Dynamics and Structure of Combustion Waves

2nd International Conference

July, 23–27, 2014, Vladivostok

Abstracts

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2nd International Conference "Dynamics and Structure of Combustion Waves" is organized by the School of Engineering of the Far Eastern Federal University with the informational support of the Russian Section of International Combustion Institute. The main purpose of the meeting is to develop existing and establish new scientific relations between researchers from Russian Far East and scientists in the field of combustion from other countries and other regions of the Russian Federation. The main topics of the conference include experimental and theoretical studies of the combustion wave dynamics in various media, the structure of combustion waves, combustion in micro channels and the development of methods for the reduction of chemical kinetic models.

The Conference is supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003).

Key words: *combustion wave, micro combustion, chemical kinetic.*

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Вторая международная конференция «Динамика и структура волн горения» проводится Инженерной школой Дальневосточного федерального университета при информационной поддержке Российской секции Международного института горения. Основной целью конференции является развитие существующих и установление новых устойчивых научных связей ученых Дальнего Востока России со специалистами в области горения из других стран и регионов Российской Федерации. Основная тематика конференции включает экспериментальные и теоретические исследования динамики волн горения в различных средах, структуры волн горения, горения в микроканалах, развитие методов редукции кинетических моделей химических реакций.

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Ключевые слова: волны горения, микрогорение, химическая кинетика.

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NUMERICAL MODELING THE RADIATIVE-CONVECTIVE-CONDUCTIVE HEAT TRANSFER

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Conductive-convective-radiative heat transfer [1] in a scattering and absorbing medium with reflecting and radiating boundaries is important for many engineering applications [2-4]. It is necessary to take into account the radiative heat transfer because in many industrial high temperature processes and applications it plays a dominant role. The P1approximation (diffusion model) is used for the simplification of the original problem. This paper considers the problem of a complex heat exchange in three-dimensional domain with reflecting boundaries. An iterative algorithm based on the use of finite elements method is proposed. Software implementation of the algorithm is carried out in the package FreeFem++.

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NUMERICAL ANALYSIS OF 2-D CLOAKING PROBLEM BASED ON THE BOUNDARY ELEMENTS METHOD

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It was proposed that perfect invisibility cloaking shells can be constructed for hiding objects from electromagnetic illumination [1]. However, the difficulty in fabricating such shells stems from the requirements on the material that composes it. Cloak obtained through such technique has anisotropic, spatially varying optical constants. In addition, some of the material parameters have infinite values at the interior surface of the cloak. In order to facilitate easier realization as well as to avoid infinities in optical constants, cloaks with simplified material parameters were proposed. Hence, perfect hiding with such a simplified cloak is not possible [2]. Another approach in cloaking material bodies consists of coating it's outer boundary with special material having the certain value of surface impedance. In this case, the cloaking problem is reduced to the choosing of the impedance such that the wave scattered by the object have certain properties.

We consider a 2-D model of scattering with impedance boundary condition. Using the optimization approach (see details in [3, 4, 5]), the cloaking problem is reduced to inverse extremal problem. The role of control is played by the surface impedance of the boundary, while the functional constraint is specified by the scattering model.

The extremal problem is studied theoretically using the Lagrange principle which leads to the construction of the optimality system. The optimality system consists of three variational relations. They describe the necessary extremum conditions including the weak statement of direct scattering problem, the dual problem for the Lagrange multiplier and the inequality for the control, i.e. for the impedance value on the boundary of scatterer.

The boundary elements method is proposed for numerical solving the direct scattering problem. Based on the optimality system and boundary elements method, the algorithm for solving the inverse problem is designed. The numerical experiments for solving the direct and inverse problems are performed. The results of numerical experiments are analyzed.

The work was supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003) and Far Eastern Federal University.

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HYDRODYNAMIC INSTUBILITY OF FLAME FRONT IN COMBUSTION OF HETEROGENEOUS MEDIA CONSISTING OF PREMIXED COMBUSTIBLE MIXTURE WITH FUEL MICRODROPLETS

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In this paper the processes of combustion of heterogeneous media consisting of a combustible mixture of fuel and microdroplets are considered. This type of fuel used in gas turbines, diesel and spark ignition engines, furnaces and hazardous environments. Experimental studies [1] showed that the surface of the divergent spherical flame gas-droplet mixtures intensively cellular structure, and in some cases, there are oscillating flame.

This thesis is a theoretical study of the hydrodynamic stability of planar wave of combustion of premixed of combustible mixture with fuel droplets. Model describing the flow of heterogeneous mixtures based on the idea of two interacting interpenetrating continua. Flame front is seen as an interface between the unburned mixture with droplets of fuel and combustion products. It is believed that the normal velocity of the combustion wave is dependent on the density of the fuel droplets in front of the flame front and the local curvature of the surface.

In this paper we analyzed the effect of the density of droplets in the fresh mixture, the coefficient of expansion and other characteristics of gas-droplet environment on the stability of the flame front. Was investigated by the limiting transition to the theory of hydrodynamic instability Darrieus-Landau conventional flame. Modes of combustion in which the flame front observed oscillations found experimentally [1].

This work was supported by the Ministry of Education and Science of the Russian Federation (contract N 14.Y26.31.0003) and Far Eastern Federal University.

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ON EFFECTIVE CONTROL FOR THE THERMALLY AND ELECTRICALLY CONDUCTIVE VISCOUS FLUID

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We consider the stationary equations of magnetohydrodynamics (MHD) of viscous fluid in the bounded three-dimensional domain under homogeneous mixed boundary conditions for the magnetic field and inhomogeneous Dirichlet condition for the velocity. Physically the homogeneous mixed boundary conditions for the electromagnetic field in correspond to the situation when the one part of the boundary of the domain of fluid flow is a perfect conductor and other part is a perfect insulator (see [1]). In author knowledge before [1] respective mixed boundary value problems for the MHD equations have not been yet considered in the mathematical literature. In [1] the global solvability of this boundary value problem under homogeneous Dirichlet condition for the velocity was proved.

The main results of this paper is to prove the global solvability of considered MHD boundary value problem under condition that normal component of the velocity vector is non zero on insulator part of the boundary. This result will allow more effective “hydrodynamic” control by velocity vector on the boundary of the fluid flow domain (suction and pumping of fluid). If the fluid is a poor conductor of heat and current then the hydrodynamic control is a unique effective mechanism of suppression of turbulence or pressure stabilization in some subdomain.

We note that on the super conductor part of the boundary we a forced to suppose that the normal component of the velocity vector is a zero.

Among them we mention [2] where the global solvability of the inhomogeneous boundary value problem for the stationary MHD equations was proved for the first time.

Next we study the control mechanisms for the model of thermally and electrically conductive viscous fluid.

The work was supported financially by the Ministry of education and science of Russian Federation (project 14.Y26.31.0003) and Far Eastern Federal University.

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ON THE STRUCTURE OF FAST COMBUSTION WAVES WITHIN POROUS/CONFINED MEDIA

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The problem of interaction of a flame – combustion wave front with walls/obstacles has become very important for understanding of the combustion phenomena both in its theoretical and in applied aspects. Downsizing of combustion engines – micro-combustors, multiplicity of possible combustion regimes and sensitivity of the flame structure to the presence of an obstacle/wall has attracted very close attention during last several decades [1-4]. Complex and non-linear interactions of heat-, momentum transfer and chemical reaction in confined-, porous media/narrow channels can be efficiently used for stabilizing reacting wave fronts for practically important applications (lean combustion systems, pulse detonation engines etc.) [3, 4]. Additionally, safety issues require better understanding the nature, limits and switching conditions of fast reacting waves propagating in confined media [5].

In the suggested talk the role of heat and momentum losses onto multiplicity of the fast sub- and super-sonic regimes of reaction waves propagating in porous media will be addressed. An overview of the problem will be given and asymptotical results conserving the quenching distance for detonation, quasi-detonation and for fast reaction waves will be established along the line suggested by Ya. B. Zel'dovich [6]. The results will be compared to those for deflagration and validated by numerical experiments using simple chemical kinetics [7, 8].

One of most interesting observations made in the study is the fact that for some mixtures flammability limits of the deflagration are smaller than those for detonation (see e.g. [9]). This means there are mixtures and geometries supporting detonation/fast reaction waves (quasi-detonations) while the deflagration quenches. The problem of the limits and sudden transition to fast reaction wave will be discussed in detail.

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MANIFOLD BASED MODEL REDUCTION STRATEGY – H_2/AIR MECHANISM OF CHEMICAL KINETICS

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Most of recently developed mechanisms of chemical kinetics for combustion systems are very large (in terms of number of species/parameters involved) and complex (non-linearity and stiffness) especially for engineering applications. In order to be a useful and predictable tool for research, chemical mechanisms have to represent the thermo-chemical state of the combustion system as accurate as possible. This means that the information about the evolution even some minor but important species/radicals (for soot formation, nitrogen oxide formation etc.) must also be available [1]. However, application of these detailed mechanisms is possible only for simple geometries (plane, cylinder etc. symmetries) within 1D spatial configuration only. Thus, developing simple reduced models in terms of complexity and dimensionality has become a crucial topic of the research last few decades (see e.g. [2]).

In the suggested talk the method of manifolds (low dimensional subsets embedded into the combustion system state/composition space) will be discussed as a major theoretical and rigorously grounded approach to proceed with the model reduction [3-6]. Within this concept any reduced model is considered as a manifold of lower dimension in the system state space. It represents all possible system states during all stages of the system evolution. In this way, the problem of model reduction transforms to the problem of definition, investigation of useful properties (fastness/slowness, attractiveness, invariance) and construction of appropriate manifolds in the detailed thermo-chemical state space of a reacting/combustion system [4, 5].

The main emphasis of the talk will be made on application of recently developed approaches to reduce the detailed mechanism of hydrogen/air combustion system. The detailed mechanism consists of 9 species and 19 reversible elementary reactions [7]. In order to address the ignition, laminar flame speed and flame structure the method of Reaction-Diffusion manifolds is applied and performance of 2D REDIMs' based reduced models (see e.g. [6]) are compared with the detailed model simulations.

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UNIQUE SOLVABILITY OF A P1 STEADY-STATE HEAT TRANSFER MODEL IN THREE DIMENSIONS

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There are a lot of applications where the conductive, convective, and radiative heat transfer mechanisms should be considered simultaneously [1-3]. The following examples can be mentioned: combustion chambers and industrial furnaces, cooling systems, glass manufacturing, production of optical fiber, etc.

The common feature of processes inherent to such applications is the radiative heat transfer occurr in gat high temperatures. The radiative heat transfer equation (RTE) is a first order integro-differential equation governing the radiation intensity. The radiation traveling along a path is attenuated as a result of absorption and scattering, and it is amplified due to emission and incoming scattering along the path.

Numerical solving the RTE is a challenging task that cannot be effectively solved in three dimensions. A way of avoiding the solution of the integro-differential RTE is the use of expansions of the local intensity in terms of spherical harmonics, with truncation to N terms in the series. This approach leads to the so called PN approximations. The odd orders are usually employed, commonly P1 and P3. Especially interesting is the use of steady state P1 approximations because they describe steady-state temperature distributions and do not require high computational efforts [4-6]. The main difficulty related to steady-state P1models is the absence of theoretical results on their unique solvability in three dimensions.

In the present paper, we close this gap. Namely, the unconditional unique solvability, without smallness or largeness assumptions, is proved in the case of Robin-type boundary conditions for the temperature and the mean intensity function. Moreover, the proof suggests an iterative algorithm for the numerical solution of the model. Numerical examples demonstrating the importance of the radiative heat transfer at high temperatures are given.

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A MULTIPURPOSE REDUCED KINETIC SCHEME FOR METHANOL COMBUSTION

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We present a multipurpose reduced chemical-kinetic mechanism for methanol combustion comprising 8 overall reactions and 11 reacting chemical species. The development starts by the investigation of the minimum set of elementary reactions that are needed to describe methanol combustion. It is found that adding only 11 elementary reactions, based on the full San Diego Mechanism [1], to the 27-step ignition submechanism proposed by Seiser et al [2] produces a sufficiently accurate skeletal mechanism that can be used in computations of autoignition, premixed-flame propagation, nonpremixed strain-induced extinction, and equilibrium composition and temperatures, giving results that compare favorably with experimental measurements in all cases. The simplification continues by the introduction of steady-state approximations for the intermediate species CH_3 , CH_4 , HCO, CH_3O, CH_2OH and O, leading to an 8-step reduced mechanism. The comparisons with experimental measurements indicate that the reduced chemistry gives results with accuracies better than 5% for autoignition times and premixed-flame propagation velocities, while somewhat larger departures on the order of 10% are observed in critical strain rates for nonpremixed flames [3]. Flame computations are also used to assess the impact of molecular transport on the accuracy of the computations of methanol combustion. In all cases considered it has been found that thermal diffusion effects are hardly noticeable and can, therefore, be neglected. Furthermore, no differences are observed in premixed-flame computations between the results obtained using a constant Lewis number approximation, the empirical mixture-averaged transport model proposed in [4], and the more accurate multicomponent transport model, following Dixon-Lewis formulation [5]. By way of contrast, for diffusion flames the constant Lewis-number approximation gives results that differ significantly from those obtained with the more involved transport models, while the differences found between the mixture-averaged and the multicomponent models are smaller.

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EXPERIMENTAL AND MODELING STUDY OF PREMIXED FLAMES STRUCTURE OF C_5 AND C_6 ALKANOIC ACID METHYL ESTERS

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Search for renewable sources of energy aimed at reducing oil consumption in energy production and transport is causing increasing interest for different oxygenated fuels. One of the most promising types of these fuels is biodiesel based on methyl esters. It is produced from plant oils and animal fats by transesterification, and thus consists of a mix of several methyl esters with 15-18 carbon atoms in the alkyl chain. It has been demonstrated in different studies that the use of biodiesel fuels can reduce generation of soot and CO in internal combustion engines [1]. Therefore, for combustion parameters to be evaluated in different systems, it is crucial to know the kinetic mechanisms of combustion for all biodiesel components. However, the high molecular weight and the complex structure of the biodiesel components significantly complicate these studies. Thus, combustion kinetics of several lighter methyl esters is being investigated to improve an understanding of methyl esters combustion and biodiesel components in particular.

In this work, structure of four premixed flames of methyl pentanoate ($C_6H_{12}O_2/O_2/Ar$, with equivalence ratios: φ = 1.0 and 1.5) stabilized at atmospheric and low (20 Torr) pressures and two premixed flames of methyl hexanoate ($C_7H_{14}O_2/O_2/Ar$, φ = 1.0 and 1.3) stabilized at low pressure has been studied with molecular-beam mass-spectrometry (MBMS) experimental technique and numerical simulations. Low pressure flames were studied by a time-of-flight mass spectrometer with a molecular beam sampling system and photoionization by tunable VUV synchrotron radiation located at the Advanced Light Source (ALS) of the Lawrence Berkeley National Laboratory [2]. Flames stabilized at atmospheric pressure conditions were studied by MBMS setup with a quadrupole mass-spectrometer and soft electron-impact ionization located in Novosibirsk [3]. Numerical simulations were performed with a PREMIX code from the CHEMKIN package. For these simulations two different detailed kinetic mechanisms were implemented. One of them was proposed earlier [4], and the other one was prepared and validated on a new obtained experimental data by authors of this work.

Temperature and mole fraction profiles of different stable and intermediate species were measured in the studied flames. The experimental results were compared with results of numerical simulations and both mechanisms have shown a good agreement with experiments for the most species, but however for a several compounds considerable discrepancies between calculated and measured mole fractions of the species were observed. Analysis of the reaction pathways has shown some noticeable differences between two mechanisms and the need of a significant improvement of a both mechanism to achieve a better agreement with an experimental results.

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FLAME PROPAGATION IN A COMPOSITE SOLID ENERGETIC MATERAL

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In a number of papers recently the possibility of developing of nanostructured composite energetic materials is discussed [1-7] in pursue for microscale power units with high energy density for microthrust and micropower generation applications such as micro–electro-mechanical systems including micropropulsion. The main idea behind this is in attempt to use the extraordinary material properties of nanostructures, which are not encountered in bulk materials, in order to modify and/or enhance the combustion characteristics of the resulting energetic materials. In [1-7] the composite consisting of an array of carbon nanotubes and combustible solids such as cyclotrimethylenetrinitramine (TNA) is considered. Here we are mainly focused on the latter system. The basic building block of such material is a shell-core nanowire which has a carbon nanotube (CNT) in its centre and is covered with a shell of energetic material (TNA).

Here we consider a thermal–diffusional model for composite energetic materials of the shell-core type which describes the propagation of combustion waves in such media of both nano and macroscopic sizes. It is demonstrated that by proper material design it is possible to substantially enhance the rate of combustion waves propagation and their stability. For macroscopic systems this opens possibilities for synthesis of new materials and creating new types of propulsion systems. For nanoscale systems we have found that the model substantially underpredicts the propagation velocities obtained in experiments thus implying that there are alternative ways for thermal energy transfer on such scales requiring further investigation.

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FILTRATIONAL COMBUSTION OF GASEOUS HYDROCARBONS INSIDE POROUS NI-AL MATERIALS

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The method of filtrational combustion consists in the combustion of a mixture of air and gaseous fuel within a chemically inert porous environment. There the outer surface of the porous environment is heated to the temperatures about 1600 K, which gives rise to generation of an IR flux. This method requires the use of specially designed high-temperature materials [1]. The purpose of this study is to investigate filtrational combustion of gas inside the porous Ni-Al materials manufactured by the combustion synthesis process.

An investigation is performed of the filtrational combustion of gaseous hydrocarbons inside a spherical nozzle manufactured from porous Ni-Al material. A combustion mode is demonstrated, wherein the combustion wave is localized inside the wall of the porous nozzle. Depending on the input power, the outer surface of the nozzle was heated to 1000÷1700 K, with a flow of nearly transparent reaction products being observed (flameless combustion mode). Radiation of the burner is controlled by the heat emitted by the porous burner and the heat emitted by the combustion products. Our investigations have shown that an increase in the specific heat output in the range $10 \div 40 W/cm^2$ results in a sharp increase in the nozzle temperature and burner radiation intensity. Beyond the upper bound of the above-mentioned range, quantities of the outer nozzle surface temperature and the total radiation power vary only a little, with a transition from the flameless mode to a combustion mode with yellow flame above the nozzle surface. At specific heat output $\approx 30 W/cm^2$, the radiative energy efficiency observed is the highest (approx. 60÷70%), the contribution from the gas phase into this energy being 20÷30%. According to the measurements performed, radiation of the burners with a spherical nozzle is isotropic in all directions, with the maximum radiative energy yield of the burners lying within the wavelength range 3÷11 μm [2].

Accurate measurements with a thermocouple demonstrated that the temperature of the yielding combustion product is by 200÷300 K lower than that of the nozzle. The effect observed is hard to interpret in terms of the conduction-convection mechanism of heat exchange between the gas phase and the solid nozzle in the course of filtrational combustion of the fuel mixture. We might assume that in the course of transformation reaction there is a relatively intensive heat release of the gas phase in the pore space, which results in its fast cooling.

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EFFECT OF METHYL PENTANOATE ADDITION ON FORMATION OF PAH PRECURSORS IN A FUEL-RICH N-HEPTANE/TOLUENE FLAME

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Using the blends of diesel fuel with biodiesel is considered to be reasonable not only because of reduction of consumption of petroleum, which is a source for diesel fuel production, but also because of the ability of biodiesel additive to lower pollutant emissions (in particular, soot and polycyclic aromatic hydrocarbons - PAH) from Diesel engines. Biodiesel represents, as a rule, a mixture of methyl esters of different fatty acids. Although many works were focused on the effect of addition of different methyl esters (as models of biodiesel) to hydrocarbon fuels on soot and PAH formation, the detailed experimental data on the effect of methyl esters on formation of PAH precursors in flames of diesel fuels (or their surrogates) are limited. Such data are vital for validation of chemical kinetic mechanisms for formation of PAH precursors in the flames of methyl ester/hydrocarbon mixtures.

The goal of this work is to investigate the effect of methyl pentanoate addition on formation of PAH precursors in n-heptane/toluene (7/3 by volumes of liquids) flame. Methyl pentanoate (MPe, 5 carbon atoms in the alkyl chain) and the mixture n-heptane/toluene are considered as surrogates of biofuel and diesel fuel, respectively. The investigation of MPe effect on formation of PAH precursors in the mixture n-heptane/toluene is an important step toward understanding processes of this kind in realistic mixtures biodiesel/diesel fuel.

Two fuel-rich flames (fuel/O_2/Ar) stabilized on a flat burner at 1 atm were studied in this work. The first flame was fueled by n-heptane/toluene mixture, and n-heptane/toluene/MPe mixture was used as a fuel for the second flame. Both flames had the same equivalence ratio equal to 1.75. Flame sampling molecular beam mass spectrometry with soft ionization by electron impact was used for measurements of mole fraction profiles of reactants, major products and different intermediates in both flames. The influence of MPe addition on absolute mole fractions of PAH precursors (acetylene, ethylene, propargyl, benzene, diacetylene, styrene) is discussed. Experimental data are compared with simulation results using PREMIX code and a detailed chemical kinetic mechanism composed of submechanisms, available in the literature, for oxidation of n-heptane, toluene and MPe in flame. Performances and deficiencies of the mechanism are discussed.

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MULTIPLICITY OF COMBUSTION WAVES IN A MODEL WITH COMPETING EXOTHERMIC REACTIONS

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Combustion waves with two-stage competing exothermic reactions A → B and A → C have been studied experimentally [1, 2], analytically [3-7] and numerically [5]. In [1, 2], the experimental observation of bistability of flame propagation is reported for combustion of Me−C−H2, where Me is either Ti or Zr.

The aim of this paper is to undertake both linear and nonlinear stability analysis for the model of flame propagation with two-stage competing parallel reactions of the first order. Our attention is mainly focused on the parametric region, where multiple solutions exist. Under these conditions, interesting dynamical behaviour can occur. Further, we focus only on pulsating instabilities; therefore, the case of Lewis numbers for fuel greater than unity is always assumed.

We investigate a diffusional-thermal model with two-step competitive exothermic reactions for premixed combustion wave propagation in one spatial dimension under adiabatic conditions. A criterion based on the crossover temperature notion was used to qualitatively predict the region in the space of parameters where three travelling combustion wave solutions coexist, which are further studied via numerical means. It is demonstrated that under certain conditions the flame speed is an 'S'-shaped function of parameters. The fast branch is either stable or is partly stable and exhibits the Andronov–Hopf (AH) bifurcation before the turning point is reached. The mid-branch is completely unstable. The slow solution branch is either unstable or partly stable and exhibits a single or a pair of AH bifurcations. The AH bifurcations are shown to be supercritical giving rise to stable pulsating waves. Bistability and hysteresis phenomena are also demonstrated.

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SIMPLIFIED MECHANISM FOR INHIBITION OF HYDROGEN AND METHANE FLAMES BY TRIMETHYLPHOSPHATE

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Combustion of solids, liquids and gases is known to be the source of fires. Fires hold a special position among other disasters, which are known to be a global problem due to their ability to cause huge damage to mankind. The development of a physico-mathematical predictive model for their initiation, propagation and suppression is of great scientific and practical importance.

At present, methods of computational fluid dynamics are being intensively developed. The methods make it possible to study 3D dynamics of the processes proceeding during fire propagation and suppression, including the case when the inhibitors and fire suppressants are used. The models used in these simulations involve fluid dynamics and also consider phase and chemical transformations of the substances. Successful application of these models is impossible without taking into account chemical transformations of the intermediate components. The chemical processes are usually described by detailed mechanisms that can include thousands of elementary reactions involving hundreds of chemical species.

On the basis of a multi-step kinetic mechanism for flames inhibition by organophosphorus compounds including more than 200 reactions, a skeletal mechanism for flames inhibition by trimethylphosphate was developed. The skeletal mechanism consists of 22 irreversible elementary reactions, involving 9 phosphorus-containing species.

The starting mechanism [1, 2] was developed by collecting the maximum number of elementary reactions involving phosphorus-containing species. Besides phosphorus-involving reactions, this mechanism includes submechanisms for combustion of hydrogen, methane and propane. Overall, the mechanism consists of 682 steps for 121 species, 44 of which contain P-atoms.

Selection of the crucial steps was performed by analyzing P-element fluxes from species to species and by calculating net reaction rates of phosphorus-involving reactions versus the flames zone. The developed mechanism was validated by comparing the modeling results with measured and simulated (using the starting initial mechanism) speed and chemical structure of H_2/O_2 and CH_4/O_2 flames doped with trimethylphosphate. The mechanism was shown to satisfactorily predict the speed of $H_2/O_2/N_2$ flames with various dilution ratios and CH_4/air flames doped with trimethylphosphate. Besides, the skeletal mechanism satisfactorily predicts the spatial variation of H and OH radicals and final phosphorus-containing products of the inhibitor combustion. Further reduction of the skeletal mechanism without modification of the rate constants recommended in the starting mechanism was shown to result in noticeable disagreement of the flames speed and structure.

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OPTIMAL CONTROL IN A MODEL OF COMPLEX HEAT TRANSFER

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Optimal control problems for models of complex heat transfer in scattering media with reflecting boundaries are of great importance in connection with engineering applications [1-4]. A considerable number of works is devoted to control problems for evolutionary models involving radiative heat transfer. There, the propagation of thermal radiation is described by a nonlocal integral-differential equation or by its local approximations. The temperature field is governed by the conventional transient heat transfer equation with additional source terms accounting for the radiative heat exchange. As for steady-state models, some preliminary results on the correctness of boundary-value problems based on the P1 approximation are recently obtained in one and three dimensions, see [5] and [6]. Nevertheless, theoretical analysis of optimal control problems for steady-state models of complex heat transfer is an open question. The main difficulty here is, in addition to nonlinearities of the governing equations, the absence of appropriate energy estimates.

This paper deals with steady-state models. The problem addressed is the design of reflection properties of the boundary of a three-dimensional domain in order to optimize a cost functional, e.g. to maximize the energy outflow from the domain. The application of the P1 approximation to the radiative heat transfer equation yields an optimal boundary multiplicative control problem for a nonlinear elliptic system. The solvability of this system is proven on the basis of new a priori estimates of solution norms. Necessary optimality conditions of first order are derived, and an analogue to the bang-bang principle of optimal control theory is obtained. Sufficient conditions ensuring the non-degeneracy of the optimality system are found in the case of heat transfer in channels (see [7]).

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SCALING FOR HIGH INTENSITY LIQUID FUEL BASED FLAMELASS COMBUSTORS

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Flameless combustion offers many advantages over conventional combustion such as uniform temperature distribution and lower emissions [1]. A new strategy is proposed and adopted to scale a flameless combustor from a heat release density of 5 to 21 MW/m^3 (thermal input 21.5 – 84.7 kW) with kerosene fuel. A swirl flow based configuration was adopted for air injection. Initially, flameless combustion was stabilized for a thermal input of 21.5 kW ($\dot{Q}'''$ = 5.37 MW/m^3) later scaled to a heat release density of 21 MW/m^3 [2, 3]. Two major difficulties were identified as possible reasons for unsustainable flameless combustion at the higher intensities (i) A constant spray cone angle and SMD increases the droplet number density (ii) Reactants dilution ratio (R_{dil}) decreased with increased thermal input [1-3]. To solve these issues, a modified combustor configuration, aided by numerical computations was adopted, providing a chamfer near the outlet to increase the R_{dil}. Detailed experimental investigations showed that flameless combustion mode was achieved at high intensities with an evenly distributed reaction zone and temperature in the combustor at all heat intensities. The emissions of CO, NO_x and HC for all heat intensities (Φ = 1 - 0.6) varied between 11 - 41, 6 - 19 and 0 - 9 ppm, respectively. These emissions are well within the range of emissions from other flameless combustion systems reported in the literature.

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ANALYSIS FOR FLAME EXTINCTIONS WITHIN MESOSCALE OPPOSED FLOW BURNERS ON NON-PREMIXED AND PARTIALLY PREMIXEDCONDITIONS

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Recently, interests on combustion phenomena within narrow combustion spaces in terms of mesoscale combustion have been increased with the development of practical small combustion systems or basic reactors. In the early study of mesoscale combustion, flame stabilization was an important issue since it could suffer large amount of heat losses due to the increased surface to volume ratio. However, the great variety of small burner configurations hindered a clear understating of mesoscale combustion phenomena. Thus, a comparison of their results to each other was difficult. Therefore, more fundamental configurations have been necessary for the evaluation of characteristic length scales in order to construct a reference database regarding mesoscale combustion phenomena. More recently, an opposed flow burner, which was horizontally installed within a mesoscale channel, was suggested as one of the fundamental burner configuration [1], and the flame stabilization characteristics were evaluated for non-premixed [1], and partially premixed conditions [2]. For non-premixed condition, the flame extinction limits could be classified into three cases; a higher-strain-rate (HSR) extinction, a lower-strain-rate (LSR) extinction and a fuel-dilution-ratio (FDR) extinction. Meanwhile, in the partially premixed conditions, flash-back was additionally observed when the equivalence ratio approaches to stoichiometry in both sides of mixtures. In the previous study, the most important issue was the flame stabilization characteristics of the LSR condition, and these results could be compared with the micro-gravity experimental results [3].

In this study, the flame behaviors near the extinction limits and their extinction mechanisms were investigated analytically for non-premixed and partially premixed conditions. For non-premixed flames, a modified strain rate was introduced as the HSR extinction criterion that could reflect the flow development in mesoscale spaces; i.e., a hydraulic diameter of the nozzle and the kinematic viscosities were considered. In order to explain the LSR extinction in mesoscale spaces, a new extinction model of a diffusion flame based on a premixed quenching theory was suggested. That model included the existence of a dead space near the wall and the heat loss through the dead space. With regard to the FDR extinction, a simple reaction rate which was coupled with the adiabatic flame temperature and the FDR was introduced. In a similar way, the extinction characteristic of partially premixed flames could be obtained by adjusting boundary conditions and thermal thickness that varied by the premixing ratios of both nozzles.

These analytic models could explain the overall trends of the experimental results of flame extinctions for non-premixed and partially premixed opposed flow flames within the mesoscale channels.

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ANALYSIS OF THE 2-PARAMETRIC CONTROL PROBLEM FOR TWO-DIMENSIONAL MODEL OF WAVE SCATTERING

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In recent years much attention has been given to constructing invisibility cloaking devices for material bodies. Beginning with the pioneering paper by J. Pendry et al. [1] the large number of publications was devoted to developing methods of solving the cloaking problems (see, e.g., paper [2] and references therein). It should be emphasized that the technical realization of solutions obtained in these papers is connected with substantial difficulties.

One of the approaches overcoming these difficulties consists of replacing the exact cloaking problem by approximate cloaking problem for which solutions admit simple technical realization. There are different approaches of replacing exact cloaking problem by approximate one which were developed in a number of papers. Among them we mention paper [3-5, 6] where the transformation optics approach proposed in [1] is used and papers [7-9] in which the optimization method is used for solving the impedance cloaking problems.

In this paper we consider control problems for 2-D electromagnetic wave scattering model which are associated with invisibility cloaking for this model. Unlike [7-9] the cloaking effect in cloaking problems under study is achieved via controlling two variable parameters entering into the scattering model: the refraction index of the medium and boundary conductivity. Using the mathematical theory developed in [7-10] for studying one-parametric control problems we prove the solvability of the control problems, derive the optimality systems describing the first-order conditions of extremum and establish sufficient conditions on the input data which provide the uniqueness and stability of optimal solutions.

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ON THE FEATURES OF 1D UNSTEADY HETEROGENEOUS COMBUSTION WAVES IN POROUS MEDIA UNDER NATURAL CONVECTION

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The work is devoted to the numerical investigation of one-dimensional unsteady processes of heterogeneous combustion in porous object under free convection. Combustion is due to the exothermic reaction between the fuel in the porous solid medium and oxidizer contained in the gas flowing through the porous object. In considered porous objects the gas pressure at object boundaries is known but the flow rate and velocity of the gas at the inlet to the porous objects are unknown, so the flow rate of oxidant, which enters into the reaction zone in porous object, regulates itself. The mathematical model is based on the assumption of interacting interpenetrating continua using the classical approaches of the theory of filtration combustion; it includes equations of state, continuity, momentum conservation, energy for each phase (solid and gas) and oxidizer concentration. The proposed mathematical model is similar to the one used in [1] and allows to describe the processes for both free convection and forced filtration.

The cocurrent wave, when the gas moves in the same direction as the combustion wave, and countercurrent wave, when the gas and the combustion wave move in opposite directions, have been numerically investigated for different parameters in the present work. It has been revealed that reaction-trailing type of wave structure, when the reaction occurs at the trailing edge of the heated region of the porous object, may not occur when the analytical criterion for reaction-trailing combustion wave takes place. The analytical criterion, which determines the reaction-leading or reaction-trailing regime of combustion wave for simple model [2-3], cannot determine types of wave structure for more complicated model. Using some different expressions of the dependence of permeability on porosity, the effect of the changing of permeability due to the changing of porosity has been numerically investigated. It has been revealed that taking into account the dependence of permeability on porosity can significantly change the solution quantitatively in one-dimensional case; it can also increase the temperature in the countercurrent combustion wave.

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NUMERICAL SOLVING THE INVERSE PROBLEM FOR THE CONVECTION-DIFFUSION-REACTION EQUATION

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In this work we consider the problem of identification of the coefficients in the differential equation for the heat transfer models using the additional information on the solution of the initial boundary value problem. The study of this problem can be reduced to the study of the corresponding extremum problem for a certain cost functional. For the theoretical study of inverse extremum problems we use methods of constrained minimization [1-4].

The purpose of our work is creation of efficient numerical algorithms of inverse coefficient extremum problems and the numerical analysis.

We consider the heat transfer model in a bounded domain with Lipschitz boundary. The boundary value problem of the heat transfer model contains a number of parameters that must be given to ensure the uniqueness of the solution. In practice, situations can arise when some of the parameters are unknown. For this reason, we need more information about the solution of boundary value problem. As this information we can use, for example, temperature measured in some subdomain of a bounded domain. For the study of identification problem we apply optimization method and reduce solution of this problem to the corresponding extremum problem (see [3, 4]).

Using the mathematical apparatus of the book [3] we obtained the optimality system. This system has the meaning of the necessary extremum condition of the first-order. The optimality system is essentially used to prove the uniqueness and stability of the solution of the extremum problem and for creation of numerical algorithms. This system consists of the direct problem, adjoint problem and variational inequality, which has the meaning of the minimum principle. The authors carried out a series of numerical experiments showing the convergence of the developed numerical algorithm based on Newton's method and the efficiency of parallelization techniques for solving inverse problems.

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COMBUSTION SYNTHSIZED β-SIALON POROUS CERAMICS FOR RADIATIVE POROUS BURNERS

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Porous penetrable ceramic materials attract wide attention of experts due to their capability of operation at high temperatures in aggressive media, for example, as parts of gas-burners, filters, catalysts, and so on. Ceramic materials based on silicon or aluminum oxynitrides known as SiAlONs are promising due to their superior thermal stability, high strength, high durability, high creep resistance and wear resistance, as well as chemical stability at room and high temperatures, good oxidation/corrosion performance, etc. By the present time, no energy-efficient technologies of fabrication of large-sized porous products from sialon or nitrides based ceramics have been developed. Sialon ceramics can be fabricated by the method of self-propagating high temperature synthesis also known as combustion synthesis (CS). The porosity parameters of products of combustion synthesis are conventionally controlled by adding components easily melting or gasifying in the combustion wave as well as by varying sizes of particles of powder reagents. These procedures are unsuitable for the combustion synthesis of porous SiAlON materials. In the present work, the possibility of realization of CS in preliminary slurry-foamed powder systems to fabricate porous SiALON materials is investigated.

In this work, we investigated Al and SiO_2 powders with particle sizes less than 10 μm. The reactive charge was mixed according to the relation $4Al + 2SiO_2 + 4N_2 + \text{diluent} \rightarrow Si_2Al_4O_4N_4$. Self-made SiAlON powder with particle size less than 10 μm was used as a diluent agent [1]. To obtain high-porosity powder samples, the method of foaming aqueous slurries made from reactive powders was used. The foamed samples were subjected to combustion synthesis in the reactor with volume of 3 L in the nitrogen atmosphere at pressures up to 1 MPa. Depending on the porosity, the combustion velocity was U_C = 1÷3 mm/s when the temperature of the process attained its maximum T_C = 1550÷1750 K. According to the data of x-ray phase analysis, the main product of synthesis is β-SiAlON. As a result of combustion synthesis, the structure of β-SiAlON materials with total porosity from 40 to 75%, size of core elements 250÷750 μm, sizes of pore channels 10÷200 μm, and specific surface 4÷15 mm^{-1} was fabricated.

It has been determined that the method of foaming of slurry can be used to organize high-porosity reactive systems for subsequent combustion synthesis of ceramic materials with retention of initial structure of pore space of foamed reactive systems during synthesis. It has been established that combustion in reactive gas flow considerably intensifies the process of synthesis.

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ON SELF-DRIFTING FLAME BALL AND FLAME BALLS ARRAY COLLECTIVE PROPAGATION

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A three-dimensional (3D) reaction–diffusion model for premixed flames with radiative heat losses is studied numerically and analytically. In accordance with previous analytical predictions and numerical simulations, it is shown that cellular flames occurring in low Lewis number premixtures can propagate at heat-loss rates greater than the maximum that extinguishes the planar flame. At sufficiently high heat losses, the flame interface breaks up into separate self-drifting flame balls while a significant portion of the fuel remains unconsumed. A method of evaluation of flame balls array propagation velocity is proposed and possibility of single self-drifting flame ball in free space is discussed. Combustion wave consisting of flame balls is specific regime observed in weak near-limit low-Lewis-number gas mixtures. The modeling of such combustion waves is important for development of eco-friendly technologies of lean gas burning and energy saving. The developed method may be also applied for pulse dynamics in an excitable reaction–diffusion system to describe a transition from a motionless reaction spot to self-drifting spot. By employing the analogy of particle motion in a conserved system, we can clarify the mechanism that the pulses undergo an elastic-like collision in a special parameter regime as observed by computer simulations even though the system is purely dissipative.

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2D LINEAR STABILITY OF TWIN STRETCHED FLAMES

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Understanding of propagation and stability of counterflow premixed flames is required for the development of new combustion technologies such as: combustion with low-NOx emission, combustion of lean mixtures, micro-scale combustion and material synthesis. While the stability of counterflow flames is not well investigated in the case of premixed gas combustion, the only stable combustion regimes can be used to obtain materials with homogeneous properties. A two-dimensional thermal-diffusive instability of stretched counterflow flames is investigated. The stability diagram and dispersion equation describing growth rate of spatial perturbations of the flame front are obtained. Regions of the flame front instability are distinguished. Our results show that three types of the instability exist. It is shown that two types of instability can lead to the flame quenching and the third one can be related with the cellular flame formation. The establishing of flammability limits and the region of cellular flames existence can be useful for practical applications of flame-synthesis methods for new material production.

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INVESTIGATION OF INFRA-RED FLUX CHARACTERISTICS FROM CYLINDRICAL POROUS BURNER

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Modern trends in development of effective and eco-friendly technologies for gas heaters, ovens, energy conversion devices and for utilization of waste and low-calorific fuels demand fundamental investigations of combustion processes in porous burners. Experimental data on porous media temperature, radiative heat flux and flame stabilization in the burners of different geometries are necessary for development of combustion based devices for industrial and domestic applications.

In present work combustion in the cylindrical porous burner are studied experimentally. The burner is a hollow porous cylinder made of NiAl alloy. The inner and outer radiuses of the burner are 15mm and 24 mm, correspondingly, the cylinder height is 52 mm. Top part of the cylinder is closed by porous NiAl semi sphere. Methane-air mixture is supplied to the inner hollow of the burner from the bottom side. Experimental setup consists of PC, digital flowmeters, FTIR spectrometer and bolometer. Set of Pt/PtRh thermocouples was embedded inside the porous medium in order to measure radial temperature distribution inside the burner. Ignition system allows to initiate the flame near both the inner and outer surface of hollow porous cylinder.

It was found that depends on ignition conditions, the flame can be stabilized inside the hollow or outside the burner. Temperature of the porous cylinder, total radiative heat flux from the burner and emission spectrum significantly differs for these two combustion regimes. From practical point of view the combustion regime with the flame stabilized near the inner radius of porous cylinder is preferable because radiative heat flux and porous medium temperature in this case is about 1.5 times higher than in the case of flame stabilization outside the burner. The dependencies of burner temperature, radiative flux and emission spectrum on mixture equivalence ratio and flow rate were studied. It was found that considered burner characteristics reach maximum for stoichiometric mixture and increases with increase of flow rate. Stable combustion was observed in the wide range of flow rates and equivalence ratios. Experimental investigations of the effect of porous layer thickness shown that porous medium temperature and burner radiation power grow with increase of cylinder thickness from 3 mm to 9 mm.

Obtained experimental results revealed some essential features of combustion processes in cylindrical porous media which should be taken into account at development of practical porous burners.

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ELECTRIC POWER GENERATION USING HEAT-RECIRCULATING MICRO-COMBUSTOR

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An experimental effort was made to extract electrical energy from the stabilized flame in micro-combustor using thermo-electric generators. The design, by virtue of lack of moving parts and hence being free from mechanical losses, stands as a demonstrator for substitution of conventional batteries with hydrocarbon fuel using micro-devices. The fuel of choice for the work was Liquefied Petroleum Gas (LPG), due to its availability and high calorific value. The micro-combustor is hollow cylindrical with three internal steps to aid in the stabilization of the flame formed using premixed fuel-air mixture at high velocities, by providing local recirculation zones at the steps and thereby, increasing the residence time of the mixture [1]. The material of choice for the micro-combustor was Mild Steel to enable the pre-heating of the fuel-air mixture. The micro-combustor was placed in a heating cup. The heating cup is a Copper cube with a cylindrical blind hole drilled through one face for the entry of the combustor. This introduces counter-flow recirculation of the exhaust gas, heating up the wall of the combustor and preheating the fuel-air mixture. These help in increasing the flammability limits. The outer wall of the Copper micro-combustor was threaded and a stopper ring was placed on it to further increase the residence time of the exhaust gases inside the cavity of the heating cup. Based on the works of Yadav et al. [2], it was realized that increasing the number of thermo-electric modules to cover four walls resulted in an increase in thermal efficiency. Hence, four Bismuth-Telluride HZ-12 thermo-electric modules were attached to four walls of the heating cup. The walls of the heating cup acted as the hot junction and the cold junction was maintained by operating a heat sink with water as the cooling fluid. Proper clamping force was provided to ensure almost gap-free contact and optimum operation of the modules. This experimental work showed high thermal efficiencies obtained in the range of 6-7% at high flow velocity conditions of up to 7 m/s. This range of efficiencies is very high compared to those obtained in other micro-combustion based power devices researched on worldwide.

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AN ITERATIVE METHOD FOR SOLVING A COMPLEX HEAT TRANSFER PROBLEM

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The study of the radiative-conductive heat transfer [1] is important for many engineering applications [2-4]. Usually this process is described by a non-linear system of two differential equations: an equation of the radiative heat transfer and an equation of the conductive heat exchange. The problem is characterized by anisotropic scattering of the medium and by specularly and diffusely reflecting boundaries. We use the diffusion approximation (also named P1 approximation) for simplifying the complex heat transfer problem. This approximation allows to describe the behavior of the temperature properly in computation in difficult cases of high temperature. Thus, this approximation be successfully applied to various heat transfer problems in which are not required high accuracy.

The aims of the current work are to present a constructive proof of the solvability of the nonlinear heat transfer problem, to find uniqueness conditions of the solution, to propose an algorithm for solving, and to show that the algorithm can be implemented in practice. The proposed approach is related to finding a fixed point of a nonlinear solution operator constructed on the base of modified form of the diffusion approximation. Based on the contraction property of the solution operator, the iterative algorithm is proposed. Sufficient conditions of existence and uniqueness of a fixed point are determined. Under these conditions the proposed iterative algorithm converges at a geometric rate. The numerical experiments were fulfilled. The efficiency of this algorithm is demonstrated. The advantage of the proposed algorithm is its guaranteed convergence. Also, there is an opportunity for finding an a priory error estimate.

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ON PROPERTIES OF SOLUTIONS OF INVERSE COEFFICIENTS PROBLEMS FOR THE CONVECTION-DIFFUSION-REACTION EQUATION

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In the study of the inverse coefficients problems for a number of well-known mathematical models the theorems of uniqueness of their solutions play very important role. We mentioned [1-3] devoted to the study of inverse coefficients problems and multiplicative control problems for the equation of convection-diffusion-reaction, models of heat convection, Maxwell equations. There are mathematical tools and detail review of these problems in [4, 5].

Due to the nonlinearity of the inverse coefficient problems the uniqueness of their solutions tend to be proved under the small condition on initial date of the corresponding boundary value problem only.

In our paper we consider the linear equation of convection-diffusion-reaction under Dirichlet condition for the concentration. The problem of recovery of the reaction coefficient by additional information on concentration of pollution in some subdomain is studied. This problem is reduced to the problem of minimization of some cost functional on the weak solution of considered boundary value problem. Our main result is a proof of uniqueness of solution of the considered inverse coefficient problem without smallness of initial data of corresponding boundary value problem. We note that the developed in our paper method is applicable to a number of other similar problems.

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SOLVING THE INVERSE PROBLEM FOR THE REACTION-DIFFUSION MODEL USING PARALLEL TECHNOLOGIES

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Modern high-tech manufacturing, medicine, ecology, and other industries require large computing resources and high-tech approach to achieve the best results in its development. Protecting the environment from human impact, and in particular the study of the propagation of the pollutant in water, is one of these areas. Modern computing resources and parallel computing technologies allow highly accurate modeling and statistical analysis of real experimental data in the modeling of mass transfer processes in the study area.

In this work we consider the problem of identification of the coefficients in the differential equation for the mass transfer models using the additional information on the solution of the initial boundary value problem.

The study of this problem can be reduced to the study of the corresponding extremum problem for a certain cost functional. For the theoretical study of inverse extremum problems we use methods of constrained minimization [1-4]. For numerical solution of the inverse problems we use a parallel computing technologies. The application of these technologies enables one to solve several sub-tasks simultaneously [5]. The application of parallel computing also is caused by processing of a large number of data and solutions of systems of equations with sparse matrices.

The purpose of our work is the theoretical analysis of inverse coefficient extremum problems and creation of efficient numerical algorithms.

Our model has the form of stationary diffusion-reaction equation with variable coefficient of the chemical reactions. This equation is considered in bounded domain under Dirichlet boundary condition. Based on the analysis of optimality system we developed a parallel algorithms for solving of our inverse problems. The testing of our programs has shown the effectiveness of our programs using parallel computing techniques with help a package of computer programs FreeFem++.The results of numerical experiments are discussed.

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COMBUSTION CHEMISTRY OF FUEL-RICH CH_4/AIR AND C_3H_8/AIR FLAMES WITH CO_2 ADDITIVE

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The reduction of pollutant emissions from combustion of fossil fuels is the world's largest problem. One of the alternative methods of solving this problem is using the technology of recirculation of flue gas, the main component of which is CO_2. The effects of CO_2 on the burning velocity, composition of final products, and other combustion characteristics of hydrocarbon/air mixtures were extensively studied. An important issue, in particular, is the influence of replacement of N_2 with CO_2 in the fresh combustion mixture on soot formation in the flame. The goal of this work is to study the effect of replacement of part of N_2 with CO_2 in fuel-rich CH_4/air and C_3H_8/air mixtures on chemical kinetics in premixed flame stabilized on a flat burner at 1 atm by measurement and numerical simulation of its thermal and chemical structure.

Fuel-rich (φ=1.2) $CH_4/O_2/N_2$, $C_3H_8/O_2/N_2$ and $CH_4/O_2/N_2/CO_2$, $C_3H_8/O_2/N_2/CO_2$ flames were stabilized on a flat burner 16 mm in diameter at 1 atm. The burner surface was kept at 95 ^oC. The linear velocity of the fresh mixture on the burner surface was 16.0 cm/s for the $CH_4/O_2/N_2$ flame, 40.2 cm/s for the $C_3H_8/O_2/N_2$ flame and 7.25 cm/s for the $CH_4/O_2/N_2/CO_2$ flame, 20.1 cm/s for the $C_3H_8/O_2/N_2/CO_2$ flame.

Mole fraction profiles of reactants (CH_4, C_3H_8, O_2, CO_2), intermediates (CH_3,CH_4, CH_2O, C_2H_2, C_2H_3, C_2H_4, C_2H_6, C_3H_3, C_3H_4) and final products (H_2O, CO, CO_2, H_2) were measured using quadrupole mass spectrometer coupled with molecular-beam sampling system. The flame structure was simulated using Premix code from the Chemkin-II collection of codes and Konnov's mechanism for hydrocarbons combustion. Experimentally measured temperature profiles were used as input data for the modeling.

The results of measurements indicate that the replacement of 15% of N_2 with CO_2 in $CH_4/O_2/N_2$ and $C_3H_8/O_2/N_2$ flames leads to reducing the post-flame temperature and decreasing maximum mole fraction of ethylene, vinyl, propargyl, allene, propyne and other intermediate hydrocarbon species in the reaction zone. Addition of CO_2 to fuel-rich methane and propane flames is shown to result in considerable reduction of mole fraction of soot precursors. Konnov's chemical kinetic mechanism, in general, adequately reproduces the experimental profiles for major flame species, however, noticeable discrepancies take place between measured and calculated mole fraction profiles for some combustion intermediates. Analysis of the results of calculating the structure of the flame under study and of the literature data has shown the effect of reducing the concentration of intermediate combustion products with partial replacement of N_2 with CO_2 to be connected with the increase of the reaction rate $CO_2+H \rightarrow CO+OH$, resulting in the growth of the ratio of OH/H in the zone of reactions in rich flames. The increase of OH concentration results in acceleration of the transformation of intermediate carbon-containing species into the final products of combustion, thus reducing the probability of soot formation.

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ON THE CORRELATION OF INVERTED FLAME BLOW-OFF LIMITS WITH THE BOUNDARY VELOCITY GRADIENT AT THE FLAME HOLDER SURFACE

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Premixed inverted flames, stabilized behind the trailing edge of a thin rod (wire) or plate installed lengthwise in a combustible mixture flow are often used for studies of flame stabilization mechanisms. Lewis and Von Elbe [1] performed experiments with wire-stabilized inverted flames of lean natural gas-air mixtures and found a correlation between the mixture burning velocity, the flame thermal thickness and the radial gradient of the axial mixture velocity ("boundary velocity gradient") at flame blow-off limits. Based on the fact that the correlation factor had a form of the Karlovitz number derived in [2] for a flame front in the velocity gradient flow, and, at the blow-off limit, had a value close to unity , Lewis and Elbe suggested that the inverted flame blow off was caused by the excessive flame stretch at the flame base. However, according to later developments of the flame stretch theory, the local extinction of the inverted flame at its base by positive flame stretch rate is not possible for mixtures with Lewis number less then unity, studied in [1]. Thus, an alternative explanation of the "boundary velocity gradient" correlation is required.

In this work, conductive heat losses from the base of a lean methane-air inverted flame, stabilized behind the trailing edge of a 1 mm diameter rod have been experimentally evaluated. Obtained experimental results favor the view that heat losses to the flame holder play a crucial role in the inverted flames stabilization and blow-off. Simple estimations have been performed, which indicate that the well-established correlation between mixture composition and boundary velocity gradient at the flame holder, usually considered as a proof of the flame stretch theory of blow-off, can be explained without involving the flame stretch concept. The suggested explanation of this correlation is based on the assumption that heat loss to the flame holder is the main factor, which determines the inverted flame blow-off behavior, and on the similarity between mechanisms of energy and momentum diffusion in gases. According to this assumption, the inverted flame blow-off occurs when heat losses to the flame holder become very small. This, in turn, suggests that, at the blow-off limit, the flame stand-off distance is of the same order of magnitude as the flame thermal thickness, and the burning velocity at the flame base is close to the burning velocity of the adiabatic flame. Then, the "boundary velocity gradient" correlation is derived by equalizing the flame thermal thickness and the estimated distance, at which the velocity of a "gas particle" traveling from the tip of the flame holder toward the flame base becomes equal by the absolute value to the mixture burning velocity.

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THE MODEL OF GAS COMBUSTION IN POROUS MEDIA

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A discrete quasi three-dimensional model of gas combustion in porous media is proposed. The porous media is represented as the set of randomly placed solid grains which are connected through the artificial solid plate to mimic thermal conductivity between grains. The propagation of the combustion wave is simulated in the frame of thermal-diffusion model with the prescribed flow field computed preliminary using Lagrangian particles method. Dependencies of combustion wave velocity on the inlet gas velocity for different equivalence ratios and porosities are obtained and compared with the continuous one-dimensional thermal-diffusion model. Our results imply that the flame propagation in the porous media can be considered as a collective process, when the actual combustion wave can be represented by a set of individual flame fronts propagating in the mutually connected micro-channels of the different diameter. The discrete structure of the combustion wave is most prominent when the inlet velocities are small and the flame propagation is accomplished with pulsations of flame front fragments. When the inlet velocities are high enough, the propagation of the combustion wave is much more regular. Our model describes the flame anchoring phenomena when the combustion wave is stabilized inside of the porous media for a range of inlet velocities.

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DEPENDENCY OF NITROGEN OXIDES FORMATION FROM MIXTURE FORMATION EFFICIENCY

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NOx emissions control is one of the most important issues to be solved when designing modern devices for combustion of organic fuels. At the stage of construction design, mathematical model is used which allows estimating with a considerable certainty technological and equipment resources for NO_x concentration reduction.

Purification of flue gases from NO_x requires considerable capital investments, comparable with the total cost of power engineering plant. One of technological ways of NO_x concentration reduction is cyclone vortex technology of burning fuel in the air of cooled cyclone vortex burners (CVB), which design allows implementing multi-stage burning with effective preliminary mixture formation.

CVB are air-cooled vortex furnaces with side and multi-lateral (3x, 4x) tangential air inlet, made through the system of nozzles. At the entrance to the burning chamber of cyclone vortex burner (CVBBC) a guide vane is installed, which is an axial swirler. Natural gas fuel is fed in various combinations, most commonly used is side and tangential feed [1].

Within the period of its operation CVB design was changed from time to time. Analysis of test results shows that NO_x emission in the CVB boilers is almost 1.5-2 times lower than in the similar boilers with factory-installed burners.

Based on experience of Okhtinskaya Combined Heat and Power Plant boiler *BKZ120-100GM* operation, as well as analysis of other boilers equipped with CVB with the purpose of NO_x emission reduction, one can use partial preliminary mixing of fuel and air. To do this, tangential gas inlets are offered to distribute over all air nozzles except the last one in the direction of gases movement. This done, conditions close to stoichiometrical will be achieved. Once deepening gas nozzles to the air nozzles, it is necessary to provide gas feed to the air flow.

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THE THEORETICAL ANALYSIS OF CLOAKING PROBLEM FOR 2-D WAVE PROPAGATION MODEL

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Cloaking of material bodies has been the subject of extensive studies for a long time. Currently cloaking problems are under active investigation. Beginning with the pioneering work [1], theoretical and numerical methods for solving problems of this type have been extensively developed.

In this paper control problems for 2-D Helmholtz equation in a bounded domain with mixed boundary conditions are studied. Helmholtz equation is considered with Dirichlet boundary condition on uncoated part of boundary and impedance boundary condition on the coated part of boundary. Impedance boundary condition is introduced for describing properties of special materials covering the boundary. This boundary condition relates acoustic pressure and normal component of oscillatory velocity in the case of acoustic waves or electric and magnetic fields in the case of electromagnetic waves via boundary coefficient called surface impedance. These problems arise when creating methods of acoustic or electromagnetic cloaking of material bodies [2, 3]. Similar control problems for Maxwell's equations considered in bounded domains are studied in [4, 5].

The problems consist of constructing approximate cloaking shell. By the optimization method these problems are reduced to study of inverse extremal (or control) problem. This approach is based on introducing quality functional which adequately corresponds to inverse problem of constructing approximate cloaking shell. The control problem under study consists of finding minimum of specific quality functional depending on the surface impedance and weak solution of the boundary value problem. In other words, one should choose surface impedance entering into impedance boundary condition on the coated part of the boundary which minimizes certain quality functional.

In the paper solvability of the control problem is proved. Existence of Lagrange multiplier for the control problem is proved and optimality system is derived. This optimality system consists of the direct problem for main state, conjugate problem for the conjugate state and variational inequality for finding desired control. Based on analysis of the optimality system sufficient conditions on the data are established which provide uniqueness and stability of specific control problems solutions.

Results of the numerical experiments are discussed.

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PARALLEL ALGORITHM FOR MODELING OF HETEROGENOUS COMBUSTION IN POROUS MEDIA

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In this paper the parallel algorithm and the parallel implementation of a numerical method for modeling heterogeneous combustion in porous media are considered [1]. The problem is solved in one-dimensional (1D) or two-dimensional (2D) formulation. Parallel processing is implemented using OpenMP multi-threaded technology.

Parallel algorithm consists of three main steps: initialization, calculation and saving results. The first step is the initialization of the physical constants, temporal and geometric parameters of the model, the initialization of the computational domain and the initial boundary conditions. Initial data for computational domain are loaded from the set of input files generated automatically for a given simulation conditions. At the second step all numerical computations are performed. At the third step, the final results are uploaded to the set of output files, which are then analyzed for a features of the combustion reaction passing in a specified porous object with the given parameters and boundary conditions.

The second step with numerical computations consists of two nested cycles. The outer loop is a time simulation cycle. The inner loop is a calculation domain space cycle. Time cycle cannot be parallelized due to the dependence between of next and previous time step. Number of iterations of time cycle is defined as a multiplication number of seconds for which simulation is to be performed, and the number of iterations in one second of simulated time. Space cycle can be parallelized using the geometric decomposition. The whole computational domain is divided into separate sub-domains, the calculation of which ones can be done simultaneously. For effective implementation of the algorithm the inner loop was in addition split into four separate cycles, running one after each other but in parallel mode itself. This partitioning is dictated by the natural structure of the numerical method of the problem, consisting of a combination of explicit and implicit schemes. The first cycle solves explicit scheme which determines the temperature of the gas, the temperature of the porous object, the gas velocity and the mass concentration of oxidizer. The second cycle calculates the boundary conditions for these parameters. The third cycle solves implicit scheme, which determines the pressure of the gas and the gas density. Each iteration in this cycle solves linear equations system using block tridiagonal matrix method, which can be parallelized. The fourth cycle calculates the boundary conditions for pressure and density. For two-dimensional solutions of the problem at the end of a space cycle vertical boundary conditions are recalculated. In the implementation each of cycles listed above is partitioned in turn into separate groups of iterations (directive omp parallel for). Each group is computed by the separate parallel thread. Thus, on each time iteration the set of parallel threads is launched, and each thread consistently participates in computing some groups of iterations of each cycles described above.

As a result, with using of parallel technologies the calculation speed decreased about 4 times in eight parallel threads. Test calculation was performed on a computing cluster node with two quad-core Intel Xeon processors.

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STABILIZATION OF COMPLEX HEAT TRANSFER PROCESS

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Complex heat transfer processes include conduction, convection and radiation heat exchanges. All these processes are presented in engineering objects such as gas turbines, combusting and cooling systems, etc. It is necessary to take into account the radiative heat transfer because in many industrial high temperature processes and applications it plays a dominant role. This paper deals with a three dimensional nonstationary complex heat transfer problem. We use the (P1) (diffusion) – approximation for the transport equation.

The results of the paper are to establish sufficient conditions for asymptotic Lyapunov stability of the dynamical system. Moreover, some numerical experiments demonstrating the stabilization of complex heat transfer process are presented. In the previous works [2-6] the authors proved the existence and uniqueness of stationary solutions.

For numerical experiment let us consider a one-dimensional problem of complex heat transfer for the layer with thickness L. Assume that physical fields may vary only in the direction which is perpendicular to the layer boundaries. A series of computational experiments was performed, which show us that the stationary fields exist, despite the sufficient conditions of stability are not fulfilled, but solution of evolution problem stabilizes. We use MATLAB software for calculations.

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NUMERICAL SOLUTION OF INVERSE HEAT TRANSFER PROBLEMS

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In the heat transfer problems if temperature values on the boundary and/or the heat sources are known, then the temperature distribution can be found. This is termed as a direct problem. However in many heat transfer situations, the surface heat flux, temperature boundary values or heat sources must be determined from temperature measurements at one or more interior locations. This is an inverse problem [1]. Another type of inverse problems associated with the parameters estimation. We mention papers [2, 3] devoted to the parameter identification in combustion processes modeled by partial differential equations. Briefly speaking one might say that inverse problems are concerned with determining causes for a desired or an observed effect.

In many cases a formal mathematical model of an inverse problem can be easily derived. However, the process of solving the inverse problem is extremely difficult and the approximate methods like iterative procedures, regularization techniques are used. In general we can say that the approximate solution of an inverse problem does not necessarily depend continuously on the measured data. Moreover, small measurement errors can be the source for unacceptable perturbations in the solution.

We consider the model of heat transfer in a viscous incompressible heat-conducting fluid. The model consists of the Navier-Stokes equation and the convection-diffusion equation for temperature that are nonlinearly related via buoyancy in the Boussinesq approximation and via convective heat transfer [4, 5]. In our work we reduce inverse heat transfer problems to corresponding minimization problems by choosing a suitable cost functional that adequately describes the given data. Then these inverse problems can be analyzed and solved by applying a unified approach based on the theory of constrained optimization. Optimality system describing first-order necessary optimality conditions is derived. It consists of three parts. First part is a weak formulation of the initial boundary problem for the velocity, pressure and temperature. Second part of the optimality system is the adjoint problem for the adjoint velocity, adjoint pressure and adjoint temperature. Third part is the optimal relations for controls.

Numerical algorithm based on Newton's method for the nonlinear optimality system was proposed. Some computational results connected with the heat source estimation using temperature measurements are given and analyzed. The proposed method will be used in solving inverse and control problems for models of reacting fluid flow. We plan to apply this optimization approach to solve new problems of the combustion theory.

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EFFICIENCY OF THERMOELECTRIC CONVERTER COMBINED WITH COUNTERCURRENT BURNER

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Efficiency of gas combustion heat conversion into electricity by thermoelectric module combined with small sized countercurrent burner is estimated. The system is two channels with gas flows coming from the opposite directions and the thermoelectric element embedded into the heat conducting wall which separate two channels. The unburned gas preheating by combustion products allows to burn very lean gas premixture. The unburned gas preheating occurs through the heat conducting wall separating combustion products and unburned mixture. The thermocouple embedded in the separating wall operates temperature difference at the wall ends. For the maximum efficiency of energy conversion in a small-size device to be reached, the properties of thermoelectric materials, the device geometry, and other parameters have to be correlated with the gas combustion characteristics. It was shown that the efficiency of energy conversion in such small-size device can be higher than that in a similar large-size device and much higher than in the conventional system operating with the heat of combustion products. Another advantage of the proposed system is the absence of special cooling system that is necessary to use in conventional system. The maximal efficiency of the proposed system can be close to the maximal efficiency of the applied thermoelement even in the case of very lean gas premixture burning. The maximal efficiency of the thermoelement is determined by maximal working temperature of the thermoelement hot side. The heat return allows to heat up the hot side of the thermoelement up to the its maximal working temperature even in the case when the adiabatic combustion temperature of incoming premixture is less than the maximal working temperature of the thermoelement.

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