFD code based on MOL for multi-dimensional reacting flows is not available to date.

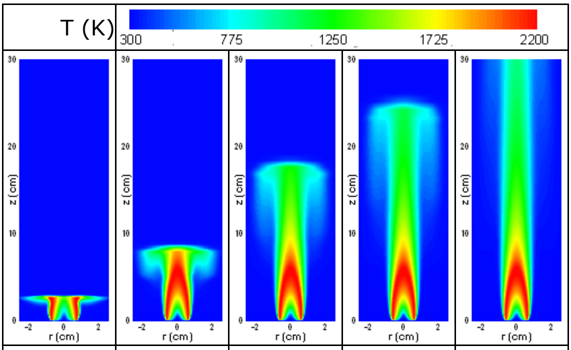


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Figure 2. Time development of temperature field.

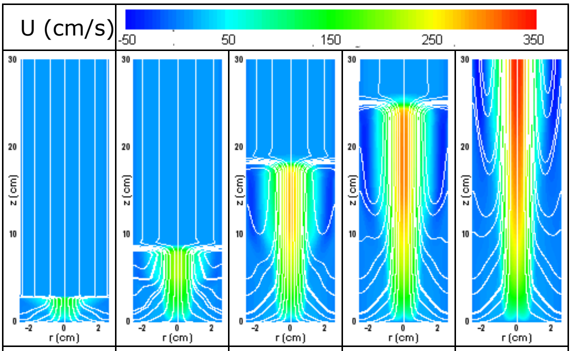

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Figure 3. Time development of axial velocity field.

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Investigation of combustion process in a Diesel engine by using KIVA-3V multi-dimensional code

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Due to stringent and continuously tightened emission standards, improvement in diesel engine technology is required. One of the methods utilised for this purpouse is to use high pressure injection system for better combustion performance in the cylinder and a selective catalytic reduction for further reduction of pollutants in the exhaust system.

In this study a multidimensional modeling has been considered as a predictive tool to investigate mixture formation and combustion process in internal combustion engines. This modelling approach has been carried out in order to understand the effects of certain parameters on NOx and soot emissions by using KIVA-3V code. Results were compared with the experimentally obtained data from Ford NHDD diesel engine which has electronically controlled common rail fuel system with 8 hole injector.

Examination of combustion process and emissions require a well predicted evolution of spray jet that takes place in a logical sequence undergoing various stages of spray atomization, breakup, collision, evaporation and mixing with surrounding air. For diesel engine applications, KIVA code solves the conservation equations for evaporating fuel sprays coupled with the three-dimensional turbulent fluid dynamics of compressible, multicomponent, reactive gases in cylinder with arbitrary shaped piston geometries. In the code, it is assumed for fast chemical reactions to be in equilibrium and for slow reactions to proceed kinetically. But, all of these processes don’t incorporate with the detailed mechanism accounting for the trimolecular processes with different third body efficiencies and chemistry/turbulence interactions. For this purpouse, these models are being implemented into the code (Golovitchev 2000).

In this study, for turbulent spray combustion modeling, enhanced eddy dissipation concept with partially stirred reactor model was used. Physical properties of diesel oil like vapor pressure, critical temperature, latent heat of vaporation were used for diesel oil #2 grade. But, chemical mechanism is of n-heptan having cetane number of aproximately ~56, which is similar to conventional diesel fuel. This reduced n-heptane mechanism consists of 68 species and 279 reactions.

PaSR

Partially stirred reactor model was proposed by Vulis as an extension of Eddy Break-Up (EBU) model. (Vulis 1961) While this model is implemented into the code, the grid size is seldom small enough to resolve the smallest turbulence scales because of excessive computational load. Thus to compansate this a computational cell is split into two different zones in this approach. One is reaction zone and in the other one no reaction occurs. The reacting zone is treated as a perfectly stirred reactor (PSR), where the composition is homogeneous.Reactor-exit concentration can be found from mass conservation as below, where κ^* is the mass fraction of the mixture

$c_1 = \kappa^* c + \left(1-\kappa^*\right) c_0$ [Eq.1] that reacts.

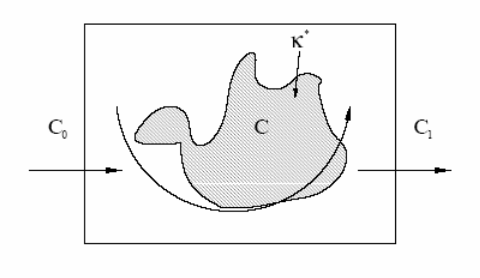

Figure 1. C0 is the initial averaged concentration in the cell.C is the unknown concentration in the reaction zone.C1 is the averaged reactor-exit concentration in the cell.. A conceptual figure of PaSR model (Nordin 2001)

Results

Comparison of predicted cylinder pressure data and measured data at different loads by using partially stirred reactor model is shown below:

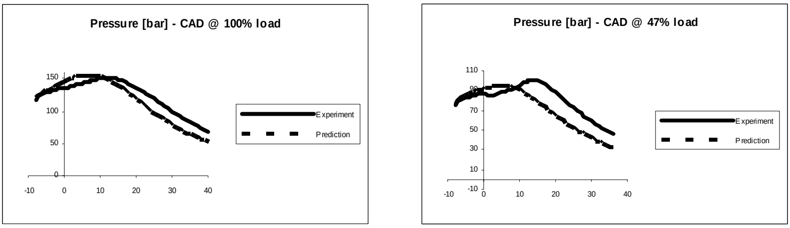

Figure 2. At different loads predicted and measured pressure vs. CAD curves

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COMPUTATIONAL MODELLING OF A TURBULENT JET DIFFUSION FLAME OF HYDROGEN

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Turbulent diffusion flames of a round jet of hydrogen into air, have been, in fact, investigated widely in literature (Jones 2002, Yamada 2002, Nicoli2003). The main difficulties are reported as that the flame retards the transition to turbulence (Torii 2001).

From the numerical point of view, the present work is concerned with the numerical simulation of interaction of the cold jet and the diffusive flame of H_2 with the air. Standard k-ε turbulence model has been used by means of the FLUENT® software.

A global exothermic reaction between H_2 and O_2 describes heat release:

$H_2+1/2O_2 \rightarrow H_2O$

To validate our model, we used the geometry reported in (Torii 2001). In this model a fuel gas jet, mixture of hydrogen (H_2) and nitrogen (N_2), spouts vertically upward from a nozzle. Surrounding air flows parallel to this jet through a coaxial circular duct. Thus the chemical reaction is as the following:

$0.6H_2+0.4N_2+0.3(O_2+3.76N_2) \rightarrow 0.6H_2O+1.528N_2$

The stochiemetric coefficients are calculated from the mixture of the fuel including H_2 and N_2 with a ratio of 1:0.68.

The turbulence related boundary conditions at the fuel and air inlets are as the following:

Turbulence intensity: 70 % for the fuel inlet (nozzle) and 20% for the air (air duct).

The second parameter of the turbulence at both of the inlets is the length scale and for this value, the hydraulic diameters of the nozzle and the air duct are used, as guided by FLUENT® (Fluent Manual 2001)

Mesh structure has been created by using T-Grid for both the cold jet interaction and combustion cases. The probability density function properties are calculated via prePDF utility of FLUENT®, previous to the main computations.

The diffusion of the fuel jet and the flame for the cold interaction and combustion cases, respectively, have been obtained, as well as the flow and temperature fields.

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