

A method of calculating of the thermodynamic properties and the composition of the explosion products of hydrocarbons and air under partial chemical equilibrium

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Abstract. We examined the approximate method to calculate composition and thermodynamic parameters of hydrocarbons–air nonequilibrium explosion products based on the assumption of the existence of a partial chemical equilibrium. With excellent accuracy of calculating thermodynamic properties and species mass fraction the respective stiff system of detailed kinetics differential equations can be replaced by the one differential equation or the two differential equations and a system of algebraic equations. This method is always consistent with the detailed kinetic mechanism. The constituent equations of the method were derived and the respective computer code written. We examine the applicability of the method by solving the test problem. The proposed method simulation results are in excellent agreement with the detailed kinetics model results corresponding the stiff ordinary differential equation solver including NO time histories.

1. Introduction

The chemical kinetics models are important for analysis and design in many chemistry and industrial processes. The composition of the explosion products changes in the course of their expansion and cooling. This evolution should be taken into account in numerical simulations of flows containing explosion products for the following reasons.

First, whatever the equation of state of the explosion products is used, its coefficients depend on the chemical composition of the medium. Even in the simplest case of the equation of state of an ideal gas, its molecular weight and heat capacity depend on the composition of the mixture.

Second, a change in the composition of the explosion products leads to an additional release of the so-called chemical component of the internal energy, which transforms into the thermal energy and the work done by the explosion products. For example, immediately during the detonation of a stoichiometric hydrogen–oxygen mixture, an energy of 7.4 MJ/kg is released, whereas the subsequent expansion of the detonation products to atmospheric pressure gives additionally 2.8 MJ/kg [1].

Third, changes in the composition are of interest in their own right, for example, when the purpose of calculations is to determine the amount of toxicants entering the atmosphere, such as nitrogen oxide, unburnt hydrocarbons, and carbon monoxide.



Since the explosion products are initially at very high temperature, one has naturally to allow for a change in specific heats of the components and their concentrations when performing gasdynamic calculations. There are several ways how to take into account variation in physical and chemical properties of expanding explosion products. One of them is a calculation of the dynamic parameters with due regard for the kinetics of chemical reactions (including both the forward and reverse ones) occurring in the expanding gas. The time evolution of the composition is calculated using a stiff system of chemical kinetics equations. This is the most general approach. This approach is very time consuming and cumbersome. At a large number of individual species in the explosion products and a large number of chemical reactions involved, calculation of the mixture composition requires a long computation time. Typically, the time it takes for calculating the mixture composition is much longer than that spent on solving the gasdynamic equations.

There are two more procedures that actually represent the extreme cases of approach, namely, the constant c_p/c_v method and fully equilibrated flow. The first procedure assumes the chemical reactions to be frozen and the second one assumes all the reactions to proceed at infinite rates.

An equilibrium approximation was used in numerical simulation of hydrogen–air combustion in [2] and hydrogen–air detonations in [3]. On the base of this approach the blast waves generated by hydrocarbons–air and hydrocarbon–oxygen explosion and detonation were numerically investigated in [4–7]. The effect of changes in the product composition on the results of calculations were thoroughly studied in [2–12] and, therefore, is not considered here.

The rate of the change in concentrations of the reaction products depends on the instantaneous values of the thermodynamic parameters and a flowing gas, its finiteness implies a certain deviation of the product composition and, consequently, of the heat released in gas, from their equilibrium counterparts. The chemical equilibrium model may be applied only in the case when this deviation is small. This defines the sufficient condition for model applicability to explosion products as shown in [13, 14].

The applicability of the chemical equilibrium mixture model to the products of explosion of fuel–oxygen and fuel–air mixtures was discussed in detail in [9, 13–17]. The applicability of the chemical equilibrium model to hydrogen–oxygen mixtures in the case of heat supply at constant density was assessed in [9]. In [13, 14] a sufficient condition for the applicability of the chemical equilibrium mixture model to gasdynamic calculations was obtained. As first noted by Borisov et al. [13] there is a substantial difference between the cases of fuel–air and fuel–oxygen detonations, and the physical dimensions of the detonation region play an important role. The authors of [17] compared the results of gasdynamic calculations performed using the system of equations of chemical kinetics for calculating the composition of the explosion products with the results of gasdynamic calculations within the framework of the chemical equilibrium mixture model and the constant composition mixture model. It was demonstrated [9, 13, 14, 16] that the process of establishment of chemical equilibrium in the products of explosion of gas mixtures proceeds in several stages. First, partial chemical equilibrium is established, without changes in the total number of molecules in the system. That is, even in cases where there is no chemical equilibrium, it suffices to know the molar mass of the mixture and two required thermodynamic parameters (for example, specific internal energy and density) to determine the composition of the mixture.

The existence of quasi-equilibrium in exchange reactions was discussed in [17]. This same assumption underlies an approximate model for calculating the molar mass of gas mixtures at high temperatures [12]. The author of [8, 12] proposed an approximate kinetic equation for calculating the molar mass of the mixture and then the thermodynamic parameters.

The origins of quasi equilibrium approach for explosions can be traced back to the pioneering studies of Strehlow [18] and Nikolaev [8]. The concept of partial equilibrium flow was used by Ramshaw [19] to derive simplified fluid dynamics equations for reactive flow.

The process of achieving chemical equilibrium in the explosion products of fuel–air mixtures involves all the components of the mixture. The process of establishing a full chemical equilibrium occurs as follows: first, the rates of the forward and reverse bimolecular reactions become close to each other. After that, the rate of change of the concentrations of the major components of the mixture decreases sharply. In what follows, the composition changes only due to changes in the number of molecules in the system. The change in the number of molecules in the system is a consequence of the reactions of dissociation and recombination, the rates of which are considerably lower than the rates of the bimolecular reactions that control the process of establishing a local chemical equilibrium without changing the number of species in the system. In other words, each time with a change in the number of molecules in the system, the chemical composition of the mixture relaxes very quickly to the state of chemical equilibrium for the available number of molecules in the system at the given moment.

The third stage of establishment of chemical equilibrium is characterized by equalizing the rates of the forward and reverse reactions that control the process of formation and decomposition of nitric oxide. This is the slowest stage of the process of establishing a complete chemical equilibrium.

Thus, the chemical equilibrium is first established among the molecules consisting of C, H, and O atoms, with the process of establishing equilibrium occurring so that the number of molecules does not change. Then, the rates of the forward and reverse reactions, including recombination and dissociation, become close to each other, except for the reactions controlling the process of formation of NO.

In [1,20,21] we made an effort to speed up directly a chemical integrator for some special case. In [1,20,21] we developed a method for calculating the changing composition of the explosion products in the case where there is no complete chemical equilibrium, but the bimolecular reactions are in equilibrium. A detailed kinetic mechanism is used, but without the need to solve the stiff system of differential equations. The core of our approach is to replace the complete system of chemical kinetics equations by an equivalent system composed of a differential and a few algebraic equations. The proposed method is based on a physically reasonable assumption that equilibrium in the bimolecular reactions is established much faster than the complete chemical equilibrium, being applicable when this assumption holds. According to [1, 20, 21] the method includes only one differential equation for calculating the change in the number of molecules per unit mass of the mixture due to the reactions of recombination and dissociation. This equation is used instead of dozens of equations of chemical kinetics. In the present work, we propose to supplement this equation with algebraic equations for calculating the equilibrium composition at given values of density, internal energy, molar mass and the linear combinations of logarithms of the concentration. The equations are derived based on the characteristic function (entropy or Helmholtz free energy) extremum method.

The applicability of the model was demonstrated by solving the test problems in [1,20,21]. It was shown that the proposed model can be used to calculate the characteristics of the explosive transformation process after the induction period in hydrogen–oxygen mixtures. The goal of the work described here was to examine the method for calculating the changes in composition of the explosion products in the case where the complete chemical equilibrium is absent but the bimolecular reactions are in quasi-equilibrium with the exception of bimolecular reactions with one of the components of the mixture. In addition we have investigated the possibility of using the method of quasi-equilibrium for mixtures of hydrocarbons and air.

This work was motivated by the author's wish to make kinetic calculations faster when our 3D-multicomponent parallel code is used. Also, the communication time between processors should be reduced. Right now 5 parameters (velocity, energy, density) and all concentrations of all species of a mixture must be sent. The author's goal is to make the latter as small as possible.

2. Equation for calculating the composition of the partial equilibrium mixture

According to [1,20,21] we obtain equations to calculate the mixture composition assuming that the entropy of the mixture reaches its maximum value at a specific internal energy U_0 , a specific volume v and additional conditions. These additional conditions are written in the general form

$$G_A(M_1, \dots, M_k) = 0,$$

$$G_B(M_1, \dots, M_k) = 0,$$

where k is the number of individual compounds in the mixture, M_i is the number of moles of the i -th substance per 1 kg of mixture. For example if the total number of moles per unit mass is known and equals M_0 then

$$G_A(M_1, \dots, M_k) = \sum_{i=1}^k M_i - M_0. \quad (1)$$

If the number of moles of the substance B per 1 kg of mixture is known and equals B_0 then we have

$$G_B(M_1, \dots, M_k) = M_B - B_0. \quad (2)$$

The entropy of a mixture of ideal gases with known dependence of the heat capacity on the temperature is given by

$$S = \sum_{i=1}^k \{S_i - R \ln[RTM_i/(vP_0)]\} M_i,$$

where R is the universal gas constant, T is the temperature of the mixture, v is the specific volume of the mixture, S_i is the standard entropy, U_i is the internal energy of one mole of mixture component i at a given temperature T .

The amount of each chemical element in the mixture is known, since it is determined by the initial composition of the mixture, remaining unchanged during chemical reactions. For chemical element j we obtain equation

$$\sum_{i=1}^k \alpha_{ij} M_i - \beta_j = 0, \quad j = 1, \dots, m,$$

where m is the number of different chemical elements in the mixture, β_j is the number of kilogram-atoms of the j -th element in 1 kg of mixture, α_{ij} is the number of atoms of the j -th element in a molecule of the i -th substance.

The specific internal energy is a preset value. This condition leads to the equation

$$\sum_{i=1}^k U_i M_i - U_0 = 0.$$

Following the Lagrange procedure, we write the function

$$L = \sum_{i=1}^k \left[S_i - R \ln \left(\frac{RTM_i}{vP_0} \right) \right] M_i + \sum_{j=1}^m \left(\sum_{i=1}^k \alpha_{ij} M_i - \beta_j \right) \lambda_j + \left(\sum_{i=1}^k U_i M_i - U_0 \right) \lambda_u + G_A \lambda_A + G_B \lambda_B,$$

where λ_j , λ_u , λ_A and λ_B are the Lagrange multipliers, which, along with M_i and T , are the independent variables of the Lagrangian. At equilibrium, the derivatives of the Lagrangian with respect to the independent variables equal to zero. So we have

$$\frac{dL}{d\lambda_j} = \sum_{i=1}^k \alpha_{ij} M_i - \beta_j = 0, \quad j = 1, \dots, m, \quad (3)$$

$$\frac{dL}{d\lambda_u} = \sum_{i=1}^k U_i M_i - U_0 = 0, \quad (4)$$

$$\frac{dL}{d\lambda_A} = G_A(M_1, \dots, M_k) = 0, \quad (5)$$

$$\frac{dL}{d\lambda_B} = G_B(M_1, \dots, M_k) = 0, \quad (6)$$

$$\frac{dL}{dM_i} = -R + S_i - R \ln \left(\frac{RTM_i}{vP_0} \right) + U_i \lambda_u + \sum_{j=1}^m \alpha_{ij} \lambda_j + \frac{dG_A}{dM_i} \lambda_A + \frac{dG_B}{dM_i} \lambda_B = 0, \quad i = 1, \dots, k, \quad (7)$$

$$\frac{dL}{dT} = \sum_{i=1}^k \left(\frac{dS_i}{dT} - \frac{R}{T} \right) M_i + \sum_{i=1}^k \frac{dU_i}{dT} M_i \lambda_u = 0. \quad (8)$$

The dS_i/dT , which depends on T , satisfies

$$\frac{dS_i}{dT} = \frac{1}{T} \left(\frac{dU_i}{dT} + R \right), \quad (9)$$

so the solution of equation (8) is

$$\lambda_u = -T^{-1}. \quad (10)$$

Substituting λ_u into the equations (7) yields

$$\frac{dL}{dM_i} = S_i - R \ln \left(\frac{RTM_i}{vP_0} \right) - \frac{H_i(T)}{T} + \sum_{j=1}^m \alpha_{ij} \lambda_j + \frac{dG_A}{dM_i} \lambda_A + \frac{dG_B}{dM_i} \lambda_B = 0, \quad i = 1, \dots, k, \quad (11)$$

where $H_i = U_i + RT$.

We have $k + m + 3$ algebraic equations (3)–(6), (11) for $k + m + 3$ independent variables T , M_i , λ_j , λ_A and λ_B .

This system of algebraic equations has no analytical solution, so it is solved approximately by the Newton method described in [22]. The Newton method requires up to 8 iterations to achieve desired accuracy. Really the number of iterations is not important because for gas dynamic calculations we traditionally use precalculated database for quasi-equilibrium species concentrations or for $\partial c/\partial t$ at given internal energy, density and molar mass. To calculate U_i , S_i , and enthalpy H_i at a given temperature, we used polynomials from [22].

Table 1. The equilibrium products composition (mole fraction) at $T = 2901$ K and $\rho = 1.17$ kg/m³. The species that are taken into account in the explosion products are CO, CO₂, H, H₂O, HO₂, H₂, O, OH, O₂, N₂.

O ₂	H ₂	OH	H ₂ O	CO
2.25×10^{-2}	4.29×10^{-3}	1.09×10^{-2}	6.34×10^{-2}	4.87×10^{-2}
H	O	CO ₂	HO ₂	N ₂
2.42×10^{-3}	3.81×10^{-3}	1.00×10^{-2}	9.29×10^{-6}	7.44×10^{-1}

3. Solving the species evolution based on detailed chemical kinetics

When the chemical kinetics equations are applied to calculating the composition of the mixture, the following system of equations is used

$$\frac{\partial c_i}{\partial t} = \omega_i, \quad (12)$$

$$\sum_{i=1}^k \nu'_{ij} \chi_i = \sum_{i=1}^k \nu''_{ij} \chi_i, \quad j = 1, \dots, J, \quad (13)$$

$$\omega_i = \sum_{j=1}^J k_j (\nu''_{ij} - \nu'_{ij}), \quad i = 1, \dots, k; \quad (14)$$

where ω_i is the rate of production of species i per unit volume; c_j are the molar concentrations of the mixture components; k_j is the rate of reaction j calculated according to the law of mass action, χ_i is the chemical formula of species i participating in the reaction j ; ν'_{ij} and ν''_{ij} are the stoichiometric coefficients of the product or reactant i in reaction j . The rate of production of the total number of moles of all species per unit volume are given by

$$\frac{\partial c}{\partial t} = \sum_{i=1}^J \omega_i. \quad (15)$$

Formally, in (15), the summation is over all reactions. However, if bimolecular reactions do not change the number of molecules, the summation can be restricted to the recombination and dissociation reactions.

4. Results of calculations for the explosion products of hydrocarbons and air

In order to validate the proposed approximate method, constant volume adiabatic computations were performed and compared to the results of simulations with the detailed reaction mechanism. We have studied the explosion products of stoichiometric acetylene–oxygen with nitrogen dilution ($C_2H_2 + 2.5O_2 + 10N_2$). The equilibrium compositions of the explosions products are given in table 1 and table 2 and correspond to the so called instantaneous (constant-volume) explosion of the initial mixture. The equilibrium compositions are calculated for an initial mixture pressure of 0.1 MPa and initial temperature of 298 K.

In order to produce significant departures from equilibrium we reduce the temperature of the explosion products from 2901 K to 2600 K at constant volume and constant (frozen) composition. The mixture relaxes to the new state of chemical equilibrium at constant density and constant

Table 2. The equilibrium products composition (mole fraction) at $T = 2875$ K and $\rho = 1.17$ kg/m³. The species that are taken into account in the explosion products are CO, CO₂, H, H₂O, HO₂, H₂, O, OH, O₂, N, N₂, NO.

O ₂	H ₂	OH	H ₂ O	CO	H
1.77×10^{-2}	4.45×10^{-3}	9.75×10^{-3}	6.39×10^{-2}	4.94×10^{-2}	2.27×10^{-3}
O	CO ₂	HO ₂	N	NO ₂	N ₂
3.09×10^{-3}	9.94×10^{-2}	7.40×10^{-6}	1.66×10^{-6}	1.16×10^{-2}	7.38×10^{-1}

specific internal energy after a disturbance. It is assumed that there are no expansion and heat loss.

A stiff ordinary differential equation solver is used to march in time from a specified nonequilibrium initial state to near-equilibrium conditions. The system of twelve differential equations (12) for the concentrations and one differential equation for the temperature is used for simulation. The detailed chemical reaction mechanism is given in table 3. The species that are taken into account in the explosion products are CO, CO₂, H, H₂O, HO₂, H₂, O, OH, O₂, N, N₂, NO. The calculations were performed by numerical solving the system of differential equations of chemical kinetics corresponding to the selected detailed mechanism. The data on the rate constants are borrowed from [23]. The rate constants of the reverse reactions were calculated from those for direct reactions using the equilibrium constants. The calculation was performed until the state of the mixture was close to the equilibrium. Temperature, molar mass and species temporal histories are shown in figures 1–5 by blue lines and symbols (lines 1). These temporal histories are used as the basis for examination of our approximate method. The approximation method should be able to reproduce these temporal histories. The initial composition is given in table 1 and initial temperature is 2600 K. The species that are taken into account in the explosion products are CO, CO₂, H, H₂O, HO₂, H₂, O, OH, O₂, N₂.

The approximation method does not use any simplified chemical reaction mechanism. We have carried out approximate numerical simulations based on the same detailed chemical reaction mechanism presented in table 3. Right parts of equations (12) and equation (15) are calculated using the rate coefficients given in table 3. The presence of NO did not significantly affect the molecular weight and the amount of energy released. If a problem is solved for which the concentration of NO is unimportant, the reactions involving nitrogen containing compounds can be excluded from the reaction scheme. Taking into account the fast reaching equilibrium in bimolecular reactions and neglecting the changes of N, N₂, NO mass fraction we find temperature and species molar fractions by solving the system of algebraic equations (1), (3)–(5), (11) at given density, temperature and molar mass of the mixture. The evolution of molar mass is solved by integrating the single differential kinetic equation (15) for the total molar concentration. Calculations of quasi-equilibrium composition are performed at each time step of equation (15) integration.

Results for the approximate method with one differential equation (15) are shown in figures 1–5 by red lines (lines 2). The proposed method gives excellent results for the temperature, mixture molar mass and H₂O temporal histories.

Examination of the species plots shows that the situation is more complex for the cases shown in figures 4, 5. Figures 5 repeats the data of figures 4 but includes only first ten μ s. From figures 3, 5 H₂O profile is in better agreement with stiff solver results than that of CO₂. It means that the extent of detailed equilibrium in bimolecular reactions R12–R15 is higher

Table 3. Reaction mechanism $k = AT^n \exp(E_a/T)$.

N	Reaction	A	n	E_a
$R1$	$O + CO + M \rightleftharpoons CO_2 + M$	5.89×10^{15}	0.0	-22090
$R2$	$O + H + M \rightleftharpoons OH + M$	7.10×10^{18}	-1.0	0
$R3$	$O + O + M \rightleftharpoons O_2 + M$	1.10×10^{14}	-1.0	900
$R4$	$H + OH + M \rightleftharpoons H_2O + M$	2.20×10^{22}	-2.0	0.0
$R5$	$H + H + M \rightleftharpoons H_2 + M$	9.00×10^{17}	-1.0	0
$R6$	$H + O_2 + M \rightleftharpoons HO_2 + M$	1.50×10^{15}	0.0	500
$R7$	$N + N + M \rightleftharpoons N_2 + M$	3.02×10^{14}	0.0	500
$R8$	$N + O + M \rightleftharpoons NO + M$	1.00×10^{20}	-1.5	0
$R9$	$OH + CO \rightleftharpoons H + CO_2$	1.51×10^7	1.3	3.88
$R10$	$HO_2 + CO \rightleftharpoons OH + CO_2$	1.51×10^{14}	0.0	-11920
$R11$	$O_2 + CO \rightleftharpoons O + CO_2$	3.16×10^{11}	0.0	-18950
$R12$	$O + H_2O \rightleftharpoons OH + OH$	5.80×10^{13}	0.0	-9.059
$R13$	$H + H_2O \rightleftharpoons OH + H_2$	8.40×10^{13}	0.0	-10116
$R14$	$H + O_2 \rightleftharpoons O + OH$	2.20×10^{14}	0.0	-8455
$R15$	$O + H_2 \rightleftharpoons H + OH$	1.80×10^{13}	1.0	-4480
$R16$	$O_2 + H_2 \rightleftharpoons H + HO_2$	1.90×10^{13}	0.0	-24100
$R17$	$O + H_2O \rightleftharpoons H + HO_2$	4.76×10^{11}	0.37	-28743
$R18$	$OH + O_2 \rightleftharpoons O + HO_2$	1.30×10^{13}	0.0	-28200
$R19$	$OH + HO_2 \rightleftharpoons O_2 + H_2O$	3.00×10^{14}	0.0	0
$R20$	$OH + OH \rightleftharpoons H + HO_2$	1.20×10^{13}	0.0	-20200
$R21$	$O + N_2 \rightleftharpoons N + NO$	5.00×10^{13}	-1.0	-37940
$R22$	$O + NO \rightleftharpoons N + O_2$	1.51×10^9	1.0	-19439
$R23$	$H + NO \rightleftharpoons N + OH$	1.70×10^{14}	0.0	-24500
$R24$	$N + HO_2 \rightleftharpoons NO + OH$	1.00×10^{13}	0.0	-1000

than that in R9–R11. We have recomputed the test problem using the approximate method with two differential equations: equation (15) for total concentration c and equation (12) for concentration of CO_2 . In this case the additional conditions are written in the form

$$G_A(M_1, \dots, M_k) = \sum_{i=1}^k M_i - M_0 = 0,$$

$$G_B(M_1, \dots, M_k) = M_{CO_2} - B_0 = 0,$$

where

$$M_0 = c/\rho,$$

$$B_0 = c_{CO_2}/\rho.$$

The calculation of CO_2 time history based on the approximate method with two differential equations improves the agreement with exact solution (curves 3 in figures 4 and 5).

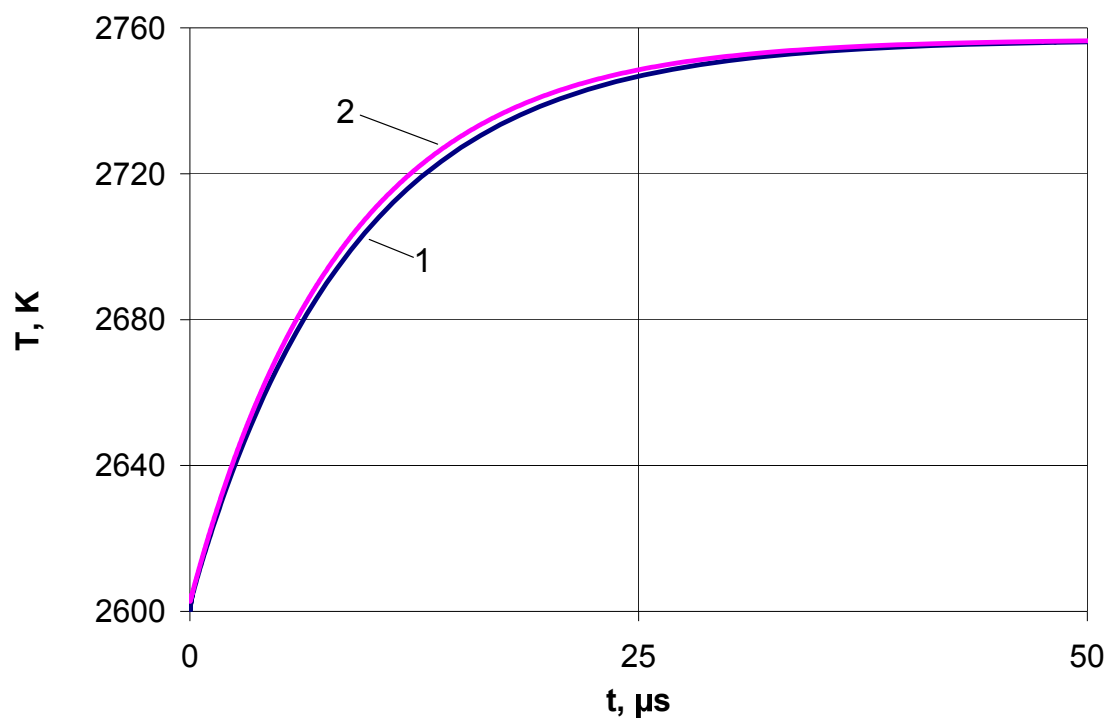


Figure 1. Temperature profile: 1—method including 10 differential equation, 2—proposed method with one differential equation (15) for c .

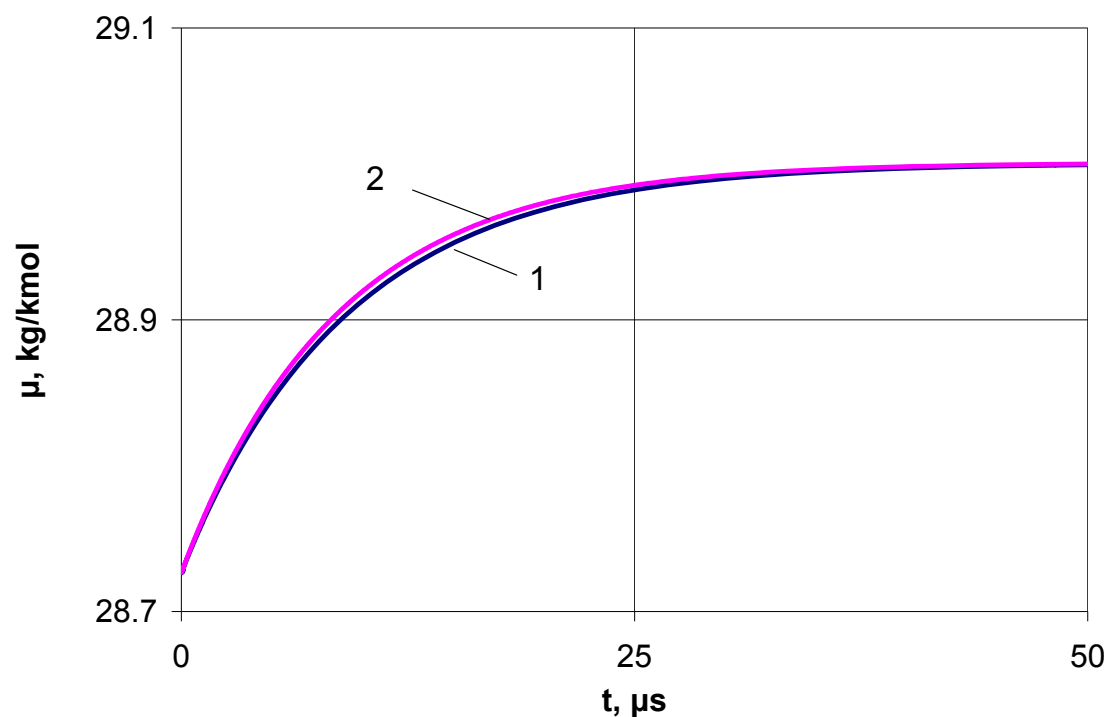


Figure 2. Molar mass profile: 1—method including 10 differential equation, 2—proposed method with one differential equation (15) for c .

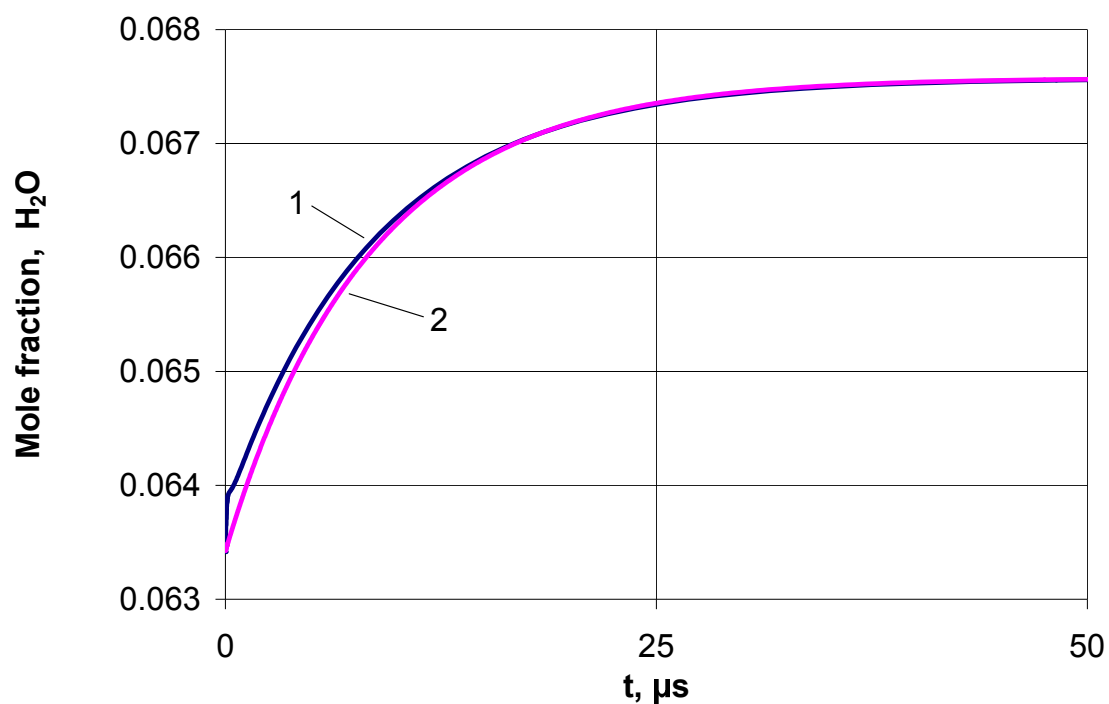


Figure 3. H₂O profiles: 1—method including 10 differential equation, 2—proposed method with one differential equation (15) for c .

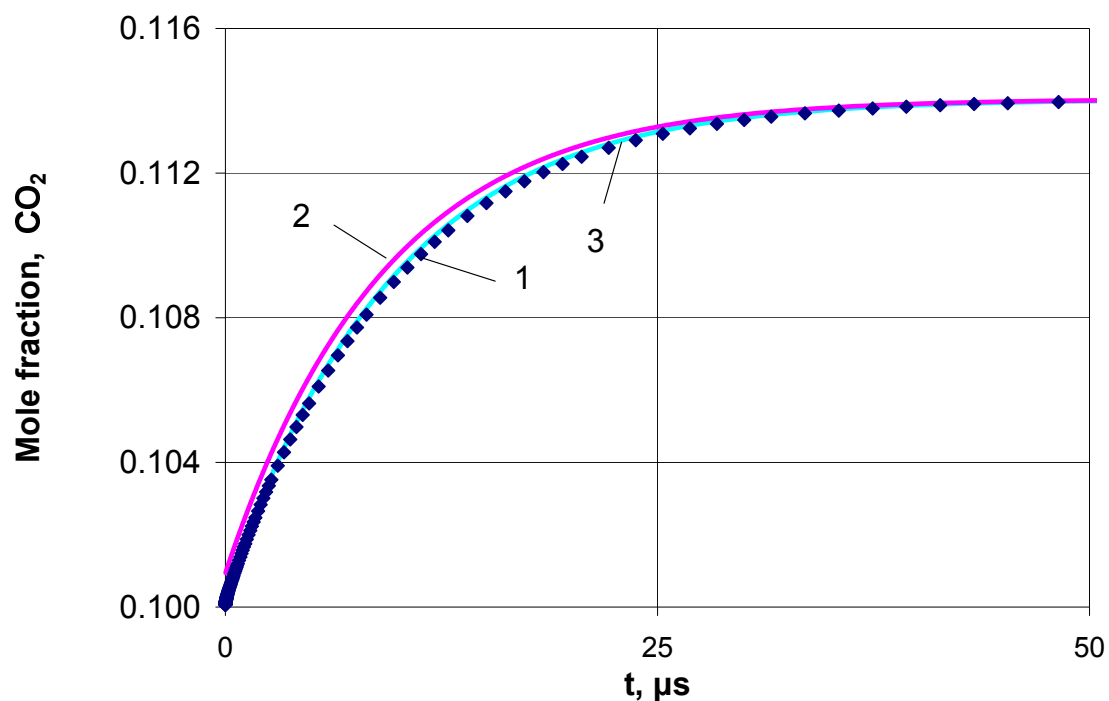


Figure 4. CO₂ profiles: 1—method including 10 differential equation, 2—proposed method with one differential equation (15) for c , 3—proposed method with two differential equations (15) for c and (12) for c_{CO_2} .

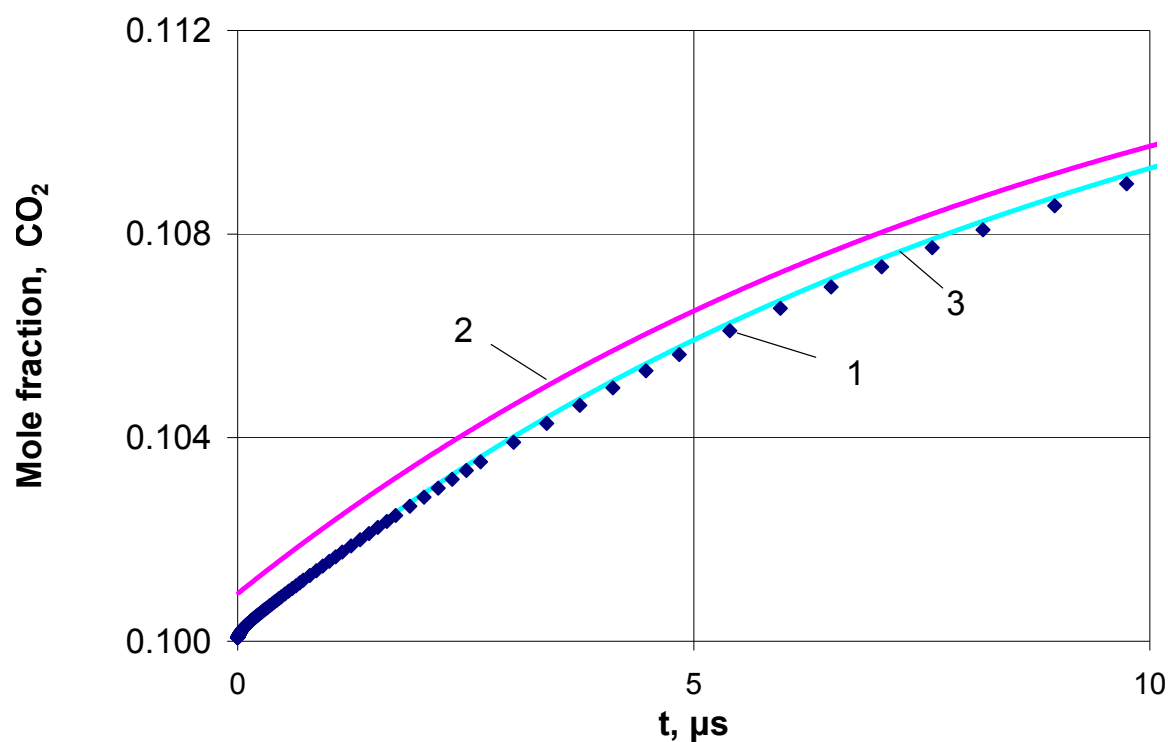


Figure 5. CO_2 profiles: 1—method including 10 differential equation, 2—proposed method with one differential equation (15) for c , 3—proposed method with two differential equations (15) for c and (12) for c_{CO_2} .

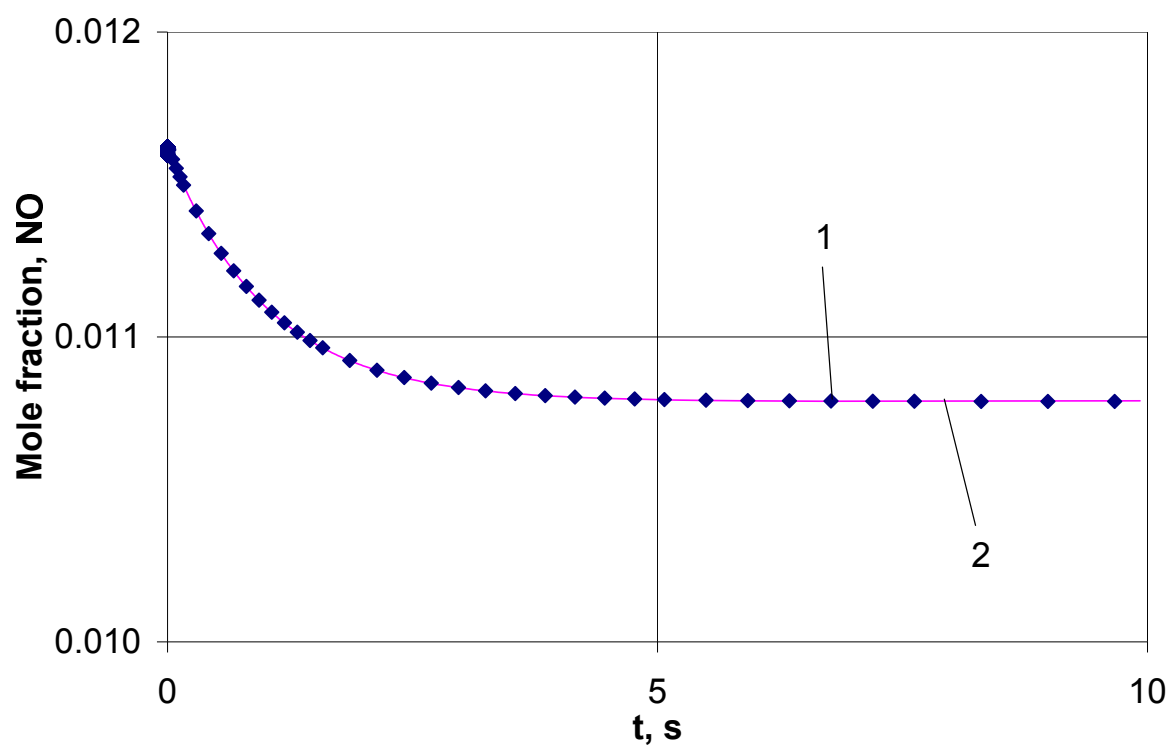


Figure 6. NO profiles: 1—method including 13 differential equation, 2—proposed method with one differential equation (12) for c_{N_2} .

Substantial nonequilibrium exists in reactions including N_2 (R7 and R21) when there is quasi-equilibrium for C–H–O system. To predict NO temporal history we used the differential equation

$$\frac{\partial c_{N_2}}{\partial t} = \omega_{N_2}$$

and assumed that the composition of detonation products can be calculated in suggestion that the entropy has the maximum value for known density, specific internal energy and mass fraction of N_2 at any given time. The temperature and the mass fractions of all species with the exception of N_2 are obtained by solving the system of the algebraic equation (3)–(5), (11) and additional relation

$$G_B(M_1, \dots, M_k) = M_{N_2} - B_0 = 0,$$

where

$$B_0 = c_{N_2}/\rho.$$

Comparison of NO profiles is shown in figures 6. The approximation method should be able to reproduce these temporal histories. The initial composition is given in table 2 and initial temperature is 2800 K. The results obtained by proposed method match excellently with the detailed kinetics model results obtained with the stiff ordinary differential equation solver.

5. Conclusions

We examined the approximate method to calculate composition and thermodynamic parameters of hydrocarbons–air nonequilibrium explosion products based on the assumption of the existence of a partial chemical equilibrium. With excellent accuracy of calculating thermodynamic properties and species mass fraction the respective stiff system of detailed kinetics differential equations can be replaced by one differential equation or two differential equations and a system of algebraic equations. This method is always consistent with the detailed kinetic mechanism. The constituent equations of the method were derived and the respective computer code written. We examine the applicability of the method by solving the test problem. The proposed method simulation results are in excellent agreement with the detailed kinetics model results obtained with the stiff ordinary differential equation solver including NO time histories.

Typically, the time this method takes for calculating the mixture composition is not longer than that spent on solving the gasdynamic equations. The comparison of the effectiveness of the method with alternative methods in the gasdynamic calculations was not discussed in the paper. All these results will be published.

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