Preface

On March 8, 2014, Yakov Borisovich Zel'dovich (1914–1987) would turn 100. The eminent scientist of the XX century, he made tremendous contribution to the combustion and detonation science and created a world-renown scientific school.

In the period from October 27 to 31, 2014, the Scientific Council on Combustion and Explosion of the Russian Academy of Sciences together with the leading Institutes of the Academy organized in Moscow the International Conference on Combustion and Detonation dedicated to the 100th birthday anniversary of Academician Ya. B. Zel'dovich to give a tribute of deep respect to his great personality. Similar to two previous international meetings dedicated to Ya. B. Zel'dovich, held in 2004 and 1994, this jubilee conference is also named Zel'dovich Memorial. The proceedings of two previous Zel'dovich Memorials were published in three books [1–3].

This volume includes condensed manuscripts of plenary lectures presented at the Conference by distinguished international experts. The contributions were edited and organized in a uniform and easily readable manner with five parts: (1) Chemical Kinetics; (2) Gas-Phase Laminar and Turbulent Flames; (3) Combustion in Porous Media; (4) Combustion and Explosion in Condensed Phase; and (5) Detonations and Shock Waves.

Part 1, *Chemical Kinetics*, includes contributions on the determining role of chemistry in evolution of combustion and detonation processes.

Korobeinichev et al. review the most important results obtained in the Combustion Kinetics Laboratory of Voevodsky Institute of Chemical Kinetics and Combustion (Novosibirsk, Russsia), dealing with the development of the ideas of Ya. B. Zel'dovich related to combustion chemistry. In particular, they address novel experimental methods for investigating combustion chemistry of gaseous and condensed systems using molecular-beam mass spectrometry, microthermocouple technique, and computer simulations based on detailed chemical kinetics; accomplishments in inhibition and promotion of chain reactions of radicals in gaseous flames; advances in combustion chemistry of condensed systems; investigations of hydrogen azide flame propagation velocity; and the effect of trimethylphosphate additive on the hydrogen–oxygen flame.

Maas and Bykov present a strategy of calculating ignition and combustion in turbulent reactive flow based on the solution of a transport equation for the probability density function of the gas phase with submodels for the chemistry–turbulence interaction and for the kinetics. The overall model allows a reliable simulation of turbulent combustion processes such as nonpremixed turbulent natural gas fames, spray flames, and engine combustion.

Mantashyan investigates the phenomenon of hydrocarbon cool flame using a technique of flame stabilization in a two-section flow reactor with sepa-

rate temperature-controlled heated sections connected via a narrow tube and equipped with devices for sampling reactive gases to register free radicals by electron spin resonance. It was found that during gas transition from the first section (preflame zone) through the connecting tube to the second section (cool flame zone), the concentration of free radicals can increase sharply by two orders of magnitude. The cool flame was shown to fade out with the increase of temperature and with transitioning the process to the NTC (negative temperature coefficient) zone because of self-heating of the rapidly developing chain exothermic oxidation.

Mansurov investigates soot formation at low-temperature conditions during transition between cool and hot flames. A number of polycyclic aromatic hydrocarbons (PAHs) such as pyrene, fluoranthene, coronene, anthanthrene, as well as 1,12-benzperylene, were identified by spectroscopic methods in soot extracts. The general scheme of conversion of hydrocarbon fuels that takes into account new experimental data on the formation of fullerenes and graphenes including the pressure effect is proposed for fuel-rich flames. Formation of fullerenes is shown to be possible at low pressures and depend on spatial orientation of PAHs. Soot surface on silicon and nickel substrates placed in a propane–oxygen flame is shown to exhibit hydrophobic properties due to the presence of soot particles in the form of nanobeads. The photovoltaic properties of solar cells coated with nickel oxide nanoparticles synthesized in a counterflow propane–air flame are explored.

Wlokas et al. conduct kinetic experiments and computer simulation aimed at better understanding the decomposition kinetics of vaporized precursor compounds, kinetics of cluster formation, potential interaction with flame chemistry, and kinetics of particle growth using shock tube reactors with optical and mass spectrometric detection of intermediate and stable product species and in flow reactors with laser-based detection of temperature, species concentration, and particle size distribution. As an example, they investigate transformations of iron pentacarbonyl as a precursor for gas-borne iron oxide nanoparticles.

Tavadyan and Martoyan apply the numerical value method to determine the critical states of a reaction system and to identify the importance of certain individual reaction steps and chemical species for critical phenomena based on extremality conditions for the appropriate Hamiltonian. As an example, critical phenomena in degenerate branching reactions of liquid-phase oxidation of hydrocarbons where branching is delayed at the chain propagation stage were considered in detail.

Azatyan revisits the importance of branched chain reactions for combustion, explosion, and detonation in gases by considering examples where the chain character of gas phase combustion at atmospheric and elevated pressures is neglected and by discussing experimental findings demonstrating the critical effect of small inhibiting additives on reactive system evolution.

Part 2, *Gas-Phase Laminar and Turbulent Flames*, includes contributions on experimental, theoretical, and computational studies of premixed laminar and turbulent flames.

Maruta et al. discuss their strategy of using low-stretched counterflow premixed flames under microgravity conditions with low convection velocity to study both propagating premixed flame and phenomena similar to the flame ball, first predicted by Ya. B. Zel'dovich in 1940s. It is implied that these studies will contribute to the development of the comprehensive combustion limit theory including the limits of propagating premixed flames and flame balls.

Sabelnikov and Lipatnikov investigate theoretically and computationally a statistically stationary, planar, one-dimensional (1D) premixed flame propagating in frozen turbulence in a form of a traveling wave, determine the spectrum of admissible flame speeds, and select a physically relevant value of the flame speed. Also, they discuss the results of three-dimensional (3D) Direct Numerical Simulation (DNS) studies of such 1D premixed flames indicating that both flame speed and mean flame brush thickness, evaluated by proper averaging the DNS data, exhibit significant large-scale oscillations with time characteristic of fingering instability.

Choi and Yang present a computational study of the stability and dynamics of the supersonic turbulent combustion in a Dual Combustion Ramjet (DCR) using high resolution numerical analysis based on the hybrid Reynolds Averaged Navier–Stokes (RANS) / Large Eddy Simulation (LES) formulation for compressible reacting flows. The approach is validated against experiments with four levels of grid refinement for three different high-resolution schemes, namely, a third-order Monotone Upstream-centered Scheme for Conservation Laws (MUSCL), a fifth-order weighted essentially nonoscillating (WENO) scheme, and a fifth-order optimized Multidimensional Limiting Process (oMLP) scheme. The time-averaged results showed the importance of fine grid resolution and a high-order accurate numerical scheme for reliable prediction, capturing the fine-scale instabilities of the supersonic turbulent combustion.

Priesching presents a novel numerical algorithm for computationally efficient 3D simulation of premixed combustion referred to as the Flame Tracking – Particle Method. The method is based on a well-balanced combination between Lagrangian and Eulerian approaches. From the Lagrangian formulation, it takes advantage of obtaining the detailed evolution of surface movement based on flame speed and local flow velocity. From the Eulerian approach, heuristic numerical stability is achieved and it is possible to compute a smooth surface normal vector field from Lagrangian particles, which is crucial in order to include all effects of turbulent combustion as accurate as possible. The model utilizes well-known correlations for the turbulent flame speed, which connect the fuel property of the laminar flame speed with local turbulence intensities. The performance of the method is demonstrated with application to academic test cases and to gasoline direct injection engine.

Skjold et al. review the development of a special class of computational fluid dynamics (CFD) tools for simulating turbulent reactive flows in large-scale complex geometries, such as offshore platforms, floating process facilities, and onshore plants. To model the influence of relatively small objects on flame acceleration and pressure buildup in large-scale conditions, they implement a pragmatic

approach based on the porosity / distributed resistance concept, which allows application of coarse computational meshes thus overcoming inherent limitations in computational resources.

Part 3, *Combustion in Porous Media*, includes contributions on filtration combustion (FC) of gases and combustion of polymers.

Babkin et al. investigate theoretically the phenomenon of superadiabatic temperature (SAT) of a poorly known type which is realized in homogeneous gaseous systems and has much in common with the phenomenon of SAT in porous media but is solely determined by competition between elementary chemical reactions in the premixed combustion zone. It is concluded that the phenomenon of SAT manifests itself in fuel-rich hydrocarbon flames with the equivalence ratio exceeding a certain critical value and is associated mostly with the superequilibrium concentration of water in the combustion products.

Aldushin investigates theoretically and computationally the propagation of exothermic reaction wave in a porous medium driven by filtration of gas reacting with the fuel component in the solid porous matrix, the process referred to as FC. The two-dimensional (2D) mathematical description of the process in a flat slot-like channel includes the equations of balance of heat and mass of solid and gaseous reactants, the kinetic equation of fuel conversion, and the dependence of characteristics of the environment on its structure. The dynamics of the FC wave propagation was shown to depend on a set of parameters among which the key role is played by the ratio (K) between the permeabilities of combustion products and initial fuel; at $K > 1$, the FC front was shown to be unstable with the development of configurations similar to Saffman–Taylor fingers in the liquid displacement problem.

Shkadinsky et al. study computationally the FC of a reasonably thin layer of a high-energy porous structure with the filtration of an active-gas reagent from outside through a slot between the porous reagent layer and the flat wall arranged in parallel to the porous layer at an adjustable distance from it, using a novel 2D transient thermal-filtration mathematical model for cellular FC front propagation. The model includes the macrokinetic law, the law of conservation of mass for gas reagent, and the equation of thermal balance, supplemented by the equation of state for gas reagent. The predicted structure of cells, critical conditions of their existence, and specific features of their motion were compared with experiments on FC of porous titanium in air.

Khalturinskij reviews the physicochemical mechanisms of fire retardant (FR) action on the processes of polymer combustion and available approaches to reducing polymer flammability, and considers the ways of determining the limiting stage of the complex process of polymer burning. In particular, it has been shown that the use of gas-phase FR, e. g., halogen-containing compounds, as inhibitors of polymer burning allows obtaining a strong effect on the rate of chemical reactions in gas phase but virtually does not affect the polymer burning process.

Part 4, *Combustion and Explosion in Condensed Phase*, includes contributions on fundamental aspects of combustion and explosion of energetic materials (EM).

Shteinberg and Knyazik discuss recent new data on kinetics and macrokinetics of combustion and explosion of EM, including the data on maximum preheating at critical conditions of thermal explosion; on kinetics of high-temperature decomposition and thermal explosion of liquid explosives; on steady-state and explosive combustion of liquid explosives; electrothermal explosion and electrothermal analysis; kinetics and macrokinetics of high-temperature reactions in systems of gasless combustion and in self-propagating high-temperature synthesis; and on fast mechanochemical interactions.

DeLuca et al. present the accomplishments of a three-year collaborative HISP (High performance solid propellants for In-Space Propulsion) project within the Seventh European Framework Program. The project was aimed at improving, in terms of both delivered performance and environmental impact, the current state-of-the-art in solid propulsion space launchers by the use of ammonium perchlorate (AP) and, sometimes, ammonium nitrate (AN) based composite formulations with a hydrocarbon inert binder and micrometric aluminum powder.

Gany et al. present a novel concept of a new class of high-energy propellants, where a liquid oxidizer in the form of small encapsulated droplets is contained within the solid propellant matrix, and the liquid capsules are spread in a way similar to the distribution of solid AP particles within the propellant binder in conventional solid propellants. It is shown that the combustion cycle of an individual oxidizer droplet represents the macroscopic combustion behavior of the propellant. Burning rate dependence on pressure is similar to that of AP-based solid propellants, whereas smaller droplets cause higher burning rates.

Mukasyan and Rogachev outline the impact of the classical works of Ya. B. Zel'dovich on the discovery of solid flame and subsequent breakthrough in a new interdisciplinary branch of combustion science, the Structural Macrokinetics (SMK), which considers the processes of structural transformations on atomic-, crystal- and microlevels in the presence of chemical reactions and intense heat and mass transfer. The development of SMK proceeds in the direction from synthesis of powders with subsequent processing for production of final materials and net-shaped articles to a single-step technology by using the combustion process.

Rogachev et al. discuss the methodology for experimental studies of gasless heterogeneous (solid-flame) combustion which allows reliable identification of homogeneous and microheterogeneous combustion modes. On the one hand, high-speed video frames of a spreading gasless reaction wave in different systems indicate that macroscopic propagation of the combustion wave proceeds solely via incipience and growth of hot spots, implying the microheterogeneous nature of gasless combustion. On the other hand, combustion wave propagation in reactive multilayer nanofilms was shown to follow the homogeneous gasless combustion mode with a uniform combustion front exhibiting no visible hot spots.

Part 5, *Detonations and Shock Waves*, includes contributions on gaseous, heterogeneous, and condensed-phase detonations and shock waves.

Hayashi et al. apply the 3D compressible Navier–Stokes equations with a detailed hydrogen/oxygen reaction mechanism to simulate flame acceleration, shock wave formation in front of the flame, and deflagration-to-detonation transition (DDT). Preflame autoignition in the course of DDT was shown to occur near the channel walls behind a smooth precursor shock wave formed ahead of the flame due to collisions of compression waves generated by the flame front, particularly, by its convexly curved portions.

Faria et al. present qualitative models and asymptotic theory, derived from the analysis of compressible reactive Navier–Stokes equations, describing the most important specific features of gaseous detonation phenomena. It was shown that a simple extension of the Burgers equation with a nonlocal forcing and appropriate damping captures, at a qualitative level, the dynamics of pulsating planar detonations, detonations with friction losses, and radially diverging detonations. Steady/quasi-steady solutions have a characteristic multiple-valued dependence of the detonation speed on the shock curvature or the friction coefficient. Unsteady solutions of the model equation reproduce the pulsating (from periodic to chaotic) solutions of 1D planar detonations and the dynamics of the point-blast initiation/failure phenomenon of radially diverging detonations. The asymptotic theory of weakly nonlinear multidimensional detonations was shown to reproduce not only the pulsating 1D detonations, but also the cellular structures of 2D detonations.

Levin et al. present the results of extensive numerical simulation of spontaneous formation of 3D cellular and spin detonations in a propane–air mixture in channels of different cross section using the software based on the modified Godunov method and computational grids with up to billion elements. The spin detonation stability is investigated concerning its transition to a wider or narrower circular channel.

Vasil'ev presents the results of investigations addressing nonclassical double-cell structures of multifront gas detonations, observed in multifuel systems, in particular, in systems with one fuel component decomposing with an exothermic effect. Experimental studies of detonation diffraction in such systems with near-stoichiometric mixtures show that the characteristic diffraction diameter is determined only by the large-scale cells; however, as the mixture composition departs from the stoichiometry, the small-scale cells begin to manifest their effect. The concentration limits for the double-cell structures are shown to be narrower than those for the classical detonation.

Frolov et al. proved experimentally that Zel'dovich thermodynamic cycle with continuous-detonation combustion of a hydrogen–oxygen mixture in the annular Liquid Rocket Engine prototype is more efficient than the Brayton cycle with continuous combustion of the same mixture, other conditions being equal. Specific impulse of the engine prototype operating in the continuous-detonation mode is shown to be 6%–7% higher than that measured when it operates in the continuous-combustion mode.

Veyssiere and Khasainov present the results of experimental and computational studies of detonability of two-phase dispersed reactive media containing

either suspended hydrocarbon droplets or suspended aluminum particles. It has been demonstrated that the detonation regime can be initiated in these heterogeneous mixtures and, in most cases, the cellular detonation structure was displayed. Detonability of fuel–air sprays may be comparable to that of homogeneous gaseous fuel–air mixtures, but only under the condition that the droplet size is sufficiently fine (less than 10 μm). On the contrary, for solid particle suspensions, the energy required to generate a detonation is much larger than that for classical hydrocarbon–air mixtures, by several orders of magnitude.

Kanel reviews the latest results of investigations into macrokinetics of high-rate inelastic deformation, fracture, and physicochemical transformations of condensed materials under shock-wave loading. Measurements of evolution of shock waves can be transformed into kinetic relationships for describing time-dependent phenomena accompanying explosive, laser and other dynamic treatments of materials. In some cases, unusual and exotic behavior of solids under shock-wave loading was observed. Due to extremely short load durations and very high strain rates, shear and tensile stresses approaching the ultimate values have been recorded. Deep penetration into the negative pressure domain opens a way to investigate phase transitions and polymorphic transformations under tension.

Bogdanov et al. present the results of the use of the microwave method to investigate detonation wave propagation, shock-wave initiation of explosives, isentropic expansion of explosion products, and processes of launching of metal plates by explosion products.

This volume is the outcome of hard work of several people who have rendered their best, and we appreciate their contribution. The editors acknowledge the concern and diligence of the TORUS PRESS staff and Drs. E. A. Salganskii and A. E. Sytschev. We thank all authors for preparing their manuscripts and spending their time and efforts with the editors on improving the text, figures, and scope of their contributions to fit the overall goals of the book.

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