

Differential Equations of Gas-Phase Chemical Kinetics

Chemked – A Program for Chemical Kinetics of Gas-Phase Reactions

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1. Introduction

Chemked [1] is a program designed for creating and editing thermodynamic and chemical kinetics databases, for formation of reaction mechanisms and simulation of problems of complex gas-phase chemistry. The program uses thermodynamic data and chemical reactions that have the CHEMKIN-II description. The information is collected in databases that are stored in files of the Microsoft Access type. The data are displayed in the tables and can be easily handled. Chemked has the multiple-document interface and can simultaneously process several reaction databases connected with a thermodynamic database. The program provides numerical and graphical information on thermodynamic functions and reaction rate constants.

Chemked incorporates a solver for integration of differential equations of gas-phase chemical kinetics at constant pressure or constant volume (density) without mass and heat transfer. The solver is a FORTRAN program based on the RADAU5 subroutines [2]. The necessary information on thermodynamics and reactions is provided for the solver directly from the databases under consideration. The solver output contains numerical and graphical information on mixture-averaged gas parameters and species concentrations.

The goal of the work presented here is the accurate derivation of equations of gas phase chemical kinetics that are used in the Chemked solver. These equations are well-known differential equations for temperature and species concentrations describing processes in a reaction vessel at constant pressure or constant volume. In addition, the definition of important gas parameters and reaction rates are given. For illustration of the discussed items, an example of chemical evolution of H₂/O₂ mixture is presented; the calculation has been made with Chemked.

More information about Chemked can be found at [3,4]. A brief list of useful literature related to topics discussed below is presented in Reference Section [5-9].

2. Gas Parameters and Variables

Here we introduce gas parameters that will be used as variables in conservation equations or will be useful for analysis of results. The choice of some of these parameters is obvious and does not require special comments. These parameters are the mixture-averaged gas parameters.

Temperature T , [K],

Pressure P , [atm],

Total gas concentration C_{tot} is a number of molecules or moles per unit of volume, [1/cm³] or [mol/cm³].

For given P and T , the C_{tot} value is found from the ideal-gas equation of state.

$$C_{tot} = \frac{P}{RT}, \quad (2.1)$$

where R is the universal gas constant.

Concentration of n th species is denoted as $[X_n]$ and has the units of $[1/\text{cm}^3]$ or $[\text{mol}/\text{cm}^3]$. The obvious formula relates the $[X_n]$ values to the total concentration C_{tot} .

$$C_{tot} = \sum_n [X_n], \quad (2.2)$$

where the summation is over all species in the gas mixture. The species concentrations can be expressed also in terms of the mole fractions X_n .

$$X_n = \frac{[X_n]}{C_{tot}}. \quad (2.3)$$

Mean mass density ρ (g/cm^3) and mean molecular weight \bar{m} (g/mol) are calculated as follows:

$$\rho = \sum_n m_n [X_n], \quad (2.4)$$

$$\bar{m} = \sum_n m_n X_n, \quad (2.5)$$

where m_n is molecular weight of the n th species.

In the following consideration, mass fraction Y_n of the n th species will be employed.

$$Y_n = \frac{m_n [X_n]}{\rho}. \quad (2.6)$$

Relation of mole fraction to mass fraction is given by

$$Y_n = \frac{X_n m_n}{\bar{m}}. \quad (2.7)$$

We define the Z_n as a number molecules or moles per unit of total mass of the gas mixture, $[1/\text{g}]$ or $[\text{mol}/\text{g}]$. Relation of Z_n to the concentration per unit of volume is

$$[X_n] = \rho Z_n. \quad (2.8)$$

Substituting Eq.(2.8) into the equation Eq.(2.6) we get

$$Z_n = \frac{Y_n}{m_n}. \quad (2.9)$$

3. Chemical Reactions

In this section, we give only a short description of chemical reactions; more detailed information on this subject can be found in literature, for example, in [5, 7-9].

3.1 Reaction Rate

The stoichiometric equation of a chemical reaction can be written in the following general form:

$$\sum_n v'_{jn} \chi_n = \sum_n v''_{jn} \chi_n, \quad (3.1)$$

where the subscript j is the reaction number, χ_n is the chemical symbol of species n , v_{jn} is the stoichiometric coefficient. The summations are over the species involved in the reaction. The superscript ' of the stoichiometric coefficients refers to the reactants, the superscript '' refers to the products. In this representation, the v_{jn} coefficients are integer positive numbers or zeros.

The forward and reverse rates and rate-of-progress of the j th reaction are

$$q_{j,for} = k_{j,for} \prod_n [X_n]^{v'_{jn}}, \quad q_{j,rev} = k_{j,rev} \prod_n [X_n]^{v''_{jn}}, \\ q_{j,net} = q_{j,for} - q_{j,rev}, \quad (3.2)$$

where $k_{j,for}$ and $k_{j,rev}$ are the forward and reverse rate constants of the j th reaction.

Remark -----

In Eq. (3.2), the powers of concentrations are reaction orders with respect to reactants. In more general expressions for reaction rates, the reaction orders are not necessarily equal to the stoichiometric coefficients v'_{jn} and v''_{jn} . Often, this situation shows up at description of non-elementary reactions, for example, gas-surface reactions. Nevertheless, in gas reaction systems, the approach used here is usually valid.

The Arrhenius form is used most frequently for calculation of the reaction rate constant:

$$k_{j,for} = A_{j,for} T^{a_{j,for}} \exp\left(-\frac{E_{j,for}}{RT}\right), \quad (3.3)$$

where $A_{j,for}$, $a_{j,for}$ and $E_{j,for}$ are the parameters that are available in chemical kinetics databases, for example [10]. The reverse rate constant is related to the forward rate constant by

$$k_{j,rev} = \frac{k_{j,for}}{K_j}, \quad (3.4)$$

where K_j is the equilibrium constant of the j th reaction. The Arrhenius form is one of the simplest expressions of the rate constant; in many cases the more sophisticated expressions are required. Description of other reaction types can be found in [7].

Remark -----

The units for the pre-exponential factor $A_{j,for}$ (A-units) depend on the units of species concentrations. In Chemked, the following units are used.

Species concentration	mol/cm ³ (moles/cm ³)	1/cm ³ (molecules/cm ³)
Designation of A-units	mol-cm-sec	cm-sec
A-units of 1 st order reaction	1/sec	1/sec
A-units of 2 nd order reaction	cm ³ /mol sec	cm ³ /sec
A-units of 3 rd order reaction	cm ⁶ /mol ² sec	cm ⁶ /sec
Reaction rate	mol/cm ³ sec	1/cm ³ sec (molecules /cm ³ sec).

The units for activation energy $E_{j,for}$ (E-units) are cal/mol, J/mol or K. Note that T is always in Kelvin.

The A-units and E-units, specified here, are most frequently used in existing databases and software [7].

Each event of the j th reaction yields the number $(v_{jn}'' - v_{jn}')'$ of species n . Then production rate of species n in the j th reaction is given by

$$w_{jn} = (v_{jn}'' - v_{jn}') q_{j,net}. \quad (3.5)$$

The sign of w_{jn} shows the actual situation. If $w_{jn} > 0$, then the species n are produced; if $w_{jn} < 0$, then the species n are consumed. The rate-of-progress $q_{j,net}$ and the species production rate w_{jn} have the units of (1/cm³ sec) or (mol/cm³ sec).

3.2 Heat of Reaction

The final products of a chemical reaction are not only new chemical compounds, but releasing (consuming) of heat as well. The last process is a result of difference in energies between products and reactants. The heat of the j th reaction Q_j is defined as an amount of heat that must be exchanged between reaction system and its surrounding to keep a fixed system temperature. Below we will consider two cases when a reaction system is at constant pressure or at constant volume.

Constant pressure, $\Delta V \neq 0$. In this case, change in the internal energy ΔU_j must be equal to a sum of heat of reaction Q_{pj} and work $-P\Delta V$ due to expansion (contraction) of the gas volume (first law of the thermodynamics). Then the heat of reaction is

$$Q_{pj} = \Delta U_j + P\Delta V, \quad (3.6)$$

where the subscript p indicates constant pressure. It is convenient to use the enthalpy instead of the internal energy. By definition, enthalpy of the n th species is

$$H_n = U_n + PV. \quad (3.7)$$

where H_n and U_n are the enthalpy and the internal energy of species n . Taking into account Eq.(3.7), we may rewrite Eq.(3.6) in the form:

$$Q_{pj} = \sum_n (v_{jn}'' - v_{jn}') H_n. \quad (3.8)$$

Constant volume, $\Delta V=0$. Under these conditions the gas does not make any work ($P\Delta V=0$) and the heat of reaction Q_{vj} is equal to change in internal energy.

$$Q_{vj} = \Delta U_j, \quad \Delta U_j = \sum_n (v_{jn}'' - v_{jn}') U_n. \quad (3.9)$$

where the subscript v indicates constant volume process.

Rate of heat production. This value is given by the expression

$$s_j = -Q_j q_{j,net}. \quad (3.10)$$

where $q_{j,net}$ is rate-of-progress of the j th reaction, Eq.(3.2). Eq (3.10) can be rewritten in terms of production rate of species involved in reaction (Eq. 3.5).

$$s_{pj} = -\sum_n w_{jn} H_n, \quad (3.11a)$$

$$s_{vj} = -\sum_n w_{jn} U_n, \quad (3.11b)$$

The sign of s_j shows the actual situation. If $s_j < 0$, then the heat is consumed; if $s_j > 0$, then the heat is released. The heat of reaction Q_j (like H_n and U_n) has the units of energy per mole, (J/mol) or (cal/mol). Correspondingly, the rate-of-progress $q_{j,net}$, as well as production rates of species w_{jn} , must have the units of molar production, (mol/cm³ sec). Then the s_j values describe the rate of heat production in the j th reaction per unit volume, (J/cm³ sec) or (cal/cm³ sec).

4. Equations of Chemical Kinetics

4.1 Problem Formulation

We will consider evolution of parameters of a gas mixture in course of chemical reactions. Schematic diagram of a reaction vessel is given in Fig. 4.1. When describing the chemical processes, the following assumptions will be used.

- There is perfect gas mixing in the vessel volume.
- The vessel walls are impermeable.
- There are no surface reactions.
- Adiabatic walls (the vessel walls are thermally insulated, i.e. there is no heat exchange between the reaction system and surrounding).

The vessel has a piston that allows us to get two types of conditions. When the piston can move freely, chemical reactions take place at constant pressure, which is equal to surrounding gas pressure, Fig. 4.1a. When the piston is fixed, chemical reactions take place at constant volume, Fig. 4.1b.

We believe that chemical reactions occurring in the gas mixture are known and their rate constants are specified. In addition, specific thermodynamic functions of species (enthalpy, internal energy and heat

capacity) are defined as well. Below we will obtain set of equations that describe parameters of the reaction system in the course of reactions.

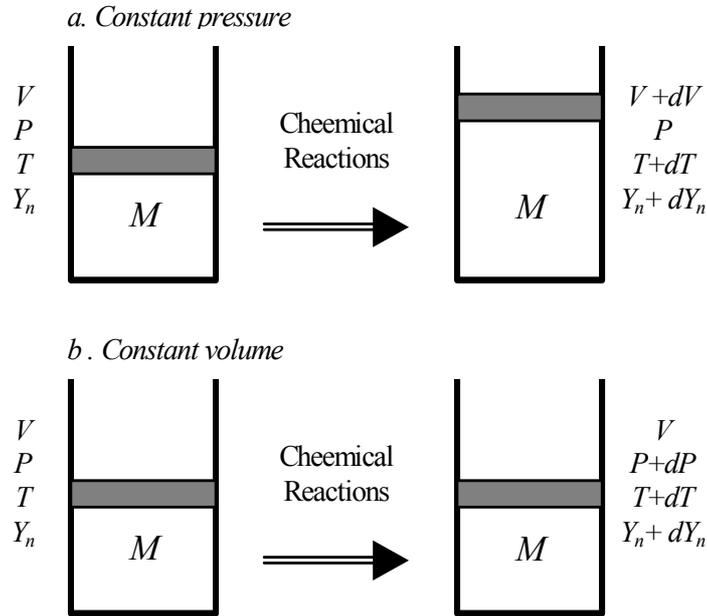


Fig. 4.1. Schematic diagram of changing parameters in reaction system

4.2 Constant Pressure Process

These conditions are met when the piston of the reaction vessel can move freely, Fig. 4.1a. The total mass of gas and volume are related by the following equation:

$$M = \rho V = \text{constant} \quad , \quad (4.1)$$

In this case, the volume changes in course of chemical reactions and consequently the mean mass density ρ changes as well.

Conservation of species. The conservation of mass of species n in the whole reaction volume can be written in the form:

$$\frac{d}{dt}(MY_n) = m_n w_n V \quad , \quad (4.2)$$

$$w_n = \sum_j w_{jn} \quad . \quad (4.3)$$

Here Y_n is mass fraction and m_n is molecular weight of the n th species, w_{jn} is molar production rate of species n in the j th reaction (Eq (3.5)), w_n is the total molar production rate of the n th species. Sum is over reactions that involve the n th species. Thus, the left-hand side of Eq (4.2) is time-derivative of the total mass of the n th species in the whole volume V and the right-hand side is the mass production rate of the same species in the same volume. Differentiating the left-hand side leads to

$$Y_n \frac{d}{dt}(M) + M \frac{d}{dt}(Y_n) = m_n w_n V . \quad (4.4)$$

If we taken into account Eq (4.1), then the differential equations for the mass fractions of species may be written as

$$\frac{dY_n}{dt} = \frac{m_n}{\rho} w_n , \quad (4.5)$$

It should be noted once again that here the mass density ρ is a time-dependent parameter, Eq (4.1).

Remark -----

When analyzing the calculation results it is desirable to know the integral production of species n by each reaction. For this purpose, the equation (4.5) can be written somewhat differently. Dividing both sides of the equation by molecular weight m_n gives

$$\frac{dZ_n}{dt} = \sum_j b_{jn} , \quad Z_n = \frac{Y_n}{m_n} , \quad b_{jn} = \frac{w_{jn}}{\rho} . \quad (4.5a)$$

where Z_n is content of species n per 1 gram of gas mixture Eq.(2.9), mol/g; b_{jn} is production rate of species n in the j th reaction in units mol/g sec. The integral production of species n on the time interval t_1-t_2 (mol/g) is

$$Z_n(t_2) - Z_n(t_1) = \sum_j B_{jn} ; \quad B_{jn} = \int_{t_1}^{t_2} b_{jn} dt .$$

The values B_{jn} provide information about the importance of the reactions in production of species n .

Conservation of energy. Under constant pressure the enthalpy of a gas mixture in a closed vessel with insulated walls is held constant.

$$\frac{d}{dt} M \bar{h} = 0 , \quad (4.6)$$

where \bar{h} is the mean specific enthalpy in mass units (J/g or cal/g).

$$\bar{h} = \sum_n Y_n h_n . \quad (4.7)$$

Here h_n is the specific enthalpy of the n th species; the summation is over all species of the gas mixture. Differentiating Eq (4.6) gives

$$\bar{h} \frac{dM}{dt} + M \frac{d\bar{h}}{dt} = 0 . \quad (4.8)$$

The first term is equal to zero (see Eq (4.1)), then Eq (4.8) can be written in the form

$$\frac{d}{dt} \sum_n Y_n h_n = 0 . \quad (4.9)$$

After differentiating, Eq (4.9) can be written as

$$\sum_n Y_n \frac{dh_n}{dt} = -\sum_n h_n \frac{dY_n}{dt}. \quad (4.10)$$

The ideal-gas enthalpy h_n is function of gas temperature only. In that case, the h_n derivative can be evaluated by

$$\frac{dh_n}{dt} = c_{pn} \frac{dT}{dt}, \quad c_{pn} = \frac{dh_n}{dT}, \quad (4.11)$$

where c_{pn} is the specific heat capacity of the n th species at constant pressure in mass units; (J/g K or cal/g K). Using these relations we get Eq (4.10) in the form:

$$\bar{c}_p \frac{dT}{dt} = -\sum_n h_n \frac{dY_n}{dt}, \quad (4.12)$$

where the summation is over all species of gas mixture. Mean specific heat capacity at constant pressure \bar{c}_p is

$$\bar{c}_p = \sum_n Y_n c_{pn}. \quad (4.13)$$

Substituting Eq (4.5) in Eq (4.12) gives us the final equation for the gas temperature.

$$\frac{dT}{dt} = -\frac{1}{\rho \bar{c}_p} \sum_n H_n w_n, \quad (4.14)$$

where H_n is the enthalpy of the n th species in molar units (J/mol or cal/mol).

$$H_n = m_n h_n. \quad (4.15)$$

Remark -----

Eq (4.14) can be also expressed in terms of the rates of heat production in chemical reactions, Eq (3.11a).

$$\frac{dT}{dt} = -\frac{1}{\rho \bar{c}_p} \sum_j s_{pj}, \quad (4.14a/)$$

where the summation is over all chemical reactions.

Initial conditions. The differential equations (4.5) and (4.14) must be accompanied by initial conditions, that is, at a time instant $t=0$ we must specify the following gas parameters in the reaction vessel:

- P_0 pressure
- T_0 temperature
- Y_{n0} species mass fractions

Remark -----

Often, species mole fractions X_n are specified as initial conditions; conversion of X_n to Y_n is made with Eq (2.7).

Hence, the equations (4.5), (4.14) with initial conditions for temperature T_0 and species mass fractions Y_{n0} at a given constant pressure P completely determine parameters of the gas mixture in reaction vessel. Some additional values (mass density ρ , total gas volume V , etc) can be found from formulae of this section and Section 2.

4.3 Constant Volume Process

These conditions are met when the piston of the reaction vessel is fixed, Fig. 4.1b. The total mass of gas and volume are related by Eq (4.1), as previously:

$$M = \rho V = \text{constant} \quad .$$

In this case, the volume is constant in course of chemical reactions and consequently the mean mass density ρ is constant as well.

Conservation of species. When deriving Eq (4.5) for species mass fractions we did not explicitly use the constant pressure assumption. So, Eq (4.5) has a general character and can be applied to the constant volume conditions as well. Under these conditions some simplification is possible. Taking into account that the mass density ρ is constant, we can rewrite Eq (4.5) in the form.

$$\frac{d [X_n]}{dt} = w_n \quad . \quad (4.16)$$

Here, the relation (2.6) between molar concentration $[X_n]$ and mass fraction Y_n was employed.

Remark -----

To obtain the integral production of species n in reactions the method described in remark to Eq.(4.5a) can be used. In constant volume process, the gas density is constant. Then the product ρB_{jn} gives the integral production in units mol/cm³.

Conservation of energy.

Internal energy of a gas mixture in a closed vessel with insulated walls is.

$$\frac{d}{dt} M\bar{u} + P \frac{dV}{dt} = 0, \quad (4.17)$$

where \bar{u} is the mean specific internal energy in mass units (J/g or cal/g).

$$\bar{u} = \sum_n Y_n u_n \quad . \quad (4.18)$$

Here, u_n is the specific internal energy of species n ; the summation is over all species of gas mixture.

Here u_n is the specific internal energy of the n th species; the summation is over all species of gas mixture. The further conversion of Eq (4.17) is similar to the conversion of Eq (4.6) (Section 4.1); this gives us the familiar equation for the gas temperature:

$$\frac{dT}{dt} = -\frac{1}{\rho\bar{c}_v} \sum_n U_n w_n \quad (4.19)$$

where \bar{c}_v is the mean specific heat capacity at constant volume in mass units (J/g K or cal/g K), U_n is the internal energy of the n th species in molar units (J/mol or cal/mol),

$$U_n = m_n u_n. \quad (4.20)$$

Initial conditions. As previously mentioned, the differential equations for species and temperature ((4.16), (4.19)) must be accompanied by initial conditions. In the reaction vessel, pressure P_0 , temperature T_0 and species mass fractions Y_{n0} must be specified at a time instant $t=0$.

5. Example of calculation

In order to illustrate the discussed above theory, we consider a simple gas-phase system consisting of H_2 , O_2 and Ar. The simulation of chemical processes was carried out with a computer program Chemked [1]. The thermodynamic data and detailed reaction mechanisms of hydrogen combustion [10] was used. We will examine constant pressure and constant volume processes that start at the identical initial conditions:

$$P_0 = 0.3 \text{ atm}$$

$$T_0 = 900 \text{ K}$$

$$X_{H_2} : X_{O_2} : X_{Ar} = 0.05 : 0.025 : 0.925$$

Results of the calculation are presented in Fig. 5.1 and 5.2. Here we call attention on some qualitative features of the results only. As seen from the figures, the gas temperature is notable greater in the constant volume process. In reaction system, the temperature elevation is a result of transformation of the heat released in chemical reactions into the internal energy of gas. At constant volume, the heat of reactions goes totally into the internal energy (Eq. (3.9)). At constant pressure, a part of the heat of reactions is used for the work of gas expansion and rest of the heat goes into the internal energy (Eq. (3.8)). For these reasons, there is a difference in the calculated temperatures in Fig. 5.1 and 5.2. One must also pay attention to the fact that the final species concentrations are greater at the constant volume.

In constant pressure process, the reaction volume changes and we can determine the degree of the expansion (contraction), Eq. (4.1). In particular, for conditions of Fig. 5.1 the volume increases by the factor 1,58.

6. Conclusion

The equations of gas phase chemical kinetics are derived. These equations are the differential equations for temperature and species concentrations describing processes in a reaction vessel at

constant pressure and constant volume, Eqs. (4.5, 4.14, 4.16, 4.19). Now we summarize the requirements for use of these equations. Let us consider a gas-phase reaction system. We select a volume inside the system. The equations will describe chemical evolution of the selected gas volume if the following conditions are satisfied.

- There are no mass fluxes through the boundary of the volume; the gas mass in the volume is constant.
- There are no heat fluxes through the boundary of the volume; well insulated boundaries.
- There are no temperature and species gradients within the volume; the gas in the volume is always uniform.
- Course of chemical reactions takes place at
 - a. constant volume
 - b. constant pressure

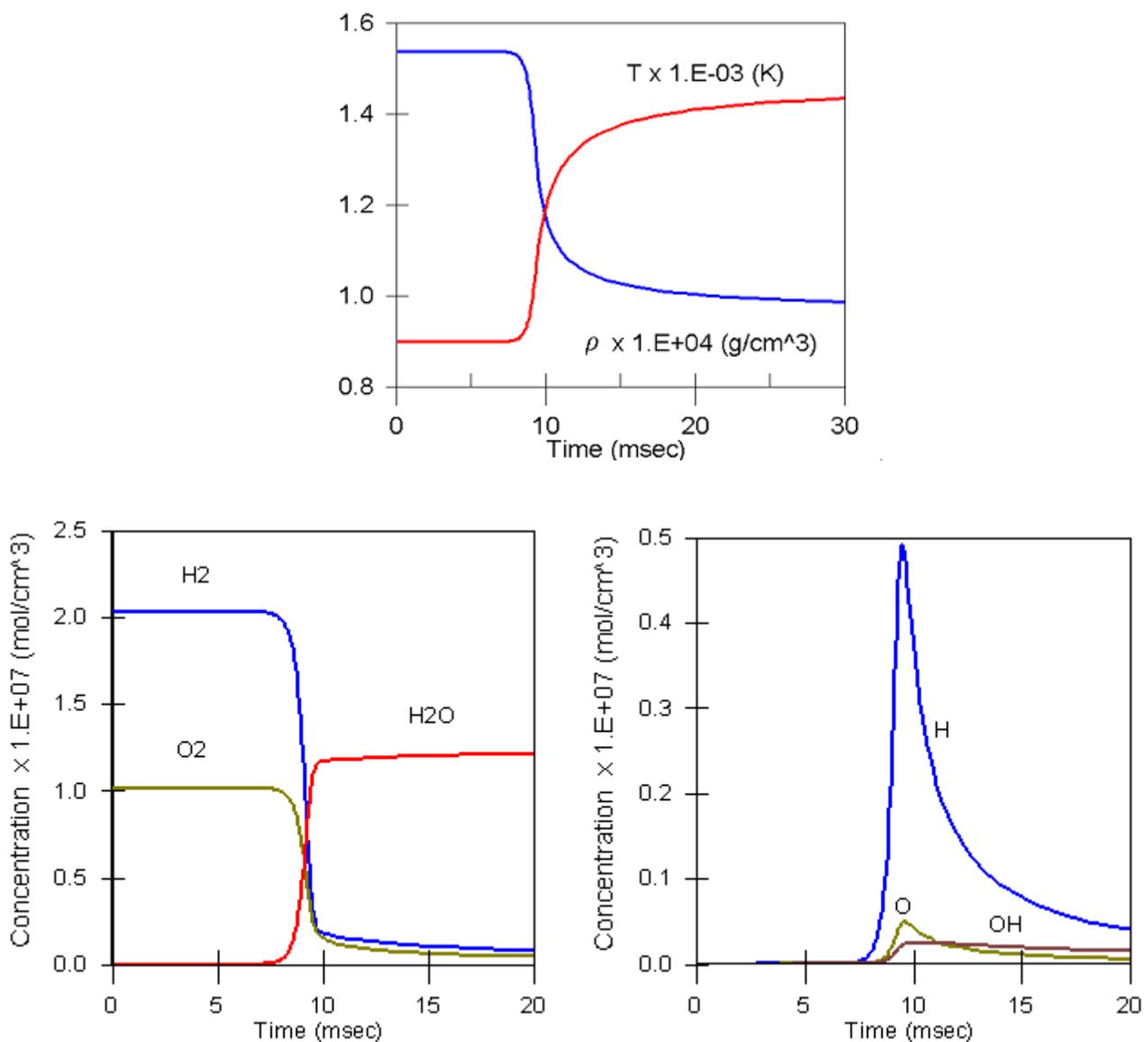


Figure 5.1. Temperature, mass density and species profiles of H₂/O₂/Ar mixture, constant pressure process

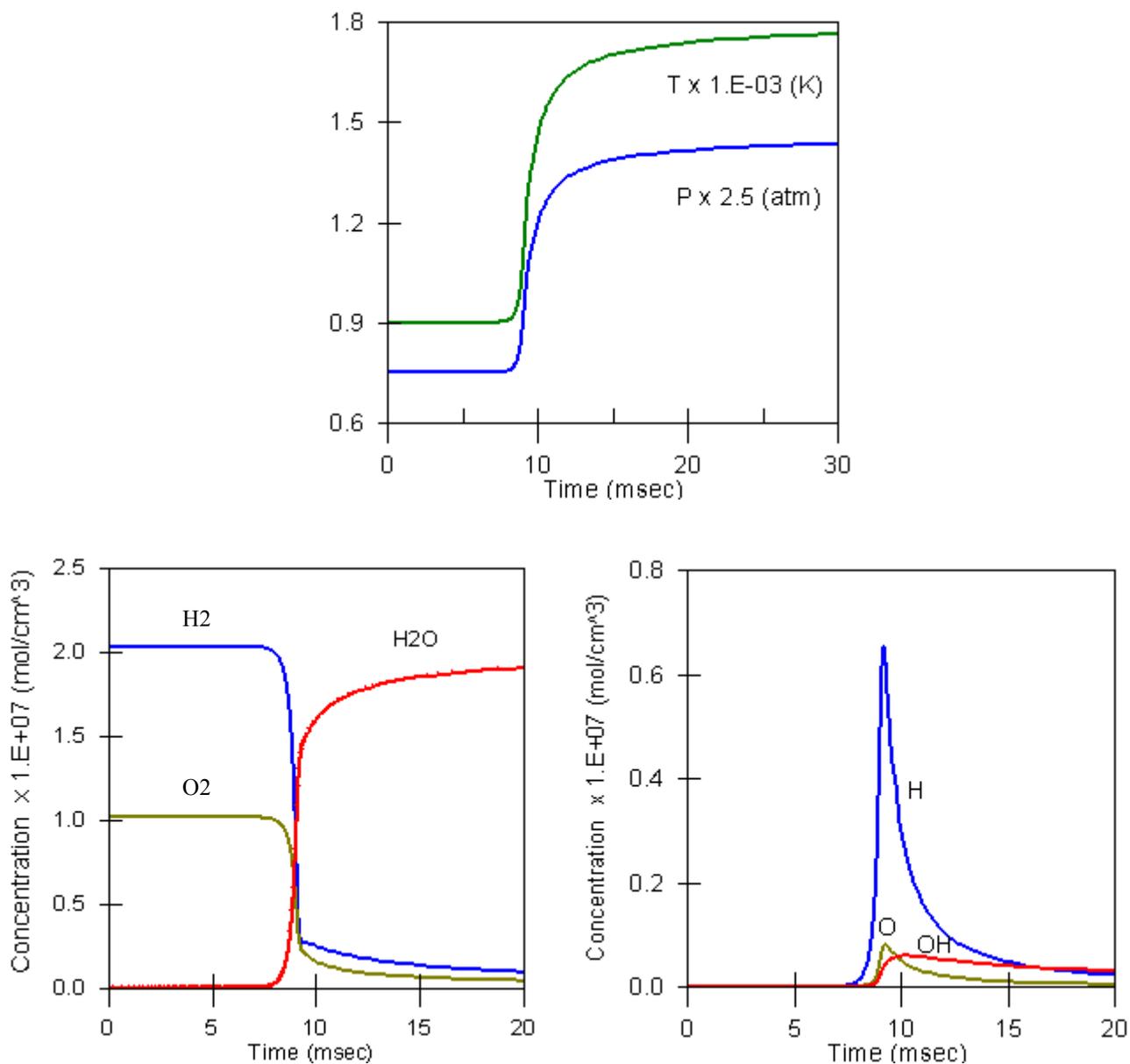


Figure 5.2. Temperature, pressure and species profiles of $H_2/O_2/Ar$ mixture, constant volume process

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Nomenclature

c_{pn}	specific heat capacity at constant pressure of the n th species	(cal/g K), (J/g K)
\bar{c}_p	mean specific heat capacity at constant pressure	(cal/g K), (J/g K)
\bar{c}_v	mean specific heat capacity at constant volume	(cal/g K), (J/g K)
C_{tot}	total gas concentration	(1/cm ³), (mol/cm ³)
h_n	specific enthalpy of the n th species	(cal/g), (J/g)
h	mean specific enthalpy of a mixture	(cal/g), (J/g)
H_n	molar enthalpy of the n th species	(cal/mol), (J/mol)
$k_{j,for}$	forward rate constant of the j th reaction	depends on reaction
$k_{j,rev}$	reverse rate constants of the j th reaction	depends on reaction
K_j	equilibrium constant for the j th reaction	depends on reaction
m_n	molecular weight of the n th species	g/mol
\bar{m}	mean molecular weight of a gas mixture	g/mol
M	total mass of gas mixture in reaction vessel	g

P	pressure	atm
$q_{j,for}$	forward rate of the j th reaction	(1/cm ³ sec), (mol/cm ³ sec)
$q_{j,rev}$	reverse rate of the j th reaction	(1/cm ³ sec), (mol/cm ³ sec)
q_j	rate-of-progress of the j th reaction	(1/cm ³ sec), (mol/cm ³ sec)
Q_j	heat of the j th reaction	(cal/mol), (J/mol)
R	universal gas constant	(cal/mol K), (J/mol K)
s_j	rate of heat production of the j th reaction	(cal/cm ³ sec), (J/cm ³ sec)
t	time	sec
T	temperature	K
u_j	rate of heat production in the j th reaction	(cal/cm ³ sec), (J/cm ³ sec)
u_n	specific internal energy of the n th species	(cal/g), (J/g)
\bar{u}	mean specific internal energy	(cal/g), (J/g)
U_n	internal energy of the n th species	(cal/mol), (J/mol)
V	volume of reaction vessel	cm ³
w_{jn}	production rate of species n in the j th reaction	(1/cm ³ sec), (mol/cm ³ sec)
X_n	mole fraction of the n th species	
$[X_n]$	concentration of the n th species per unit volume	(1/cm ³), (mol/cm ³)
Y_n	mass fraction of the n th species	
Z_n	concentration of the n th species per unit mass	(1/g), (mol/g)
ν_{jn}	stoichiometric coefficient of the n th species in the j th reaction	
χ_n	chemical symbol of species n	
ρ	mass density	g/cm ³

Subscripts

p	constant pressure process
v	constant volume process
n	species number
j	reaction number