Introduction

This volume includes the extended abstracts of the International Conference on Micromixing held in Moscow, May 14–17, 2004. The Conference had the ambition of making a contribution to one of the most challenging fields in the turbulent combustion science that is the simulation of mixing and reaction phenomena occurring at the smallest spatial and temporal turbulence scales. As the experimental studies of these phenomena are faced with essential difficulties, any valuable contribution from the simulation side would be considered as an important step forward in understanding complex relationships between turbulence and chemistry.

The technical program of the Conference included various aspects of turbulent reacting flows with a special emphasis on the dynamics of small-scale turbulence responsible for mixing of chemical species and triggering chemical activity. In addition to fundamental issues relevant to the problem, a number of modeling efforts and computational approaches to the prediction of turbulent combustion for practical applications have been reported.

The common feature of most of the contributions is that the description of the turbulent mixing process, either deterministic or stochastic, tends to become more detailed in terms of using a spectrum of mixing frequencies rather than a single frequency or using a two-point rather than a single-point Probability Density Function (PDF). The claim or hope of the authors is that this increased level of sophistication is rewarded by an increased accuracy of the methods. This is illustrated by applications to flow patterns of fundamental interest and those found in industry. The scope of the Conference is widened considerably by the inclusion of the contributions on heterogeneous systems, shock waves, and environmental flows.

This understanding of the conference scope made it possible to subdivide the material of the book into three Sections: Fundamentals Modeling, and Applications.

The aim of this introduction is to provide a reader with a quick overview of the notable aspects of each contribution.

Section 1: Fundamentals. A large number of chemical variables with highly diverse molecular weights and other properties inherent in turbulent reactive flows imply that multicomponent molecular diffusion processes can manifest themselves in micromixing phenomena. This issue is addressed by *Frolov & Basevich* who discuss the role of multicomponent diffusion in premixed and nonpremixed laminar flames. They provide several examples demonstrating the importance of the issue and pose a question on the range of validity of relevant Direct Numerical Simulation (DNS) studies involving a single progress variable to represent chemical transformation.

Due to thinness of most flames relative to turbulent length scales, there is a need for flame-zone submodels in turbulent combustion models. *Lipatnikov et al.* propose such a submodel based on considering a laminar flame propagating along a vortex tube — tube-like intense vortical structures. They use the model to put forward a possible explanation of experimentally observed high turbulent burning velocities for lean hydrogen–air flames.

An important issue in turbulence theory is the effect of boundary conditions. *Pavelyev* considers a class of turbulent flows with local turbulence properties determined by flow geometry and history and eventually decoupled from the local mean velocity profile. Referring to such flows as nonequilibrium turbulent flows, the author claims their potential importance for controlling turbulent transport in various applications.

Renou et al. report their initial experimental results obtained on the setup designed to represent the ideal Partially Stirred Reactor (PaSR) — a useful tool for validating turbulent models. Valuable statistical information on turbulence in a nonreactive medium has been obtained by using simultaneous Particle Image Velocimetry (PIV) and Planar Laser-Induced Fluorescence (PLIF).

Lipatnikov has identified the conditions when a generalized balance equation for a progress variable in the turbulent reacting flow can be reduced to a simple equation widely used in simulations of premixed turbulent flames, thus providing a fundamental substantiation for the latter. Moreover, it has been shown that the reduced equation can be applied to both developing and fully-developed flames with well-pronounced countergradient transport.

Hierro et al. conducted an interesting study of the effect of isoscalar surfaces curvature on scalar diffusion in turbulent flow field. They examined the difference between the full Laplacian of the species mass fraction entering the general diffusion equation and the one-dimensional

(1D) second derivative of the same variable used in most relevant studies for modeling micromixing processes. It has been shown that the use of the 1D representation is equivalent to the neglect of the isoscalar surfaces curvature, which is proved to be correct only for almost unpremixed scalar fields. However, as the scalar field gets more and more mixed, the effects of curvature cannot be neglected. In another contribution, *Hierro et al.* study the evolution of the correlation function of a scalar field in homogeneous, isotropic, incompressible turbulence by comparing the results of modeling with DNS. As the availability of the correlation function provides a closure for micromixing, this effort is noteworthy, despite the model used still needs improvements.

Valiño et al. investigate quasi-stationary approximate solutions for a single scale PDF in statistically homogeneous turbulent flows aimed at developing improved micromixing models. The quasi-stationarity of scalar diffusion was checked against the DNS data.

Section 2: Modeling. *Frost et al.* suggest the extension of the coalescence/dispersion (C/D) micromixing model to an arbitrary number of independent variables. The micromixing rate constant is derived on the basis of the equation for a two-point correlation function. The results of calculations are compared against the DNS results for statistically homogeneous turbulent flow field without and with chemical reactions.

Scalar intermittency in turbulent flow field is the issue studied by *Frost et al.* This phenomenon is characterized by a large number of marginal scalar values, which manifest themselves as a singularity in the corresponding PDF. The authors explore a possibility to develop a statistical model of mixing processes taking into account discontinuities in the scalar field, like flame fronts and contact surfaces, typical for turbulent combustion. The model is based on the two-point passive scalar PDF with the closures based on "weak connection approximation."

The first contribution of *Soulard & Sabel'nikov* is concentrated on two new micromixing models accounting for turbulent frequency scale distribution. These models are based on multiscale extension of the classical Interaction by Exchange with the Mean (IEM) and Langevin models and are referred to as Extended IEM (EIEM) and Extended Langevin (EL) models. Both models were tested against DNS results for the decay of a statistically homogeneous scalar field in isotropic homogeneous turbulence. In their second contribution, *Sabel'nikov & Soulard* propose an alternative approach for deriving hyperbolic stochastic partial differential equations based on the concept of stochastic characteristic. The numerical implementation of the Eulerian Monte Carlo method for solving the PDF equation has been discussed and the accompanying problems have been identified.

Babenko & Chorny consider the joint statistics of scalar and its gradient in the turbulent flow field to link the scalar length scale PDF with the joint PDF of the scalar and its gradient in the form of the integral relation. Application of DNS data for the coefficients entering the relation allowed the average length and time scales as well as length-scale variance to be determined.

Fedotov et al. derive a time-discrete nonlinear integral equation for the PDF of the random conserved scalar ensuring the relaxation from an arbitrary initial distribution to delta-function and the decay of the variance resembling the empirical power-law decay. The mixing model suggested is based on the law of large numbers. The Lagrangian mixing process is modeled by a stochastic differential equation with the exchange rate and ambient concentration as random variables.

Heinz discusses advantages and drawbacks of various stochastic models of turbulent scalar mixing. He compares the performance of the Refined IEM (RIEM) model and Stochastic IEM (SIEM) model (neglecting memory effects), on the one hand, and DNS data, on the other hand. It has been shown that the RIEM model exhibits a very good performance in predicting the temporal evolution of PDF of two scalars.

Smirnov applies the spectral approach based on the Random Flow Generation (RFG) model to simulate micromixing in turbulent flames. The phenomenon of his interest is the acceleration of turbulent flame propagation due to engulfment of unburned mixture. With the model applied, the increase in the flame propagation speed due to turbulent fluctuations has been obtained and the entrainment of unburned mixture pockets into the regions occupied by combustion products has been captured.

Babenko & Petrovich compare the performance of three Lagrangian models of micromixing of passive scalar in the isotropic turbulence field, namely, mapping closure (MC), Linear Mean-Square Estimation (LMSE), and C/D models with the deterministic model based on the joint PDF of scalar and its gradient, on the one hand, and with DNS data, on the other hand. It is shown that the deterministic model shows in general good agreement with DNS data, while the Lagrangian models exhibit the largest disagreement with DNS at the initial stage of mixing.

Turbulence–chemistry interaction in the limit of fast chemistry is the issue addressed by *Vorotilin.* The reacting medium is represented as an ensemble of independent turbulent vortices with mixing occurring due to their random roaming in the reactor. The author's approximation takes into account only those mixing events, which lead to chemical reactions and ignore chemical reactions occurring without turbulent mixing. Within this approximation, mixing between inert species is excluded from the analysis. Despite the resultant mathematical formulation contains an unknown constant, the model allows the analysis of different reaction regimes in the turbulent flow field.

Section 3: Applications. *Beishuizen et al.* apply transported scalar PDF and velocity-scalar joint PDF approaches for the numerical simulation of turbulence–chemistry interaction in the benchmark turbulent piloted jet diffusion flame "Delft Flame III." The sensitivity of predictions to the choice of micromixing submodels is studied.

Huai et al. apply Large-Eddy Simulation (LES) and DNS for modeling scalar mixing in jet in cross-flow configurations relevant to industrial furnaces and gas-turbine combustors. As subgrid scale models for scalar field, the Eddy Diffusivity, Dynamic Procedure, and Scale Similarity models were implemented. The main idea of the study was to analyze and optimize the mixing process in terms of the "mixedness" parameter characterizing the portion of mixed fluid in the entire computational domain. Various mixing enhancement means were examined including introduction of swirl, variation of jet angle, and positioning of obstacles in the flow.

Mura & Demoulin study the effect of micromixing models on the combustion of natural gas in a Homogeneous Charge Compression Ignition (HCCI) engine. In such engines, ignition of a fuel-lean premixed charge is mainly controlled by finite-rate kinetics. To take into account the effect of imperfect premixing of fuel and oxidizer of HCCI engine performance, the authors apply the joint scalar PDF of composition and enthalpy approach with a detailed methane oxidation chemistry. Within this approach, the effect of small-scale fluctuations of mixture composition on the ignition and pressure evolution in HCCI engine is examined.

Zabaikin et al. report their experimental studies on hydrogen–air mixing and combustion in a supersonic flow. The effect of periodic wave structures inherent in jet-mixing flows on the dimensions of the mixing zone between fuel and oxidizer was also studied.

Jonker et al. apply LES for studying variance spectra of chemically active species in a dry convective atmospheric boundary layer. The objective of their study is to quantify the impact of chemistry on the spatial fluctuations in the concentration field. As a characteristic length scale of the species concentration variability, a "variance-dominating length scale" (VDLS) is used which demonstrates a clear dependence on the reaction rate: an increase in the reaction rate leads to a significant decrease in the species VDLS. To better understand these results, a conceptual spectral shell-model is developed, which incorporates multiple scales, chemistry, turbulence production, etc.

Ershov et al. study computationally in two-dimensional approximation the mixing mechanisms in heterogeneous gaseous systems under the impact of the propagating shock wave. Two computer codes are used: a gasdynamic code solving for gasdynamic equations with and without turbulence, and a code solving for the lattice Boltzmann equation. The mixing is shown to be enhanced considerably by hydrodynamic instabilities of the contact surfaces between different gases.

The analytical study of *Velikodnyi et al.* is focused on the structure of a shock wave in a microporous liquid representing a liquid fuel saturated with gaseous microbubbles. It is shown that liquid fuel preconditioning with barbotage followed by processing in a cavitator makes it possible to attain partial conversion, cracking, and oxidation of the fuel behind a relatively weak shock wave, which is important for propulsion applications.

We have tried to highlight the contents of the various articles in the book to enable easy selection of the subject of choice by the reader. As can be seen, the contributions involve exploring new micromixing modeling issues and approaches, variants of existing models, testing of models with DNS data, computation of complex flows, and experimental findings. The impressive fact is that scientists from different nations (Belarus, France, Russia, and Spain) worked together using the same DNS database developed by the group of Prof. Dopazo for validating their models. Such a cooperation proved to be very fruitful for improving our knowledge on the mixing phenomena. We believe, the articles represent the cutting edge of science and do hope that this book will contribute to the literature on the micromixing in turbulent reactive flows.

Editors