CP1
Large Eddy Simulation of Turbulent Flame Kernels

A combustion LES code has been developed to investigate the effects of a premixed turbulent flame kernel. The code solves the fully compressible governing equations for mass, momentum, progress variable and energy on a structured Cartesian grid. Smagorinsky eddy viscosity model with dynamic procedure is used as a subgrid scale turbulence model. A flame surface density model based on the flamelet concept is employed on the subgrid scale reaction rate. Results from LES will be compared with existing DNS results, and investigations will be carried out on flame surface evolution statistics.

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CP1
A Low-Dimensional Stochastic Closure Model for Combustion Large-Eddy Simulation

A novel formulation for the Large-Eddy Simulation (LES) of turbulent combustion is presented. It is based on coupling LES equations for mass and momentum, with 1-D stochastic governing equations using the One-Dimensional Turbulence (ODT) model. ODT domains, on which fine-grained ODT simulations are implemented, are embedded in the flow to represent unresolved scalar and momentum statistics. The formulation addresses important coupling between turbulent transport and molecular processes over a wide range of length and time scales.

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CP1
Improvement to the Eddy Dissipation Concept (edc) Turbulent Combustion Model for Application to Low Reynolds Number Wall-Bounded Reactive Flows

Accurate prediction of wall-bounded reactive flows characterized by flame-wall interactions require a turbulent combustion model that must be able to account for effects associated with low Reynolds numbers. The widely used standard version of Magnussens Eddy Dissipation Concept (EDC) assumes high Reynolds number and highly turbulent flow conditions. The present work provides an assessment about the performance of the standard EDC model in representing premixed turbulent combustion at low Reynolds numbers in the near-wall regions of the flow and suggests a modification to the standard version of the model to improve its performance and extend its applicability range. The model benchmarking analysis consists in comparing results from Direct Numerical Simulation (DNS) of a low Reynolds number premixed flame-wall interaction test case against Reynolds Averaged Navier-Stokes (RANS) simulations. The RANS simulations are performed with a Finite Volumes code that includes, together with the EDC, low Reynolds number $k-\epsilon$ turbulence modeling while the DNS database is built with a state-of-the-art massively parallelized Finite Differences code for direct simulation of reactive flows. A relatively simple modification to the EDC expression that defines the turbulent fine-structures regions of the flow (γ^*) considerably improves the near-wall performance of the model, reducing its notorious tendency to over-prediction of the local burning rate in the near-wall regions of the flow.

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CP1
LES of 3D Nonpremixed Flames Submitted to Transverse Acoustic Modulations

This research aims at developing predictive tools for combustion instabilities. The case of turbulent diffusion flames is of interest for many applications. Nonpremixed injection raises difficulties in the estimation of reaction rates which can be handled in the compressible LES framework by making use of flame surface density concepts. Results of simulations are evaluated using the data from the "H3" case of the TNF Workshop. Dynamics induced by transverse acoustic modulations is investigated in a second step.

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CP1
Linear Eddy Modeling of N-Heptane Combustion in Hcci Engines

HCCI engines have the potential advantage to combine high thermal efficiencies with low emissions. Autoignition of premixed systems with non-homogeneous conditions exhibit different combustion modes including spontaneous ignition front propagation and deflagrations. In this work we apply the linear eddy model (LEM) to simulate n-heptane auto-ignition under thermal stratification. Resolving all spatial and temporal scales in a one dimensional domain we investigate the influence of initial temperature fluctuations and turbulent scales on the combustion mode under typical HCCI engine conditions.

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CP1
Large Eddy Simulation of a Methane-Air Turbulent

Jet Flame in a Vitiated Co-Flow.

A new turbulent combustion model for Large Eddy Simulation of non-premixed flames stabilized by hot products is proposed. To tackle both auto-ignition and diffusion phenomena, chemistry is tabulated from unsteady diffusion flamelets. Filtered quantities are estimated from presumed probabilities density functions. The proposed approach is used to numerically predict a lifted jet flame issuing in a vitiated co-flow. Results are compared with experimental data.

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CP2

The Effects of Adding Dimethyl Ether and Ethanol to Coflow Ethylene/Air Diffusion Flames: A Computational and Experimental Study

Several laminar coflow ethylene/air diffusion flames are examined computationally and experimentally to determine the effects of adding various amounts of dimethyl ether and ethanol to the fuel stream. Computationally, the local rectangular refinement method solves the fully coupled nonlinear conservation equations in 2D. The model includes a C6 chemical mechanism, detailed transport, and optically thin radiation. Experimental techniques measure temperature and species along each flame's centerline. Computational and experimental results show very good agreement.

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CP2

Three-Dimensional Simulation of Flames on a Spinning Burner

Numerical simulations are carried out to model a flame supported by a spinning porous plug methane burner. Earlier experiments by others reveal interesting dynamical behavior: the emergence of holes; a single-arm spiral wave; a dual-arm spiral wave. These phenomena are captured by the simulations. These are edge-flames that might be relevant in turbulent combustion simulations.

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CP2

Effect of Radiation on the Determination of Laminar Flame Speed Using Propagating Spherical Flames

The laminar flame speed is one of the most important parameters of a combustible mixture since it affects the burning rate in internal combustion engines and it is an important target for kinetic mechanism development. Recently, the technique using propagating spherical flames is the most favorable method for measuring flame speed, especially at high pressures. In this study, the effect of radiation on the accurate determination of laminar flame speed is investigated theoretically and numerically.

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CP2

The Impact of Multicomponent Transport and Thermal Diffusion Effects on Soot Formation in Coflow Ethylene/Air Diffusion Flames

Coflow laminar diffusion ethylene/air flames are investigated numerically using complex chemistry, detailed transport and sectional soot models. All transport coefficients, including thermal diffusion coefficients, are evaluated using cost-effective, accurate algorithms derived from the kinetic theory of gases. The numerical results presented here provide a quantitative assessment of the effects of detailed multicomponent transport and thermal diffusion on soot concentrations in the coflow geometry as a function of equivalence ratio.

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CP2

Investigation of Flame Extinction and Reignition Modes in Nonpremixed Ethylene Jet Flames Using Direct Numerical Simulation

Modes of flame extinction and reignition in nonpremixed ethylene jet flames are investigated using DNS. A validated, reduced ethylene mechanism consisting of 19 transported species is used. Flame extinction occurs in regions of high strain, and allows mixing of fuel, oxidizer and combustion products prior to reignition. A parametric study is performed with varying Damkohler number to alter the extent of extinction, and shift the balance between possible reignition modes including flame propagation and autoignition.

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CP2

Reaction Layer of Rich Premixed Flame Disturbed by Vigorous Turbulence in a Hydrogen Jet Lifted Flame

The authors have succeeded in capturing a hydrogen jet lifted flame by highly resolved detailed numerical simulation. The rich premixed flame, located at the inner side of the lifted flame, is affected by vigorous turbulence of the hydrogen jet, and the flame internal structure is largely disturbed. The modified chemistry will be discussed by investigating the statistical relations between variables in the reaction layers, such as, a relation between temperature and fuel consumption rate.

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CP3

An Eulerian Model for the Dynamics of Polydisperse Evaporating Sprays: Combining the Multi-Fluid Model with the Quadrature Method of Moments

As the computational cost of a particle-based Lagrangian solver is too high for polydisperse sprays in unsteady configurations, we propose a novel approach combining the efficiency of Eulerian multi-fluid models with the accuracy of the quadrature method of moments in order to capture the dynamics of polydisperse sprays undergoing evaporation and combustion. The resulting computational algorithm strongly relies on the theory of moments and dedicated numerical methods.

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CP3

Pulsated Free Jets with Evaporating Spray Injection : Eulerian Multi-Fluid Modelling And Simulation Versus Experimental Measurements

Eulerian models appear as an interesting alternative to Lagrangian methods in polydisperse unsteady configurations. Dynamics of round free jets submitted to upstream modulations provide an interesting configuration. In this contribution, we provide an evaluation of eulerian models through a series of detailed comparisons with experimental measurements. Beyond the validation of this model and robustness of the numerical method, it yields an interesting insight into the dynamics of evaporating sprays in coherent vortical structures.

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CP3

Oscillations of An Edge Flame with Fuel Spray

The nature of gaseous edge flames in a variety of configurations is fairly well understood. However, in a wide range of practical problems the fuel is introduced as a polydisperse spray of droplets; yet the role played by sprays in the context of edge flames has not been investigated. Here some preliminary examples of the way in which fuel spray parameters induce oscillatory behavior of edge flames is discussed.

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CP3

An Evaluation of Eulerian Models Versus Lagrangian for the Description of the Dynamics of Polydisperse Evaporating Sprays in Free Jet Configuration

The computational cost of Lagrangian approaches to describe evaporation and dynamics of polydisperse sprays in unsteady configurations is too large for many combustion applications. Eulerian models have been developed in order to describe the dispersed liquid phase, among which the Multi-fluid one. In this presentation, we provide an evaluation of Eulerian models versus Lagrangian solvers in the configuration of a multidimensional free jet. We provide a detailed study in terms of accuracy and computational cost.

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CP3

Droplet Formation Mechanism with the Effect of Finite-Length Ligament Tip

A microgravity droplet formation experiment is simulated to understand in further detail a newly proposed droplet formation mechanism including the effect of finite-length ligament tip and dynamic capillary wave motion. The results show that the tip capillary waves play an important role in droplet pinch-off and a different pinch-off wavelength is observed compared to the classical predictions. The present mechanism is to be incorporated into a case of liquid jet injection of practical scale.

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CP3

Numerical Study on Ignition of Droplet Array for Fuel with Different Volatility

Ignition phenomena of a droplet array in a high-temperature stagnant air were investigated numerically for n-hexadecane and n-heptane. Effects of the droplet span on ignition delay time were studied. As the span narrowed, the interaction between droplets became significant and ignition time increased monotonously for hexadecane. On the other hand, in the case of heptane, ignition time had a minimum at certain span; and shorter than that of a single droplet can be obtained.

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CP4

Incorporating Unsteady Effects in Flamelet Gener-

ated Manifolds

Detailed simulations are performed for (un)steady diffusion type flames. We show that both a 2D and a 3D manifold exists, which are used during unsteady flame simulations. The 2D manifold is generated from steady flame simulations and when the 2D FGM is applied, species mass-fractions show a phase-shift compared to the detailed simulations. The 3D manifold is generated from unsteady reaction-trajectories in state-space. Consequently, the phase-shift in species mass-fractions, using Z, c2 and c3, disappears.

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CP4

A Strategy for Tabulating NOx from Detailed Chemistry and Coupling with Flow Solver

Tabulation of detailed chemistry based on species trajectories evolving in chemical sub-space constructed from progress variables has been found successful in Large-Eddy Simulation to reproduce temperature and major species. The extension to slowly evolving species, as NO_x, is discussed. The large difference in characteristic time between NO_x and major species imposes the definition of both a new progress variable and a novel strategy for coupling the chemical table with the flow solver.

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CP4

Large Eddy Simulation of Methane-Air Premixed Swirl Burner Using Tabulated Detailed Chemistry

The PCM-FPI strategy, which consists of introducing flame tabulated detailed chemistry into a fully compressible Navier-Stokes solver, is discussed. Different coupling are considered for methane-air combustion and evaluated in terms of thermochemical behavior. Large-Eddy Simulations of the Tecflam premixed turbulent swirl burner have been performed and comparisons against temperature measurements are reported. An improved closure for the scalar dissipation rate is evaluated.

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CP4

Mild Combustion of H2-Enriched Fuels: A Numerical and Experimental Study

Mild combustion represents a very appealing technology to reduce the large NOx emissions related to H2-based fuels combustion in conventional systems. The present work shows a numerical and experimental investigation of a burner operating in mild combustion mode and fed with H2-enriched fuels. Particular attention is devoted to the validation of the combustion model, in order to properly address the complex turbulence-chemistry interactions which characterize the mild combustion regime.

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CP4

Optimization-Based Model Reduction in Chemical Kinetics

We present a general framework in model reduction, based on the minimization of chemical forces along state trajectories subject to given constraints including the choice of progress variables. Using this approach some remedies for common problems of other model reduction approaches can be found. It especially avoids the necessity of clear timescale separation, as the computation optimal solutions to the underlying variatonal boundary value problem is always feasible, independent of the desired reduced dimension.

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CP4
HCCI Modelling for Gasoline Surrogates

HCCI (Homogeneous Charge Compression Ignition) is still a promising concept to optimize future engines with respect to emissions. Modelling this seems relatively simple, even using large chemical mechanisms. However, predicting the correct time of ignition and the correct pressure-rise rate as a function of fuel composition is still a challenge. In this work we will present results from a modelling study for several (gasoline) surrogates using large (¿1200 species) and small mechanisms (¡200). The effect of several heat-loss model is investigated and compared to experimental results from several sources. Using the smaller mechanisms a multi-zone approach is pursued to assess the correct pressure rise rate applying both composition and temperature distributions.

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CP5
Simulation of Unstable Hydrogen Combustion with Flamelet Generated Manifolds

Premixed plane laminar hydrogen combustion at lean conditions shows unstable behavior. This unstable behavior manifests itself in cellular cusp-like structures in which small cusps are squeezed out by larger ones. In between the cusps there is local extinction. This was observed in previous studies by means of DNS with detailed chemistry. It will be demonstrated that this behavior can be simulated with DNS using flamelet generated manifolds to reduce the chemistry.

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CP5
Simulation of Turbulent Spray Flames Using Coupled PDF and Spray Flamelet Modeling

A joint mixture fraction - enthalpy probability density function (PDF) is proposed for the simulation of turbulent spray flames. Standard spray and turbulence models are used to describe the remaining gas flow characteristics and the liquid phase. Detailed chemistry is implemented to model the chemical reactions through the spray flamelet model. Pre-calculated spray flamelet libraries for methanol/air and for ethanol/air combustion are considered. The simulations are compared with both experimental data and with RANS simulations.

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CP5
Flamelet-Based Large Eddy Simulation of LO_x/GH_2 Shear-Coaxial Jet Flame at Supercritical Pressure

A large eddy simulation is conducted for liquid oxygen (LO_x) and gaseous hydrogen (GH_2) shear-coaxial jet flame at supercritical pressure. In the present simulation, a flamelet-based modeling is employed for chemistry model. One of our objectives is to evaluate the validity of flamelet model for LO_x/GH_2 flame at surpercritical pressure. We simulate the test case RCM-3 conducted on the MASCOTTE facility by the ONERA, and obtained results are compared with experimental results.

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CP5
Numerical Modeling of Non-adiabatic Heat-recirculating Combustors

A two-dimensional numerical models of a spiral counterflow "Swiss roll" was developed including the effects of temperature-dependent properties, viscous laminar/turbulent flow, surface-to-surface radiation, one-step gas phase chemical reaction, and heat loss. Extinction limits were determined over a wide range of Reynolds numbers (2 ¡ Re ¡ 5000) and were showed quantitative agreement with experiments. At the high Re (above 500), it was found that turbulent flow effects must be included in the model to obtain results in agreement with experiments. It is shown that heat conduction along the burner wall has a major impact on the performance and that the optimal wall thermal conductivity is smaller than air thermal conductivity. The effect of surface-to-surface radiation was shown to be similar to the effect of heat loss and had to be included when calibrating a macroscale models. The out-of-center limit of chemical reaction was also predicted by numerical model in agreement with experiments. Both the number of turns and size of the reactor were also examined;,it is found that more turns of the spiral heat exchanger is not always beneficial to burner performance. Studies of size effects showed decreased range of Re supporting combustion at smaller scales, in agreement with experiments.

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CP5

Strongly Stretched Flamelets Equations for Propagating Flames

We introduce the strongly stretched flamelets equations (SSFE), which is a quasi-one-dimensional system of conservation laws for laminar flames based on a moving, curvilinear coordinate system attached to the flame. Integral analysis is applied to the SSFE to investigate the propagation properties of premixed, stretched flames. In particular, we derive a model for the mass burning rate. As special cases, we consider a plane stagnation flame and a spherically expanding flame.

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CP5

Predicting Pollutant Formation with Steady Flamelet Models

With the increasing tightness of emission limits, models for pollutant formation become more and more important. Steady flamelet models have proven to be very efficient methods to model combustion. However, formation of nitrogen oxide and soot are relatively slow chemical processes, which cannot be assumed in quasi-steady state. In this study, a post-processing method is applied using chemical source terms obtained from steady flamelet tables. The results are compared with detailed simulations.

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CP6

Transport Properties of Inert Gas/metal Mixtures in a Wide Temperature Range

A detailed model to compute molecular transport properties developed recently is applied to Ar/metal and N2/metal mixtures used in arc welding. The model is universally applicable with respect to pressure, temperature and degree of ionization. The numerical details of our efficient calculation procedure will be presented. Results will be shown for the thermal conductivity the electrical conductivity, and the viscosity of argon mixtures containing copper, iron or aluminum, and nitrogen mixtures containing copper.

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CP6

Direct Numerical Simulation of Turbulent Nonpremixed Flame Quenching by Water Spray

This paper presents our recent progress in two and three dimensional simulations of non-premixed counterflow flames with turbulence and spray droplet loading. Our high fidelity terascale codes incorporate advanced submodels of soot formation, radiation, spray injection and dynamics. The flow configuration corresponds to two and three dimensional counterflow non-premixed ethylene-air flames. Turbulence is sustained by means of an inflow-forcing technique, and subsequently evolves into homogenenous turbulence that interacts with the strained non-premixed flame. Spray loading is turned on once the flames have been moderately wrinkled by the turbulence. The baseline non-spray results are compared to the results at moderate to heavy spray loading, thereby assessing the effects of spray loading on the local and global flame extinction characteristics. The scientific objective is to understand the fundamental characteristics of flame suppression and extinction due to the interaction of turbulence, spray, chemistry and radiative heat transfer. In particular, this study seeks to explain how the interaction of water spray affects the chemistry and structure of the flame. Investigation is also made on flame weakening caused by increased radiation losses from water-vapor, and the dynamics of soot formation under these conditions.

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CP6

Multidimensional Numerical Modeling of Smoldering Combustion

Numerical simulations of smoldering combustion in cylindrical coordinates are presented. Azimuthal symmetry is assumed. The discretized set of equations describing the physics of the system is solved in a fully-coupled manner using a Newton-GMRES solver. Computational strategies are discussed.

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CP6

Simulation and Modeling of Wood Gasification in Fluidized Beds

Wood can be gasified with hot air mainly into syngas, char, and tar. In this work we present two different modeling approaches for the simulation of wood gasification in fluidized beds: An Euler-Euler continuum approach and an Euler-Lagrange method with 4-way coupling using the discrete element method for dense particulate flow. We compare the two modeling approaches against each other and against experimental data of a laboratory scale fluidized bed gasification reactor.

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CP6

Spectroscopic Approach to Condensed Phase Combustion Modeling

The combustion modeling of energetic materials still involves a guess- ing step due to the lack of knowledge in the condensed phase. Quantum dynamical calculations are presently the only way to predict the ini- tial reaction but require tremendous computing power, thus limiting their application. An empirical method was devised which uses spec- troscopic data of energetic molecules as the source for the complete modal molecular picture. The method enables a qualitative prediction of the rst combustion reaction.

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CP6

Dns of Aluminum Agglomeration in Metallized Propellant Combustion

The DNS method of aluminum agglomeration in metallized propellant combustion is developed. The simulation has three stages. On the first stage, a simulation of propellant structure is performed. On the second stage, the thermal conductivity of propellant is calculated. On the third stage the evolution of aluminum particles above the propellant burning surface is considered. The results of calculation are dynamically represented and compared with high-speed movies taken on combustion of metallized propellants.

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CP7

Numerical Study of Detonability Limits

Detonability limits result from the adverse effects of boundary condi- tions on the propagation mechanism of a self-sustained detonation. In this study, the failure mechanism due to flow divergence in the reaction zone from the negative boundary layer displacement is studied numeri- cally for both stable and unstable detonations. For stable detonations, failure is due to quenching of chemical reactions. For unstable detona- tions, it is due to suppression of the intrinsic cellular instability of the detonation.

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CP7

Flames As Surfaces: An Asymptotic Hierarchical Multi-Layer Approach

Describing flames as surfaces is numerically efficient since flame structures must not be resolved but are replaced by jump conditions. However, strong stretch/curvature leads to inaccuracies of weak-stretch asymptotic models. We propose a new asymptotic hierarchical multi-layer approach (preheat-, inner-, oxidation layer) which automatically selects layers to be replaced by jump conditions yielding the most efficient model for desired accuracy. Model parameters are evaluated from detailed one-dimensional flame structures and turbulent DNS-data.

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CP7

Operator Splitting Techniques for Multi-Scale Reacting Waves And Application to Low Mach Number Flames with Complex Chemistry

In this contribution, we propose an analysis of order reduction of operator splitting techniques for time integration of reacting waves in the presence of stiffness due to both a large spectrum of time scales and high spatial gradients. We then propose a new strategy in order to use the obtained results for the simulation of the dynamics of flames with detailed transport and complex chemistry in the low Mach number limit.

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CP7

A High Order Projection Method for Premixed Low Mach-Number Combustion

On typical grid sizes for LES and RANS computations of low Mach-number premixed combustion the flame front can be treated as a discontinuity. In this work we present a projection method for low Mach-number combustion with subcell resolution using a level-set approach. We explicitely incorporate jump conditions for the dynamic pressure and its gradient over the flame front into the pressure Poisson equation to obtain a locally second order method.

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CP7

Numerical Study of Spark Based Flame Propagation Using High-Order Schemes

Flame kernel propagation produced by an electric spark in quiescent methane-air mixture at atmospheric pressure is analyzed in depth. High-order explicit time marching scheme in combination with a high-order WENO scheme are applied to solve species, momentum, and energy conservation equations in a two dimensional inviscid chemically reacting fluid. Different reduced and detailed chemical kinetics are used to show timing and magnitude of chemical heat release are very important for sustainable flame initiation.

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CP7

Extended Finite Element Methods for the Computation of Premixed Turbulent Combustion

The eXtended Finite Element Method (X-FEM) provides an attractive numerical method to simulate premixed turbulent combustion based on the G-function approach. First of all, X-FEM allow for an accurate capturing of the flame interface as no interpolation is needed. Further, by locally enriching the FEM space, discontinuities encountered in the velocity and pressure across the flame interface can be represented without smoothing. Results will be presented for various one-dimensional flames and a Bunsen burner.

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CP8

Influence of Flame Wrinkling on the Upstream Disturbance Field of An Acoustically Excited Premixed Flame

Acoustic wave interaction with a flame sheet involves the mutual interaction between the flow disturbances on the flame position, and the feedback of the exothermic, wrinkled front on the acoustic disturbance. These lead to flame wrinkles that convect downstream and impart a convective feature to the upstream disturbance field. This paper presents a computational study of this problem, using a level set solver for the flame sheet position coupled to a compressible Euler flow solver.

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CP8

Dns Study of V-Flame/Wall Interactions

In a combustion chamber interaction between a flame and a wall play a major role in the production of unburnt hydrocarbon (HC). The objective of this DNS study is to analyse the heat transfers between a wall with a prescribed temperature and a statistical stationary flame. Laminar and turbulent configuration have been set up by using an isooctane 29 species chemical Kinetics scheme. Evolution of HC concentration level is scrutinized for various wall temperatures and turbulent intensities.

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CP8

Large Eddy Simulation of Turbulent Swirling Flames

Large Eddy Simulation (LES) has been applied to predict swirling flames based on the Sydney swirl burner. In the numerical methods, the governing equations for mass, momentum and mixture fraction have been solved on a structured Cartesian grid. Smagorinsky eddy viscosity model with localised dynamic procedure of Piomelli and Liu is used as a subgrid scale turbulence model. The conserved scalar mixture fraction based thermo-chemical variables are described using a steady laminar flamelet model. With appropriate boundary conditions and relatively fine grid resolutions, LES predict the vortex breakdown and recirculation zones for swirling flames with high level accuracy.

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CP8

Premixed V-Shaped Flame Response to Equivalence Ratio Perturbations: Investigations on the Flame Kinematics

The response of a rod-stabilized V-shaped premixed flame to upstream velocity and equivalence ratio perturbations was characterized as a function of excitation frequency, flame angle, and mean equivalence ratio. Self-excited oscillations in low emission, premixed combustion systems are often caused by feedback between unsteady heat release rates and reactive mixture equivalence ratio perturbations. Using an analytical model based on linearization of the G-equation for inclined flames, the kinematics of a V-flame anchored on a central obstacle is investigated. It is shown that V-flames behave as an amplifier for upstream velocity and equivalence ratio perturbations in a certain range of frequencies and they are more susceptible to combustion instabilities than the conical flames.

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CP8

High-Fidelity Flame Front Capturing for the Compressible LES of Premixed Combustion

A high-fidelity flame front capturing scheme for the compressible large-eddy simulation of turbulent premixed combustion is presented. The flame front is captured using an efficient high-order localized level set/G-equation method in conjunction with a novel constrained reinitialization scheme. A dual-mesh approach is used to discretize the compressible Navier-Stokes equations and the G equation on different grids. The ghost fluid method is applied to implicitly resolve the flame front.

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CP8

Modeling Differential Diffusion with Conditional Moment Closure

In the context of conditional moment closure (CMC) modeling of turbulent reacting flows it is customary to make equal-diffusivity assumptions. Here an alternative derivation of the CMC equations is provided without making such assumptions. The appicability of the typical closure models is assessed, and it is found that substantial deviations occur. A new modeling approach is presented based on the relative diffusion of the mixture fraction and the scalar.

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CP9

The Effect of Reynolds Number on Extinction and Reignition in Syngas Jet Flames: A Direct Numerical Simulation Study

Terascale Direct Numerical Simulations have been performed to study extinction and reignition in nonpremixed syngas jet flames (Hawkes, et al. (2007), Proc. Combust. Inst. 31: 1633-1640). We characterise extinction using a metric based on the flame surface area having a reacting scalar less than a threshold value. The motion of edge-flames separating extinguished and burning regions is studied using a massively parallel analysis tool. Here, the joint probability density function of the edge-flame speed and scalar dissipation is used to study the effect of Reynolds number on extinction and reignition.

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CP9

Capturing Extinction and Reignition in Turbulent Flames: a Principal Component Analysis Approach

In the present paper, a novel methodology based on Principal Component Analysis (PCA) is developed for the construction of a combustion model for the description of

turbulence-chemistry interactions in flames. The ability of the model to parameterize the state variables describing the system and their source terms is assessed by means of high fidelity data, available from DNS simulations of a CO/H2 flame with increasing degrees of local extinction and reignition.

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CP9

Direct Numerical Simulation and Analysis of Stratified Turbulent Methane-Air Flames

Direct numerical simulations have been conducted for turbulent propagation of a flame spanning a mixture stratification layer. The stratification layer is composed of two co-flowing methane-air mixtures with differing equivalence ratios containing decaying turbulence. Combustion is simulated using a reduced methane-air mechanism. Several combinations of inlet composition, and turbulence levels are imposed permitting study of their effects on the stratified flame structure and propagation in the statistically stationary flow.

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CP9

Dns of Ignition and Propagation of Turbulent H2/air, Ch4/air and N-Heptane/air Premixed Flames

Direct numerical simulations of ignition and propagation of turbulent premixed flames in homogeneous isotropic turbulence have been conducted for hydrogen/air, methane/air and n-Heptane/air mixture to investigate effects of turbulence on ignition and propagation process. Detailed kinetic mechanism is used for hydrogen/air and methane/air mixture and several reduced kinetic mechanisms are used for n-Heptane/air mixture. Effects of pressure and fuel species on both processes are discussed with the investigation of local extinction of hydrocarbon flames.

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CP9

Direct Numerical Simulation of Premixed Flames Impinging on Isothermal Wall

Direct numerical simulations of interactions between premixed flame and isothermal wall have been conducted to investigate quenching mechanism of turbulent premixed flames near the wall. Near-wall behaviors of hydrogen/air, methane/air and n-Heptane/air premixed flames were investigated for different wall-temperature, mixture temperature and pressure by considering detailed kinetic mechanism for hydrogen/air and methane/air flames, and several reduced kinetic mechanisms for n-Heptane/air flames. Effects of fuel species on the heat flux at the wall are also discussed.

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CP9

DNS of Stabilization of Turbulent Lifted Nonpremixed Jet Flames in Vitiated Coflow

The stabilization of a turbulent lifted nonpremixed jet flame in a vitiated coflow is investigated using 3D direct numerical simulations (DNS) in a slot burner configuration at jet Reynolds numbers in excess of 10,000. Detailed hydrogen-air and reduced ethylene-air chemical kinetic mechanisms are used with mixture averaged transport properties. The effects of auto-ignition and coherent jet structures on the stabilization mechanism are investigated. A comparison of the flame base dynamics for hydrogen and hydrocarbon fuels will be made.

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CP10
Numerical Simulation of Initial Perturbation Effects on the Detonation Cell Size

One of the most important contributions of linear detonation stability analysis is the presentation of the perturbations growth rate versus perturbations wave number for a given set of detonation parameters. The objective of this work is to establish a relation between the unstable wave numbers of the linear results and the actual detonation cell size. Using the reactive Euler equations we have studied the effect of initial perturbation wavelength on the final cell structure of weakly unstable detonations with low activation energy and regular cellular pattern.

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CP10
Linear Stability of Detonations

This study focuses on the linear stage of the detonation instability of an initially steady, one-dimensional ZND model base flow. We have investigated the linear stability characteristics of a single reversible reaction kinetics model using a generalized form of the normal modes method of Lee and Stewart [H.I. Lee, D.S. Stewart, J. Fluid Mech., 216 (1990) 103-132] and Short [M. Short, SIAM J. Appl. Math, 57 (2) (1997) 307-326]. We have then validated our results with direct Euler simulations by concentrating on the linear stage of the unsteady growth.

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CP10
Kinematics of Multi-Dimensional Shock Fronts with Application to Numerical Solution of the Reactive Euler Equations

Evolution of multi-dimensional shock fronts is analyzed and is represented by a pair of partial differential equations for the shock position. A high-order numerical algorithm is proposed that solves the shock evolution equations coupled with the reactive Euler equations for the flow behind the lead shock. Application to detonation simulations is discussed.

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CP10
The Macroscopic View on Deflagration-to-Detonation Transitions in Thermonuclear Supernovae

As astrophysical objects, thermonuclear supernovae feature a prohibitively vast range of length scales to investigate deflagration-to-detonation transitions (DDTs) in a single numerical approach. Thus, the problem can be tackled from two perspectives. Complimentary to microscopic studies of the mechanism of DDTs is the macroscopic approach which will be discussed here. Large-scale simulations determine the conditions under which DDTs may occur and ultimately provide the overall picture resulting from thermonuclear supernovae with delayed detonations.

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CP10
Critical Energies and Conditions for Initiation of Detonation in Explosives

We consider the classic problem of initiation of detonation in an explosive from a hot spot. The hot spot can be regarded as point source deposition of energy that is the result of a rapid energy flux from a boundary or from the rapid energy release from a smaller charge, such as a primary explosive in a detonator. Since the reaction zone that contributes to the explosive, in the domain from the lead shock to the trailing sonic locus is very small compared to the radius of the shock, small curvature asymptotics can be use to compute reduce evolution equations. These are compared to direct numerical simulation for the cases of gaseous and condensed explosives, and critical energies and condition are computed.

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CP10
Mode Selection in Unstable Two-Dimensional Detonation

A novel formulation of the reactive Euler equations in the shock-attached frame is used to study the transition to instability of weakly unstable two-dimensional detonation in confined channels through direct numerical simulation. The results are shown to agree with the predictions of linear stability analysis with remarkable accuracy. The long-time, nonlinear behavior and detonation cell spacing are studied by Fourier decomposition of the shock-displacement function in the transverse spatial domain.

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CP11

Radiation Using Higher-Order Spherical Harmonics Method for DNS of Turbulent Reacting Flows

The inherent complexity of the radiative transfer equation (RTE) makes the exact treatment of radiative heat transfer impossible even for idealized situations and simple boundary conditions. Here a third-order spherical harmonics method (P_3 approximation) is used to decompose the RTE into a set of six coupled second-order partial differential equations with general boundary conditions. The solution is coupled with Direct Numerical Solution (DNS) of turbulent reacting flows to isolate and quantify turbulence−radiation interactions.

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CP11

Partially Premixed Flames in a Centerbody Burner

Chemical and physical processes that govern soot formation and growth in a flame (nonpremixed or premixed) occur simultaneously. A novel flame system utilizing a naturally formed recirculation zone for trapping soot precursor particles has been designed for studying soot growth process. A recirculation zone is created behind a 4.6-cm-diameter disc with an annular airflow of 1-4 m/s. Fuel, a mixture of ethylene and air, is injected through a 0.76-cm-diameter hole made at the center of the disc. Calculations are made using UNICORN code.

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CP11

A Simplified Model for the Simulation of Soot Formation in Shock Tube Experiments

The direct description of the soot formation in CFD simulations based on many equations is computationally prohibitive. Therefore a simplified soot model (2-equation model) was developed and calibrated. This model was tested for shock tube conditions. The results of the simplified soot model are compared to those of the detailed model of soot formation which was used for the calibration. Results will be presented for fuels like n-heptane and toluene.

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CP11

Master Equation Formulation of Radiative Transfer In Clumpy Statistical Mixtures

A stochastic Liouville equation approach is proposed for modeling radiative transfer and material temperature response in clumpy random mixtures. Sub-ensemble averaging is shown to produce doubly unclosed, coupled Master equations for the conditional probability densities of the radiation intensity and material temperature. Closures are proposed and numerically tested for the mean intensity and temperature in the linearized regime. Reduced-order models valid in certain asymptotic limits are also presented in the linear case.

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CP11

Radiation-Driven Flame Extinction in Sooting Turbulent Diffusion Flames

The present study uses direct numerical simulation to bring basic information on the structure of turbulent luminous non-premixed flames, with a particular emphasis on flame extinction and soot mass leakage. The numerical configuration corresponds to an ethylene-air, wall-jet diffusion flame in which the Planck mean absorption coefficient of soot particles is artificially increased by a factor 10. The resulting optically-thickened flames feature low-burning-intensity spots that are similar to the radiative extinction events observed in microgravity combustion.

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CP11

Comparison of Different Radiative Heat Transfer Models in Large Eddy Simulation of Turbulent Combustion

The influence of the radiative heat transfer model on the dynamics of a turbulent flame is investigated coupling a large eddy simulation combustion solver and a radiation code through a dedicated language. Results using three different radiation models (Optical thin model, Discrete Ordinate Method and Monte-Carlo technique) are discussed and compared both in terms of physical behavior of the flame and in computational aspects (memory requirement,

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CP12

A Level-Set Flamelet Model for the Prediction of Nitrogen Oxides in Homogeneous Charge and Spray-Guided Spark-Ignited Engines

The level set flamelet model of Peters [Turbulent Combustion, Cambridge Univ. Press, Cambridge, UK, 2000] for turbulent premixed combustion was recently extended to comprise pollutant models. The formation of nitrogen oxides (NO_x) is predicted using the extended Zeldovich mechanism. An efficient NO_x model is presented which incorporates local turbulence-chemistry interactions. Numerical simulations of engines running in homogeneous charge and spray-guided (SG) operating modes highlight that the commonly involved laminar chemical equilibrium assumption is valid for premixed mixtures only. It is shown that in spray-guided engines turbulence-chemistry interactions have to be considered due to distinctive mixture fraction fluctuations occurring during the main NO_x formation phase.

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CP12

Modeling of the Low Temperature Oxidation of Large Alkanes

A modeling study of the low-temperature oxidation of alkanes from C10 to C16 has been performed from low to intermediate temperature (550-1050 K). Detailed kinetic mechanisms have been developed using computer-aided generation (EXGAS) with improved rules for the writing of secondary reactions. These mechanisms reproduce correctly autoignition delay times and experimental data obtained in flow reactors. A considerable improvement of the prediction of the formation of products is obtained compared to our previous models.

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CP12

Auto-Ignition of Nonpremixed N-Heptane in Unsteady Counterflow

As a model problem to understand the effect of turbulence on autoignition behavior in diesel engines, autoignition of n-heptane in a nonpremixed counterflow configuration subjected to a time-varying scalar dissipation rate is studied numerically with detailed chemistry. Fuel and air temperatures are chosen so that two-stage ignition occurs in the negative temperature-coefficient regime. The mean and the fluctuation amplitude of the scalar dissipation rate is carefully chosen based on the steady condition such that the second stage ignition is suppressed for a duration over the cycle. The response of ignition delay for various frequencies is investigated. It is found that the first stage ignition behavior is hardly irresponsive to the scalar dissipation rate fluctuation at all frequencies. On the other hand, the second stage ignition is found to be sensitive to the frequency of the scalar dissipation rate fluctuation. Furthermore, the response of the ignition delay to the increasing frequency is found to be nonmonotonic: as the frequency increases, the ignition delay decreases first and increases, and finally decreases again asymptotically towards the steady ignition delay. This non-monotonic response of the second stage ignition delay is attributed to the combined effects of the phasing of the instantaneous scalar dissipation rate at the ignition kernel as well as the changes in the spatial location of the ignition kernel.

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CP12

Towards a Detailed Soot Model for Internal Combustion Engines

We integrate previously developed models for engine combustion and soot formation, namely, the Stochastic Reactor Model (SRM) engine code, which features detailed chemistry, heat transfer, and mixing, with SWEEP, a Monte Carlo population balance solver. The combined model provides not only averaged quantities like soot mass, aggregate diameter, and number of primary particles per aggregate, but also aggregate/primary particle size distributions, aggregate structure/composition, and TEM-images. Simulated distributions and their time evolution qualitatively agree with measurements.

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CP12

Theoretical Study of the Thermal Decomposition of a Jet Fuel Surrogate

In a scramjet, the fuel can be used to cool down the engine walls. The thermal decomposition of the jet fuel changes the reacting mixture before its combustion. A numerical study of the pyrolysis of norbornane, a jet fuel surrogate, has been performed. Rate constants of some sensitive reaction channels have been based on theoretical calculations. The mechanism has been validated against experimental results and important and/or sensitive pathways have been derived.

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CP12

A Nitrogen Pollutants Prediction Scheme for Combustion of a Hydrocarbon Fuels

This paper presents a modelling of nitrogen oxide (NO) reaction mechanisms with appropriate combustion and radiation modelling, which are required to accurate predict NO formation. A piloted jet flame was simulated and predictions are compared with experimental data. Combustion was modelled by stationary laminar flamelet model (SLFM) and radiation was modelled by the conservative discrete transfer radiation method (DTRM). The NO formation was predicted with post-processing computation using converged solution of flame structure.

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CP13

Comparisons Between Eulerian and Lagrangian Pdf Methods for Turbulent Reacting Flows

Eulerian field methods have been proposed as alternatives to Lagrangian particle methods for solving modeled probability density function (PDF) equations for chemically reacting turbulent flows. Systematic comparisons among three approaches to solving modeled PDF equations are reported to assess their relative strengths, weaknesses, and limitations: a stochastic Eulerian field method, a deterministic Eulerian field method using DQMOM closure, and a Lagrangian particle method.

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CP13

A Partially Premixed Combustion Approach for Presumed-PDF LES

Methods of dealing with partially premixed combustion in the context of presumed-PDF large eddy simulation (LES) are considered. A partially premixed model consistent with both the non-premixed flamelet progress variable approach and the premixed level set approach is presented. This model distinguishes between combustion regimes by examining how chemical source terms are balanced. The model is applied in a simulation of a laminar triple flame and in an LES of a low swirl burner.

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CP13

Efficient Coupled Les / Transported Pdf Approach Using a Second Order Accurate Eulerian Monte-Carlo Scheme

An Eulerian Monte-Carlo PDF (MC-PDF) method coupled with LES has been extended to second order accuracy in space using a TVD-scheme based model proposed by [Chen, J.Y.; Comb. Theory and Modelling Vol.11, No.5 (2007)]. The order of the time discretization is increased by integrating the MC-PDF transport into the three step Runge-Kutta scheme of the LES time stepping. The method is validated by simple transport test cases. Finally, the method is used to simulate the well investigated piloted jet flame Sandia Flame D [Barlow, R.S. and Frank, J.H.; Proc. Comb. Inst. 27 (1998)].

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CP13
PDF Modeling for PCCI Engines

Transported probability density function (PDF) methods have shown promise in applications to canonical flames and simple internal-combustion-engine (ICE) configurations. The combustion event in a realistic ICE is highly non-stationary, involves two-phase combustion, and creates difficult situations for experimental diagnostics. In this work, skeletal-level chemistry, a transported composition PDF method, and a liquid fuel spray model are integrated to compute autoignition and emissions for a real engine with comparison to experimental data.

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CP13
Composition Pdf Modeling of a Turbulent Ethylene/Air Jet Flame with Soot Formation

A composition PDF method for gas-phase thermochemistry is coupled with a method of moments for soot formation is used to simulate experimental ethylene/air jet flame. A simplified nucleation mechanism and a modified surface growth mechanism for soot and reduced mechanism for ethylene consisting of 33 species and 205 elementary reactions is used. The soot formation mechanism is coupled directly with the transported PDF approach to account for turbulence–chemistry interactions, with optically thin approximation for radiation. Simulation results are compared with experimental data.

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CP13
The Multi-Environment Conditional Pdf Model, Recent Progress

The multi-environment conditional PDF model for non-premixed turbulent combustion was developed to describe the regime where mixing timescales and reaction timescales overlap to the degree that the flame experiences local extinction and re-ignition. Recent developments include a numerical procedure for stable solution to the equations for the weights, and model extension to arbitrary number of reacting species and variable density. A validation study comparing to direct numerical simulations will be presented.

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CP14
Effects of Lewis Number on the Scalar Flux in Turbulent Premixed Flames

The effects of Lewis number Le on scalar transport in turbulent premixed flames have been studied using 3D DNS. It is demonstrated that a Le¡1 flame may show counter-gradient transport below a threshold value of Le, whereas the transport remains gradient-type in Le≥1 flames under similar turbulence conditions. The mean pressure gradient term of the scalar flux transport equation is shown to be strongly affected by Le, and is predominantly responsible for this behaviour.

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CP14
The Effects of Initial Kernel Radius on the Surface Density Function Transport in Turbulent Flame Kernels

The effects of initial radius on the Surface Density Function (SDF = magnitude of progress variable gradient) transport in turbulent flame kernels have been studied based on 3D-DNS. The global flame curvature is shown to have profound influence on the mean and local behaviour of the SDF and on the different terms of its transport equation. The local curvature effects on the relevant terms have been studied in terms of their joint pdfs with curvature.

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CP14
Flame Surface Density Distribution in Turbulent Flame Kernels: Influence of the Initial Energy Spectrum

DNS are used to assess the influence of the initial turbulent energy spectrum on the distribution of Flame Surface Density during the early stages of growth. Significant variation in the surface mean velocity and displacement is found between individual isosurfaces of the reaction progress variable, and a bias is shown to exist in the distribution of the Surface Density Function. The developing fresh gas turbulence properties are evaluated from an independent ensemble of cold-flow simulations.

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CP14
An Algebraic Model for Scalar Dissipation Rate in Turbulent Premixed Flames

An algebraic model for the Favre averaged scalar dissipation rate (SDR) is derived by balancing the leading order terms in SDR transport equation for high Damkhler number turbulent premixed flames. This model is obtained us-

ing the recent models for several terms of the SDR transport equation. Turbulent flame speed obtained from the KPP analysis based on this model is found to be in very good agreement with wide range of experimental data.

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CP14

Comparison of an a priori Tabulation of Turbulent Flame Speeds with DNS and Algebraic Models

The authors recently presented a technique for an a priori tabulation of turbulent flame speeds (TFST). Statistically stationary turbulent flame structures are computed by solving the incompressible one-dimensional Navier-Stokes equations and turbulent transport via the linear eddy model (LEM). The evaluated turbulent flame speeds are stored in a data base that could be used by, e.g., front tracking schemes. Here we focus on a comparison between the tabulated results with DNS and modern algebraic models.

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CP14

Three Dimensional Calculations of Supersonic Combustion Using LU-SGS-GE Scheme

An implicit LU-SGS-GE time-marching method in combination with high-order shock-capturing schemes is proposed for solving the three dimensional compressible Navier-Stokes, species and two equation $q - \omega$ turbulence model equations in a fully coupled and very efficient manner. In compare with existing methods, the present scheme, LU-SGS-GE, leads to faster convergence and better stability. To demonstrate the validity of this method, various experimental cases are numerically studied, and, the obtained results are compared with existing experimental data.

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CP15

Using Cartesian Embedded Boundary Methods for Simulating Potential Hydrogen Explosions in the Nuclear Industry

We demonstrate the use of a Cartesian grid, cut-cell method for simulating accidental hydrogen detonations in scenarios for the nuclear safety industry. The numerical scheme is based on conservative, finite-volume methods for Cartesian grids. To handle the complex geometry present the industrial problems we consider, we use an embedded boundary method of Colella, et. al. in which geometry is allowed to cut the background Cartesian grid. The cut-cells are then handled using special algorithms. We present several simulations using the EBChombo code, developed by the ANAG group at Lawrence Berkeley Laboratory and demonstrate that cut-cell methods can accurately and efficiently handle the complex geometry arising in industrial applications.

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CP15

Numerical Simulation of Propagating Flames Using Locally Adaptive Mesh

High-fidelity numerical simulation is currently a productive research tool in combustion science. In this study, the locally adaptive mesh is employed in simulation to overcome the current simulation limitations caused by mesh number. The details on A-SURF, developed for Adaptive Simulation of Unsteady Reactive Flow, are resented and it is utilized to carry out high-fidelity numerical simulations of the propagating flames in a closed chamber.

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CP15

A Compressible Navier-Stokes Solver for Non-Premixed Combustion on Unstructured Hexahedral Grids

A compressible Navier-Stokes solver on unstructured hexahedral grids, for the simulation of non-premixed combustion is presented. Since the solution scheme is density-based, a preconditioning technique is used when incompressible or low Mach number flows are simulated. To

ensure efficent convergence properties, several algorithms, such as agglomeration multigrid, implicit residual smoothing and parallelization with automatized domain decomposition have been developped. The coupling of mixture fraction based models for non-premixed combustion to a preconditioned solution scheme is shown and the means to ensure monotonous and bounded solutions are explained. A comparison of the computational results obtained for well-established fundamental academic test cases with experimental data confirms the validity of the implemented combustion models. The computational results for industrial test cases are used to discuss the capabilities and the limitations of the applied combustion models based on the mixture fraction approach.

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CP15

Numerical Study of Various Flame Stabilization Methods in Supersonic Combustion

The effects of various methods on flame stabilization in the supersonic combustion of hydrogen are considered here using numerical approaches. Non-active flame holders, cavity and backward facing step, are compared with oxygen and nitrogen plasma jets. The effects of combining above methods on flame stabilization are also analyzed in depth. The solutions to the governing equations are brought in using high-order numerical schemes. Results clearly demonstrate the superiority of oxygen plasma jet for flame stabilization.

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CP15

Adaptive Software Design for Discretization-Independent Multiphysics Simulations

Achieving adaptive simulations where models (including governing equations themselves) may change dynamically requires advanced software designs. Often, the complex physical dependencies among various terms in the governing equations require strict orderings that produce rigid algorithms. This talk will present a software development approach that is independent from the spatial discretization scheme and which naturally allows increasing complexity. A key characteristic of this approach which facilitates adaptivity is the lack of a user-defined algorithm.

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CP15

Distributed Fast Marching Methods

Fast Marching Methods (FMM) are very efficient algorithms for the numerical solution of evolution equation arising, for instance, from the front propagation problems. The classical FMM are theoretically optimal in terms of operation count (O(NlogN)), sequential by nature and hence not straightforward to parallelize. We present several parallel implementations of the FMM combining Fast Sweeping with Fast Marching, in such a way that allows fast convergence. We illustrate the power of these approaches with a series of benchmarks which include the study of the convergence and the error estimates, and show the monotonicity and stability properties of the algorithms.

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CP16

Numerical Simulation of Turbulent Combustion Using Urans and Les

Large-eddy simulation (LES) has become an attractive approach for the numerical simulation of turbulent combustion while the use of unsteady Reynolds-averaged Navier-Stokes (URANS) is still subject of debate. Although extensive research, regarding the numerical simulation of turbulent combustion, has been carried out, there are still many fundamental questions that have to be addressed. The goal of the present investigation is to highlight the fundamental differences between LES and RANS combustion models, for turbulent combustion.

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CP16

Acoustic Timescale Detonation Initiation - Part I: 1-D Theory and Modeling

This is the first of two talks on modeling and simulation of detonation initiation following localized, spatially- and time- resolved thermal power deposition. Momentary, partial inertial confinement resulting from localized heat addition on time scales comparable with the local acoustic time causes high pressure and temperature reaction centers. Subsequent relaxation produces compression waves that condition neighboring gas, leading to additional reaction centers. Computational results based on adaptive wavelet collocation methods confirm earlier solutions ob-

tained from a MacCormack-based approach.

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CP16

Probability Density Function Approach for Large-Eddy Simulation of Turbulent Spray Combustion

Large-eddy simulation (LES) of spray combustion requires detailed modeling of the spatial correlation between the spray droplets and the gas-phase at the sub-filter scale. For this purpose, Direct numerical simulations (DNS) of spray combustion are used here to study the spray-gas phase interactions. A planar spray jet and a homogeneous isotropic turbulent flow are considered. The mixing process is found to be substantially different for droplets with near-unity and non-unity droplet Stokes numbers. Further, sub-grid modeling assumptions used in the context of mixture-fraction based combustion modeling are found to be inaccurate when the evaporation time-scale is comparable to the mixing time-scale. A new transported probability density function method is proposed as a viable route for modeling the gas-phase evolution. Modeling and numerical issues will be discussed.

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CP16

Reverse Monte-Carlo Ray-Tracing Method Combined with Full-Spectrum K-Distribution Method for Radiative Heat Transfer

In this paper, the Reverse Monte-Carlo Ray-Tracing (RMCRT) method is used to solve the RTE and combined with the Full-Spectrum k-Distribution (FSK) for non-gray radiative properties. The RMCRT method has advantages over the Forward Monte-Carlo Ray-Tracing (FMCRT) method in that it uses less memory and is easier to parallelize for domain decomposition. The accuracy and efficiency of this combined method is demonstrated by sample calculations in multidimensional, inhomogeneous combustion problems. The results are compared to line-by-line calculations.

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CP16

Self Sustained Oscillations in a Lumped Parameter Pulse Combustor Model

A Lumped parameter model of pulse combustion is developed which employs a submodel for the reactant mass flow that modifies the usual model based on the orifice flow equations. A complete numerical study of the model is presented and the results are compared with earlier work based on the orifice flow equation submodel. Among the parameters varied in the numerical study are the length of the tailpipe, the air-fuel ratio, and the cross-sectional area of the air and gas valves.

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CP16

Acoustic Timescale Detonation Initiation - Part II: Numerical Approach and 2-D Simulations

This is the second of two talks on modeling and simulation of acoustic timescale detonation initiation. This talk discusses the Adaptive Wavelet Collocation Method used to perform one and two-dimensional simulations and describes the results of 2-D simulations in a channel initiated by thermal power deposition into a small circular region. Multidimensional gasdynamic processes including wave reflections lead to the appearance of numerous reaction centers that promote the development of an overdriven detonation, like that seen in the 1-D simulation.

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CP17

Structure of Nonpremixed Methane Flames in Twin-Jet Counterflow

Structure of nonpremixed flame in a twin-jet counterflow has been simulated by using reduced and detailed mechanisms for methane fuel diluted with nitrogen. A nonpremixed flame with an advancing edge was stabilized with a trail flame similar to a conventional counterflow flame. At large strain, the trailing flame becomes extinguished, such that a petal-shaped flame existed, which had a retreating edge. The structure of the stationary retreating edge flame will be discussed.

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CP17
On the Modeling of the Conditional Variance Equation for Autoignition

Compressible three-dimensional Direct Numerical Simulation of autoignition of a non-premixed mixture has been analyzed to validate the sub-models for the conditional covariance equation. The mixture has been assumed to react according to a one-step irreversible reaction. Standard sub-models, developed for flame calculations have a limited predictivity in case of autoignition and flame propagation. This work intends to study the limitation of the present sub-models in the aim of an application of CMC in LES in the context of a progress variable approach for autoignition and flame propagation.

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CP17
A Partially-Premixed Coherent Flame Model (pcfm) for Turbulent Combustion

Partially-premixed combustion occurs in many combustion devices of practical interest. Aiming at simulating these combustors, a PCFM model is developed by modifying the coherent flame model. It solves a flame area density equation for the primary premixed flame and uses a laminar flamelet methodology for the subsequent non-premixed zone. The model is validated against the experimental data on a turbulent lifted flame issuing into a vitiated coflow. Its capabilities are further demonstrated by practical cases.

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CP17
Reactive Rayleigh-Taylor Turbulence

We study reactive Rayleigh-Taylor turbulence in the regime of slow reactions (thick laminar fronts). Numerical simulations show that the typical velocities of the Rayleigh-Taylor instability are essentially unaffected by reaction, while the temperature distribution transitions from well-mixed to partially-mixed state. In the partially mixed state we observe regions of pure reacted and unreacted fluid separated by the reaction zone. While both the size of pure regions and the reaction zone grow in time, on average the system becomes less mixed. The numerical simulations become a source of inspiration for a phenomenological "Obukhov-Corrsin"-type theory which explains the observed behavior, makes the further predictions, and suggests a number of diagnostic routines. The building blocks of the phenomenology are not restricted to the Rayleigh-Taylor instability and theoretical results could be applied to various two-phase systems such as turbulent combustion or turbulent flow of immiscible fluids with surface tension.

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CP17
The Turning Points on a Dn-kappa Curve

An explicit asymptotic solution derived for the Dn-kappa curve of a quasi-steady detonation shows that besides the two possible under-driven turning points, there is another turning point on the over-driven portion. It seems to mean that when a sonic locus is embedded in the flow, a limiting value of the detonation velocity exists such that a quasi-steady detonation may exist only when its propagation speed is below this value.

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MS1
Low-Dimensional Manifolds in the Spatial Dynamics of Steady One-D Premixed Flames

Spatial dynamics of steady one-dimensional H2/O2 flames are studied from a geometric perspective. The geometry is studied via low-dimensional sub-manifolds that describe the longer spatial dynamics on the stable manifold of a saddle point. The saddle point of the flame dynamics corresponds to an equilibrium point of a time-dependent chemical-kinetic system that is adiabatic and isobaric The low-dimensional manifolds of the flame system are compared to the low-dimensional manifolds of the chemical-kinetic system.

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MS1
The Effect of Diffusion on Simple Paradigm Chemical Kinetic Problems

In joint work with L. Kalachev, H. Kaper, N. Popovic, and A. Zagaris, the speaker has analyzed reduction for a

paradigm problem of three coupled reaction-diffusion (R-D) equations. It is shown that, depending on the ratios of the diffusivities and the rates of the reaction kinetics, reduction is possible to a system of ODEs or to a single R-D equation. The effects of different types of boundary conditions are also explored analytically. This paradigm problem serves as a good benchmark problem for numerically-based reduction procedures.

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MS1

Transport-chemistry Coupling in the Reduced Description of Reactive Flows

In this talk, we address the issues arising from the use of chemistry-based slow manifolds in calculations of inhomogeneous reactive flows. In particular we describe three different mechanisms that can pull compositions off the chemistry-based slow manifolds, namely, non-invariance, dissipationcurvature, and differential diffusion. We demonstrate that these three seemingly small perturbations introduce three generally nontrivial terms into the governing equations for the reduced compositions, which in general are of leading order.

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MS1

Calculation of Invariant Manifolds for Reacting Systems

We discuss the construction of invariant manifolds for a reacting system. A model of hydrogen-oxygen combustion will be considered with special attention given to finding all equilibria, including points at infinity, and identifying any and all trajectories which link these equilibria. This will first be considered for a spatially homogeneous system; extensions to reacting flow will be discussed.

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MS2

An Adaptive Numerical Method for Compliant Confinement in Shock Desensitized High Explosives

The dynamics of detonations in charges of high explosive can be drastically altered by the type of material which confines it. Accurate modeling of this confining material and its interaction with the detonation front is critical for complete understanding of detonation dynamics, even far from the reactive/inert interface. Here we present an adaptive numerical method to treat the two material interface in charges of high explosive which may or may not be desensitized by shocks.

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MS2

Accurate Simulation of Transient Mach-reflection Structures in Gaseous Detonations with an Adaptive High-resolution Method

Multi-dimensional instabilities, intrinsic to gaseous detonations, lead to the formation of evolving Mach-reflection patterns at the detonation front. Dynamic mesh adaptation is an indispensable tool to resolve such patterns accurately. We describe a Riemann-solver-based finite volume scheme for detailed kinetics, that has been incorporated into a parallel blockstructured mesh adaptation method with immersed boundary capability, which enabled numerical investigations of Mach-reflection structures in three-dimensional and transient two-dimensional detonations in low-pressure hydrogen-oxygen-argon mixtures at unprecedented detail.

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MS2

Accuracy Improvement of Flux-corrected Transport Algorithms for an Adaptive Cartesian Mesh

A multidimensional fourth-order flux-corrected transport algorithm, using a flux limiter based on local characteristic variables, has been implemented on a dynamically adaptive mesh based on the fully-threaded tree data structure. We solve a series of numerical test problems, including flame-shock interactions, and use these to illustrate the effect of the high-order flux, the dissipation term, and the limiter.

The result shows the fourth-order FCT can accurately resolve smooth profiles as well as discontinuities.

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MS2
An Adaptive Method for a Model of Two-phase Reactive Flow on Overlapping Grids

A two-phase model of heterogeneous explosives is handled computationally by a new numerical approach that is a modification of the standard Godunov scheme. The approach generates well-resolved and accurate solutions using adaptive mesh refinement on overlapping grids, and treats rationally the nozzling terms that render the otherwise hyperbolic model incapable of a conservative representation. The evolution and structure of detonation waves for a variety of one and two-dimensional configurations will be discussed with a focus given to problems of detonation diffraction and failure.

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MS3
Turbulent Flames in Type Ia Supernovae

Over the past few years Type Ia (thermonuclear) supernovae received considerable attention because this subgroup is the brightest and most homogeneous and their light curves and spectra are all very similar. Therefore, they are used as cosmic distance indicators with great success. The model favored by astrophysicists explains Type Ia supernovae with thermonuclear explosions of white dwarf stars, composed of carbon and oxygen and disrupted by the explosive fusion of carbon and oxygen to iron-group elements, predominantly radioactive ^{56}Ni. It has been shown that the physics involved is very similar to that of premixed chemical flames. Here we discuss recent attempts to model the explosions by means of large-eddy simulations.

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MS3
Discussion

The speakers of the previous three presentations, and others in the audience, will discuss the properties of turbulence in Type Ia supernovae, the structure of distributed flames, and how these set the stage for the explosion process.

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MS3
Distributed Flames and DDT in Supernovae

Type Ia supernovae are nature's grandest thermonuclear explosions and a laboratory to study combustion in unusual circumstances - enormous Reynolds number, large Karlovitz and Lewis numbers, very temperature-sensitive reactants, long time scale, and large length scales. So long as a well-defined flame exists, detonation will not occur, but as the flame moves into a regime where turbulence can tear the flame, numerical and analytic considerations suggest a transition to detonation may be possible.

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MS4
Turbulent combustion modelling using tabulated chemistry based on self-similar properties of turbulent premixed flames

Chemical databases are widely developed to incorporate complex chemistry features in turbulent combustion simu-

lations, for example in the framework of ILDM or related approaches. Unfortunately, the size of these databases may become a crucial issue for efficient implementation on massively parallel computers. Several reduction stategies, taking advantage of the self-similarity behavior of turbulent premixed flames, are proposed and compared, both in terms of precision and computational efficiency, in simulations of a turbulent jet flame.

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MS4

Implementation of ILDM- and REDIM- reduced kinetics in PDF calculations

Intrinsic low-dimensional manifolds (ILDM) and reaction-diffusion manifolds (REDIM) are two approaches to reduce detailed kinetic schemes for subsequent use in reacting flow calculations. The low-dimensional manifolds are calculated beforehand, and they are tabulated together with the chemical reaction rates and other information in terms of the reaction progress variables. In this work we discuss the tabulation and the implementation in transported probability density function (PDF) models for turbulent flames.

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MS4

Construction of Optimal Artificial Neural Networks for Tabulated Chemistry Using Pattern Search Algorithms

A pattern search optimization method is applied to the generation of optimal artificial neural networks (ANNs) for chemistry tabulation. Optimization is performed using a mixed variable extension to the generalized pattern search method. This offers the advantage that categorical variables, such as neural transfer functions and nodal connectivities, can be used as parameters in optimization. When used together with a surrogate, the resulting algorithm is highly efficient in providing accurate low memory chemistry tables.

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MS4

Tabulation of detailed chemistry for LES predictions of non-premixed burners ignition maps

An accurate description of chemistry is needed for simulating ignition of nonpremixed mixtures. The tabulation of detailed methane/air chemistry for spark ignition simulations is discussed. Nonpremixed mixture is considered and the impact of both spark location on the equivalence ratio map and scalar dissipation rate are studied. The obtained chemical table is applied to Large-Eddy Simulation to build nonpremixed burner ignition maps and results are compared with experiments.

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MS5

On the Use of Elemental Flux Graphs for Developing Adaptive Reduced Representations of Complex Reaction Mechanisms

Integration of complex CFD and comprehensive kinetic models consumes substantial amount of CPU. We explore the possibility of associating reactive conditions, and hence reduced mechanisms, with elemental flux graphs accounting for the reactive propensity of the mixture. We propose an integrated framework for the generation and mining of such graphs and demonstrate the advantages of the approach in the context of low-temperature oxidation of nPentane in predicting auto-ignition delays and simulating PMSR reactors.

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MS5

Reacting Flow and Control Theory

Model reduction of reacting flows begins with a set of ODEs and searches for "slow manifolds"—by exploiting the fast/slow speed gap—so that some of the ODEs can

be replaced by algebraic equations. Control theory begins with a set of ODEs with unknown control forces, and determines them to honor some user-specified behaviors—such as staying on a phase space surface (i.e. manifold). Model reduction methodologies for reacting flows can be applied to control theory.

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MS5

Coupling of Kinetics and Transport in the Context of Intrinsic Low-dimensional and Reaction/diffusion Manifolds

Manifold methods have proven to be an efficient and accurate method to reduce detailed chemical models. One important effect that has to be accounted for in the construction of the low-dimensional manifolds is the fact that there is a strong coupling of molecular transport with the chemical kinetics. We shall discuss how this is accounted for by a projection of the transport terms in the context of ILDM, and how the REDIM concept accounts for the coupling explicitly in the construction of the manifolds.

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MS5

Time Integration of Reacting Flows using Adaptive CSP Tabulation

We present a tabulation strategy for the adaptive numerical integration of chemically reacting flow using Computational Singular Perturbation (CSP). The strategy stores and reuses CSP quantities required to filter out fast processes, resulting in a non-stiff chemical source term. This enables efficient time integration of reaction-diffusion systems without operator-splitting. The use of the CSP homogeneous correction enables efficient manifold identification and subsequent time integration. We demonstrate the method and evaluate its performance on model systems.

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MS6

Requirements for Adaptive Detailed Simulation of Premixed Turbulent Flames in the Corrugated Flamelet Regime

Recently, we reported detailed simulations of laboratory-scale turbulent premixed methane flames in the corrugated flamelet regime. While the grid spacings used in these simulations were too coarse to definitively resolve the finest scales of the turbulence, flame-related diagnostics were indeed grid-independent and agree with available laboratory measurements. Here we validate our simulation approach formally, demonstrating the meshing requirements of a well-designed adaptive-mesh numerical discretization to reproduce experimentally relevant features of a refined DNS flame solution.

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MS6

Large Eddy Simulation of Turbulent Premixed Flames Using Parallel Block-based Adaptive Mesh Refinement

A parallel block-based adaptive mesh refinement (AMR) scheme is described for performing large eddy simulations (LES) of turbulent premixed combustion on body-fitted multi-block hexahedral mesh. Key elements of the proposed algorithm will be discussed and include a hierarchical data structure that permits local anisotropic mesh refinement, efficient and scalable parallel implementation via domain decomposition, a parallel implicit time-marching scheme based on a Newton-Krylov-Schwarz (NKS) approach, and subfilter scale models based on thickened flame and flame surface density (FSD) approaches.

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MS6

Performance of a High-order Projection Scheme for AMR Computations of Chemically Reacting Flows

A high-order projection scheme was developed for the study of chemically reacting flows in the low-Mach number limit. This scheme is coupled with an operator-split stiff approach for the species and energy equations. The code employs a block-structured high-order adaptive mesh refinement approach to tackle the challenges posed by the large spectrum of spatial scales encountered in reacting flow computations. Results for canonical configurations

are used to examine the performance of the construction.

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MS6
Fully Adaptive Multiresolution Methods for 3d Thermodiffusive Combustion Instabilities

We present numerical simulations of planar, circular, and spherical thermo-diffusive flames in three space dimensions. Attention is focused on the interaction of spherical flames with adiabatic walls or equivalently on their interaction with their mirror image. The numerical scheme is based on a fully adaptive multiresolution discretization which allows self-adaptive grid refinement in regions of the thin reaction zone. We show that the Lewis number determines the behaviour of the flame-wall interaction. When the flame is approaching the wall, we observe for Lewis numbers smaller than unity that the reaction rate is decreased, for unitary Lewis number the reaction rate neither increases nor decreases, and for Lewis numbers larger than unity the reaction rate increases. Due to tangential diffusion the flame front curvature is also modified, i.e. for small Lewis numbers the spherical flame contracts, for large Lewis numbers it spreads out, while for a unitary Lewis number the flame front remains perpendicular to the wall. The observed phenomena present similarities with capillarity effects in fluid mechanics when a droplet hits a wall.

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MS7
Mechanisms of DDT in Type Ia Supernovae

Thermonuclear explosions of degenerate carbon-oxygen stars that produce Type Ia supernovae are currently believed to involve both deflagrations and detonations. It is unclear, however, how and when the detonation appears in this large unconfined system, since the problem of unconfined DDT is still unsolved even for terrestrial combustion. Analysis of DDT phenomena in terrestrial systems and properties of thermonuclear reaction waves involved in supernova explosions provide some insights into possible mechanisms of thermonuclear DDT.

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MS7
Discussion of DDT

The speakers in this session, and others in the audience, will discuss mechanisms of the deflagration to detonation transition and its relevance to Type Ia supernovae.

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MS7
DDT in Terrestrial Systems

Abstract not available at time of publication.

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MS7
Observational Constraints on DDT in Type Ia Supernovae

The spectral evolution of Type Ia supernovae does not show unburned carbon either deep within nor in the outermost layers of the expanding ejecta. This is difficult to reconcile with models of the thermonuclear explosion based solely on subsonic deflagration. Deflagration alone also tends to produce insufficient velocities and energetics. Models in which a detonation is initiated after a period of deflagration-induced expansion provide a good agreement with observations over a large range in wavelengths.

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MS8
Compressible Multiphase Flow Simulations Using Accurate Unsteady Drag Force Models

Accurate modeling of detonating enhanced blast explosives requires accurate models for the drag and heat transfer of small metal particles evolving in the blast flow field. We present results from fundamental studies on the unsteady drag force on spherical particles in subcritical compressible flow and their use in compressible multiphase flows. The unsteady drag-force studies are novel in that they extend previously available results for the added-mass force in incompressible flow to the compressible regime.

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MS8

Towards the Development of a Complete Computational Design System for Practical Combustion Devices

Computational design process in engineering is an emerging technology. Design optimisation in combustion is in its infancy, and hence a preliminary study of the trade-off between 1D laminar flame speed and thickness is investigated for single- step Arrhenius kinetics. The computational design system comprises the Multi- Objective Tabu Search (MOTS) optimisation toolkit for efficient navigation to the complicated design space and Direct Numerical Simulation (DNS) for the detailed evaluation of all the combustion metrics under consideration.

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MS8

Premixed Flames on Porous-Plug Burner: Influence of the Plug Properties on Flame Standoff Distance and Stabilization

The flat premixed on a porous-plug burner has been reexamined using (i) a flame sheet model suggested by the asymptotic limit of high activation energy, and (ii) a numerical approach using finite-rate chemistry. Of particular interest in this study is the influence of the plug properties, such as its thickness and porosity, on the flame standoff distance and the onset of instabilities in the form of planar oscillations or cellular structures. The flame-sheet model allows to determine all possible steady states and their dependence on the physicochemical parameters including the mass flow rate, the effective Lewis number of the mixture, the overall activation energy of the chemical reaction and the extent of heat release. For Lewis numbers that are sufficiently large the analysis determines the critical conditions for the onset of pulsations. We show that by decreasing the mass flow rate below a critical value a steady stable flame starts to oscillate back and forth for a limited range of velocities but when further decreasing the mass flow rate the flame is again stabilized. The phenomenon of flame restabilization is, in this case, a consequence of the fuel mass flux fraction fluctuations inside the plug. We also discuss the effect of the plug properties ion the onset of cellular flames, for mixtures with sufficiently low Lewis numbers.

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MS8

A Paradigm Shift in the Interaction of Experiments and Computations in Combustion Research

A different approach to comparing experimental data to numerical computations is presented. Traditionally, experimentalists seek to measure the same fundamental quantities that are calculated when making comparisons with computations. This approach often requires measurement of many variables in order to arrive at the desired quantity, and uncertainty may accumulate with each additional measurement. With recent advances in computations, more complete information is available within the computations, which allows for the possibility of using calculated values to derive measured signals rather than measuring many quantities to derive a single calculated quantity. Three examples of comparing measured and calculated signals are presented: NO laser-induced fluorescence (LIF) in both non-sooting and sooting diffusion flames, and luminosity images of sooting diffusion flames. For illustration, the non-sooting LIF data and the soot luminosity data are treated both by the traditional method of comparing specific quantities and by comparing measured and computed signals.

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MS9

Shock Fitting Algorithms in Advanced Detonation Shock Dynamics Simulations

A general formulation for shock fitting will be presented in regards to applications in detonation modeling. Solutions, where applicable, will be compared to traditional high resolution schemes. It will be shown that shock fitting can lead to a computational savings of several orders of magnitude for practical problems, when compared to shock capturing. Furthermore, for certain applications of higher-order Detonation Shock Dynamics modeling, shock fitting is a prerequisite.

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MS9

Reduced Detonation Models for Insensitive High Explosives

We explore the level of modeling complexity required to describe the propagation of detonations in insensitive high explosives (IHE), specifically PBX 9502. We examine models with sufficient complexity to capture the main properties of detonations in IHE, yet simple enough to remain, to a large extent, analytically tractable. Examples include mixture models based on Stiffened-Gas equations of state. Computations of the reduced IHE detonation models are compared against predictions from more complex models like Ignition & Growth.

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MS9

Higher-order Detonation Shock Dynamics Methods for Reactions with Disparate Time Scales

A new higher-order extension of detonation shock dynamics methods is described. The extension can describe the relaxation process of detonations for which the chemical heat release occurs over two disparate time-scales. Such chemical heat release profiles typically occur in insensitive high explosives, or when slow burning metallic particles (e.g. aluminium) are added to explosives. The work shows that the relaxation dynamics of the detonation front are determined by the solution of initial/boundary value PDEs in the slow heat release layer.

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MS9

Programmed Burn for Non-Ideal High Explosives: Pseudo-Reaction Zone Model

The pseudo-reaction zone model was proposed to improve engineering scale simulations with high explosives that have a slow reaction component. A detonation velocity dependent extension was developed for non-ideal explosives that propagate well below their steady-planar Chapman-Jouguet (CJ) velocity. The pseudo-reaction rate is calibrated to the experimentally obtained normal detonation velocityshock curvature relation. The normal detonation velocity from DSD then provides the measure of departure from CJ for a state-dependent like term.

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MS10

Analysis of Uncertainty in Model Prediction with Data Collaboration

Data Collaboration is a framework designed to make inferences from experimental observations in the context of an underlying (complex, dynamic) model. The methodology allows one to determine realistic uncertainty bounds on model prediction, which experiment/parameter uncertainty contributes the most to these uncertainty bounds, rank such effects, consider new experiments to perform, and combine the uncertainty analysis with the cost of uncertainty reductionthereby providing guidance in selecting an experimental/theoretical strategy for future action.

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MS10

Uncertainty Quantification in Chemical Systems using Polynomial Chaos Constructions

Uncertainty quantification (UQ) is necessary for model validation and for assessing confidence in computational predictions. It is important in inverse problems for model construction, and in forward predictive computations. Chemical systems pose specific UQ challenges, given their nonlinearity. We discuss the utilization of Polynomial Chaos constructions for UQ in chemical systems, including forward and inverse problems, and both intrusive and nonintrusive methods. We illustrate these methods using homogeneous ignition and one-dimensional flame systems.

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MS10

The Role of Verification and Validation Metrics in Quantifying Predictivity in Buoyancy-Driven Plumes

The practical utility of the results of a numerical simulation are proportional to the degree to which the error and uncertainty in the simulation results have been quantified. We have used large eddy simulations (LES) to study heat flux to objects in or near large JP-8 pool fires. We have built a hierarchical verification and validation framework for quantification of error and uncertainty in buoyancy driven flames and plumes which forms the basis for our non-linear, multi-physics, sensitivity and uncertainty quantification analysis. Computational and experimental data are integrated through a range of experimental scales and through a hierarchy of complexity levels. The simulation and experimental data are analyzed together to quantify the predictivity of our fire simulation. Our approach is to draw on prior information on error and to exploit a consistency requirement among the available experimental data sets and the simulations of these sets to quantify the uncertainty in model parameters, boundary conditions and experimental error and simulation outputs. From this analysis we produce validation metrics for the uncertainty of the simulation predictions for the intended use of the computation. We have used this validation process to demonstrate how to identify and improve the models and parameters among the multi-physics components of our simulation that contribute the largest error.

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MS10

Spectral Optimization and Uncertainty Quantification in Detailed Kinetic Modeling of Hydrocarbon Combustion

Accuracy of a combustion kinetic model may be ensured, in principle, by a multi-parameter optimization. However, because of the inherent uncertainties in the combustion experiments, the resulting optimized model is characterized by a finite kinetic parameter space in which each point may be valid. Recently, advances have been made in the use of multidimensional polynomial chaos representations to quantify the uncertainty of kinetic models. The topic

of discussion will be the application of these techniques to multi-parameter optimization and mechanism reduction.

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MS11

Direct Numerical Simulation of Premixed Flame Kernel-vortex Interactions in Hydrogen-air Mixtures

The unsteady interaction between a vortex and a premixed hydrogen-air flame kernel is investigated using DNS with a detailed reaction mechanism. The interactions are characterized by different regimes: the laminar and the wrinkled kernel regimes, the break-through regime and the global extinction regime. Operation at a given regime is based on the vortex parameters as well as the kernel maturity at the onset of interactions. A regime diagram is presented to illustrate the different regimes.

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MS11

Cross-Diffusion in Freely Propagating Premixed Lean Hydrogen Flames

Simulations of freely propagating premixed lean hydrogen flames with detailed chemistry can be performed economically in two-dimensions using software developed at Lawrence Berkeley National Laboratory. Consequently it is possible to investigate in detail how the flame chemistry responds to changes in flame shape caused by instabilities and by turbulent forcing. This paper examines the differences in predictions of flame behavior resulting from the mixture-averaged diffusion model and from the multicomponent diffusion model with Dufour and Soret cross-diffusion effects.

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MS11

Lean Flame Modeling

A two-step reduced mechanism including a thermally sensitive branching reaction and an exothermic recombination reaction is used to describe the structure and propagation velocity of lean and stoichiometric hydrogen-air flames. It is seen that the activation temperature of the branching step is sufficiently large that branching occurs in a relatively thin layer at a temperature slightly above the crossover value, whereas radical recombination occurs in a distributed manner both upstream and downstream from this layer, yielding a leading-order solution that can be integrated numerically to give burning rates in agreement with detailed-chemistry computations. The analysis is modified as the adiabatic flame temperature approaches the crossover value near the flammability limit, when branching and recombination are seen to occur simultaneously in a relatively thin layer, which is preceded by a radical-free preheat region. The analysis of the resulting reactive layer provides the fuel burning rate, to be used in stability analyses of lean flames. The applicability of this weakly burning regime to the investigation of observable flame balls will be discussed.

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MS11

Reaction Mechanisms and H-Atom Transport Issues in Lean Hydrogen Combustion

The state of knowledge in the reaction mechanisms of hydrogen combustion will be discussed. Emphasis will be given to the reactions of the HO2 free radical and their influence on the combustion processes of hydrogen at high pressures. Additionally the transport parameters of the H atoms will be examined in terms of their uncertainty and impact on hygrogen combustion simulations.

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