"The book is well organized and the presentation is excellent. The material logically follows from the fundamental concepts and proceeds to the deeper and deeper peculiarities of the theoretical and mathematical modeling and numerical simulation."

Vladimir Semak
Signature Science, LLC

Chemical Kinetics in Combustion and Reactive Flows

Following elucidation of the basics of thermodynamics and detailed explanation of chemical kinetics of reactive mixtures, readers are introduced to unique and effective mathematical tools for the modeling, simulation, and analysis of chemical nonequilibrium phenomena in combustion and flows. The reactor approach is presented considering thermochemical reactors as the focal points. Novel equations of chemical kinetics compiling chemical thermodynamic and transport processes make reactor models universal and easily applicable to the simulation of combustion and flow in a variety of propulsion and energy generation units.

Readers will find balanced coverage of both fundamental material on chemical kinetics and thermodynamics, and detailed description of mathematical models and algorithms, along with examples of their application. Researchers, practitioners, lecturers, and graduate students will find this work valuable.

Dr. V. I. Naoumov is a professor of mechanical and aerospace engineering at the Central Connecticut State University, USA. His research interests are chemical kinetics, aerothermochemistry, and combustion in aerospace propulsion systems and automotive engines. He has 35 years of teaching experience, and in performing research for leading aerospace companies. Dr. Naoumov is Distinguished Scientist of the Russian Republic of Tatarstan and a recipient of the ASME 2018 Distinguished Engineer of the Year Award.

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Chemical Kinetics in Combustion and Reactive Flows

Modeling Tools and Applications

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To our families for their support in all our endeavors.
To the Department 22 of the Kazan Aviation Institute,
one of the best Russian academic centers, where we worked
in the exciting atmosphere of creativity, integrity, and friendship.

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Preface

The combustion and reactive flows analysis has demonstrated some new trends in the past several decades:

- in-depth study of the contribution of detailed chemical mechanisms to combustion performances
- a dramatic increase in the number of chemical reactions involved in the analysis of combustion and reactive flows
- the expansion of the range of problems and objects where mathematical models of combustion built around detailed chemical kinetics are applied (gasifiers, tube furnaces, fuel cells, ozone holes, etc.)
- development of mathematical model support tools: the comparison and transfer of data on species between various databases, sensitivity analysis, application of eigenvalues, reduction of reaction mechanisms, selection of the rate constants from experimental data, automatic control over the balance of chemical elements, etc.
- construction of highly sophisticated mathematical models and algorithms of combustion and reactive flows to provide the accurate and reliable prediction and optimization of operating performances of combustion devices.

However the development of such models is complicated by the necessity of integration therein and appropriate simulation of three complex phenomena – namely turbulent flow and interaction of multiphase media, heat and mass exchange between phases with due allowance for multidimensionality of these processes, and chemical interaction in the flow of reactants and combustion products. The multidimensional nature of the flows characteristic of propulsion and power generation systems, the presence of chemically and thermally nonhomogeneous regions, and complex mechanisms of chemical interaction in a gas phase under conditions sometimes far from chemical equilibrium render a detailed numerical simulation of the entire complex of aerothermochemical processes an extremely complex problem.

One of the governing of matters in simulation of such complex of processes consists in the selection of an approach and base models for their detailed simulation. At present two basic approaches may be isolated. In compliance with the first one, “gas-dynamic,” physical schemes of processes are designed for multidimensional, mainly turbulent flows while 2-D and 3-D equations of nonreactive and reactive gas mixes motion are basic equations. Calculation algorithms comprise the procedures involving division of the solution region into finite elements, formation of finite-difference equations and

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their solutions. To solve the combustion problems, the following approximations are used: eddy dissipation, flamelet, global reactions, or detailed chemical kinetics. The latter is used very seldom because of a considerable amount of calculations. The example of implementation of gas-dynamic approach is the FLUENT software tool.

The second one, the thermochemical or “reactor” approach, considers single reactors or sets of interconnected reactors as the focal points, while basic equations are detailed chemical kinetics equations. Calculation algorithms are built on implicit methods capable of solving stiff differential equations. This approach allows one to consider reactive systems involving hundreds of species and thousands of reactions. Reaction mechanisms can incorporate the nonstandard reactions of Landau–Teller, Troe, etc. Besides, it is possible to simulate two-temperature medium and surface kinetics reactions.Various tools are widely used in this approach for development of models of combustion and flow.Software tools CHEMKIN and KINETICUS are the examples of thermochemical or reactor approach implementation.

This book brought to public notice has been aimed at describing the thermochemical approach (hereinafter, the authors would use the “reactor” approach term) in case the constructing of numerical models rests on procedures and algorithms of detailed calculation of chemical composition and properties of combustions products in various types of reactors.

The gas-dynamic component of the models is designed on the basis of relatively simple working medium flow schemes, some assumptions for the formation of the system of integrated reactors, and a priori known data on the flow pattern features in working volumes of combustion and power generation systems.

Specific features of presentation consist in well-balanced description of both basic material on thermochemistry of high-temperature reactive mixtures and detailed description of unique models and algorithms for calculation of combustion and flow. Such approach makes the book material available for not only specialists in chemical thermodynamics and chemical kinetics, in application to combustion theory to combustion and flow problems solution, but also for graduate students who have limited knowledge in these fields and plan the in-depth study of aerothermochemistry and its application to the simulation of complex aerothermochemical processes. For this, in the authors’ opinion, the reader should command, as a minimum, the entry graduate-level or graduate-level knowledge in thermodynamics, chemical thermodynamics, fluid mechanics, and heat and mass-transfer, as well as some skills in computational and numerical methods. However, the authors considered it apt to add the materials related to basic principles of chemical thermodynamics as well.

While considering the basis reactor schemes, equations, and algorithms, the reader learns the modeling tools that allow constructing far more complex mathematical models, algorithms, and computer codes. Besides, it helps to develop original invariant models of the processes including not only nonequilibrium chemical interaction in the gas phase but also mass exchange processes accompanying combustion and multiphase flows.

The book may well aid the creation, analysis, and application of proper models of combustion and flows in quite different high-temperature systems, provided the adequate original mathematical apparatus is used. Examples of constructing such models, their use for the analysis, and the optimization of parameters of various high-temperature units are presented as well for all interested parties.

Structurally, the book is divided into three parts. Part I (Chapters 1–3) contains the required material from chemical thermodynamics, chemical kinetics, and fundamentals of combustion, and describes in detail the original basic mathematical models and algorithms for calculation of chemical nonequilibrium composition in separate idealized reactors. Special attention is given to the description of tools designed to maintain the chemical interaction and combustion simulation – that is, the presentation of information on thermodynamic properties of chemical species and the transfer of this information between different databases, sensitivity analysis, the application of eigenvalues, and the selection and reduction of reaction mechanisms. Examples of application of these tools to the analysis of combustion and chemical interaction problems in reactors and reacting flows are also given.

Part II (Chapters 4–6) describes the application of basis schemes, models and algorithms to simulation of separate standard physicochemical processes characteristic for high-temperature units – e.g., a model of combustion and nonequilibrium effects in the flame front, a novel model of vapor conversion and interaction under the conditions of chemical nonequilibrium in the boundary layer of a single droplet, and unique models of multifractional droplet evaporation and droplet evaporation at supercritical pressures. Every cited model is provided along with useful examples of its application.

Part III (Chapters 7–10) incorporates the set of applied models designed for the simulation of combustion processes and chemical nonequilibrium working medium flows in high-temperature unit – that is, combustion chambers for the generation of high-temperature gas, gas generators of liquid-propellant rocket engines, liquid-propellant rocket engine tanks, and internal combustion engines. These models are mainly multireactor systems and allow for, along with nonequilibrium variation of chemical composition, the important accompanying processes, such as evaporation, heat exchange, condensation, diffusion, the availability of turbulent flows and reverse flows, heat and mass exchange, ionization of combustion products, etc. The potential of these models and algorithms is verified by the examples of numerical analysis and optimization of the operating parameters of these units.

I. Basic Components of Chemical Nonequilibrium Models: Chapters 1–3

Chapter 1 illuminates main combustion schemes in idealized reactors and separate combustion process fragments in high-temperature units. The principal concepts of thermochemistry and thermodynamic properties of the working medium as well as the methods and procedures of their calculations are given. The structures and characteristics of most frequently used databases are described. The model and algorithm of calculation of chemical equilibrium systems are presented as well as the elements of detailed gas-phase chemical kinetics model along with corresponding equations in their traditional form. The other models of calculation of chemical composition are described as well – e.g., the instant response model, the global kinetic model, and the model of nonequilibrium chemical kinetics. The reactor approach idea is presented while its applications to combustion and flow simulation are defined.

Chapter 2 derives in detail the chemical kinetics equations in exponential form for model reactors such as batch reactor, perfectly stirred reactor, and plug flow reactor. The concept is presented along with the examples of "accompanying" equations. The method of "large molecules" is described to allow extending the nonequilibrium models to heterogeneous systems. The procedure of mass exchange processes' presentation as "mass exchange reactions" is disclosed. Examples of the formation of these "reactions" and the determination of their "rate constants" are given. Classical and advanced explicit integration schemes of ordinary differential equations are proposed. Implicit schemes incorporating the Jacobian matrix are described (Gear, Pirumov, and spline integration). The algorithm for the formation of invariant computer codes for the calculation of chemical nonequilibrium systems is described. The structure of coordinating matrices, species enthalpy, and entropy presentation and the determination procedure of rate constants of reverse directions of chemical reactions are disclosed. Analytical formulas of the Jacobian matrix partial derivatives are obtained for their advantages to be analyzed. Separate single-reactor models have been verified.

Chapter 3 describes the procedure of conversion and comparison of thermodynamic properties of chemical species given in independent databases. Three databases, – IVTANTERMO, BURCAT, and TTR – are disclosed and compared. The algorithm of sensitivity coefficient determination to be applied to the perfectly stirred reactor is defined. Equations and procedure of analytical calculation of these coefficients are presented to allow analyzing the sensitivity nearby the "extinction line." The algorithm of chemical kinetics equations eigenvalue calculation is described. Relations between the nature of variation of these values and combustion stages have been established and applied to the batch reactor. The method for determination of integration steps at application of explicit schemes is proposed along with its application to the calculation of processes in specific high-temperature units. With the use of Jacobian eigenvalues applied to perfectly stirred reactor, the range of self-oscillation modes of pure kinetic nature was defined for complex reaction mechanisms. Three independent methods of reaction mechanism reduction – that is, the method of engagement with an adaptive threshold, the method of direct sounding, and the directed relation graph with error propagation method (DRGEP) – have been illuminated, along with the number of their efficient combinations that provides an automatic generation of reduced mechanisms. Examples are given for the efficient reduction of reaction mechanisms for "CH_4 + air" reacting systems for both rich and lean mixtures, as well as for propellants "O_2 + kerosene" and "unsymmetrical dimethylhydrazine + N_2O_4."

II. Mathematical Modeling of Selected Typical Modes of Combustion: Chapters 4–6

Chapter 4 describes the physical scheme, mathematical model, and algorithm of calculation of parameters in the premixed laminar flame front based on the front heat model at increased pressures and using the basic model of plug flow reactor. The results of numerical experiments aimed at predicting the flame propagation rates of different propellants and ecological parameters prediction are presented.

Chapter 5 examines the dispersed fuel combustion problems and presents a model of chemical interaction and heat and mass exchange in the boundary layer on the basis of the reactor model at combustion of a single liquid droplet in a high-temperature reactive flow. The methodology of applying the perfectly stirred reactor scheme and the mathematical apparatus discussed in Part I in regard to the development of a model of chemical nonequilibrium evaporation and reacting in the boundary layer is described in detail. A detailed derivation of conservation equations characteristic of the process under consideration is given. Results of numerical analyses showing the mathematical model adequacy and cited along with the advantages of chemical nonequilibrium model application to simulation of the processes in the boundary layer at droplet evaporation under high temperatures of external flow are described.

Chapter 6 depicts several models of liquid droplet evaporation in a reactive gas-liquid flow at comparatively low temperatures of the flow when vapors failed to react within the boundary layer. The traditional Priem–Haidmann model of single-component liquid droplet evaporation at subcritical pressures is presented. Also, a novel droplet evaporation model at supercritical pressures proposed is, which – unlike traditional models – allows for nonuniform droplet heating over the radius. The third model is a unique one as well and simulates the multifractional liquid droplet evaporation. Its specific feature consists in the modeling of uneven evaporation of liquid fractions, which causes a stepwise increase in droplet temperature with its heating. Numerical analyses of multifractional propellant evaporation and evaporation at supercritical pressures are presented to underline the relevance of applying these nontraditional models to the creation of complex models of combustion and flow in high-temperature units.

III. Simulation of Combustion and Nonequilibrium Flows in Propulsion and Power Generation Systems: Chapters 7–10

Chapter 7 examines simulation of high-temperature heterogeneous reacting flows in combustion chambers at multifractional propellant droplet evaporation in the presence of recirculation using the multireactor scheme. A unique iteration algorithm is presented to allow a sequential cyclic solution of individual problems for the prediction of gas-dynamic parameters, properties of the dispersed evaporating multifractional liquid phase, and those of chemical interaction at conversion of reactants into combustion products. Examples of calculation are shown aiming to optimize the design and performance of combustion chambers of different propulsion and energy generation systems.

Chapter 8 presents the model for calculation of two-phase flows in gas generators of liquid-propellant rocket engines. It examines chemical nonequilibrium processes in the gas phase, droplet atomization polydispersity, slip velocity, and droplets' non-steady-state heating and evaporation at both subcritical and supercritical pressures, and it considers the channels of the variable cross-section area. To calculate fuel-rich working medium properties at the combustion of hydrocarbon propellants, the authors worked out the kinetic mechanism supplemented by the original mechanism of soot participles formation via polyacetylenes and their radicals. The results of numerical experiments are given.

Chapter 9 describes the application of multireactor model to the creation of that for pressurization of liquid-propellant rocket engine tanks, and it presents the results on numerical analyses of complex set of aerothermochemical processes in the tank gas ullage. Whereas the comparatively low level of reacting medium temperature in the ullage, chemical nonequilibrium approach application is necessitated, which is confirmed by numerous results of numerical experiments analyzed in detail in the chapter. Cited material features a detailed mathematical description of complex schemes of gas flows in the ullage as well as heat and mass exchange processes and the analysis of their significant influence on the parameters of gas mixture in the ullage at the feeding of propellant into the thrust chamber of the rocket engine.

Chapter 10 describes the model of combustion and chemical nonequilibrium processes in spark ignition engines at the ignition and power stroke, with a focus on the combustion product ionization. The necessity of the application of chemical nonequilibrium model is caused by a notable effect of chemical nonequilibrium on the ionization of combustion products. The perfectly stirred reactors scheme and basic mathematical tools described in the first part of the book have shown their efficiency at simulation and predicting the ion current resulting from chemical and thermal ionization and its application for possible prediction of the engine working and ecological performances.

Acknowledgments

Work over the development of base reactor models, methods, algorithms, and other tools; their analysis; computer-code writing; their application to the development of applied models; and numerical analyses took several decades. For a number of reasons, not all applied models built around the base universal models and algorithms were included in this book. Particularly, multiple models and algorithms were omitted from the book scope: the model of calculation of ionized nonequilibrium heterogeneous flows in nozzles, the model of solid-propellant rocket engine thrust cut by coolant injection, the model of concurrent burnout of propellant and thermal insulation in the thrust chambers of solid propellant rocket engines, the model of low-emission pulverized coal burning in furnaces, the model of combustion processes in the combustion chamber of air jet engines, the model of two-dimensional axially symmetric chemical nonequilibrium reacting internal flows, and others.

Therefore, the authors consider their duty to mention their colleagues who provided invaluable contribution in creation of separate models, algorithms, computer programs, research and preparation of information for databases, and numerical analysis performance. We acknowledge with appreciation the following colleages who have contributed in these efforts: R. Khasanov, R. Iskhakova, I. Zenukov, R. Mukhammedzyanov, G. Glebov, T. Trinos, V. Kotov, R. Valeev, D. Sokolov, M. Nikandrova, V. Gasilin, K. Berezovskaia, and I. Safiullin, as well as untimely passing A. Senyukhin, R. Khairullin, and I. Naidyshev.

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V. Glushko, chaired lately by V. Alemasov, the Academician of the Russian Academy of Sciences, Twice the USSR State Prize Winner, who developed, along with his associates A. Tishin and A. Dregalin, the first in the Soviet Union methods, universal mathematical models, and software tools for the calculation of chemical equilibrium high-temperature systems. Exactly these persons made the authors of this book scientists and professionals in the field.

Nomenclature

Latin Letters

A_s^+	pre-exponential factor in Arrhenius equation written for forward direction of the s-th reversible chemical reaction, $s = 1 \ldots m_c$, depends on the order of reaction*
A_j	pre-exponential factor in Arrhenius equation written for the j-th chemical reaction, $j = 1 \ldots 2m_c + r_c$, depends on the order of reaction*
C_i	molar concentration of specie i, $gmol/cm^3$ or $kmol/m^3$
C_{pi}	molar specific heat at constant pressure of the specie i, $cal/(gmol \times \mathrm{K})$
c_{pi}	mass specific heat at constant pressure of the specie i, $J/(kg \times \mathrm{K})$
$\bar{C}_p = \sum_i C_{pi} r_i$	molar specific heat of mixture at constant pressure, $cal/(gmol \times \mathrm{K})$
$\bar{c}_p = \sum_i c_{pi} g_i$	mass specific heat of mixture at constant pressure, $J/(kg \times \mathrm{K})$
C	total molar concentration of gas mixture, mol/cm^3
c_{pV}	mass specific heat of vapor at constant pressure, $J/(kg \times \mathrm{K})$
$\bar{c}_{liq}$	average specific heat of liquid, $J/(kg \times \mathrm{K})$
$\bar{c}_{pq}$	average specific heat of the vapor of liquid component q at constant pressure, $J/(kg \times \mathrm{K})$
D_{im}	binary diffusion coefficient of the i-th substance in gas mixture, m^2/s
E_j	activation energy in Arrhenius equation written for the j-th chemical reaction, $j = 1 \ldots 2m_c + r_c$, $cal/gmol$
E_s^+	activation energy in Arrhenius equation written for forward direction of the s-th reversible chemical reaction, $s = 1 \ldots m_c$, $cal/gmol$
F	area, m^2
F_x	drag force acting on the droplet moving in gas flow, N
g_i	mass fraction of specie i
h	integration step, s or m

---

* Dimension of the reaction rate constant is defined by the reaction order:

- for zeroth-order reaction, $[k_j, A_j] = gmol/(cm^3 \times s)$
- for first-order reaction, $[k_j, A_j] = 1/s$
- for second-order reaction, $[k_j, A_j] = cm^3/(gmol \times s)$
- for third-order reaction, $[k_j, A_j] = cm^6/(gmol^2 \times s)$

(The units are *cm*, *gmol*, K, and *sec*.)

h	convection heat transfer coefficient, $W/(m^2 \times \mathrm{K})$
H	total enthalpy, J
H_i	molar enthalpy of i-th specie, $J/kmol$ or $cal/gmol$
H_Σ	molar enthalpy of mixture, $J/kmol$
h_i	mass specific enthalpy of the i-th substance, J/kg
h_Σ	mass specific enthalpy of mixture, J/kg
h_{fuel}	enthalpy of fuel, J/kg
h_{ox}	enthalpy of oxidizer, J/kg
h_p	enthalpy of propellant, J/kg
h^+	specific enthalpy of reactants, J/kg
h_{liq}	specific enthalpy of liquid, J/kg
h_z	specific enthalpy of reacting mixture in the z-th reactor, J/kg
$\bar{h}$	average enthalpy of liquid, J/kg
h_g	specific enthalpy of gas, J/kg
h_d	enthalpy of liquid droplet, J/kg
J	Jacobian matrix
$\dot{J}$	mass flux, $kg/(m^2 \times s)$
$\dot{J}_V$	vapor mass flux from the droplet surface, $kg/(m^2 \times s)$
$\dot{J}_{qV}$	mass flux of the vapor of component q through the boundary layer, $kg/(m^2 \times s)$
k_m^o	mass stoichiometric ratio of propellant components (stoichiometric oxidizer- fuel ratio), $kg\ oxidizer/kg\ fuel$
k_m	mass ratio of propellant components (oxidizer-fuel ratio), $kg\ oxidizer/kg\ fuel$
k_s^+	rate constant of forward direction of the s-th reversible chemical reaction, $s = 1 \ldots m_c$, depends on the order of reaction*
k_s^-	rate constant of reverse direction of the s-th reversible chemical reaction, $s = 1 \ldots m_c$, depends on the order of reaction*
k_j	rate constant of the j-th reaction, $j = 1 \ldots 2m_c + r_c$, depends on the order of reaction*
K_s^c	equilibrium constant of s-th reaction based on molar concentrations, $\left(\frac{gmol}{cm^3}\right)^{\sum_i \left(\nu''_{is} - \nu'_{is}\right)}$
k	thermal conductivity, $W/(m \times \mathrm{K})$
$k_{i,}$	thermal conductivity of the i-th specie, $W/(m \times \mathrm{K})$
k_{gV}	average thermal conductivity of vapor–gas mixture in the boundary layer, $W/(m \times \mathrm{K})$
k_{liq}	thermal conductivity of liquid, $W/(m \times \mathrm{K})$
L_V	latent heat of evaporation, J/kg
L_{qV}	specific heat of evaporation of the q-th liquid component, J/kg
m_c	number of reversible reactions in reacting medium
M	mass, kg
$\dot{m}$	mass flow rate, kg/s
m_i^+, m_i^-	inflow and outflow of substance i, kg/s

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M_z	mass of reacting mixture in the *z*-th reactor, *kg*
n_a	number of atoms in reacting mixture
n_b	number of reacting substances (species)
n_s^+	temperature factor in Arrhenius equation written for the forward direction of the *s*-th reversible chemical reaction, $s = 1 \ldots m_c$
n_j	temperature factor in Arrhenius equation written for *j*-th chemical reaction, $j = 1 \ldots 2m_c + r_c$
n	number of integration step
Nu	Nusselt number
Nu_D	diffusion Nusselt number
Nu_T	thermal Nusselt number
n_z	total number of reactors
n_{sd}	the number of droplets groups in the droplet sizes distribution
n_q	number of the components in multicomponent droplet
p	pressure, *Pa*
p_i	partial pressure of the *i*-th substance in the gas mixture, *Pa*
p_{sat}	pressure of saturated vapor, *Pa*
Pr	Prandtl number
p_{Vsd}	vapor partial pressure above the surface of the *sd*-th group of droplets, *Pa*
$p_{V\infty}$	vapor partial pressure beyond the reduced film, *Pa*
Q	total heat transfer, *J*
$\dot{q}$	heat flux, W/m^2
q	heat flow rate, *W*
q	number of liquid fractions in multicomponent droplet
$R_0 = 8314.6$	universal gas constant, $J/(kmol \times \mathrm{K})$
$R_0 = 1.987$	universal gas constant, $cal/(gmol \times \mathrm{K})$
r_i	mole fraction of the *i*-th specie
r_i^+	mole fraction of the *i*-th substance in reactants
r_c	number of mass exchange reactions
Re	Reynolds number
R_d	droplet radius, *m*
R_{sd}	droplet radius of *sd*-th group of droplets, *m*
S_i^0	molar entropy of the specie *i* at $p = 1$ atm, $J/(kmol \times \mathrm{K})$ or $cal/(gmol \times \mathrm{K})$
Sc	Schmidt number
sd	number of the group of droplets
T	temperature, K
T_g	temperature of gas, K
T_{boil}	boiling temperature, K
T^+	temperature of reactants, K
T_d	temperature of droplet, K
T_{eq}	chemical equilibrium temperature, K

T_f	temperature at the exit of the reactor or channel, K
T_∞	temperature of external gas flow, K
T_z	temperature of reacting mixture in the z-th reactor, K
T_0	initial temperature, K
T_{cr}	critical temperature, K
T_w	wall temperature, K
T_{gV}	average temperature of vapor–gas mixture in the boundary layer, K
T_{rf}	reference temperature, K
T_{sd}	temperature of the sd-th group of droplets, K
U	total internal energy, J
U_i	molar internal energy of the i-th substance, $J/kmol$
u_i	specific internal energy of the i-th substance, J/kg
V_g , u_g	velocity of gas, m/s
u_{sd}	velocity of sd-th group of droplets, m/s
V	volume, m^3
V_z	volume of z-th reactor, m^3
W_j	rate of the j-th reaction, $gmol/(cm^3 \times s)$
$W_{ij} = \left(\frac{dC_i}{d\tau}\right)_j$	rate of substance i concentration variation in j-th reaction, $gmol/(cm^3 \times s)$
x, y	coordinates, m
z	number of reactor

Greek Letters

$\alpha_{ox} = \frac{k_m}{k_m^o}$	oxidizer–fuel equivalence ratio
$\gamma_i = -\ln r_i$	logarithm of mole fraction of the i-th specie
γ	relative variation of droplet volume at evaporation
δ	thickness of reduced film, m
ε/k	depth of the potential well in the Lennard–Jones potential
ζ_s	reduction threshold for substances
ζ_R	reduction threshold for reactions
ζ_d	reduction threshold of DRGEP method;
η_i	dynamic viscosity of the i-th substance, $N/(m^2 \times s)$
θ	parameter of approximation ($\theta = 0.4 \dots 0.5$)
λ_i	eigenvalues of matrix
μ_i	molecular mass of the i-th specie, $kg/kmol$
μ_m, μ_g	average molecular mass, $kg/kmol$
μ_V	molecular mass of vapor, $kg/kgmol$
μ_q	molecular mass of the q-th liquid fraction, $kg/kmol$
ν_k	valence of the atomic element k
ν'_{is}	stoichiometric coefficient at i-th substance in forward direction of the s-th reversible chemical reaction

ν''_{is}	stoichiometric coefficient at *i*-th substance in reverse direction of the *s*-th reversible chemical reaction
$\nu_{ij} = \nu''_{is} - \nu'_{is}$	difference of stoichiometric coefficients in the right-hand side and left-hand side for forward direction of the s-th reversible chemical reaction, $j = s$
$\nu_{ij} = \nu'_{is} - \nu''_{is}$	difference of stoichiometric coefficients in the right-hand side and left-hand side for reverse direction of the *s*-th reversible chemical reaction, $j = s + m_c$
ρ	density, kg/m^3
ρ_i	partial density of the *i*-th substance, kg/m^3
ρ_g	density of the gas phase, kg/m^3
ρ_V	vapor density, kg/m^3
ρ_q	density of the *q*-th liquid fraction, kg/m^3
ρ_{liq}	density of liquid,kg/m^3
σ_{im}	collision diameter of the Lennard–Jones potential
τ_f	integration interval or process time, *s*
τ_p	residence time, *s*
$\phi = \frac{k_m^o}{k_m}$	fuel–oxidizer equivalence ratio
$\Omega_j = W_j/C$	ratio of the *j*-th reaction rate to the total molar concentration,$1/s$
Ω_{im}	reduced collision integral for the *i*-th specie and mixture

Acronyms

PSR	perfectly stirred reactor
BR	batch reactor
PFR	plug flow reactor
SR	the system of interconnected reactors
LPRE	liquid-propellant rocket engine
SPRE	solid-propellant rocket engine
ABE	air-breathing engine
ICE	internal combustion engine
LM	large molecule
ODE	ordinary differential equations
DRG	Directed Relation Graph (method)
DRGEP	Directed Relation Graph with Error Propagation (method)