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Part I

Basic Components of Chemical Nonequilibrium Models

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1 Approaches to Combustion Simulation

Patterns, Models, and Main Equations

1.1 Standard Combustion Patterns

Combustion processes (that is, conversion of chemical energy of propellant components into thermal energy of combustion products) are typical for various engineering systems. Working volumes wherein these processes can occur may be represented by combustion chambers of liquid-propellant rocket engines (LPRE), solid-propellant rocket engines (SPRE), air-breathing engines (ABE) steam-gas generators, magnetohydrodynamic generators (MHD generators), boiler furnaces of thermal electric power stations, and cylinders of internal combustion engines (ICEs) [1]. Besides, further conversion of combustion products with chemical conversions can proceed also in aircraft and rocket engine nozzles, ICE exhaust systems, LPRE gas ducts, etc.

Working volumes of these propulsion and power generation systems feature the availability of a multiphase working medium, a wide range of temperature variation (from hundreds to some thousands of degrees) and pressure (from several tenths of MPa to tens of MPa), chemical conversions not only in gas phase but in condensed phase as well, changes of parameters of state of working medium against the background of intraphase and interphase heat-and-mass transfer and multidimensional flow of working medium, a high degree of turbulence, and nonuniformity of parameters over the working volume. The history of these processes defines, in the end, the energetic and ecological characteristics of a particular propulsion and power generation system. One of the ways of simulating the latter consists in the development of mathematical models of combustion processes along with subsequent computational experiments [2].

Models of processes that occur in propulsion and power generation systems are usually based on mathematical models of some standard combustion modes for propellant components (oxidizer and fuel) in the working volumes. In the following paragraphs, some of these modes are considered in brief.

Combustion in homogeneous zones (Figures 1.1, 1.2, and 1.3). This is the simplest mode of combustion that can be considered as a process of conversion of ideally mixed reactants (propellant components) into combustion products in a sample reactor. Working medium composition and state parameters are uniform at any two points of a reactor but can vary in time [3, 4]. Heat exchange (Q – heat flow) of a reactor and an environment is also possible. Two patterns are most frequently used for simulation of combustion in homogeneous zones:

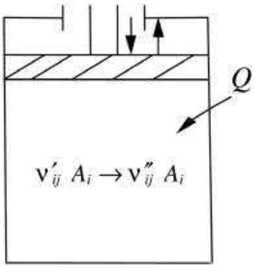

Figure 1.1 Combustion pattern in batch reactor. Q – heat flow.

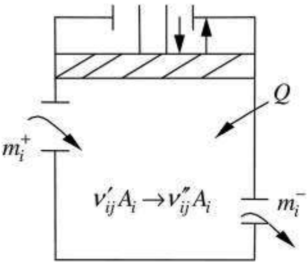

Figure 1.2 Combustion pattern in a perfectly stirred reactor (m_i^+ and m_i^- – mass flows at inlet and outlet).

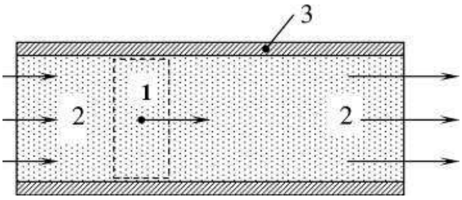

Figure 1.3 Combustion process in plug flow reactor (PFR): (1) moving batch reactor (BR); (2) one-dimensional gas flow; (3) tube wall.

1. Combustion in the batch reactor (BR; Figure 1.1) at no mass exchange with the environment ($m_i^+ = m_i^- = 0$). Problems usually solved in the framework of this procedure involve the assumption that the reactor originally houses the reactants that convert into chemically equilibrium combustion products at combustion.
2. Combustion in perfectly stirred reactor (PSR; Figure 1.2), with obligatory occurrence of mass exchange with environment ($m_i^+ \neq 0; m_i^- \neq 0$). Note here that reactants fed into the reactor are assumed to mix instantly with combustion products. It is usually assumed for the models using PSR [5] that $m_i^+ = m_i^-$ and variation of chemical composition of reacting mixture and state parameters proceed until a certain stationary state is reached, which can be both chemical equilibrium and chemical nonequilibrium.

Apart from these patterns, most frequently used is the approximation of moving BR – plug flow reactor (PFR; Figure 1.3) for simulation of combustion in one-dimensional

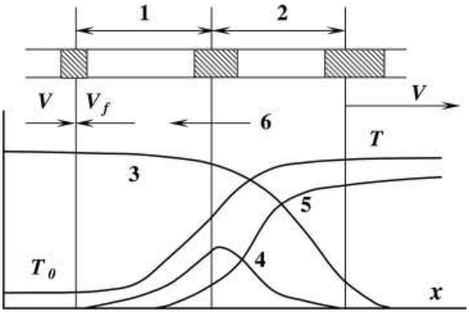

Figure 1.4 Flame front of premixed reactants: (1) heating zone; (2) combustion zone; (3) reactants; (4) intermediate substances; (5) combustion products; (6) heat transfer and diffusion.

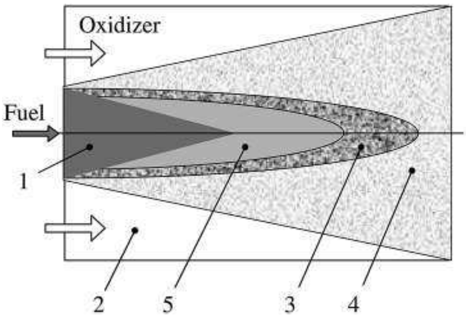

Figure 1.5 Diffusion combustion mode: (1) fuel; (2) oxidizer; (3) combustion zone; (4) nonuniform mixture of oxidizer and combustion products; (5) nonuniform mixture of fuel and combustion products.

reacting flows. In compliance with this procedure, it is assumed that neighboring moving working medium layers (volumes) are not mixed. Now, a thin layer of reacting gas (1) can be arbitrarily isolated, and combustion process can be described in said layer with application of the BRs moving at the gas velocity. In case the gas flow is transient, the combustion will be described by whatever system of BRs is used, while stationary flow may be represented by single BR using a reference system of coordinates.

Combustion in a flame front (deflagration) (Figure 1.4) occurs within a narrow zone, as premixed reactants being fed at its inlet while, at its outlet, combustion products are formed [6, 7]. The flame front is formed at the interaction of three phenomena: chemical reactions of combustion; heat transfer from combustion products to reactants; and diffusion of substances over the front (reactants diffuse with the flow, and combustion products diffuse against the flow). This interaction brings about the formation of a self-sustaining combustion zone displacing relative to fresh mixture at the flame speed (for example, $u_n \approx 1$ m/s). In turbulent flow, magnitude u_n increases notably because of the intensification of transport processes.

Diffusion combustion in parallel flows (Figure 1.5) originates when reactants are fed into the combustion zone separately and react with each other as they are being

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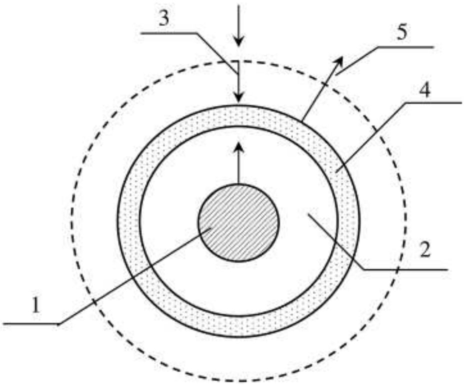

Figure 1.6 Combustion of a liquid fuel droplet in atmosphere of oxidizer: (1) droplet; (2) fuel vapor diffusion toward combustion zone; (3) oxidizer diffusion toward the combustion zone; (4) combustion zone; (5) combustion products diffusion toward the environment.

mixed [7]. Here, chemical reactions in the gas phase as well as diffusion and heat transfer are the governing processes that, unlike flame front, occur both along and across the flow. Several zones may be introduced in diffusion combustion: fuel; oxidizer; combustion zone; and zones of nonuniform mixes of propellant components with combustion products. The problem of simulation of this combustion process should be solved in at least a two-dimensional approximation. This is why it is more complicated than a deflagration mode.

Multiphase Combustion

Several combustion patterns may be introduced in this combustion mode subject to composition and properties of particles of liquid (or solid) phases. Some of them are considered in the following section on the assumption that phases are fixed relative to each other.

Combustion of a liquid fuel droplet in the atmosphere of oxidizer. The example of this pattern of combustion is shown in Figure 1.6 when droplets of fuel with inferior boiling temperature (for example, $T_{boil} \approx 500\,\mathrm{K}$) are injected into oxidizing reacting medium (for example, $T_g > 1000$ K) to get gaseous products of their chemical interaction.

Combustion in this system occurs in some thin layer around the droplet. Gaseous oxidizer diffuses into said layer from the environment while vaporous of fuel diffuses from the droplet. Heat released at combustion propagates on both sides from the combustion layer to heat the oxidizer and to facilitate the droplet heating and evaporation [8].

Combustion of metal particles in the atmosphere of oxidizer. This combustion pattern is shown in Figure 1.7 [9]. A metal particle (for example, an aluminum particle) getting into the high-temperature oxidizing medium with temperature T_g converts into a liquid droplet (1) and, if T_g is higher than the metal ignition temperature (T_{ign} = 2323 K), then the combustion process proceeds at contact with gaseous oxidizer (2) to produce refractory oxides (for example, Al_2O_3). If T_g is lower than oxide boiling temperature

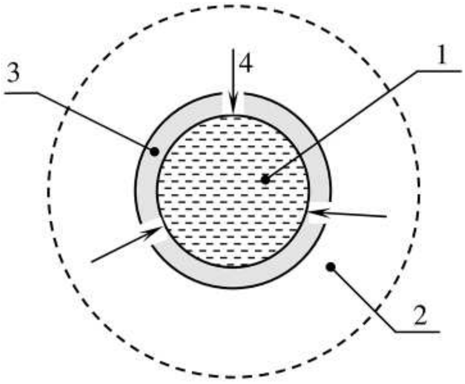

Figure 1.7 Combustion of metal particles in the atmosphere of oxidizer: (1) liquid metal; (2) oxidizing gas medium; (3) refractory oxide film; (4) fractures in oxide film.

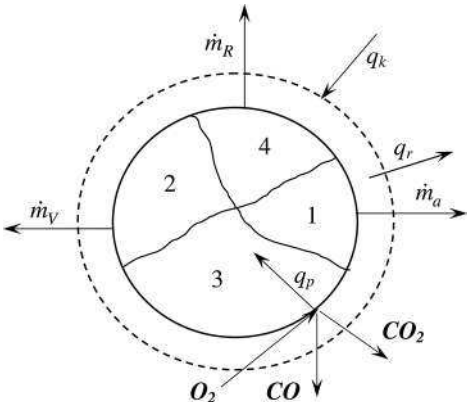

Figure 1.8 Coal particle structure and pattern of its combustion. (1) moisture; (2) volatile matters; (3) fixed carbon; (4) impurities; $\dot{m}_a, \dot{m}_V, \dot{m}_R$ – mass flows of steam, volatile matters, mineral impurities; q_κ, q_r, q_p – heat flows from gas to particle (convection), radiative flow, heat flow into the particle.

T_{boil}, (for example, $T_g = 2500$ K, while $T_{boil} = 3253$ K), then it remains on the particle surface and forms the oxide film (3). Film thickness increases as combustion proceeds to impede oxidizer contact with the metal surface – hence, to retard the combustion process. However, thermal stresses originating in the oxide film cause fractures (4) through which the oxidizer penetrates the metal surface to make the combustion proceed.

Combustion of coal particles. Figure 1.8 shows the coal particle combustion process and processes that occur at the particle surface and in a boundary layer [10]. At particle heating, first, water contained therein is evaporated (flow $\dot{m}_a$). Then, volatile matters are formed (flow $\dot{m}_V$), carbon is ignited, and mineral impurities are released (flow $\dot{m}_R$). Here, particle temperature (T_p) increases and its density changes. Carbon combustion produces carbon monoxide (CO) and dioxide (CO_2); the ratio between the rates of

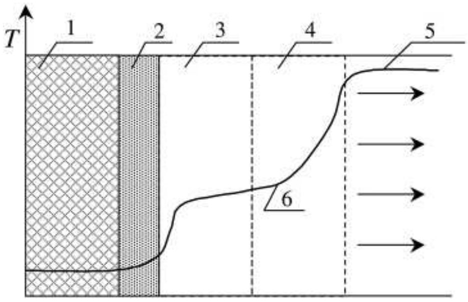

Figure 1.9 Combustion of solid-propellant grain: (1) solid-propellant grain; (2) reaction zone in condensed phase; (3) gasification zone; (4) zone of basic reactions; (5) zone of combustion products; (6) temperature variation.

formation of said substances depends on temperature T_p. Heat flow (q_p) for heating of the particle results from conversion of carbon into CO (or CO_2) on its surface. Multiple reactions – particularly, reactions of combustion of volatile matters – occur outside the particle (in the gas medium). The particles may be heated nonuniformly and are porous and nonspherical. The size of the particles may increase at the release of volatile matters. Heat exchange between particles and gases occurs via convection and radiation. The rates of volatile matter release and carbon are significantly different, but sometimes these processes can overlap.

Combustion of solid propellant (Figure 1.9). In this case, the fuel and oxidizer are in a solid phase and are almost perfectly stirred (in fact, a solid propellant could be treated as a monopropellant), and combustion occurs in the combustion zone similar in essence to the flame front of the premixed gaseous fuel and exider [11] with heat transfer from high-temperature combustion products to the solid-propellant grain. However, phase transitions (and possibly pyrolysis) of both the fuel and the oxidizer occur inside the combustion zone in addition to the processes inherent in a common flame front.

Detonation [12] is the mode of combustion of premixed reactants including the shock wave and zone of chemical conversions next thereto. Unlike flame front (deflagration), the detonation propagates at supersonic speed (V) while diffusion and heat transfer processes are of minor importance. Detonation is a self-sustaining process wherein a shock wave raises the temperature of reactants while the next chemical reactions maintain said shock wave. Figure 1.10 describes the distribution of basic flow parameters in the detonation wave. The motion rate starts to increase in the combustion zone to drop notably after the shock wave. Pressure distribution features an opposite dynamics while the temperature increases continuously. At detonation (unlike flame front), a significant nonequilibrium energy distribution over the degrees of freedom is observed at a certain section after the shock wave.

Combustion in high-temperature propulsion and power generation systems is normally a sophisticated process complicated by a nonuniform distribution of working medium parameters over the working volume, and it comprises several standard

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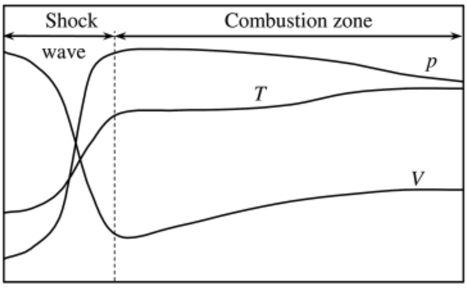

Figure 1.10 Variation of flow parameters at detonation.

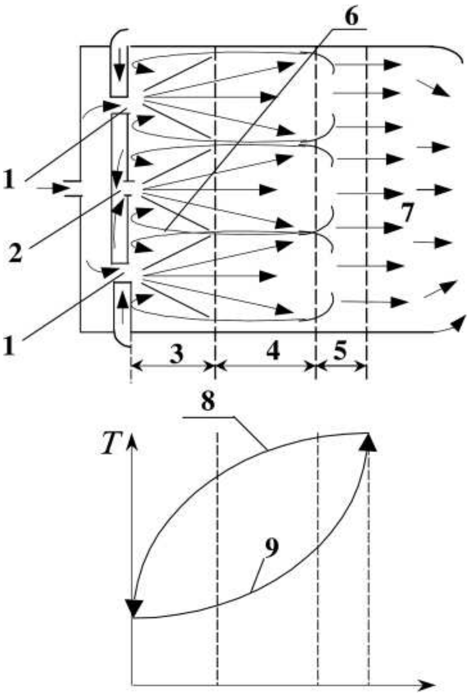

Figure 1.11 Diagram of processes in LPRE combustion chamber: (1) oxidizer injectors; (2) fuel injectors; (3) droplet formation zone; (4) evaporation and mixing zone; (5) combustion zone; (6) recirculation zone; (7) release of combustion products into a nozzle; (8) temperature of the reverse flow; (9) straight flow temperature.

patterns. Let us consider, for example, the processes in the LPRE combustion chamber [1] designed for the conversion of chemical energy of the propellant into thermal energy of combustion products (Figure 1.11). The combustion chamber's main unit is the injector plate composed of the set of fuel and oxidizer injectors; thereof, the injector plate design defines chamber efficiency. Immediately after injection of the components (fuel and oxidizer), different-diameter droplets are formed. These droplets drive the gas mixture located near the injector plate into the combustion zone.

High-temperature combustion products are fed from this zone, in their turn, to the injector plate to produce recirculating flows to maintain the combustion process. Moving droplets of liquid component evaporate, while vapors of fuel and oxidizer stir and react, and convert into combustion products. Thus, the following combustion processes in the LPRE combustion chamber are observed: combustion in the two-phase system; combustion in homogeneous zones; diffusion combustion. At the same time, the key method of maintaining the combustion is implemented by the flame front combustion mode with the replacement of molecular heat-and-mass transfer by the convective transfer.

1.2 Basic Characteristics of Working Medium

Working medium in propulsion and power generation systems, as a rule, is the mixture of individual substances with a predominance of the gas phase, but some of them can be in a condensed (liquid or solid) state. Such substances in combustion analysis are considered to be atoms, molecules, and radicals. Generally, let us identify them by index i, but in some formulas (related to the calculation of chemical equilibrium systems), index k is assigned to atoms while index q is assigned to radicals and molecules. Their composition is described by factors a_{kq}; for example, we obtain for a CO_2 molecule: $a_{C,CO_2} = 1\ a_{O,CO_2} = 2$. Let us denote the valence of atoms by symbol ν_k. Hereinafter, gas components and their mixtures will be considered as ideal gases.

Working medium gas phase composition is described by various magnitudes: C_i, n_i, p_i, ρ_i interrelated by following formulas:

$$C_i = n_i/V; \quad p_i = C_i R_0 T; \quad \rho_i = p_i \mu_i/(R_0 T); \quad i = 1 \ldots n_b, \tag{1.1}$$

where V is the volume occupied by the gas mixture; $C_i,\ n_i,\ p_i,\ \rho_i,\ \mu_i$ are partial molar concentration, number of moles in volume V, partial pressure, partial density, and molecular mass of i-th substance, respectively; R_0 is universal gas constant; T is temperature; n_b is number of reacting substances.

In many instances, working medium composition is described by relative magnitudes molar r_i or mass g_i fractions, as well as by mole-mass concentrations χ_i. At the variation of state parameters only, these magnitudes (unlike ρ_i, p_i, C_i) remain unchanged. These can vary if chemical reactions proceed in the system or if mass exchange processes occur between the gas and condensed phase or between the system and environment. For ideal gases, these relative values are defined by known formulas:

$$r_i = \frac{n_i}{N_m} = \frac{C_i}{C} = \frac{p_i}{p}; \quad g_i = \rho_i/\rho; \quad \chi_i = g_i/\mu_i, \tag{1.2}$$

where ρ is mixture density; N_m is total number of gas phase moles in volume V, $C = N_m/V$ is total molar concentration.

Average working medium gas phase molecular mass μ_g and interrelation between magnitudes r_i, g_i, χ_i are defined by formulas listed in the Table 1.1.