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On the analytic calculation of premixed flames

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Technische Hogeschool Delft

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SUMMARY

In the present report, a method is presented which allows for the analytic calculation of temperature, concentration, and velocity profiles in premixed flames. The method is based on two, physically tractable assumptions:

- i heat transfer is only a determining factor at the cold boundary
- ii the temperature rise in the major portion of the flame is a linear function of the relative concentration of reactants.

As a result of these assumptions, a simple quadrature for the temperature can be derived which is related to the location where that temperature is reached.
A necessary requirement for the analytic solution is that the combustion can be described by an overall arbitrary order Arrhenius reaction, but there are no restrictions on the value of the stoichiometric coefficient.
The method also immediately allows to see the effect of various parameters, such as pressure, pre-exponential factor, stoichiometric coefficient, and molar mass on the temperature profile.

To verify the validity of the method, the results of the analytic calculations are compared with the results of a numerical integration of the differential equations, describing the flame.

In general there is an excellent agreement between the two methods.

Results are presented in graphical and tabular form, which also allows to see the effect of just one parameter on the temperature, concentration and velocity profiles, the flame temperature and the temperature gradients.

CONTENTS

NOMENCLATURE

A - Frequency Factor
C_1 - Mass flow rate
C_p - Molar heat capacity
C_{p_k} - Molar heat capacity of reactants
C_{p_p} - Molar heat capacity of products
E - Activation energy
ΔH_f^o - Molar heat of formation of products
H_k^o - Enthalpy of the reactants
k - Reaction rate
K - Concentration of reactants
K_o - Concentration $K + \nu P$
m - Order of reaction
$\bar{M}$ - Mean molar mass of mixture
M_k - Molar mass of reactants
M_p - Molar mass of products
p - Pressure
P - Concentration of products
p_t - total pressure
q - Heat transfer rate
r - Burning rate of propellent
R_o - Universal Gas Constant
T - Temperature
T_F - Flame temperature
V - Gas velocity
x - Distance from burning surface

ε - Parameter in energy equation
λ - Heat conduction coefficient
ν - Stoichiometric coefficient
ρ - Density
ρ_b - Propellant density
θ - Activation temperature
τ - Temperature ratio θ/T

Subscripts:

S - Location at the burning surface
F - Location at x_F: distance from burning surface where flame temperature

T_F is achieved.

The specific variables used in the program description in Chapter 5 are defined within the text.

1. INTRODUCTION

For a long time in the history of mankind flames and fire must have fascinated and intrigued men. Evidence for this is found in the records of historical and findings from prehistorical times. The ancient Greek had their god Prometheus and considered fire as one of the four basic elements; the germanic people worshipped the goddess Frig, the goddess of mariage but also the fire was devoted to her. Someone, such as a blacksmith in those days, who was able to control fire and use it for his own benefit or the interest of mankind was highly esteemed by his society.
One of the reasons for ancient people to be fascinated by, and afraid for fire may have been their inability to understand the phenomenon.

With the advent of the physical sciences, flames for a long time remained an area not well understood, although fire found many industrial applications. It should be recalled that, while the solid and liquid states of aggregation were known for a long time, on a historical time scale the existance of a gasphase was realized only recently. The concept was introduced by Stevin, who derived the name from the greek "chaos", indicating that the constituing elementary particles were organized in a chaotic way. As gas is a major and essential constituant of flames, people could not have a grasp for the nature and character of flames before obtaining some elementary understanding about the nature of gases. Even nowadays flames are only understood poorly, especially if one means by 'understanding' ones ability to describe in detail all relevant aspects and mutual relations between the variables that govern combustion.

Nowadays we are well aware that one may distinguish between two basic types of flames:
premixed flames, which are primarily governed by chemical kinetics, and
diffusion flames, where diffusion of species largely controls the flame.
Of course most 'real' flames are neither purely premixed flames nor pure diffusion flames but somewhere 'in between'.

At present it does not seem possible to analyze in detail all relevant aspects of flames. An excellent example is found in a recent paper by Gardiner(1), which illustrates that even for a simple type of flames, such as the H_2-O_2 flame, so much information about the detailed reaction mechanism is still lacking that such a flame escapes precise analysis. However, it is possible nowadays to approach the problem of describing flames by assuming overall reaction mechanisms, while minute analyses of the occurring flow patterns have become possible. Whether one deals with a premixed flame or a diffusion flame, the flow phenomena strongly affect the flame and its structure, and it is not surprising therefore that many of the contributions to the advance of combustion science have been and still are being made by aerodynamicists.

In the present work we deal with the overall analysis of a premixed flame. Although premixed flames are not the ones encountered most commonly, they still form an important class of flames. Such flames may arise in the combustion of rockets and gun propellants. Especially if a homogeneous propellant is used, the pyrolysis products are a homogeneous mixture of fuel and oxidizer and the resulting flame belongs to the purest type of premixed flames that occur in practical situations.

In an early analysis of such a type of flame, von Kàrmàn(2) had to use a so-called ignition temperature, because he considered the entire space $-\sim < x < \sim$ and hence he had to impose his boundary conditions as:

$$x \to -\sim \qquad T = T_o \ , \ dT/dx = 0,$$
$$x \to \ \ \sim \qquad T = T_F \ , \ dT/dx = 0.$$

This introduced a basic difficulty: as it was observed, or posed for the problem that at $x = 0$ there were no products present, and according to elementary kinetic theory reactions should have taken place in the halfspace $-\sim < x \leq 0$, a contradiction resulted. This contradiction could be solved by assuming that reactions would only occur for $T > T_i$, the ignition temperature. Now if $T_i > T\ (x=0)$ the contradiction was abolished. Nevertheless, the ignition temperature is an arbitrary and, as will turn out an unnecessary artificial concept. Hirschfelder(3) et al. did not use the concept of an ignition temperature, but instead used the concept of a flameholder, acting as a heat sink which is held at a constant temperature. Behind the heat sink no appreciable reactions are assumed to take place, and a reactive mixture is thought to emanate from the flameholder. This model seems to approach the physical reality better than the concept of an ignition temperature.

For a buring homogeneous solid propellant the flameholder concept looks very realistic as indeed a heat flow from the hot flame is required to heat up, decompose and/or vaporize the propellant. It is therefore perhaps not surprising that one of the first attempts(4) to describe a premixed flame in detail has been made for burning solid propellants. As the resulting system of differential equations, even for a planar, or one-dimensional flame is highly non-linear, Denison et al.(4) approximated their solution for the case of an (extremely) large activation energy. This approach has been followed by many other investigators such as Carrier et al.(5), Buckmaster et al.(6) and Kassoy et al.(7), to name a few. Carrier et al(5) discarded the idea of the flameholder concept and had to modify their kinetics artificially to overcome the cold boundary difficulty. Buckmaster et al(6) and Kassoy et al(7) do not make use of artificial concepts such as 'ignition temperatures' or 'modified kinetics' but correctly assume some form of heat transfer at the cold wall. In all cases, however, asymptotic expansions accompanied by complicated mathematical analyses are necessary to obtain solutions. Often these analyses have been limited to first order unimolecular reactions, be it that this is not always a necessary condition.

The present work shows that in those cases where diffusion effects may be neglected, a simple analytic solution may be obtained for flames which can be described by an overall gasphase reaction:

$$\nu K \overset{k}{\rightarrow} P \ , \tag{1.1}$$

of arbitrary order of reaction, while no conditions have to be imposed on the activation energy. The analysis turns out to yield accurate results, independently of the magnitude of the activation energy. An important assumption is that for the major part of the flame, the ratio of the concentration of products and the initial concentration of reactants is a linear function of a temperature difference. Although this follows from an approximate solution of the governing differential equations, it is basically a statement that conductive heat transfer is negligible as compared to the heat generated by the combustion reaction. This conclusion is not new in itself. It has been drawn before by Denison et al(4) and Williams(8), although its implications have not been pursued. In fact Denison et al. and Williams allow for diffusion effects, which have been neglected in the present work, and then too the assumption that the heat generation by combustion by far exceeds heat flow rates due to diffusion and conduction seems to hold for the major part of the flame. In cases that this assumption fails, the analytic method may lead to erroneous results.
To check the validity of the newly developed approach, the results of the analytic solution have been compared with numerical solutions. It turns out that for a very wide range of parameters, the analytic solution yields results that very

closely match the numerical solution, indicating the validity of the method.

The importance of the analysis is that it is now possible to give analytic relations between the various parameters that determine the flame, i.c. temperature-, concentration-, and velocity-distributions, while it also shows that if the solution is known for one combination of parameters, solutions for other combinations of parameters may be obtained by a simple coordinate transformation. It therefore yields a clear insight in the effects of various physical parameters on the flame structure.

In how far this approach yields valuable results for 'real' flames is difficult to say as the combustion reaction is modeled as an overall reaction, and it is known(1) that actual reactions are far more complicated. In this respect the new approach is neither better nor worse than many existing methods for describing premixed flames, but it is more tractable, and not limited by the condition of large activation energies.

One final remark should be made. It has been common practice in flame theory to consider the 'flame-stand-off distance' or 'flame thickness'. It appears from the present analysis that this concept in reality does not exist. Reactions take place in the half space $0 \leq x < \sim$ and a flame thickness or flame stand-off-distance could only be defined as the location where only α percent reactants are still present or where the temperature ratio $(T_f - T)/(T_F - T_s) = \beta$.
Whether this still is a useful concept is doubtful. It may be that one has to consider 'flame thickness' as artificial a concept as 'ignition temperature' or 'cold boundary difficulty', namely a concept that has been introduced by an ill-posed question or statement.

2. GOVERNING EQUATIONS

We consider one very simple case of a gaseous flame where a binary mixture of ideal gases undergoes a direct one-step reaction:

$$\nu K \rightarrow P \ . \qquad (2.1)$$

The reactant concentration is denoted by K; the product concentration by P. In fact this may be regarded as an elementary model for a premixed flame. If the reactant consists of a mixture of gases, K represents the mean reactant concentration; similar arguments apply for the product concentration, P. For the reaction itself, an arbitrary order Arrhenius law may be applied. In the present analysis we will only concern ourselves with planar flames, so that a one-dimensional analysis suffices. In addition we will ignore any effects of diffusion; this at the same time limits the applicability of the present model to those types of flames, where diffusion velocities are much smaller than the mean flow velocities. We do account specifically for heat conduction. To keep the treatment simple the thermal properties, i.e. λ, C_{p_K}, C_{p_P} and ΔH_f^o are assumed to be independent of the temperature. The heat capacities of the reactant, C_{p_K} and of the product, C_{p_P}, are assigned different values; in fact we take

$$C_{p_P} = \nu C_{p_K} = \nu C_p \ .$$

The conservation equations for a steady state flame are:

$$\text{Conservation of mass: } \frac{d}{dx}(\rho v) = 0 \ . \qquad (2.2)$$

$$\text{Conservation of reactants: } \frac{d}{dx}(Kv) + \nu k K^m = 0 \ . \qquad (2.3)$$

$$\text{Conservation of products: } \frac{d}{dx}(Pv) - k K^m = 0 \ . \qquad (2.4)$$

In these equations, the order of reaction is m while k represents the (forward) reaction rate, usually represented by an Arrhenius law.
Although the pressure usually does not change significantly over the flame, there may be (very) large pressure gradients, causing changes in gas velocity. Therefore, the equation for conservation of momentum is retained:

$$\rho v \frac{dv}{dx} + \frac{dp}{dx} = 0 \ , \qquad (2.5)$$

and finally the energy equation for the whole flame may be written as:

$$\frac{d}{dx}\left[v \left\{ (K + \nu P) H_K^o + P \, \Delta H_f^o \right\} \right] - v \frac{dp}{dx} + \frac{dq}{dx} = 0 \ . \qquad (2.6)$$

In this equation H_K^o is the enthalpy of the reactants at a temperature, T, and as we assumed C_p to be independent of T, $H_K^o = C_p(T - T_{ref})$. Because $C_{p_P} = \nu C_{p_K}$

it is most simple to refer to only one heat capacity $C_p = C_{p_K}$. Moreover, ΔH_f^o is the heat of formation of one mol of product P, and q represents the heat flow rate, which in our case is assumed to be purely due to conduction. Finally, some additional equations are required to relate the variables to each other. The equation of state relates concentrations, temperature and pressure:

$$p = (P + K)R_oT \ , \tag{2.7}$$

the density, ρ, follows from

$$\rho = KM_k + PM_p = (K + \nu P)M_K \ , \tag{2.8}$$

and an Arrhenius law is applied for the reaction rate:

$$k = A \exp\left(\frac{-\theta}{T}\right) \ , \tag{2.9}$$

where θ is the activation temperature,

$$\theta = E/R_o \ . \tag{2.10}$$

Finally the heat transfer rate is given by

$$q = -\lambda\frac{dT}{dx} \ . \tag{2.11}$$

By solving this system of Equations for the appropriate boundary conditions, one obtains the temperature-, velocity-, concentration- and, if required, pressure profiles for the flame.

3. APPROXIMATE ANALYTIC SOLUTION

3.1. Boundary Conditions

We will assume that there is only heat transfer at the cold boundary. At the cold boundary gaseous reactants flow into the system, which ensures that we enter the flame with 100 % reactants. For a premixed, laminar flame, this would be a fairly difficult situation to realize in practice, as always some reactions, however slow, must be taking place. One practicable way to achieve physically a 100 % concentration of reactants is to have a pyrolyzing, homogeneous propellant at the cold boundary, or an evaporating liquid or solid. Buchmaster, Kapila and Ludford have analyzed this problem for the case of a large activation energy(1). Others, like Von Kàrmàn(2) have used the concept of an ignition temperature to ensure that at the cold boundary (and beyond) no reactions take place. Bush and Fendell(3) modified the Arrhenius pre-exponential factor to ensure that at the cold boundary no reactions would take place. For a cold boundary consisting of a pyrolyzing or evaporating solid or liquid one indeed has the physical situation of 100 % reactants at the cold boundary. In that case a temperature gradient is required to ensure the necessary heat flow rate into the cold boundary for the evaporation, heating and/or pyrolysis of the cold material. If a premixed gas, via a flameholder is injected into the flame, one has to realize that the reactant concentration might be slightly less than 100 %, but again there will be a temperature and concentration gradient at the cold boundary, and the flameholder acts as a heat sink. This concept has been used before by Hirschfelder, Curtiss and Campbell(3). Therefore the cold boundary conditions are:

$$x = 0 \ : \ \left.\begin{aligned} T &= T_s \ , \\ \frac{dT}{dx} &= \left(\frac{dT}{dx}\right)_s \ , \\ P_s &= o \ , \end{aligned}\right\} \qquad (3.1)$$

and also the mass flow rate is given:

$$\rho v = (\rho \ v)_s = (M_k \ K \ v)_s = C_1 \ . \qquad (3.2)$$

The index s denotes cold boundary conditions. The cold boundary is situated at the location x = 0 while the temperature gradient still is undetermined.

After that complete combustion has been achieved, one obtains

$$\left.\begin{aligned} T &= T_F , \\ \left(\frac{dT}{dx}\right)_F &= 0 \ , \\ K &= 0 \ , \end{aligned}\right\} \qquad (3.3.)$$

It should be realized that the boundary conditions (3.1) and (3.3) are not independent of each other. Moreover, complete combustion will only be achieved for $x \rightarrow ∿$.

3.2. Solutions

Integration of the Eqs. (2.2) and (2.5) yields for the mass flow rate, C_1:

$$C_1 = \rho v = \rho_F v_F = \rho_s v_s \, , \tag{3.4}$$

and for the momentum equation:

$$\rho v^2 + p = \frac{C_1^2}{\rho} + p = \frac{C_1^2}{\rho_F} + p_F = \frac{C_1^2}{\rho_s} + p_s = p_t \, , \tag{3.5}$$

which states that the total pressure is constant.
Together with the Equation of State, Eq. (2.7) we immediately note:

$$v_F = \frac{C_1}{M_p p_F} R_o T_F \quad ; \quad v_s = \frac{C_1}{M_K p_s} R_o T_s \, , \tag{3.6}$$

which yields the ratio of the gas velocities at the flame and the cold boundary:

$$\frac{v_F}{v_s} = \frac{1}{\nu} \frac{T_F}{T_s} \frac{p_s}{p_F} \, . \tag{3.7}$$

Although the pressure gradients may be very large, the pressure itself, in many cases does not change significantly; therefore in many cases one may, for a first approximation put

$$\frac{v_F}{v_s} \approx \frac{1}{\nu} \frac{T_F}{T_s} \, . \tag{3.8}$$

The pressure follows from

$$p_F + \frac{C_1^2 R_o T_F}{M_p p_F} = p_s + \frac{C_1^2 R_o T_s}{M_K p_s} = p_t \, , \tag{3.9}$$

and usually

$$p >> \frac{C_1^2 R_o T}{\bar{M} p} \, .$$

One is free to choose one of the variables ρ_s, p_F or p_t as the "known" pressure; the other pressures then follow. Usually, and especially for rocket motor applications where one often deals with a pyrolyzing propellant or an evaporating liquid, the pressure at or after the flame, or the total pressure is measured.
So from a practical point of view it is most simple to assume p_F or p_t as being known. Assuming p_t to be known, the cold boundary pressure, p_s, follows from:

$$p_s = \frac{1}{2}\left(1 + \sqrt{1 - 4\,\frac{C_1^{\,2}\;R_o T_s}{p_t^{\,2}\;M_K}}\right) p_t \quad . \tag{3.10}$$

It is convenient to introduce a new variable, K_o, the overall concentration:

$$K_o = K + \nu P \quad . \tag{3.11}$$

At the cold boundary: $P = 0$, $K_o = K$, while at flame conditions: $K = 0$, $K_o = \nu P$. It is immediately seen that $K_o = \rho/M_K$, and hence by virtue of Eq. (3.4)

$$K_o v = C_1/M_K = \text{constant} \quad . \tag{3.12}$$

The energy equation, Eq. (2.6) may be written in the following form, which is most convenient:

$$c_p \frac{dT}{dx} - \frac{\Delta H_f^{\,o}}{\nu K_o v}\frac{d\,Kv}{dx} + \frac{1}{2} M_K \frac{d\,v^2}{dx} - \frac{\lambda}{K_o v}\frac{d^2\,T}{dx^2} = 0 \tag{3.13}$$

Use has been made of the assumption that c_p, λ and $\Delta H_f^{\,o}$ do not depend on the temperature, while the pressure gradient has been replaced by the gradient of kinetic energy with the help of the momentum equation. It is seen that Eq. (3.13) may be integrated once to yield:

$$c_p T - \frac{\Delta H_f}{\nu}\frac{K v}{K_o v} + \frac{1}{2} M_K\, v^2 - \frac{\lambda}{K_o v}\frac{dT}{dx} = c_p T_s - \frac{\Delta H_f}{\nu} + \frac{1}{2} M_K v_s^{\,2} - \frac{\lambda}{K_o v}\left(\frac{dT}{dx}\right)_s = c_p T_F + \frac{1}{2} M_K v_F^{\,2} \quad . \tag{3.14}$$

In most cases the kinetic energy, and especially the change in kinetic energy is very small as compared to the change in thermal energy due to the temperature rise as a result of combustion. To obtain an approximate analytic solution, we therefore neglect the kinetic energy term and we are left with

$$c_p T - \frac{\Delta H_f}{\nu}\frac{K v}{K_o v} - \frac{\lambda}{K_o v}\frac{dT}{dx} = c_p T_F \quad . \tag{3.15}$$

Integration of Eq. (3.15) together with (2.3), the appropriate boundary conditions and the equations that provide the relationship between the other variables gives the temperature-, concentration-, velocity- and pressure profiles over the flame.

Now for all practical problems, λ, the heat conduction coefficient, is a very small number. However, as heat conduction plays a major role at the cold boundary we cannot just neglect this term. At the cold boundary there is a substantial heat transfer rate while in many cases the reaction rates are only minute. For those parts of the flame where there is a substantial heat release due to combustion, heat conduction, although very large due to the large temperature

gradients hardly affects the flame structure.
Therefore the problem may be split into two parts: a high temperature regime where temperature changes are primarily due to combustion reactions, and a low temperature regime where hardly any combustion takes place and temperature changes are primarily due to conductive heat transfer.
After a, often slow, temperature rise near to the cold boundary, reactions are going to take place at ever greater pace and very soon heat conduction effects become negligible as far as the temperature profile itself is concerned. At the end of the flame, all reactants have been consumed and $Kv \rightarrow 0$ like the temperature gradient as a constant flame temperature is achieved.
Therefore, let us rewrite Eq. (3.15) in terms of a small parameter ε, undefined as yet:

$$C_p \frac{dT}{dx} - (1-\varepsilon)\frac{\Delta H_f^o}{\nu K_o v}\frac{dKv}{dx} - \varepsilon\frac{\Delta H_f^o}{\nu K_o v}\frac{dKv}{dx} - \frac{\lambda}{K_o v}\frac{d^2T}{dx^2} = 0 \qquad (3.16)$$

where $|\varepsilon| << 1$ and ε should be related to $\lambda/K_o v$.
The first two terms of Eq. (3.16) constitute a differential equation with zeroth order coefficients. So Eq. (3.16) may be split into two parts which have to be satisfied simultaneously:

$$C_p \frac{dT}{dx} - (1-\varepsilon)\frac{\Delta H_f^o}{\nu K_o v}\frac{dKv}{dx} = 0 , \qquad (3.17)$$

and

$$-\varepsilon\frac{\Delta H_f^o}{\nu K_o v}\frac{dKv}{dx} - \frac{\lambda}{K_o v}\frac{d^2T}{dx^2} = 0 \qquad (3.18)$$

This model therefore assumes that the conductive heat flow immediately causes reactions to occur.
Equation (3.17) has the extremely simple solution

$$\frac{K}{K_o} = -\frac{\nu C_p (T_F - T)}{(1-\varepsilon)\,\Delta H_f^o} , \qquad (3.19)$$

and as for $T = T_s$, $K = K_{os}$, we have

$$T_F - T_s = \frac{-\Delta H_f^o}{\nu}\frac{1-\varepsilon}{C_p} , \qquad (3.19a)$$

and

$$\frac{K}{K_o} = \frac{Kv}{K_o v} = \frac{T_F - T}{T_F - T_s} . \qquad (3.20)$$

This is a very important result. It tells us, that independently of the reaction mechanism, the concentration ratio is a linear function of the actual and maximum temperature rise. With the definition of K_o, Eq. (3.11), one immediately obtains:

$$\frac{P}{K_o} = \frac{1}{\nu}\frac{T - T_s}{T_F - T_s} . \qquad (3.21)$$

Integration of Eq. (3.18) yields

$$\varepsilon \frac{\Delta H_f}{\nu} \frac{Kv}{K_o v} + \frac{\lambda}{K_o v} \frac{dT}{dx} = \text{constant}, \qquad (3.21a)$$

and by substituting Eq. (3.19) we obtain

$$\frac{\varepsilon}{1-\varepsilon} C_p (T_F - T) - \frac{\lambda}{K_o v} \frac{dT}{dx} = \text{constant} .$$

Now as for $T \rightarrow T_F$, $\frac{dT}{dx} \rightarrow 0$ we finally get

$$\frac{T_F - T}{T_F - T_s} = \exp \left\{ - \frac{C_p K_o v \varepsilon}{\lambda(1-\varepsilon)} x \right\} , \qquad (3.22)$$

as for $T = T_s$ the cold boundary, $x = 0$. The small parameter ε has still to be determined. For the determination of ε we have to apply the reaction mechanism. Therefore, Eq. (3.19) is substituted in the equation for conservation of reactants, Eq. (2.3), where it should be recalled that $K_o v$ is constant. This leads to

$$\frac{dKv}{dx} = \frac{\nu C_p K_o v}{(1-\varepsilon)\Delta H_f^o} \frac{dT}{dx} = - \nu k K^m = - \nu A \exp \left(\frac{-\theta}{T}\right) K^m ,$$

or

$$\frac{dT}{dx} = \frac{-(1-\varepsilon)}{C_p} \frac{\Delta H_f}{K_o v} A K_{os}^m . \exp \left(\frac{-\theta}{T_s}\right) \left[\exp \left(\frac{\theta}{T_s} - \frac{\theta}{T}\right) . \left(\frac{K}{K_{os}}\right)^m \right], \qquad (3.23)$$

and with Eq. (3.22) we obtain

$$\frac{dT}{dx} = (T_F - T_s) \frac{C_p K_o v \varepsilon}{\lambda(1-\varepsilon)} \left[\exp \left(\frac{-C_p K_o v \varepsilon}{\lambda(1-\varepsilon)} x \right) \right] . \qquad (3.24)$$

Obviously, these expressions have to be "more or less" identical. Now at the cold boundary, i.e. at $x = 0$, $T = T_s$ and $K = K_{os}$ and the terms between brackets, in Eq. (3.23) as well as in Eq. (3.24) go to unity. At flame conditions, i.e. $x \rightarrow \sim$, $T = T_f$ and $K = 0$, the terms between brackets in the Eqs. (3.23) and (3.24) both approach zero as is requested. Therefore, the temperature gradients behave in a similar way at the two boundaries. To encertain that for $x = 0$, both the temperature gradients, as given by the two equations, are the same, we have to require that

$$\frac{-(1-\varepsilon) \Delta H_f^o}{C_p K_o v} A K_{os}^m \exp \left(\frac{-\theta}{T_s}\right) = \frac{C_p K_o v \varepsilon}{\lambda(1-\varepsilon)} (T_F - T_s) , \qquad (3.25)$$

which determines the small parameter ε.
Eliminating the heat of formation, ΔH_f^o, we obtain

$$\varepsilon = \frac{\dfrac{\lambda}{C_p(K_o v)^2}\ \nu A \exp\left(\dfrac{-\theta}{T_s}\right) K_{os}^{\ m}}{1 + \dfrac{\lambda}{C_p(K_o v)^2}\ \nu A \exp\left(\dfrac{-\theta}{T_s}\right) K_{os}^{\ m}} \tag{3.26}$$

and the analysis will hold provided that

$$\frac{\lambda}{C_p(K_o v)^2}\ \nu A \exp\left(\frac{-\theta}{T_s}\right) K_{os}^{\ m} << 1 \tag{3.27}$$

This parameter may be regarded as a quantity which tells us how fast (or slow) a relative change in the composition, initially takes place as compared with the relative contribution of heat conduction to the initial enthalpy change. For small values of ε this implies that initially there is hardly any change in the composition and the change in enthalpy is mainly due to conduction. This condition may be satisfied for a large class of laminar flames. Usually, even for small activation temperatures and high cold wall temperatures, the change in composition initially remains small, and for most gases, λ is a fairly small number, while the molar heat capacity, C_p, is very large. It is seen that, as long as the condition, in eq. (3.27) is satisfied, there is no restriction as to the magnitude of the activation temperature. The effect of heat transfer is felt through a reduction in the flame temperature, as compared to the adiabatic flame temperature. The flame temperature follows from

$$T_F = T_s - \frac{\Delta H_f^{\ o}/\nu}{C_p + \dfrac{\lambda}{(K_o v)^2}\ \nu A \exp\left(\dfrac{-\theta}{T_s}\right) K_{os}^{\ m}} , \tag{3.28}$$

and for $\lambda = 0$, one obtains the adiabatic flame temperature. Obviously, for $\lambda = 0$, the temperature gradient at the cold boundary is reduced and the reaction is "not helped" by heat conduction to initially raise the temperature.
The temperature gradient follows from substituting Eq. (3.26) into Eq. (3.23) which yields

$$\frac{dT}{dx} = \frac{-\Delta H_f^{\ o}}{C_p K_o v + \dfrac{\lambda \nu A}{K_o v} \exp\left(\dfrac{-\theta}{T_s}\right) K_{os}^{\ m}}\ A \exp\left(\frac{-\theta}{T}\right) K^m . \tag{3.29}$$

An analytic expression for the temperature as a function of location is obtained by integrating Eq. (3.29) w.r.t. x. To this end it is convenient to express the concentration K explicitly as a function of temperature. Combining the Eqs. (2.5), (2.7), (3.4), (3.11), (3.12) and (3.20), we obtain

$$\frac{K_o - (1-\nu) K_o \dfrac{T_F - T}{T_F - T_s}}{\nu} R_o T + \frac{C_1^{\ 2}}{K_o M_K} = P_t ,$$

which yields a quadratic equation for K_o. Although the exact solution could be taken, it is more convenient to use an approximate solution which if fairly accurate,

$$K_o = \frac{p_t \, \nu (T_F - T_s)}{R_o T \, [T - T_s + \nu (T_F - T)]} - \frac{C_1^2}{p_t M_K} , \tag{3.30}$$

and for K we obtain

$$K = \frac{p_t \, \nu (T_F - T)}{R_o T \, [T - T_s + \nu (T_F - T)]} - \frac{C_1^2}{p_t M_K} \, \frac{T_F - T}{T_F - T_s} . \tag{3.31}$$

After substitution of Eq. (3.31) into Eq. (3.29) we arrive at a simple quadrature:

$$- \int_{\theta/T_s}^{\theta/T} \frac{\exp(\tau) \, d\tau}{\tau^2 \left[\tau \left(\frac{T_F}{\theta} - \frac{1}{\tau} \right) \left\{ \frac{1}{\frac{1}{\tau} - \frac{T_s}{\theta} + \nu \left(\frac{T_F}{\theta} - \frac{1}{\tau} \right)} - \frac{C_1^2 R_o \theta}{p_t^2 \, \nu M_K \, \tau \left(\frac{T_F}{\theta} - \frac{T_s}{\theta} \right)} \right\} \right]^m} =$$

$$= \left(\frac{\nu p_t}{R_o \theta} \right)^m \cdot \frac{\nu M_K}{C_1} \cdot \left(\frac{T_F}{\theta} - \frac{T_s}{\theta} \right) . \, A \, . \, x , \tag{3.32}$$

where the flame temperature, T_F, follows from Eq. (3.28).
The quadrature of Eq. (3.32) is easily calculated on a computer or a (programmable) calculator.
The solution, Eq. (3.32), however shows some interesting properties. First of all it should be remarked that the term

$$\frac{C_1^2 \, R_o \theta}{p_t^2 \, \nu M_K \, \tau \left(\frac{T_F}{\theta} - \frac{T_s}{\theta} \right)}$$

is a very small number that hardly affects the numerical value of the quadrature. This is mainly because for most flames $p_t \geq 10^5$ N/m^2 so $p_t^2 \geq 10^{10}$ N^2/m^4. So the value of the quadrature is mainly determined by $\frac{T_F}{\theta}$, $\frac{T_s}{\theta}$, $\frac{T}{\theta}$, m, and ν.
This implies that for these parameters being constant, the value of the integral is constant, and hence, the right hand side of Eq. (3.32) must also be a constant. Denoting the distance to the cold boundary where the temperature has reached a value T*, by x*, it follows that

$$\left(\frac{p_t}{\theta} \right)^m \cdot \frac{M_K}{C_1} \, . \, A \, . \, x^* = \text{constant} .$$

So if a solution is known for one value of these parameters, the solution for another combination of parameters may directly be obtained by a simple coordinate transformation.
It should be recalled in this respect however, that to obtain reliable results two conditions have to be met:

i the kinetic energy has to remain negligibly small, as this contribution was neglected in the derivation

ii $|\varepsilon| << 1$.

The concentration and velocity profiles follow immediate now that the temperature distribution over the flame is known.

4. NUMERICAL SOLUTIONS

In the previous Section, an analytic solution for the temperature profile in a flame has been given. From the temperature profile, the other profiles are found directly.
As to compare the analytic solution with a numerical one, the differential equations are to be integrated numerically. In fact only two equations have to be integrated numerically, as the other equations yield for the one dimensional case, state, algebraic equations, relating the various variables. The two differential equations that are to be integrated are:

$$\frac{dT}{dx} = \frac{C_p K_o v \, (T - T_F)}{\lambda} - \frac{\Delta H_f^o}{\nu\lambda} Kv + \frac{1}{2} \cdot C_1 \cdot (v^2 - v_F^2) \; , \qquad (4.1)$$

and

$$\frac{dKv}{dx} = - \nu k K^m \; . \qquad (4.2)$$

The integration of the equation for conservation of reactants does not yield any difficulty. Integration of the energy equation, Eq. (4.1) however is not straight forward. In fact we have to meet boundary conditions at two ends

$x = 0 \quad K = K_o \quad T = T_s$
$x \rightarrow$ ∿ $\quad K = 0 \quad T = T_F$

We may replace the boundary conditions at $x \rightarrow$ ∿, however, by a statement about the temperature gradient at the cold boundary. To this end we will apply Eq. (3.29) for $T = T_s$ and $K = K_{os}$, and by virtue of Eq. (3.28), T_F is known so that v_F may be calculated from Eq. (3.8).
Nevertheless, one faces a practical difficulty. To illustrate this, one may consider the following differential equation:

$$\frac{dy}{dx} = Dy + G(x) \; , \qquad (4.3)$$

with the boundary condition that y remains limited for $x \rightarrow$ ∿.
The obvious homogeneous solution of Eq. (4.3) is

$$y = E.\exp(Dx) \; ,$$

and as y has to be a finite number for $x \rightarrow$ ∿ clearly $E \equiv 0$. This does not yield any difficulty for an analytic solution but for a numerical integration, the difficulties occur because, due to rounding-off errors the homogeneous solution will always be generated, and grow exponentially. Especially for large values of D, this will occur rapidly.
As in Eq. (4.1), $D = \frac{C_p K_o v}{\lambda}$, we deal here with a very large number, so that a direct numerical integration will blow up immediately. One way out of this dilemma, is to replace Eq. (4.3) (or Eq. (4.1)) by another differential equation that will generate the same particular solution, but not the homogeneous one.
The complete solution of Eq. (4.3) is

$$y = E.\exp(Dx) - \sum_{i=0}^{\sim} \frac{1}{D^{i+1}} \frac{d^iG}{dx^i} , \qquad (4.4)$$

where $\frac{d^iG}{dx^i}$ is the i-th derivative of the function G with respect to x and $G = \frac{d^oG}{dx^o}$
For large values of D, the series in Eq. (4.4) will converge rapidly if G is a well behaving function. For $E \equiv 0$, we hence obtain the solution for y, which indeed is bounded:

$$y = - \sum_{i=0}^{\sim} \frac{1}{D^{i+1}} \frac{d^iG}{dx^i} , \qquad (4.5)$$

and the replacing differential equation for Eq. (4.3) hence is

$$\frac{dy}{dx} = - \sum_{i=1}^{\sim} \frac{1}{D^i} \frac{d^iG}{dx^i} . \qquad (4.6)$$

A simple example may clarify this concept. For example suppose G(x) = B exp(-x), then Eq. (4.3) becomes

$$\frac{dy}{dx} = Dy + B\exp(-x) .$$

The complete solution is

$$y = E . \exp(Dx) - \frac{B}{D+1} \exp(-x) ,$$

and if one requires $\lim_{x \to \sim} y = 0$, then obviously

$$y = \frac{-B}{D+1} \exp(-x) .$$

On the other hand, we obtain from Eq. (4.5)

$$y = - \sum_{i=0}^{\sim} \frac{1}{D^{i+1}} \frac{d^iG}{dx^i} = - \frac{B.\exp(-x)}{D} \sum_{i=0}^{\sim} \left(\frac{-1}{D}\right)^i = - \frac{B\exp(-x)}{D+1} .$$

So, for the numerical integration of Eq. (4.1) this equation is replaced by the following differential equation:

$$\frac{dT}{dx} = - \sum_{i=1}^{\sim} \left(\frac{\lambda}{C_p K_o v}\right)^i \frac{d^i \left\{\frac{-\Delta H_f^o}{\nu\lambda} Kv + \frac{1}{2} . C_1 . (V^2 - V_F^2)\right\}}{dx^i} . \qquad (4.7)$$

which allows for a simple, direct integration. As $\frac{\lambda}{C_p K_o v}$ is a very small number, the series is converging rapidly, and usually two or three terms in the series will suffice to obtain the required accuracy.

5. PROGRAM DESCRIPTION

The computer program that has been develloped serves two purposes. Primarily it calculates the temperature, concentrations, concentration ratios, and gas velocities according to the analytic solution for a premixed gaseous flame, such as has been discussed in Section 3. Second, it integrates the differential equations describing such a flame numerically, as to allow for comparison of the analytic solutions with the numerical ones. One should bear in mind that this yields only information about the reliability of the analytic solution within the framework of the model.
The model necessarily is only a crude approximation of a real premixed gaseous flame, as the reaction kinetics will probably be much more complicated than has been assumed for this model. In addition diffusion has been neglected and also various thermodynamic properties have been assumed to be independent of the temperature.

If one integrates the differential equations for the flame, the x-coordinate is the independent variable, while the temperature and the reactant concentration ratio are the dependent variables. On the other hand, for calculating the quadrature, i.e. the analytic solution, the temperature is the independent variable while the x-coordinate becomes the dependent variable.

To allow for comparison between the numerical and analytic results, the differential equations are integrated over an interval Δx which yields the temperature $T(x+\Delta x)$.
Now the quadrature is calculated by integrating from $T(x)$ to $T(x+\Delta x)$, which yields the analytically obtained coordinate increment, Δx_a. Now for the same temperature, $T(x+\Delta x)$, we may compare $x + \Delta x$ with $x_a + \Delta x_a$.

A general outline of the program is given in Section 5.1, while the various procedures that are used in the program, and which require some clarifications are discussed in Section 5.2. Finally, a listing of the program that has been written in ALGOL60, is given in Section 5.3.

5.1. General outline

Generally the numerical solutions are calculated by means of the procedure Runner, which uses a Runge Kutta's method to integrate simultaneously the energy equation (4.1) and the equation for conservation of reactants (4.2). The resulting temperature and concentration of reactants are used to calculate the concentration of products and the gasvelocity.

The analytic solution of the problem as shown by equation (3.32) is calculated by procedure Intsig, using Simpsons rule for integration. In order to facilitate comparison of the numerical and analytic solutions, the procedure Intsig uses the temperature outputdata of procedure Runner as upper- and lower boundary for the integration of Eq. (3.32).

A general outline of the program is given in Fig. (1).

Numerical solutions (procedure Runner)

The functions to be integrated by the procedure Runner are

$$\frac{d\lambda T}{dx} = \frac{C_p K_o v}{\lambda} (\lambda T - \lambda T_F) - \frac{\Delta H_f}{\nu} K_o v \frac{Kv}{K_o v} + \frac{1}{2} \rho_b r (v^2 - v_F^2) \quad , \quad (5.1.1)$$

$$\frac{d\,\frac{Kv}{K_o v}}{dn} = -\nu e^{-\lambda\theta/\lambda T}\ (K)^m/K_o v \ . \tag{5.1.2}$$

For reasons discussed in Chapter 4, the integration of the energy equation (5.1.1) is not straight forward.

If we define

$$\varphi = \lambda T - \lambda T_F \quad , \tag{5.1.3}$$

$$\alpha = \frac{C_p\ K_o v}{\lambda} \quad , \tag{5.1.4}$$

$$\Gamma = -\frac{\Delta H_f}{\nu}\ K_o v\ \frac{K v}{K_o v} + \frac{1}{2}\ \rho_b r\ (v^2 - v_F^{\,2}) \ , \tag{5.1.5}$$

we may rewrite Eq. (5.1.1) as

$$\frac{d\varphi}{dx} = \alpha\varphi + \Gamma \ . \tag{5.1.6}$$

As shown in Chapter 2 we may replace Eq. (5.1.6) by

$$\frac{d\varphi}{dx} = -\frac{1}{\alpha}\frac{d\Gamma}{dx} - \frac{1}{\alpha^2}\frac{d^2\Gamma}{dx^2} - \frac{1}{\alpha^3}\frac{d^3\Gamma}{dx^3} - \ldots . \tag{5.1.7}$$

Neglecting terms of higher order, Eq. (5.1.7) may be rewritten as

$$\frac{d\varphi}{dx} = -\frac{1}{\alpha}\frac{d\Gamma}{dx} - \frac{1}{\alpha^2}\frac{d^2\Gamma}{dx^2} - \frac{1}{\alpha^3}\frac{d}{d\varphi}\left(\frac{d^2\Gamma}{dx^2}\right)\frac{d\varphi}{dx} \ ,$$

which is equivalent to

$$\frac{d\varphi}{dx} = -\frac{1}{\alpha}\left[\frac{d\Gamma}{dx} + \frac{1}{\alpha}\frac{d^2\Gamma}{dx^2}\right] \Bigg\| \left[1 + \frac{1}{\alpha^3}\frac{d}{d\varphi}\left(\frac{d^2\Gamma}{dx^2}\right)\right] \ . \tag{5.1.8}$$

From Eq. (5.1.3) we obtain

$$\frac{d\varphi}{dx} = \frac{d\lambda T}{dx} \ , \tag{5.1.9}$$

and with $\alpha = \frac{C_p\ K_o v}{\lambda}$, Eq. (5.1.8) gives

$$\frac{d\lambda T}{dx} = -\frac{\lambda}{C_p\ K_o v}\left[\frac{d\Gamma}{dx} + \frac{\lambda}{C_p\ K_o v}\frac{d^2\Gamma}{dx^2}\right] \Bigg\| \left[1 + \left(\frac{\lambda}{C_p\ K_o v}\right)^3 \frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right)\right] \ . \tag{5.1.10}$$

Concerning Eq. (5.1.10) the program uses the following procedures:

Real Procedure DFUN, which calculates the derivative $d\Gamma/dx$,
Real Procedure D2FUN, which calculates the derivative $d^2\Gamma/dx^2$,
Real Procedure D3FUN, which calculates the derivative $\frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right)$.

For the evaluation of these three procedures the program uses also

Real Procedure V, which calculates the gasvelocity V,
Real Procedure DVDX, which calculates the velocity derivative dv/dx,
Real Procedure D2VDX2, which calculates the 2nd derivative d^2v/dx^2.

To evaluate the procedure Runner, the following procedures are used:

Real Procedure k, which calculates the concentration of reactants K,
Procedure F(G,z), which contains Eq. (5.2.55) and (5.2.56), and which is called by procedure Runner itself.

A diagram of the procedures needed for procedure Runner is given in Fig. (2).

The construction of the main program is very simple. So it will suffice to give a description of the procedures used by the program.

5.2. Description of Procedures

Real Procedure V(TL, kko).

This procedure calculates the gasvelocity as a function of λT and $Kv/K_o v$.

From Eq. (2.2) we have

$$\rho v = \rho_b r = M_k K_o v = \text{constant} , \qquad (5.2.1)$$

while Eq. (2.5) together with Eq. (2.7) yields an expression for the gasvelocity:

$$M_k K_o v . v + p = M_k K_o v . v_s + p_s = p_{t_s} = \text{constant} . \qquad (5.2.2)$$

The equation of state, Eq. (2.7), may be rewritten as

$$p = (K + P) R_o T = \frac{K_o - (1-\nu)K}{\nu} R_o T . \qquad (5.2.3)$$

Combining Eqs. (5.2.1), (5.2.2) and (5.2.3) yields:

$$\rho_b r \, v2 + \frac{K_o v - (1-\nu) Kv}{\nu} R_o T - p_{t_s} v = 0$$

from which follows

$$v = \frac{p_{t_s}}{2\rho_b r}\left[1 \pm \sqrt{1 - \frac{4\rho_b r}{p_{t_s}^2}\,\frac{K_o v - (1-\nu)Kv}{\nu} R_o T}\right] .$$

For $T = T_s$, $Kv = K_o v$ and it follows that the correct solution is obtained by taking the - sign:

$$V = \frac{p_{t_s}}{2\rho_b r}\left[1 - \sqrt{1 - \frac{4\rho_b r}{p_{t_s}^2}\left(\frac{K_o v - (1-\nu)Kv}{\nu}\right)R_o T}\;\right] . \qquad (5.2.4)$$

Now

$$K_o v = \frac{\rho_b r}{M_k} ,$$

$$T = \frac{\lambda T}{\lambda} ,$$

which gives

$$V = \frac{p_{t_s}}{2\rho_b r}\left[1 - \sqrt{1 - \frac{R_o \lambda T\ (1 - (1-\nu)\ K/K_o)}{\lambda \nu M_k\ (p_{t_s}/2\rho_b r)^2}}\;\right] . \qquad (5.2.5)$$

If we define

$$\frac{p_{t_s}}{2\rho_b r} = \mathrm{PROBR} , \qquad (5.2.6)$$

$$\lambda \nu M_k \left(\frac{p_{t_s}}{2\rho_b r}\right)^2 = \mathrm{VCON} , \qquad (5.2.7)$$

$$\lambda T = \mathrm{TL} , \qquad (5.2.8)$$

$$K/K_o = \mathrm{KKO} , \qquad (5.2.9)$$

the equation for V then becomes

$$V = \mathrm{PROBR} * \left[1 - \sqrt{1 - \frac{\mathrm{TL} * R_O * (1 - (1-\nu)\ \mathrm{KKO})}{\mathrm{VCON}}}\;\right] \qquad (5.2.10)$$

<u>Real Procedure DVDX (TL, KKO, DTL, DKKO)</u>

This procedure calculates the derivative dV/dx, which is a function of λT, K/K_o, $d\lambda T/dx$ and $d(Kv/K_o v)/dx$.

Assuming $P/P_{t_s} \approx 1$ we may rewrite Eq. (5.2.4) in the following way

$$V = \frac{R_o}{\nu P_{t_s}}\left[K_o v - (1-\nu)\ Kv\right] T , \qquad (5.2.11)$$

and

$$\frac{dv}{dx} = \frac{R_o}{\nu p_{t_s}} \frac{K_o v}{\lambda} \left[\frac{d\lambda T}{dx} - (1-\nu) \frac{Kv}{K_o v} \frac{d\lambda T}{dx} - (1-\nu)\lambda T \frac{d\ Kv/K_o v}{dx} \right]. \quad (5.2.12)$$

If we define

$$\frac{R_o}{\nu p_{t_s}} \frac{K_o v}{\lambda} = \mathrm{RUPNU}\ , \quad (5.2.13)$$

$$\frac{d\lambda T}{dx} = \mathrm{DTL}\ , \quad (5.2.14)$$

$$\frac{d\ Kv/K_o v}{dx} = \mathrm{DKKO}\ , \quad (5.2.15)$$

the equation for dV/dx then becomes

$$\frac{dv}{dx} = \mathrm{RUPNU} * (\mathrm{DTL} - (1-\nu) * \mathrm{KKO} * \mathrm{DTL} - (1-\nu) * \mathrm{TL} * \mathrm{DKKO}). \quad (5.2.16)$$

Real Procedure D2VDX2 (TL, KKO, DTL, DKKO)

This procedure calculates the 2nd derivative d^2V/dx^2 as a function of λT, K/K_o, $d\lambda T/dx$ and $d(Kv/K_o v)/dx$. This procedure is used by procedure D2FUN.

The calculation is based on the energy equation (3.13):

$$C_p \frac{dT}{dx} - \frac{\Delta H_f}{\nu K_o v} \frac{dKv}{dx} + \frac{1}{2} M_k \frac{dV^2}{dx} - \frac{\lambda}{K_o v} \frac{d^2T}{dx^2} = 0\ ,$$

or, since $M_k K_o v = \rho_b r$,

$$\frac{d^2T}{dx^2} = \frac{C_p K_o v}{\lambda} \frac{dT}{dx} - \frac{\Delta H_f}{\lambda\nu} \frac{dKv}{dx} + \frac{\rho_b r V}{\lambda} \frac{dV}{dx}\ . \quad (5.2.17)$$

Applying the same technique as described in Chapter 2 yields,

$$\frac{d^2T}{dx^2} = -\frac{\lambda}{C_p K_o v} \frac{d\Gamma}{dx} - \left(\frac{\lambda}{C_p K_o v}\right)^2 \frac{d^2\Gamma}{dx^2} - \ldots\ , \quad (5.2.18)$$

$$\text{where } \Gamma = -\frac{\Delta H_f}{\nu\lambda} \frac{dKv}{dx} + \frac{\rho_b r V}{\lambda} \frac{dV}{dx}\ , \quad (5.2.19)$$

Truncating Eq. (5.2.18) after the first term gives

$$\frac{d^2T}{dx^2} = \frac{-\lambda}{C_p K_o v} \left[-\frac{\Delta H_f}{\nu\lambda} \frac{d^2Kv}{dx^2} + \frac{\rho_b r}{\lambda} * \left(\frac{dV}{dx}\right)^2 + \frac{\rho_b r V}{\lambda} \frac{d^2V}{dx^2} \right], \quad (5.2.20)$$

which may be rewritten as

$$\frac{d^2V}{dx^2} = \frac{\Delta H_f}{\nu\rho_b r V}\,\frac{d^2Kv}{dx^2} - \frac{1}{V}\left(\frac{dV}{dx}\right)^2 - \frac{C_p\,K_o v}{\rho_b r V}\,\frac{d^2T}{dx^2} \quad . \tag{5.2.21}$$

On the other hand differentiating of Eq. (5.2.12) leads to

$$\frac{d^2V}{dx^2} = \frac{\nu-1}{\nu}\,\frac{R_o}{Pt_s}\left[\left(\frac{K_o v}{\nu-1} + Kv\right)\frac{d^2T}{dx^2} + T\,\frac{d^2Kv}{dx^2} + 2\,\frac{dT}{dx}\,\frac{dKv}{dx}\right] . \tag{5.2.22}$$

Subtracting Eq. (5.2.22) from Eq. (5.2.21) yields

$$\frac{d^2T}{dx^2} = \frac{\left(\Delta H_f/\nu\rho_b r V + \frac{1-\nu}{\nu}\,\frac{R_oT}{Pt_s}\right)\frac{d^2Kv}{dx^2} - \frac{1}{V}\left(\frac{dV}{dx}\right)^2 + 2\,\frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,\frac{dT}{dx}\,\frac{dKv}{dx}}{\left(\frac{C_p\,K_o v}{\rho_b r V} - \frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\left(Kv - \frac{K_o v}{1-\nu}\right)\right)} \quad . \tag{5.2.23}$$

Replacing T and Kv by λT and $Kv/K_o v$ transforms Eq. (5.2.23) into

$$\frac{d^2\lambda T}{dx^2} = \frac{\left(\frac{\lambda\Delta H_f}{\nu} + \frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,\rho_b r V \lambda T\right)\frac{d^2(Kv/K_o v)}{dx^2}\,K_o v \; + }{\left(C_p K_o v - \frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,\rho_b r V K_o v\left\{\frac{Kv}{K_o v} - \frac{1}{1-\nu}\right\}\right)} \quad .$$

$$\frac{-\lambda\rho_b r\left(\frac{dV}{dx}\right)^2 + 2\,\frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,K_o v\,\rho_b r V\,\frac{d\lambda T}{dx}\,\frac{d(Kv/K_o v)}{dx}}{} \quad . \tag{5.2.24}$$

We now define

$$\text{NURP} = (\nu - 1)\,\frac{R_o}{\nu Pt_s} \quad , \tag{5.2.25}$$

$$\text{CO1} = \frac{\Delta H_f\lambda}{\nu} + \frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,\rho_b r\;V\lambda T \quad , \tag{5.2.26}$$

$$\text{CO2} = C_p - \frac{1-\nu}{\nu}\,\frac{R_o}{Pt_s}\,\rho_b r\;V\left(\frac{Kv}{K_o v} - \frac{1}{1-\nu}\right) \quad , \tag{5.2.27}$$

$$\text{CO3} = \text{CO1}/\text{CO2} \quad . \tag{5.2.28}$$

Then Eq. (5.2.24) now is rewritten as

$$\begin{aligned} \frac{d^2\lambda T}{dx^2} = \text{CO3}\,\frac{d^2(Kv/K_o v)}{dx^2} - \frac{\lambda\rho_b r}{K_o v\ \text{CO2}}\left(\frac{dV}{dx}\right)^2 - \\ - 2\,\frac{\text{NURP}}{\text{CO2}}\,\rho_b r\;V\,\frac{d\lambda T}{dx}\,\frac{d(Kv/K_o v)}{dx} \quad . \end{aligned} \tag{5.2.29}$$

We still have to evaluate $d^2(Kv/K_ov)/dx^2$ in terms of the procedure parameters. From Eqs. (2.3) and (2.9) we know that

$$\frac{dKv}{dx} = -\nu A\, e^{-\theta/T} K^m \quad ,$$

leading to

$$\frac{d^2Kv}{dx^2} = \frac{\theta}{T^2}\frac{dKv}{dx}\frac{dT}{dx} - \nu A\, e^{-\theta/T}\, m\, K^{m-1}\frac{dK}{dx} \quad .$$

Furthermore

$$\frac{dK}{dx} = \left(\frac{dKv}{dx} - K\frac{dv}{dx}\right)/v \quad ,$$

which yields

$$\frac{d^2Kv}{dx^2} = \frac{\theta}{T^2}\frac{dKv}{dx}\frac{dT}{dx} + \frac{m}{Kv}\left(\frac{dKv}{dx}\right)^2 - \frac{m}{v}\frac{dKv}{dx}\frac{dv}{dx} \quad ,$$

or, using λT and Kv/K_ov instead of T and Kv

$$\frac{d^2(Kv/K_ov)}{dx^2} = \frac{\lambda\theta}{(\lambda T)^2}\frac{d\lambda T}{dx}\frac{d\,Kv/K_ov}{dx} + \frac{m}{Kv/K_ov}\left(\frac{d\,Kv/K_ov}{dx}\right)^2 + - \frac{m}{v}\frac{d\,Kv/K_ov}{dx}\frac{dv}{dx} \quad . \qquad (5.2.30)$$

Combining the Eqs. (5.2.29) and (5.2.30) yields

$$\frac{d^2(\lambda T)}{dx^2} = CO3\,\frac{\lambda\theta}{(\lambda T)^2}\frac{d\lambda T}{dx}\frac{d\,Kv/K_ov}{dx} + CO3\,\frac{m}{Kv/K_ov}\left(\frac{d\,Kv/K_ov}{dx}\right)^2 + - CO3\,\frac{m}{v}\frac{d\,Kv/K_ov}{dx}\frac{dv}{dx} - \frac{\lambda\rho_b r}{CO2\;K_ov}\left(\frac{dv}{dx}\right)^2 + - 2\,\frac{NURP}{CO2}\,\rho_b rV\,\frac{d\lambda T}{dx}\frac{d\,Kv/K_ov}{dx} \quad . \qquad (5.2.31)$$

We now rewrite Eq. (5.2.22) in the following way:

$$\frac{d^2v}{dx^2} = \frac{(\nu-1)}{\nu}\frac{R_o}{p_{t_s}}\frac{K_ov}{\lambda}\left[\left(\frac{Kv}{K_ov} - \frac{1}{1-\nu}\right)\frac{d^2\lambda T}{dx^2} + \lambda T\,\frac{d^2Kv/K_ov}{dx^2} + + 2\,\frac{d\lambda T}{dx}\frac{d\,Kv/K_ov}{dx}\right] \quad . \qquad (5.2.32)$$

Combining the Eqs. (5.2.31) and (5.2.32) gives

$$\begin{aligned}\frac{d^2v}{dx^2} = \frac{R_o}{\nu Pt_s}\,\frac{K_ov}{\lambda}\Bigg[&\Bigg\{\left(1-(1-\nu)\,\frac{Kv}{K_ov}\right)\left(CO3\,\frac{\lambda\theta}{(\lambda T)^2}-2\ \mathrm{NURP}\rho_b r\ v\right)+\\ &-(1-\nu)\left(2+\frac{\lambda\theta}{\lambda T}\right)\Bigg\}\,\frac{d\lambda T}{dx}\,\frac{d\ Kv/K_ov}{dx}+\\ &-\frac{dv}{dx}\,\frac{d\ Kv/K_ov}{dx}\left\{\left(1-(1-\nu)\,\frac{Kv}{K_ov}\right)\frac{m}{v}\,CO3-(1-\nu)\,\frac{m}{v}\,\lambda\ T\right\}+\\ &+\left(\frac{d\ Kv/K_ov}{dx}\right)^2\left\{\left(1-(1-\nu)\,\frac{Kv}{K_ov}\right)\frac{m}{Kv/K_ov}\,CO3-(1-\nu)\,\frac{m}{Kv/K_ov}\,\lambda T\right\}+\\ &-\left(\frac{dv}{dx}\right)^2\left\{\left(1-(1-\nu)\,\frac{Kv}{K_ov}\right)\frac{\lambda\rho_b r}{K_ov\ CO2}\right\}\Bigg]\ . \end{aligned} \qquad (5.2.33)$$

We define

$$\mathrm{RUPTS} = \frac{R_o}{Pt_s}\,\frac{K_ov}{\lambda}\ , \qquad (5.2.34)$$

$$\mathrm{KKONU} = \left\{1-(1-\nu)\,\frac{Kv}{K_ov}\right\}/\nu\ , \qquad (5.2.35)$$

$$\mathrm{NUONE} = (1-\nu)/\nu\ , \qquad (5.2.36)$$

$$\mathrm{TAL} = \lambda\theta\ . \qquad (5.2.37)$$

In addition we make use of procedure V(TL,KKO) to calculate the gas velocity V and procedure DVDX(TL, KKO, DTL, DKKO)

V = SPEED = V(TL,KKO) ; DV = dV/dx = DVDX(TL,KKO,DTL,DKKO).

Then Eq. (5.2.33) may be written as

$$\begin{aligned}\frac{d^2v}{dx^2} = {} & \mathrm{RUPTS} * ((\mathrm{KKONU} * (\mathrm{CO3} * \mathrm{TAL}/(\mathrm{TL} * \mathrm{TL})-2 * \mathrm{NURP} * \mathrm{ROBR} * \mathrm{SPEED}) - \\ & \mathrm{NUONE} * (2+\mathrm{TAL}/\mathrm{TL})) * \mathrm{DTL} * \mathrm{DKKO} - \\ & (\mathrm{KKONU} * m * \mathrm{CO3}/\mathrm{SPEED} - \mathrm{NUONE} * m * \mathrm{TL}/\mathrm{SPEED}) * \mathrm{DV} * \mathrm{DKKO} + \\ & (\mathrm{KKONU} * m * \mathrm{CO3}/\mathrm{KKO} - \mathrm{NUONE} * m * \mathrm{TL}/\mathrm{KKO}) * \mathrm{DKKO} * \mathrm{DKKO} - \\ & (\mathrm{KKONU} * \mathrm{ROBR} * \lambda/(\mathrm{CO2} * \mathrm{KNV})) * \mathrm{DV} * \mathrm{DV})\ . \end{aligned} \qquad (5.2.38)$$

Real Procedure DFUN(TL,KKO,DTL,DKKO)

This procedure calculates the derivative $d\Gamma/dx$ and is called by procedure F(G,Z) to evaluate the procedure Runner.

According to Eq. (5.2.19) we know that

$$\Gamma = - \frac{\Delta H_f}{\nu} K_o v \frac{Kv}{K_o v} + \frac{1}{2} \rho_b r \left(v^2 - v_F{}^2\right) \quad ,$$

leading to

$$\frac{d\Gamma}{dx} = - \frac{\Delta H_f}{\nu} K_o v \frac{d(Kv/K_o v)}{dx} + \rho_b r v \frac{dv}{dx} \quad , \tag{5.2.39}$$

or

$$\mathrm{DFUN} = \frac{d\Gamma}{dx} = - \mathrm{DHKNU} * \mathrm{DKKO} + \mathrm{ROBR} * \mathrm{V(TL,KKO)} * \mathrm{DVDX(TL,KKO,DTL,DKKO)} \, , \tag{5.2.40}$$

where

$$\mathrm{DHKNU} = \frac{\Delta H_f}{\nu} K_o v \quad . \tag{5.2.41}$$

<u>Real Procedure D2FUN (TL,KKO,DTL,DKKO)</u>

This procedure calculates the 2nd derivative $\frac{d^2\Gamma}{dx^2}$ which is used in procedure F(G,Z) for the evaluation of $d\lambda T/dx$.

From Eq. (5.2.39) we know that

$$\frac{d\Gamma}{dx} = - \frac{\Delta H_f}{\nu} K_o v \frac{d(Kv/K_o v)}{dx} + \rho_b r v \frac{dv}{dx} \quad ,$$

leading to

$$\frac{d^2\Gamma}{dx^2} = - \frac{\Delta H_f}{\nu} K_o v \frac{d^2(Kv/K_o v)}{dx^2} + \rho_b r \left(\frac{dv}{dx}\right)^2 + \rho_b r v \frac{d^2 v}{dx^2} \, . \tag{5.2.42}$$

We define

$$\frac{\Delta H_f}{\nu} K_o v = \mathrm{DHKNU} \quad , \tag{5.2.43}$$

$$\frac{C_p K_o v}{\lambda} = \mathrm{KNCL} \quad , \tag{5.2.44}$$

$$\mathrm{DV} = \mathrm{DVDX(TL,KKO,DTL,DKKO)} \quad , \tag{5.2.45}$$

$$\rho_b r = \mathrm{ROBR} \quad . \tag{5.2.46}$$

Then Eq. (5.2.42) becomes

$$\frac{d^2\Gamma}{dx^2} = -\mathrm{DHKNU} * \frac{d^2(Kv/K_o v)}{dx^2} + \mathrm{ROBR} * (\mathrm{DV} * \mathrm{DV} +$$

$$+ \mathrm{V(TL,KKO)} * \mathrm{D2VDX2(TL,KKO,DTL,DKKO))}\ . \qquad (5.2.47)$$

We obtain from Eq. (5.2.30)

$$\frac{d^2(Kv/K_o v)}{dx^2} = \frac{d(Kv/K_o v)}{dx}\left[\frac{\lambda\theta}{(\lambda T)^2}\frac{d\lambda T}{dx} + \frac{m}{K_v/K_o v}\frac{d(Kv/K_o v)}{dx} - \frac{m}{v}\frac{dv}{dx}\right] ,$$

Or, using the same notations as above

$$\frac{d^2(Kv/K_o v)}{dx^2} = \mathrm{DKKO} * (\mathrm{TAL} * \mathrm{DTL}/(\mathrm{TL} * \mathrm{TL}) + m * \mathrm{DKKO}/\mathrm{KKO} -$$

$$m * \mathrm{DV}/\mathrm{V(TL,KKO)} \qquad . \qquad (5.2.48)$$

Combining Eqs. (5.2.47) and (5.2.48) yields

$$\mathrm{D2FUN} = \frac{d^2\Gamma}{dx^2} = -\ \mathrm{DHKNU} * \mathrm{DKKO} * (\mathrm{TAL} * \mathrm{DTL}/(\mathrm{TL} * \mathrm{TL}) + m * \mathrm{DKKO}/\mathrm{KKO} +$$

$$- m * \mathrm{DV}/\mathrm{V(TL,KKO))} + \mathrm{ROBR} * (\mathrm{DV} * \mathrm{DV} + \mathrm{V(TL,KKO)} *$$

$$\mathrm{D2VDX2(TL,KKO,DTL,DKKO))} \quad . \qquad (5.2.49)$$

Real Procedure D3FUN (TL,KKO,DTL,DKKO)

This procedure calculates the derivative $\frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right)$ which is used by procedure F(G,Z) for the evaluation of $d\lambda T/dx$.

The third derivative may be written as the derivative of the second derivative:

$$\frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right) = \lim_{\substack{\Delta\lambda T \to 0 \\ \frac{\Delta Kv}{K_o v} \to 0}} \left[\frac{(d^2\Gamma/dx^2)_{\lambda T + \Delta\lambda T} - (d^2\Gamma/dx^2)_{\lambda T - \Delta\lambda T}}{2\Delta\lambda T} + \right.$$

$$\left.\frac{(d^2\Gamma/dx^2)_{Kv/K_o v + \Delta Kv/K_o v} - (d^2\Gamma/dx^2)_{Kv/K_o v - \Delta Kv/K_o v}}{2\Delta(K\ /K_o v)}\left(\frac{d\ Kv/K_o v}{d\lambda T}\right)\right] .$$

(5.2.50)

For our purposes it will be sufficient to take

$$\Delta\lambda T = 0.5 \qquad ,$$

$$\Delta(Kv/K_o v) = .001\ (Kv/K_o v) \quad .$$

Then Eq. (5.2.50) becomes

$$\frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right) = \left(\frac{d^2\Gamma}{dx^2}\right)_{\lambda T + 0.5} - \left(\frac{d^2\Gamma}{dx^2}\right)_{\lambda T - 0.5} +$$

$$\left(\left(\frac{d^2\Gamma}{dx^2}\right)_{1.001\,\frac{Kv}{K_o v}} - \left(\frac{d^2\Gamma}{dx^2}\right)_{.999\,\frac{Kv}{K_o v}}\right) * \frac{1}{.002\,\frac{Kv}{K_o v}} * \frac{d\ Kv/K_o v}{dx} * \frac{1}{\frac{d\lambda T}{dx}} \quad . \qquad (5.2.51)$$

or

$$\text{D3FUN} = \frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right)$$

= D2FUN(TL + .5,KKO,DTL,DKKO) -

D2FUN(TL - .5,KKO,DTL,DKKO) +

(D2FUN(TL,1.001 * KKO,DTL,DKKO) -

D2FUN(TL,.999 * KKO,DTL,DKKO)) *

DKKO/(DTL * .002 * KKO) . (5.2.52)

Procedure Runner (Z,N,STEP,F)

This procedure, which is a catalogued procedure of the DUT computer system, integrates a set of N first order ordinary differential equations, using the Runge-Kutta's method.
The procedure uses the following variables:

Z	input: array Z(|0:N|) containing the initial values of the variables Z_o, Z_1 ... Z_n In this case, where N = 2, we have $Z_o = x$ $Z_1 = \lambda T$ $Z_2 = Kv/K_o v$ output: the calculated values of the variables after a stepsize 'STEP'.
N	input: the number of equations.
STEP	input: the stepsize.
F	input: procedure F(G,Z), which contains the set of differential equations that are to be integrated.

Procedure F(G,Z)

This procedure contains by means of array G(|1:2|) the two differential equations that are to be integrated by procedure Runner:

$$G(|1|) = \frac{1}{A}\frac{d\lambda T}{dx} = -\frac{\lambda}{C_p K_o v}\left[\frac{d\Gamma}{dx} + \frac{\lambda}{C_p K_o v}\frac{d^2\Gamma}{dx^2}\right] \Bigg| \left[1 + \left(\frac{\lambda}{C_p K_o v}\right)^3 \frac{d}{d\lambda T}\left(\frac{d^2\Gamma}{dx^2}\right)\right] , \tag{5.2.53}$$

$$G(|2|) = \frac{1}{A}\frac{d(Kv/K_o v)}{dx} = -\nu\, e^{-\theta/T}\, K^m/K_o v \tag{5.2.54}$$

These equations are equivalent to those described by Eq. (4.1) and (4.2) with one exception: for numerical reasons the program integrates

$$\frac{1}{A}\frac{d\lambda T}{dx} \quad \text{and} \quad \frac{1}{A}\frac{d\ Kv/K_o v}{dx} .$$

So in the right hand side of Eq. (5.2.54) the frequency factor A is missing.

If we make use of the procedures already mentioned above then Eq. (5.2.53) and (5.2.54) may be written as

$$\begin{aligned} G(|1|) = {} & -(\mathrm{DFUN}(Z(|1|),\ Z(|2|), \mathrm{AFG1},\ \mathrm{AFG2}) + \\ & \mathrm{D2FUN}(Z(|1|),\ Z(|2|),\ \mathrm{AFG1},\ \mathrm{AFG2})/\mathrm{KNCL}/\mathrm{KNCL}/ \\ & (1 + \mathrm{D3FUN}(Z(|1|),\ Z(|2|),\ \mathrm{AFG1},\ \mathrm{AFG2})/(\mathrm{KNCL})^3)) \end{aligned} \tag{5.2.55}$$

$$G(|2|) = -\nu * \mathrm{EXP}(-\lambda\theta/Z(|1|)) * (K(Z(|1|),\ Z(|2|)))^m/K_o v \tag{5.2.56}$$

Here

$$Z(|1|) = \lambda T$$

$$Z(|2|) = Kv/K_o v$$

being the outputdata of the foregoing integration step of procedure Runner, and

$$\mathrm{AFG1} = \frac{1}{A}\frac{d\lambda T}{dx} ,$$

$$\mathrm{AFG2} = \frac{1}{A}\frac{d\ Kv/K_o v}{dx} ,$$

being the previous values of the derivatives.

Consequently the program needs the initial values $(\mathrm{AFG1})_S$ and $(\mathrm{AFG2})_S$ being the gradients at the burning surface.

It is easily shown from Eq. (4.1) that

$$\left(\frac{d\lambda T}{dx}\right)_S = (\mathrm{AFG1})_S = \frac{C_p K_o v}{\lambda}(\lambda T_S - \lambda T_F) - \frac{\Delta H_f}{\nu} K_o v + \frac{1}{2}\rho_b r(v_S{}^2 - v_F{}^2) . \tag{5.2.57}$$

The calculation of TF will be dealt with below; to calculate the velocity at the burning surface V_S we make use of Eq. (3.6):

$$V_S = \frac{C_1}{M_K P_S} R_o T_S = \frac{\rho_b r}{M_K} \frac{R_o T_S}{P_S} \quad , \tag{5.2.58}$$

The variables at the right hand side all are inputdata of the main program.

From Eq. (3.8) we know that, assuming a constant pressure:

$$V_F = \frac{V_S * T_F}{\nu * T_S} \tag{5.2.59}$$

So it only remains to estimate the flame temperature T_F.
Using the burning surface as boundary value in the energy equation, we find:

$$C_p (T_F - T_S) + \frac{1}{2} M_K (V_F^2 - V_S^2) + \frac{\Delta H_f}{\nu} + \frac{\lambda}{K_o v} \left(\frac{dT}{dx}\right)_S = 0 \quad . \tag{5.2.60}$$

From Eqs. (3.19a) and (3.21a) we know that:

$$\frac{\lambda}{K_o v} \left(\frac{dT}{dx}\right)_S = -\varepsilon \frac{\Delta H_f}{\nu} \quad , \tag{5.2.61}$$

and

$$C_p (T_F - T_S) = - \frac{\Delta H_f}{\nu} (1-\varepsilon) \quad , \tag{5.2.62}$$

where we have neglected the kinetic energy .

So

$$\frac{\lambda}{K_o v} \left(\frac{dT}{dx}\right)_S = C_p (T_F - T_S) \frac{\varepsilon}{1-\varepsilon} \tag{5.2.63}$$

Combining Eq. (5.2.59), (5.2.60) and (5.2.63) yields:

$$T_F^2 + \left(\frac{\nu T_S}{V_S}\right)^2 \frac{2}{M_K} \frac{C_p}{1-\varepsilon} T_F - \left(\frac{\nu T_S}{V_S}\right)^2 \frac{2}{M_K} \left[\frac{C_p T_S}{1-\varepsilon} + \frac{1}{2} M_K V_S^2 - \frac{\Delta H_f}{\nu} \right] = 0 \quad . \tag{5.2.64}$$

Defining

$$C_p/(1-\varepsilon) = HT1 \quad , \tag{5.2.65}$$

$$(\nu T_S/V_S)^2/M_K = HT2 \quad , \tag{5.2.66}$$

$$HT3 = HT1 * HT2 \quad , \tag{5.2.67}$$

will give the following solution for the flame temperature:

$$T_F = -HT3 + \sqrt{(HT3)^2 + 2 * HT2 * \left[T_S * HT1 + \frac{1}{2} M_K V_S^{\,2} - \frac{\Delta H_f}{\nu}\right]} \quad . \qquad (5.2.68)$$

Furthermore

$$(AFG2)_S = \frac{1}{A}\left(\frac{d\ Kv/K_o v}{dx}\right)_S = -\nu e^{-\theta/T_S} K_S^{\ m}/K_o v \quad , \qquad (5.2.69)$$

where

$$K_S = \frac{K_o v}{V_S} = \frac{\rho_b\ r}{M_K\ V_S} \quad . \qquad (5.2.70)$$

The concentration of reactants K is calculated within Real Procedure K(TL,KKO) by the simple expression:

$$K = \frac{Kv}{K_o v} * \frac{K_o v}{V} \quad . \qquad (5.2.71)$$

So

$$K = KKO * K_o v/V(TL,KKO) \quad . \qquad (5.2.73)$$

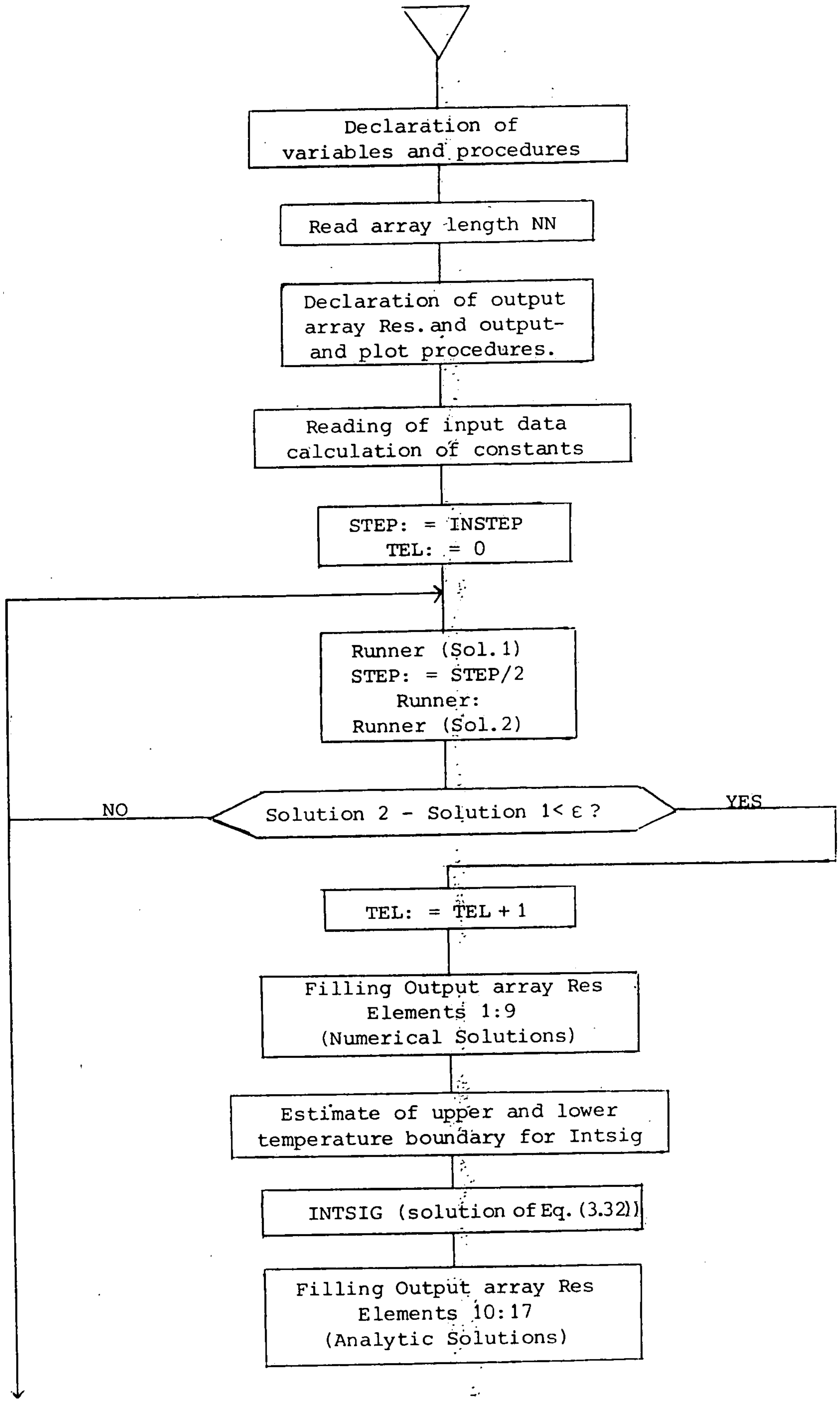
Real Procedure Intsig (A,B,Y,EPS)

This procedure integrates a function using a 5 points Simpsons Rule. Intsig, which is a catalogued procedure of the DUT computer system, uses the following variables:

A	input:	lower boundary of the integral
B	input:	upper boundary of the integral
Y	input:	the procedure Y which contains the function that has to be integrated
EPS	input:	the accuracy for each step.

Real Procedure Y(X)

This procedure contains Eq. (3.32) that has to be integrated by procedure Intsig.


Declaration of variables and procedures
Read array length NN
Declaration of output array Res. and output- and plot procedures.
Reading of input data calculation of constants
STEP: = INSTEP
TEL: = 0
Runner (Sol. 1)
STEP: = STEP/2
Runner:
Runner (Sol. 2)
NO
Solution 2 - Solution 1< ε ?
YES
TEL: = TEL + 1
Filling Output array Res
Elements 1:9
(Numerical Solutions)
Estimate of upper and lower temperature boundary for Intsig
INTSIG (solution of Eq. (3.32))
Filling Output array Res
Elements 10:17
(Analytic Solutions)

/./

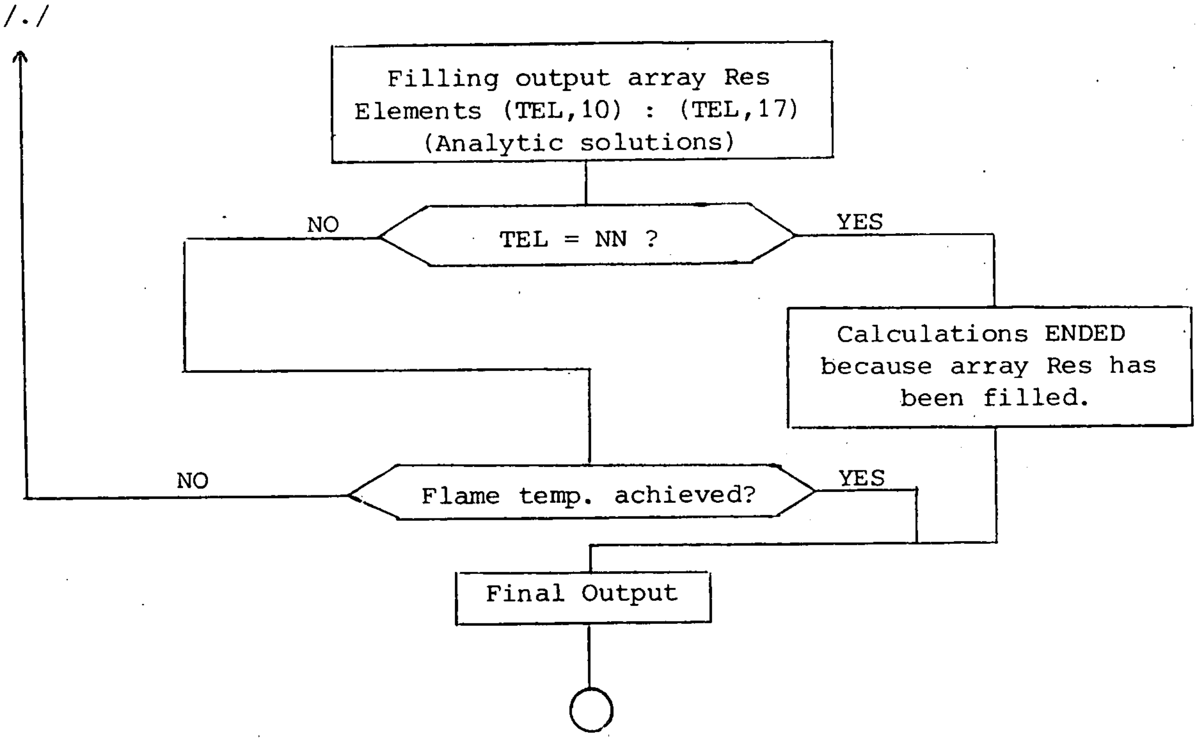


Fig. 5.1. General outline of the Algorithm.

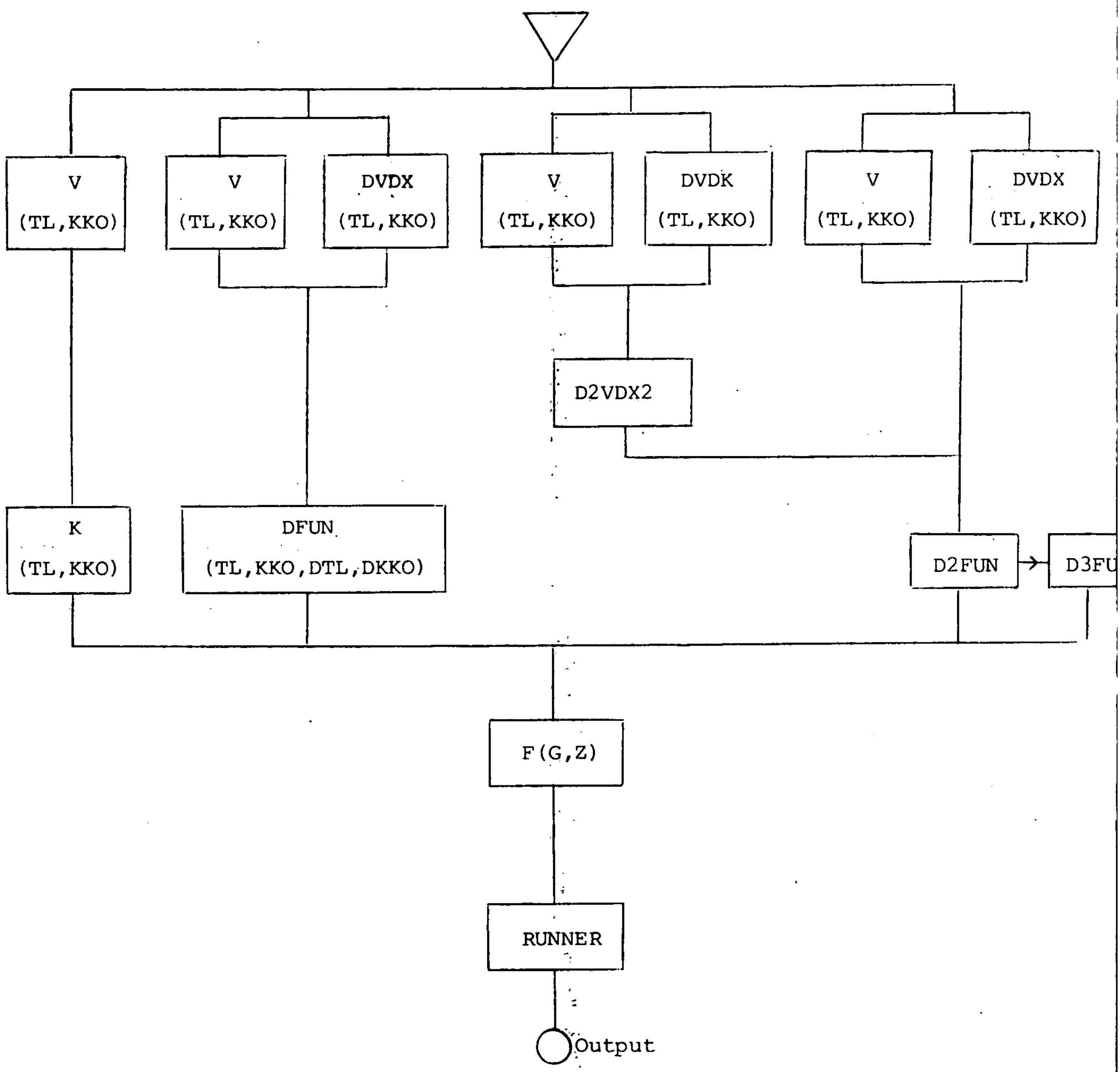


Fig. 5.2. Chart of procedures involved in procedure "Runner".

5.3. Listing of the computer program

In this Section the computer program for the numerical and analytic solution of premixed flames is listed. The program is written in ALGOL 60 and has been run on the AMDAHL 470 V/7B of Delft University of Technology.

```
'BEGIN'
'COMMENT'*************************************************************
 THIS PROGRAM CALCULATES FLAME TEMPERATURE,CONCENTRATIONS AND
 GAS VELOCITIES FOR A PREMIXED LAMINAR FLAME. DIFFUSION EFFECTS
 ARE NOT ACCOUNTED FOR. HEAT CONDUCTION EFFECTS ARE ACCOUNTED FOR.

 THE CALCULATION IS DONE IN TWO DIFFERENT WAYS.
 FIRST: BY A NUMERICAL INTEGRATION OF THE DIFFERENTIAL EQUATIONS.
        THE INITIAL CONDITIONS ARE ESTIMATED FROM AN ANALYTIC
        APPROXIMATE SOLUTION, ALSO THE FINAL FLAME TEMPERATURE IS
        ESTIMATED FROM THIS APPROXIMATE ANALYTIC SOLUTION.
 SECONDLY: AN ANALYTIC APPROXIMATE SOLUTION IS CALCULATED.

 THE PROGRAM VARIABLES ARE:
 A        FREQUENCY FACTOR   (KG**(1-M).KMOL**(M-1).M**(3M-3)/S)
 CP       MOLAR HEAT CAPACITY OF REACTANTS (KG.M**2/(S**2.KMOL.K))
 DH       MOLAR HEAT OF FORMATION OF PRODUCTS (KG.M**2/(S**2.KMOL))
 DHKNU    DH*KNV/NU    (KG/S**3)
 DHLN     DH*L/NU    (KG**2.M**3/(S**5.KMOL.K))
 DKKOS    RELATIVE CONCENTRATION FLUX GRADIENT AT THE
          BURNING SURFACE   (1/M)
 DNK      DH/(NU*KCT)    (S*M**2/KMOL)
 DTS      GRADIENT OF THE TEMPERATURE TIME THE HEAT CONDUCTION
          COEFFICIENT AT THE BURNING SURFACE   (KG.M/S**3)
 E        ARRAY E(/0:2/) WITH RESULTS OF ONE INTEGRATION STEP
 E1       ARRAY E1(/0:2/) WITH RESULTS OF TWO SUCCESSIVE INTEGRATION
          STEPS
 FACT     FACTOR
 FACT2    FACTOR
 FACT3    FACTOR
 G        ARRAY G(/1:2/) FUNCTION VALUES FOR INTEGRATION
 INSTEP   INITIAL VALUE OF INTEGRATION STEP IN RUNNER   (M)
 KCT      KNV*CP*TF      (KG/(S**3))
 KNV      MOLAR CONCENTRATION FLUX   (KMOL/(M**2.S))
 KNVL     RATIO OF MOLAR CONCENTRATION FLUX AND HEAT CONDUCTION
          COEFFICIENT   (KMOL.K.S**2/(KG.M**3))
 KS       REACTANT CONCENTRATION AT BURNING SURFACE   (KMOL/M**3)
 L        HEAT CONDUCTION COEFFICIENT  (KG.M/(S**3.K))
 M        ORDER OF REACTION
 MK       MOLAR MASS REACTANTS   (KG/KMOL)
 NN       LENGTH OF ARRAY RES(/0:NN,1:17/) WITH RESULTS OF COMPUTATIONS
 NU       STOICHIOMETRIC COEFFICIENT
 NURP     CONSTANT    (M**3/(KMOL.K))
 NURPK    CONSTANT    (S**2/KG)
 PS       PRESSURE AT THE BURNING SURFACE   (PA)
 PTS      TOTAL PRESSURE AT THE BURNING SURFACE   (PA)
 RB       PROPELLANT BURNING RATE   (M/S)
 RES      ARRAY RES(/0:NN,1:17/) WITH FINAL RESULTS OF ALL COMPUTATIONS
    RES(/I,1/)= X   (INTEGRATION)
```

```
    RES(/I,2/)= T           ,,
    RES(/I,3/)= K           ,,
    RES(/I,4/)= KO          ,,         (CONCENTRATION K+NU.P)
    RES(/I,5/)= K/KO        ,,         (CONCENTRATION RATIO REACTANTS)
    RES(/I,6/)= PR          ,,         (CONCENTRATION PRODUCTS)
    RES(/I,7/)= PR/KO       ,,         (PRODUCT CONCENTRATION RATIO)
    RES(/I,8/)= V           ,,         (GAS VELOCITY)
    RES(/I,9/)= V/VS        ,,         (VELOCITY RATIO)
    RES(/I,10/)= X     ANALYTIC
    RES(/I,11/)= K          ,,         (CONCENTRATION REACTANTS)
    RES(/I,12/)= KO         ,,         (CONCENTRATION K+NU.P)
    RES(/I,13/)= K/KO       ,,         (CONCENTRATION RATIO RECTANTS)
    RES(/I,14/)= PR         ,,         (CONCENTRATION PRODUCTS)
    RES(/I,15/)= PR/KO      ,,         (PRODUCT CONCENTRATION RATIO)
    RES(/I,16/)= V          ,,         (GAS VELOCITY)
    RES(/I,17/)= V/VS       ,,         (VELOCITY RATIO)
 ROB      PROPELLANT DENSITY  (KG/M**3)
 RU       UNIVERSAL GAS CONSTANT  (KG.M**2/(S**2.KMOL.K))
 S        ARRAY S(/0:2/) WITH STARTING VALUES FOR EVERY INTEGRATION
          STEP
 STEP     INTEGRATION STEP IN RUNNER  (M)
 TA       ACTIVATION TEMPERATURE  (K)
 TAS      TA/TS
 TB       UPPER TEMPERATURE BOUNDARY FOR INTEGRATION IN INTSIG  (K)
 TEL      COUNTER
 TF       ESTIMATED FLAME TEMPERATURE  (K)
 TFTS     TF-TS   (K)
 TFA      TF/TA
 TO       LOWER TEMPERATURE BOUNDARY FOR INTEGRATION IN INTSIG  (K)
 TS       TEMPERATURE AT THE BURNING SURFACE  (K)
 TSA      TS/TA
 VF       GAS VELOCITY AT FLAME TEMPERATURE  (M/S)
 VS       GAS VELOCITY AT BURNING SURFACE  (M/S)
 VV       GAS VELOCITY  (M/S)
 Z        ARRAY Z(/0:2/) WITH VALUES FOR INTEGRATION
          Z(/0/)= X       Z(/1/)= T        Z(/2/)= KV
*******    PROCEDURES    *********************************************
 DFUN
 D2FUN
 D3FUN          PROCEDURES FOR CALCULATION OF FIRST, SECOND AND
                THIRD DERIVATIVES TO BE USED IN PROCEDURE F(G,Z)
 DVDX           PROCEDURE FOR CALCULATION OF FIRST DERIVATIVE
                OF SPEED
 D2VDX2         PROCEDURE FOR CALCULATION OF SECOND DERIVATIVE
                OF SPEED
 F(G,Z)         PROCEDURE FOR RUNGE KUTTA INTEGRATION
 INTSIG(A,B,Y,EPS)    PROCEDURE FOR CALCULATION OF INTEGRAL BETWEEN
                      BOUNDARIES A AND B  (SIMPSON)
 K(TL,KKO)      PROCEDURE FOR CALCULATION OF CONCENTRATION
                OF REACTANTS
 RUNNER(Z,N,STEP,F)   INTEGRATION PROCEDURE FOR DIFFERENTIAL
                      EQUATIONS  (RUNGE KUTTA)
 V(TL,KKO)      PROCEDURE FOR CALCULATION OF THE GAS VELOCITY
 Y(X)           PROCEDURE FOR FUNCTION TO BE INTEGRATED IN INTSIG
*********************************************************************;
```

```
'REAL' A,AFG1,AFG2,CP,DH,DHKNU,DHLN,DIST,DISTM,DKKOS,DNK,DTS,EPS,
       FACT,FACT2,FACT3,FT,HT1,HT2,HT3,INSTEP,KNCL,KNV,KNVL,KS,L,
       M,MK,NODIS,NU,NUA,NURP,NURPK,PARAM,PLH,PLV,PROBR,PS,PTS,
       RB,ROB,ROBR,RU,RUPNU,RUPTS,STEP,TA,TAL,TAS,TB,TDIF,TF,TFA,
       TFL,TFTS,TLOG,TS,TSA,TO,VCON,VF,VS,VV,TF2AN;
'INTEGER' ARFIL,CUT,FIRST,FLAME,I,KWANT,LAST,NN,
          TEL,TELAN,TELMIN;
'REAL''ARRAY' E,E1,S,Z(/0:2/),G(/1:2/);
'REAL''PROCEDURE' V(TL,KKO);'REAL'TL,KKO;
    'BEGIN'  'REAL' QQ;
     QQ:=RU*TL*(1-(1-NU)*KKO)/VCON;
    'IF'QQ>1'THEN'
       'BEGIN'
        PRINT(1,'('NEGATIVE FACTOR IN SQRT PROC. V ')');
        LINE(1,1);
        PRINT(1,'('TEMP= ')',TL/L);LINE(1,1);
        PRINT(1,'('KKO= ')',KKO);LINE(1,1);
        PRINT(1,'('VCON= ')',VCON);LINE(1,1);
        PRINT(1,'('FACT= ')',1-QQ);LINE(1,1);
       'END';
     V:=PROBR*(1-SQRT(1-QQ));
'END'V;
'REAL''PROCEDURE' K(TL,KKO);'REAL'TL,KKO;
    'BEGIN'
    'REAL' QQ;
     QQ:=KKO*KNV/V(TL,KKO);
    'IF'QQ<0.0'THEN'QQ:='-15;
     K:=QQ;
'END'K;
'REAL''PROCEDURE'DVDX(TL,KKO,DTL,DKKO);'REAL'TL,KKO,DTL,DKKO;
    'BEGIN'
    'REAL' QQQ;
     QQQ:=RUPNU*(DTL-(1-NU)*KKO*DTL-(1-NU)*TL*DKKO);
    'IF'ABS(QQQ)<'-60'THEN'QQQ:=0.0;
     DVDX:=QQQ;
'END' DVDX;
'REAL''PROCEDURE'D2VDX2(TL,KKO,DTL,DKKO);'REAL'TL,KKO,DTL,DKKO;
    'BEGIN'
    'REAL' CO1,CO2,CO3,SPEED,DV,KKONU,NUEEN;
     SPEED:=V(TL,KKO);
     CO1:=DHLN-NURP*TL*ROBR*SPEED; CO2:=CP+NURP*KKO*ROBR*SPEED;
     CO3:=CO1/CO2; DV:=DVDX(TL,KKO,DTL,DKKO);
     KKONU:=(KKO*(NU-1)/NU)+1/NU; NUEEN:=(NU-1)/NU;
     D2VDX2:=RUPTS*((KKONU*(TAL*CO3/(TL*TL)-2*ROBR*SPEED
             *NURP/CO2)+(TAL/TL+2)*NUEEN)*DTL*DKKO-
             (KKONU*CO3*M/SPEED+M*TL*NUEEN/SPEED)*
             DV*DKKO+(KKONU*CO3*M/KKO+M*TL*NUEEN/KKO)*
             DKKO*DKKO-(KKONU*ROBR*L/(KNV*CO2))*DV*DV);
'END' D2VDX2;
'REAL''PROCEDURE' DFUN(TL,KKO,DTL,DKKO);
    'REAL' TL,KKO,DTL,DKKO;
     DFUN:=-DHKNU*DKKO+ROBR*V(TL,KKO)*DVDX(TL,KKO,DTL,DKKO);
'REAL''PROCEDURE' D2FUN(TL,KKO,DTL,DKKO);
    'REAL' TL,KKO,DTL,DKKO;
    'BEGIN'
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    'REAL' DV; DV:=DVDX(TL,KKO,DTL,DKKO);
     D2FUN:=-DHKNU*DKKO*(TAL*DTL/TL/TL+M*DKKO/KKO-M*DV/V(TL,KKO))+
              ROBR*(DV*DV+D2VDX2(TL,KKC,DTL,DKKO));
'END' D2FUN;
'REAL''PROCEDURE' D3FUN(TL,KKO,DTL,DKKO);
      'REAL' TL,KKO,DTL,DKKO;
      'BEGIN'
       D3FUN:=D2FUN(TL+.5,KKO,DTL,DKKC)-D2FUN(TL-.5,KKO,DTL,DKKC)+
             ('IF'ABS(DTL*.002*KKO)>'-50'THEN'
             (D2FUN(TL,KKO-(.5/(L*IFTS)),DTL,DKKO)-
              D2FUN(TL,KKO+(.5/(L*IFTS)),DTL,DKKO))*
              (-L*TFTS)*DKKO/DTL 'ELSE' 0);
'END' D3FUN;
'PROCEDURE' F(G,Z); 'ARRAY'G,Z;
    'BEGIN'
    'IF' FIRST=1 'THEN'
     'BEGIN'
      AFG1:=DTS/A; AFG2:=DKKOS/A;
     'END';
     G(/1/):=-(DFUN(Z(/1/),Z(/2/),AFG1,AFG2)+
             D2FUN(Z(/1/),Z(/2/),AFG1,AFG2)/KNCL)/KNCL/
             (1+D3FUN(Z(/1/),Z(/2/),AFG1,AFG2)/(KNCL*
             KNCL*KNCL));
     G(/2/):=-NU*EXP(-TAL/Z(/1/))*((K(Z(/1/),Z(/2/)))**M)/KNV;
     AFG1:=G(/1/);  AFG2:=G(/2/);
    'IF'ABS(AFG1)<'-60'THEN'AFG1:='-60*SIGN(AFG1);
'END' F;
'REAL''PROCEDURE' INTSIG(A,B,Y,EPS);'VALUE'A,B,EPS;
    'REAL'A,B,EPS; 'REAL''PROCEDURE'Y;'CODE';
'PROCEDURE' RUNNER(Z,N,STEP,F);'VALUE'N,STEP;'INTEGER'N;
    'REAL' STEP; 'ARRAY'Z; 'PROCEDURE'F; 'CODE';
'REAL''PROCEDURE' Y(X);'REAL'X;
    'BEGIN'  'REAL' IX,TFAX; IX:=1/X; TFAX:=TFA-IX;
     Y:=-EXP(X)/(X*X*(X*TFAX*(1/(IX-TSA+NU*TFAX)-FACT2*TA/
        (X*(TFA-TSA)*FACT3)))**M);
'END' Y;
'PROCEDURE' HEAD(J); 'INTEGER' J;
 'BEGIN' 'SWITCH' S:=S1,S2,S3,S4,S5; 'GOTO'S(/J/);
  S1: TXT1;
  PRINT(1,'('     CONCENTRATION K           CONCENTRATION KO')');
  PRINT(1,'('      CONCENTR.RATIO K/KO')'); LINE(1,1);
  TXT2; TXTN; LINE(1,1); TXT3;
  PRINT(1,'('          KMOL/M**3                  KMOL/M**3      ')');
  PRINT(1,'('               (-)')'); LINE(1,3); 'GOTO' FIN;
  S2: TXT1;
  PRINT(1,'('     CONCENTRATION P        CONCENTR. RATIO P/KO   ')');
  PRINT(1,'('      GAS VELOCITY')'); LINE(1,1);
  TXT2;TXTN; LINE(1,1); TXT3;
  PRINT(1,'('          KMOL/M**3                  (-)          ')');
  PRINT(1,'('             M/S')'); LINE(1,3); 'GOTO' FIN;
  S3: TXT1;
  PRINT(1,'('      VELOCITY RATIC                LOCATION       ')');
  PRINT(1,'('      CONCENTRATION K')'); LINE(1,1); TXT2;
  PRINT(1,'('         NUMERICAL                   ANALYTIC      ')');
  PRINT(1,'('          ANALYTIC')'); LINE(1,1); TXT3;
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  PRINT(1,'('              (-)                        M      ')');
  PRINT(1,'('                KMOL/M**3')'); LINE(1,3); 'GOTO' FIN;
  S4: TXT1;
  PRINT(1,'('     CONCENTRATION KO      CONCENTR. RATIO K/KO ')');
  PRINT(1,'('     CONCENTRATION P')'); LINE(1,1); TXT2; TXTA;
  LINE(1,1);
  TXT3;
  PRINT(1,'('         KMOL/M**3                   (-)      ')');
  PRINT(1,'('            KMOL/M**3')'); LINE(1,3); 'GOTO' FIN;
  S5: TXT1;
  PRINT(1,'('   CONCENTR. RATIO P/KO        GAS VELOCITY      ')');
  PRINT(1,'('      VELOCITY RATIO')'); LINE(1,1); TXT2; TXAN;
  LINE(1,1);
  TXT3;
  PRINT(1,'('             (-)                         M/S      ')');
  PRINT(1,'('                (-)')'); LINE(1,3);
  FIN:
'END' HEAD;
'PROCEDURE' TXT1;
      PRINT(1,'('       LOCATION              TEMPERATURE       ')');
'PROCEDURE' TXT2;
      PRINT(1,'('       NUMERICAL              NUMERICAL       ')');
'PROCEDURE' TXT3;
      PRINT(1,'('          M                      K            ')');
'PROCEDURE' TXTN;
     'BEGIN'
      PRINT(1,'('        NUMERICAL                 NUMERICAL  ')');
      PRINT(1,'('             NUMERICAL        ')');
'END' TXTN;
'PROCEDURE' TXTA;
     'BEGIN'
      PRINT(1,'('         ANALYTIC                   ANALYTIC  ')');
      PRINT(1,'('             ANALYTIC        ')');
'END' TXTA;
'PROCEDURE' TXAN;
'BEGIN'
 PRINT(1,'('          ANALYTIC                 ANALYTIC')');
 PRINT(1,'('                 ANALYTIC')');
'END' TXAN;
   SETTING(1,132,60);
   READ(0,NN);PAGE(1);
   PRINT(1,'('ARRAY LENGTH NN =')',NN);LINE(1,2);
'COMMENT' ************** BEGIN SECOND BLOCK ************************;
  'BEGIN'
  'REAL''ARRAY' RES(/0:NN,1:17/);
  'INTEGER' J;
'COMMENT' ***************** BEGIN OUTPUT PROCEDURE *****************;
  'PROCEDURE' OUT;
       'BEGIN' 'INTEGER' J,TEL50;
        J:=1;
  LOOP2:   TEL:=0;
  LOOP1:   'IF' (TEL+49)<=NN'THEN' TEL50:=TEL+49 'ELSE' TEL50:=NN;
        PAGE(1); HEAD(J);
       'FOR' TEL:=TEL'STEP'1'UNTIL'TEL50'DO'
       'BEGIN'
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      PRINT(1,RES(/TEL,1/),RES(/TEL,2/),RES(/TEL,3*J/));
      PRINT(1,RES(/TEL,3*J+1/),RES(/TEL,3*J+2/)); LINE(1,1);
     'END';
     'IF' TEL50<NN'THEN'
     'BEGIN'
      TEL:=TEL50+1;
     'GOTO' LOOP1;
     'END'  'ELSE'
     'BEGIN'
     'IF'J<5'THEN'
     'BEGIN'
        J:=J+1; 'GOTO' LOOP2;
     'END';
     'END';
 'END' OUT;
'COMMENT' ***************** BEGIN PLOT PROCEDURES *****************;
  'PROCEDURE'FRAME;
   'BEGIN'
    PLOT(10,0,3);PLOT(10,8.3,2);PLOT(0,8.3,2);PLOT(0,0,3);
   'FOR'J:=0'STEP'1'UNTIL'10'DO'
   'BEGIN' PLOT(J,0,2);PLOT(J,-.2,2);PLOT(J,0,3);
   'END';PLOT(0,0,3);
   'FOR'J:=0'STEP'1'UNTIL'8'DO'
   'BEGIN' PLOT(0,J,2);PLOT(-.2,J,2);PLOT(0,J,3);
   'END'; PLOT(0,8.3,2);PLOT(0,0,3);
   'END'FRAME;
   'PROCEDURE' REFER;
   'BEGIN'
    FACTOR(.3937);
    PLOT(2,0,2);PLOT(28,0,3);PLOT(30,0,2);PLOT(30,2,2);
    PLOT(30,20,3);PLOT(30,23,2);PLOT(28,23,2);PLOT(2,23,3);
    PLOT(0,23,2);PLOT(0,21,2);PLOT(0,2,3);PLOT(0,0,2);
    'END' REFER;
  'PROCEDURE'TEXT(D); 'INTEGER'D;
  'BEGIN''SWITCH'S:=S1,S2,S3,S4; 'GOTO'S(/D/);
   S1:    SYMBOL(-1.8,PLV/4-1.5,.2,'('TEMPERATURE (K)')',90,15);
          SYMBOL(PLH/4-1.2,-.8,.2,'('LOCATION (M)')',0,12);
         'GOTO'LAB7;
   S2:    SYMBOL(-1.8,PLV/4-1.9,.2,'('CONCENTR.RATIO P/KO')',90,19);
          SYMBOL(PLH/4-1.2,-.8,.2,'('LOCATION (M)')',0,12);
         'GOTO'LAB7;
   S3:    SYMBOL(-1.8,PLV/4-1.9,.2,'('VELOCITY RATIO V/VS')',90,19);
          SYMBOL(PLH/4-1.2,-.8,.2,'('LOCATION (M)')',0,12);
         'GOTO'LAB7;
   S4:    SYMBOL(-1.8,PLV/4-1.9,.2,'('CONCENTR.RATIO P/KO')',90,19);
          SYMBOL(PLH/4-1.5,-.8,.2,'('TEMPERATURE (K)')',0,15);
   LAB7:
  'END'TEXT;
  'PROCEDURE' CONST;
  'BEGIN'
   SYMBOL(6,22.5,.4,'('FLAME NO ')',0,9);
   NUMBER(999.0,999.0,.4,FLAME,0,0);
  'END' CONST;
  'REAL''PROCEDURE'FACM(XMAX);'REAL'XMAX;
  'BEGIN'
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'REAL' NUMB,BOUND,EXPON;
   NUMB:=LN(XMAX)/TLOG;
   EXPON:=(10**(ENTIER(NUMB)));
   BOUND:=(ENTIER(2*XMAX/EXPON+1))/2;
   FACM:=BOUND*EXPON;
'END'FACM;
'PROCEDURE' PLT(AR,NN);'ARRAY'AR;
'INTEGER' NN;
'BEGIN' 'REAL' DELT1,VERT2,VERT7,VERT9,VERT22,
                 MAX1,MAX2,MAX7,MAX9,LMAX1,MANTX1,EXPX1;
'INTEGER' QU,POWER;
    PLH:=10; PLV:=8;
    MAX1:=FACM(AR(/NN,1/)); MAX2:=FACM(AR(/NN,2/));
    MAX7:=FACM(AR(/NN,7/)); MAX9:=FACM(AR(/NN,9/));
    LMAX1:=LN(MAX1)/TLOG;
    EXPX1:=(10**(ENTIER(LMAX1)));
    POWER:=ENTIER(LMAX1);
    MANTX1:=MAX1/EXPX1;
    PLOTS(1,20); REFER; CONST; PLOT(3,2,-3);  FRAME;
    DELT1:=PLH/MAX1;
    VERT2:=PLV/MAX2;VERT7:=PLV/MAX7;
    VERT9:=PLV/MAX9; VERT22:=PLH/MAX2;
    QU:=1;TEXT(QU);
    NUMBER(-1.0,0,.2,0.0,0,1);
    NUMBER(-1.4,PLV/2,.2,MAX2/2,0,0);
    NUMBER(-1.4,PLV,.2,MAX2,0,0);
    NUMBER(-.2,-.8,.2,0.0,0,1);
    NUMBER(PLH/2-.4,-.8,.2,MANTX1/2,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
    NUMBER(999.0,999.0,.2,POWER,0,0);
    NUMBER(PLH-.8,-.8,.2,MANTX1,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
    NUMBER(999.0,999.0,.2,POWER,0,0);
    PLOT(DELT1*AR(/0,1/),VERT2*AR(/0,2/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
    PLOT(DELT1*AR(/J,1/),VERT2*AR(/J,2/),2);
    PLOT(DELT1*AR(/0,10/),VERT2*AR(/0,2/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
   'BEGIN'
   'IF'AR(/J,10/)>MAX1 | AR(/J,10/)<AR(/J-1,10/)
   'THEN' 'GOTO' LAB10;
    PLOT(DELT1*AR(/J,10/),VERT2*AR(/J,2/),2);
   'END';
LAB10:
    PLOT(0,10,-3); FRAME;
    QU:=2;TEXT(QU);
    NUMBER(-1.2,0,.2,0.0,0,2);
    NUMBER(-1.2,PLV/2,.2,MAX7/2,0,2);
    NUMBER(-1.2,PLV,.2,MAX7,0,2);
    NUMBER(-.2,-.8,.2,0.0,0,1);
    NUMBER(PLH/2-.4,-.8,.2,MANTX1/2,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
    NUMBER(999.0,999.0,.2,POWER,0,0);
    NUMBER(PLH-.4,-.8,.2,MANTX1,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
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    NUMBER(999.0,999.0,.2,POWER,0,0);
    PLOT(DELT1*AR(/0,1/),VERT7*AR(/0,7/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
    PLOT(DELT1*AR(/J,1/),VERT7*AR(/J,7/),2);
    PLOT(DELT1*AR(/0,10/),VERT7*AR(/0,15/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
   'BEGIN'
   'IF'AR(/J,10/)>MAX1 | AR(/J,10/)<AR(/J-1,10/)
   'THEN' 'GOTO' LAB20;
    PLOT(DELT1*AR(/J,10/),VERT7*AR(/J,15/),2);
   'END';
LAB20:
    PLOT(14,0,-3); FRAME;
    QU:=3;TEXT(QU);
    NUMBER(-1.2,0,.2,0.0,0,2);
    NUMBER(-1.2,PLV/2,.2,MAX9/2,0,2);
    NUMBER(-1.4,PLV,.2,MAX9,0,2);
    NUMBER(-.2,-.8,.2,0.0,0,1);
    NUMBER(PLH/2-.4,-.8,.2,MANTX1/2,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
    NUMBER(999.0,999.0,.2,POWER,0,0);
    NUMBER(PLH-.4,-.8,.2,MANTX1,0,2);
    MARK(999.0,999.0,.2,125,0,-1);
    NUMBER(999.0,999.0,.2,POWER,0,0);
    PLOT(DELT1*AR(/0,1/),VERT9*AR(/0,9/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
    PLOT(DELT1*AR(/J,1/),VERT9*AR(/J,9/),2);
    PLOT(DELT1*AR(/0,10/),VERT9*AR(/0,17/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
   'BEGIN'
   'IF'AR(/J,10/)>MAX1 | AR(/J,10/)<AR(/J-1,10/)
   'THEN' 'GOTO' LAB30;
    PLOT(DELT1*AR(/J,10/),VERT9*AR(/J,17/),2);
   'END';
LAB30:
    PLOT(0,-10,-3); FRAME;
    QU:=4;TEXT(QU);
    NUMBER(-1.2,0,.2,0.0,0,2);
    NUMBER(-1.2,PLV/2,.2,MAX7/2,0,2);
    NUMBER(-1.2,PLV,.2,MAX7,0,2);
    NUMBER(-.2,-.8,.2,0.0,0,1);
    NUMBER(PLH/2-.4,-.8,.2,MAX2/2,0,0);
    NUMBER(PLH-.4,-.8,.2,MAX2,0,0);
    PLOT(VERT22*AR(/0,2/),VERT7*AR(/0,7/),3);
   'FOR' J:=1'STEP'1'UNTIL'NN'DO'
    PLOT(VERT22*AR(/J,2/),VERT7*AR(/J,7/),2);
    PLOT(VERT22*AR(/0,2/),VERT7*AR(/0,15/),3);
   'FOR'J:=1'STEP'1'UNTIL'NN'DO'
   'BEGIN'
   'IF' AR(/J,15/)<AR(/J-1,15/)'THEN' 'GOTO'LAB60;
    PLOT(VERT22*AR(/J,2/),VERT7*AR(/J,15/),2);
   'END';
LAB60:
    LASPLO;
'END' PLT;
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'COMMENT' ****************** END PLOT PROCEDURES *****************;
'COMMENT' ******************READING OF INPUT DATA ****************;
  READ(0,A,CP,DH,INSTEP,L,M,MK,NU,PS,RB,ROB,RU,TA,TS,FLAME);
  PRINT(1,'('FREQUENCY FACTOR A =')',A); LINE(1,1);
  PRINT(1,'('HEAT CAPACITY REACTANTS CP =')',CP); LINE(1,1);
  PRINT(1,'('HEAT OF FORMATION PRODUCTS DH =')',DH); LINE(1,1);
  PRINT(1,'('INITIAL INTEGRATION STEP INSTEP=')',INSTEP);LINE(1,1);
  PRINT(1,'('HEAT CONDUCTION COEFFICIENT L =')',L); LINE(1,1);
  PRINT(1,'('ORDER OF REACTION M =')',M); LINE(1,1);
  PRINT(1,'('MOLAR MASS OF REACTANTS MK =')',MK); LINE(1,1);
  PRINT(1,'('STOICHIOMETRIC COEFFICIENT NU =')',NU); LINE(1,1);
  PRINT(1,'('PRESSURE AT BURNING SURFACE PS =')',PS); LINE(1,1);
  PRINT(1,'('BURNING RATE RB =')',RB); LINE(1,1);
  PRINT(1,'('PROPELLANT DENSITY ROB =')',ROB); LINE(1,1);
  PRINT(1,'('UNIVERSAL GAS CONSTANT RU =')',RU); LINE(1,1);
  PRINT(1,'('ACTIVATION TEMPERATURE TA =')',TA); LINE(1,1);
  PRINT(1,'('TEMPERATURE AT BURNING SURFACE TS =')',TS);LINE(1,2);
  PRINT(1,'('CALCULATED CONSTANTS')'); LINE(1,2);
  ARFIL:=KWANT:=LAST:=TELAN:=0;
  TLOG:=LN(10);
  FIRST:=1;
  ROBR:=ROB*RB;  KNV:=ROBR/MK;  VS:=KNV*RU*TS/PS;
  PTS:=PS+ROBR*VS;  KS:=KNV/VS;  TAS:=TA/TS;
  HT1:=CP+L*NU*A*EXP(-TAS)*(KS**M)/KNV/KNV;
  HT2:=NU*NU*TS*TS/MK/VS/VS;
  HT3:=HT1*HT2;
  TF:=-HT3+SQRT(HT3*HT3+2*HT2*(MK*VS*VS/2+TS*HT1-DH/NU));
  VF:=VS*TF/(NU*TS);  TFA:=TF/TA;  TSA:=TS/TA;
  FACT:=((NU*PTS/(RU*TA))**M)*NU*A*(TFA-TSA)*MK/ROBR;
  FACT2:=ROBR*ROBR/PTS/MK;  FACT3:=PTS*NU/RU;
  TFTS:=TF-TS;
  DNK:=DH*KNV/NU;
  PROBR:=PTS/2/ROBR; VCON:=NU*MK*L*PROBR*PROBR; NUA:=NU*A;
  KNCL:=KNV*CP/L; TAL:=TA*L; TFL:=TF*L;
  NURP:=(NU-1)*RU/NU/PTS;
  KNVL:=KNV/L; DHLN:=DH*L/NU; DHKNU:=DH*KNV/NU; NURPK:=NURP*KNVL;
  RUPTS:=RU*KNVL/PTS; RUPNU:=RUPTS/NU;
  DTS:=KNCL*(TS*L-TFL)-DNK+ROBR*(VS*VS-VF*VF)/2;
  DKKOS:=-NUA*EXP(-TAS)*(KS**M)/KNV;
  PARAM:=-DKKOS*L/(CP*KNV);
  PARAM:=PARAM/(1+PARAM);
  TF2AN:=TS-((DH/NU/CP)*(1-PARAM));
  PRINT(1,'('MASS FLUX ROBR =')',ROBR); LINE(1,1);
  PRINT(1,'('MOLAR CONCENTRATION FLUX KNV =')',KNV); LINE(1,1);
  PRINT(1,'('REACTANT CONCENTRATION AT BURNING SURFACE KS =')',KS);
  LINE(1,1);
  PRINT(1,'('VELOCITY AT BURNING SURFACE VS =')',VS); LINE(1,1);
  PRINT(1,'('TOTAL PRESSURE AT BURNING SURFACE PTS =')',PTS);
  LINE(1,1);
  PRINT(1,'('FLAME TEMPERATURE (ESTIMATED) TF =')',TF); LINE(1,1);
  PRINT(1,'('FLAME VELOCITY (ESTIMATED) VF =')',VF); LINE(1,1);
  PRINT(1,'('TEMPERATURE RISE (ESTIMATED) TFTS =')',TFTS);
  LINE(1,1);
  PRINT(1,'('TEMPERATURE RATIO TAS =')',TAS); LINE(1,1);
  PRINT(1,'('TEMPERATURE RATIO TFA =')',TFA); LINE(1,1);
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   PRINT(1,'('TEMPERATURE RATIO TSA =')',TSA); LINE(1,1);
   PRINT(1,'('FACTORS ARE,FACT=')',FACT,'('FACT2=')',FACT2);
   PRINT(1,'('FACT3 =')',FACT3); LINE(1,1);
   PRINT(1,'('CONSTANT,DNK=')',DNK); LINE(1,1);
   PRINT(1,'('GRADIENT REL.CONC.FLUX AT BURNING SURFACE, DKKOS= ')'
        ,DKKOS);LINE(1,1);
   PRINT(1,'('GRADIENT TEMP*HEAT COND. COEF DTS= ')',DTS);LINE(1,1);
   PRINT(1,'('CONSTANT NURP= ')',NURP); LINE(1,1);
   PRINT(1,'('CONSTANT NURPK= ')',NURPK); LINE(1,1);
   PRINT(1,'('CONSTANT DHKNU= ')',DHKNU); LINE(1,3);
   PRINT(1,'('TF2AN= ')',TF2AN);LINE(1,1);
   PRINT(1,'('PARAMETER EPSILON= ')',PARAM); PAGE(1);
   TEL:=0;
  'FOR'I:=1'STEP'1'UNTIL'17'DO' RES(/0,I/):=0;
   RES(/0,2/):=TS;
   RES(/0,3/):=RES(/0,4/):=RES(/0,11/):=RES(/0,12/):=KS;
   RES(/0,5/):=RES(/0,9/):=RES(/0,13/):=RES(/0,17/):=1;
   RES(/0,8/):=RES(/0,16/):=VS;
   STEP:=INSTEP;
   VV:=VS;
   S(/0/):=Z(/0/):=0;
   S(/1/):=Z(/1/):=L*TS;
   S(/2/):=Z(/2/):=1;
REPEAT:
   RUNNER(Z,2,STEP,F);
  'FOR'I:=0'STEP'1'UNTIL'2'DO'
  'BEGIN'
     E(/I/):=Z(/I/);
     Z(/I/):=S(/I/);
  'END';
   STEP:=STEP/2;
   RUNNER(Z,2,STEP,F); FIRST:=0; RUNNER(Z,2,STEP,F);
  'FOR'I:=0'STEP'1'UNTIL'2'DO'
   E1(/I/):=Z(/I/);
  'IF'ABS(AFG1)<'-60'THEN'
     'BEGIN'
      NODTS:=1;'GOTO' FOLLOW;
     'END';
   NODTS:=ABS(DTS/AFG1);
FOLLOW:
  'IF' (ABS((E1(/1/)-E(/1/)))>5'-2*('IF'NODTS
   >1'THEN'1'ELSE'NODTS)) |
   (ABS((E1(/2/)-E(/2/)))>5'-2*('IF'NODTS>1'THEN'1'ELSE'NODTS))
  'THEN'
  'BEGIN'
    'FOR'I:=0'STEP'1'UNTIL'2'DO'
     Z(/I/):=S(/I/);
    'IF' TEL=0 'THEN' FIRST:=1;
    'GOTO' REPEAT;
  'END';
   TDIF:=Z(/1/)/L-RES(/TEL,2/);
CHECK:
  'IF'(((TDIF>TFTS/1000) | LAST=1) | (Z(/1/)/L
   >.95*TF)) 'THEN'
  'BEGIN'
```

```
'COMMENT' *********** SET UP ARRAY RES CONTAINING OUTPUT DATA *****;
  TEL:=TEL+1;
  VV:=V(Z(/1/),Z(/2/));
  RES(/TEL,1/):=Z(/0/)/A;
  RES(/TEL,2/):=Z(/1/)/L;
  RES(/TEL,3/):=Z(/2/)*KNV/VV;
  RES(/TEL,4/):=KNV/VV;
  RES(/TEL,5/):=Z(/2/);
  RES(/TEL,6/):=(RES(/TEL,4/)-RES(/TEL,3/))/NU;
  RES(/TEL,7/):=(RES(/TEL,6/)/RES(/TEL,4/));
  RES(/TEL,8/):=VV;
  RES(/TEL,9/):=VV/VS;
  EPS:=(RES(/TEL,1/)-RES(/TEL-1,1/))*FACT*'-3;
  TO:=TAL/(RES(/TEL-1,2/)*L);   TB:=TAL/Z(/1/);
 'IF'RES(/TEL,2/)<.999*TF & LAST=0'THEN'
 'BEGIN'
  RES(/TEL,10/):=INTSIG(TO,TB,Y,EPS)/(FACT)+RES(/TEL-1,10/);
  FT:=Z(/1/)/L*(Z(/1/)/L-TS+NU*(TF-Z(/1/)/L));
  RES(/TEL,11/):=FACT3*(TF-Z(/1/)/L)/FT-FACT2*(TF-Z(/1/)/L)/TFTS;
  RES(/TEL,12/):=FACT3*TFTS/FT-FACT2;
  RES(/TEL,13/):=RES(/TEL,11/)/RES(/TEL,12/);
  RES(/TEL,14/):=(RES(/TEL,12/)-RES(/TEL,11/))/NU;
  RES(/TEL,15/):=(RES(/TEL,14/)/RES(/TEL,12/));
  RES(/TEL,16/):=ROBR/MK/RES(/TEL,12/);
  RES(/TEL,17/):=RES(/TEL,16/)/VS;
 'END' 'ELSE' TELAN:=TELAN+1;
 'IF'LAST=1'THEN' 'GOTO' READY;
 'END';
  STEP:=3.4*STEP;
 'IF'TEL=NN'THEN'
 'BEGIN'
    ARFIL:=1;
    LINE(1,3);
    PRINT(1,'('PROGRAMME ENDED BECAUSE ARRAY RES HAS BEEN FILLED')');
    LINE(1,1);
    PRINT(1,'('TF-RES(/TEL,2/)= ')',TF-RES(/TEL,2/));
   'GOTO' READY;
 'END';
  'IF' 1/NU-RES(/TEL,7/)<'-9 |
  RES(/TEL,2/)/TF>.9999  &  M>1.5
 'THEN' 'BEGIN' LAST:=1; 'GOTO' CHECK; 'END' 'ELSE'
 'BEGIN'
   'FOR'I:=0'STEP'1'UNTIL'2'DO' S(/I/):=Z(/I/);
   'GOTO' REPEAT;
 'END';
 READY:
  PRINT(1,'('*******************************')');LINE(1,2);
 'IF'ARFIL=0'THEN'
 'BEGIN'
    PRINT(1,'('FLAME TEMP ACHIEVED  RES(/TEL,2/)-TF= ')',
    RES(/TEL,2/)-TF); LINE(1,1);
    PRINT(1,'('TEMP RES(/TEL,2/)= ')',RES(/TEL,2/));LINE(1,1);
    PRINT(1,'('CONTROL FACT= ')',ABS(RES(/TEL,7/)-1/NU));
    LINE(1,1);
    PRINT(1,'('NUMBER OF NUMERICAL DATAPOINTS= ')',TEL);
```

```
    LINE(1,1);
    PRINT(1,'('NUMBER OF ANALYTIC DATAPOINTS=  ')',TEL-TELAN);
    LINE(1,1);
 'END';
  PRINT(1,'('*******************************')');LINE(1,1);
  NN:=TEL;
  TELMIN:=10;DIST:=RES(/NN-TELMIN,1/);
  DISTM:=100*DIST; CUT:=0;
CUTTING:
 'IF'RES(/NN-CUT,1/)>DISTM'THEN'
 'BEGIN'
    CUT:=CUT+1; 'GOTO'CUTTING;
 'END';
  LINE(1,6);
  PRINT(1,'('INFORMATION CONCERNING PLOTPROCEDURE')');LINE(1,1);
  PRINT(1,'('NUMBER OF CANCELLED ELEMENTS OF ARRAY RES')',
        CUT);LINE(1,1);
  PRINT(1,'('TEMP.RANGE HAS BEEN CUT OFF AT T= ')',
        RES(/TEL-CUT,2/));LINE(1,1);
  PRINT(1,'('AT DISTANCE X= ')',RES(/TEL-CUT,1/));LINE(1,1);
  PRINT(1,'('TEMPERATURE DIFFERENCE= ')',
        RES(/TEL,2/)-RES(/TEL-CUT,2/));LINE(1,1);
'COMMENT'*** PRINTOUT OF RESULTS IN SUCCESSIVE TABLES  ************;
  OUT; NN:=TEL-CUT-1;TEL:=TEL-CUT-1;
  PLT(RES,NN);
 'END'; 'COMMENT' *************** END SECOND BLOCK ****************;
 'END'
```

6. RESULTS

6.1. General remarks

Temperature, concentration and velocity profiles have been calculated for a variety of flames. In addition the product concentration ratio, P/K_o, has been calculated as a function of temperature. According to a fundamental assumption, this concentration ratio should be a linear function of the temperature. Any deviation from linearity is an indication that this basic assumption is violated.

The parameter ε which is required to be small follows from a combination of independent variables according to Eq. (3.26):

$$\varepsilon = \frac{\dfrac{\lambda}{C_p (K_o v)^2}\, \nu\, A \exp\left\{\dfrac{-\theta}{T_s}\right\} K_{os}^{\ m}}{1 + \dfrac{\lambda}{C_p (K_o v)^2}\, \nu\, A \exp\left\{\dfrac{-\theta}{T_s}\right\} K_{os}^{\ m}} \quad . \qquad (6.1)$$

It is seen from this equation that ε will increase with increasing values for λ, ν and A, decrease with increasing values for C_p and θ.

The factor $K_o v$ represents the mass flow as

$$K_o v = m_s / M_K \qquad (6.2)$$

where m_s is the mass flow rate per unit surface area, which is constant. Increasing mass flow rates therefore will decrease the value of ε.
K_{os} stands for the initial concentration of reactants. It is related to the pressure and temperature by the equation of state:

$$p_s = K_{os} R_o T_s \quad . \qquad (6.3)$$

It is seen that the effect of pressure therefore enters the value of ε through the concentration K_{os}. For a zeroth order of reaction, no effect of pressure is felt. For unity order of reaction, i.e. $m = 1$, ε will increase linearly with pressure, while for $m > 1$, ε will increase more than linearly with pressure.

Table 6.1 lists the parameter values for which calculations have been made. It is seen that the frequency factor A varies between 6.10^5 and 6.10^{12} $(\text{kMol/m}^3)^{1-m}$./s. The order of reaction varies between 1 and 2, the stoichiometric coefficient ν varies between 0,25 and 1, the pressure between 0,1 and 5 MPa, the mass flow rate varies between 0,16 and 128 kg/(m^{2}s), the ratio of the activation temperature and the surface temperature varies between 1 $^2/_3$ and 25, while the ratio of activation temperature and flame temperature varies between 1/3 and 12,5. For first order reactions the reaction rate, k, based on the surface temperature varies between $2{,}78.10^{-3}$ and $3{,}86.10^5.\text{s}^{-1}$ while based on the flame temperature k varies between $4{,}8.10^4$ and $2{,}24.10^7$/s. Altogether this is a fairly wide variation of parameters. The corresponding parameter ε varies between $1{,}11.10^{-9}$ and $1{,}34.10^{-1}$.

Two types of calculations have been made:
i. by numerical integration
i.i. according to the analytic approach outlined in the present studies.

Table 6.1. Combinations of Parameters for Flame Calculations.

Pre-exponential Factor, A, ($S^{-1}.(kMol/m^3)^{1-M}$)	Heat of formation, ΔH_f^o, ($Kg.m^2/(kMol.S^2)$)	Order of Reaction, M (-)	Stoichiometric Coefficient, ν (-)	Pressure P, (N/m^2)	Mass flow rate, m_s, ($kg/(m^2.S)$)	Activation Temperature, θ (K)	Surface Temperature, T_S (K)	Flame Temperature, T_F (K)	Flame velocity, V_F (m/s)	Parameter ε, (-)	Plotted in Fig.
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	7500	600	1799,64	29,92	$2,99.10^{-4}$	6.2
4.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	7500	600	1799,28	29,92	$5,97.10^{-4}$	6.3
6.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	7500	600	1798,93	29,91	$8,96.10^{-4}$	6.4
2.10^8	$-\ 1,2.10^8$	1	0,25	2.10^5	10	7500	600	2999,28	49,86	$2,99.10^{-4}$	6.5
2.10^8	$-\ 6.10^7$	2	0,25	2.10^5	10	7500	600	1799,99	29,93	$1,20.10^{-5}$	6.6
5.10^6	$-\ 1,2.10^8$	1	0,25	5.10^6	16	7500	600	2999,82	3,19	$7,29.10^{-5}$	6.7
5.10^6	$-\ 1,2.10^8$	1,5	0,25	5.10^6	16	7500	600	2999,82	3,19	$7,30.10^{-5}$	6.8
2.10^8	$-\ 6.10^7$	1	0,50	2.10^5	10	7500	600	1198,28	9,96	$5,97.10^{-4}$	6.9
2.10^8	$-\ 6.10^7$	1	0,25	4.10^5	10	7500	600	1799,28	14,96	$5,97.10^{-4}$	6.10
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	20	7500	600	1799,91	59,83	$7,47.10^{-5}$	6.11
6.10^5	$-\ 6.10^7$	1	0,25	10^5	16	500	300	1479,07	78,62	$1,74.10^{-2}$	6.12
6.10^5	$-\ 6.10^7$	1	0,25	10^5	64	500	300	1498,67	313,77	$1,11.10^{-3}$	6.13
6.10^{12}	$-\ 6.10^7$	1	1	10^5	128	7500	300	600,00	63,77	$8,16.10^{-7}$	6.14
6.10^{12}	$-\ 6.10^7$	1	1	10^5	16	7500	300	599,98	7,98	$5,22.10^{-5}$	6.15
5.10^6	$-\ 1,2.10^8$	1	0,25	5.10^6	64	7500	600	2999,99	12,77	$4,56.10^{-6}$	6.16
5.10^6	$-\ 1,2.10^8$	1	0,25	$5,10^6$	128	7500	600	2999,99	25,54	$1,14.10^{-6}$	6.17
$1,2.10^7$	$-\ 1,2.10^8$	1	0,25	5.10^6	0,16	10.000	600	2936.57	$3,13.10^{-2}$	$2,64.10^{-2}$	6.18
$1,2.10^7$	$-\ 1,2.10^8$	1	0,25	5.10^6	1,6	10.000	600	2999,35	0,32	$2,71.10^{-4}$	6.19
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	3750	600	1639,15	27,25	$1,34.10^{-1}$	6.20
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	10.000	600	1799,99	29,93	$4,63.10^{-6}$	6.21
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	15.000	600	1799,99	29,93	$1,11.10^{-9}$	6.22
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	7500	300	1500,00	24,94	$2,23.10^{-9}$	6.23
2.10^8	$-\ 6.10^7$	1	0,25	2.10^5	10	7500	1200	2313,80	38,47	$7,18.10^{-2}$	6.24
2.10^8 *	$-\ 6.10^7$ *	1 *	0,25 *	2.10^5 *	10 *	7500 *	600 *	1799,96 *	29,93 *	$2,99.10^{-5}$ *	6.25 *
2.10^8 **	$-\ 6.10^7$ **	1 **	0,25 **	2.10^5 **	10 **	7500 **	600 **	1799,28 **	29,92 **	$5,97.10^{-4}$ **	6.26 **

Heat Capacity Reactants,	$C_p = 2.10^5\ kg.m^2/(S^2,Kmol.K)$
Heat Conductivity Combustion Gases,	$\lambda = 0,08$ (*$\lambda = 0,008$,**$\lambda = 0,16$) $kg.m/(S^3.K)$
Molar Mass Reactants,	$M_K = 100$ kg/kMol

* $\lambda = .008$

** $\lambda = .16$

In most cases the difference between the two solutions can hardly be distinguished. Only for some larger values of ε one can distinguish between the two cases.

The first variable where one can distinguish between the analytical and numerical solutions is the velocity profile. It should be recalled that effects of velocity were dropped from the energy equation for the analytic solution on the argument that kinetic energy in general is negligible. Therefore the analytically obtained velocity may deviate from the numerically obtained value, even when one cannot distinguish between the numerically and analytically obtained temperatures and concentrations. If one can distinguish between the two concentration ratios, it turns out that the analytically determined concentration ratio P/K_o always exceeds the numerically determined one, when plotting P/K_o versus T.

6.2. Accuracy

By Eq. (3.28) the flame temperature may be calculated before a complete (numerical) integration has been performed:

$$T_f = T_s + \frac{-\Delta H_f/\nu}{C_p + \dfrac{\lambda}{(K_o v)^2}\,\nu\, A \exp\left(\dfrac{-\theta}{T_s}\right) K_{os}^{\;m}} \tag{6.4}$$

This flame temperature may be compared with the flame temperature that follows from a numerical integration. The difference between the two flame temperatures is a measure for the accuracy of the analytic solution. The results are given in Fig. 6.1. It is seen that in all cases the error is smaller than 1 % for $\varepsilon < 10^{-3}$. The scatter in Fig. 6.1 is caused by the combination of the analytic accuracy and the accuracy of the numerical integration which is not the same for every calculation.

6.3. Effect of the various parameters

In addition to comparing the new analytic and the numerical solution for premixed flames, the figures 6.2 through 6.26 also allow to see the effect of the various parameters.

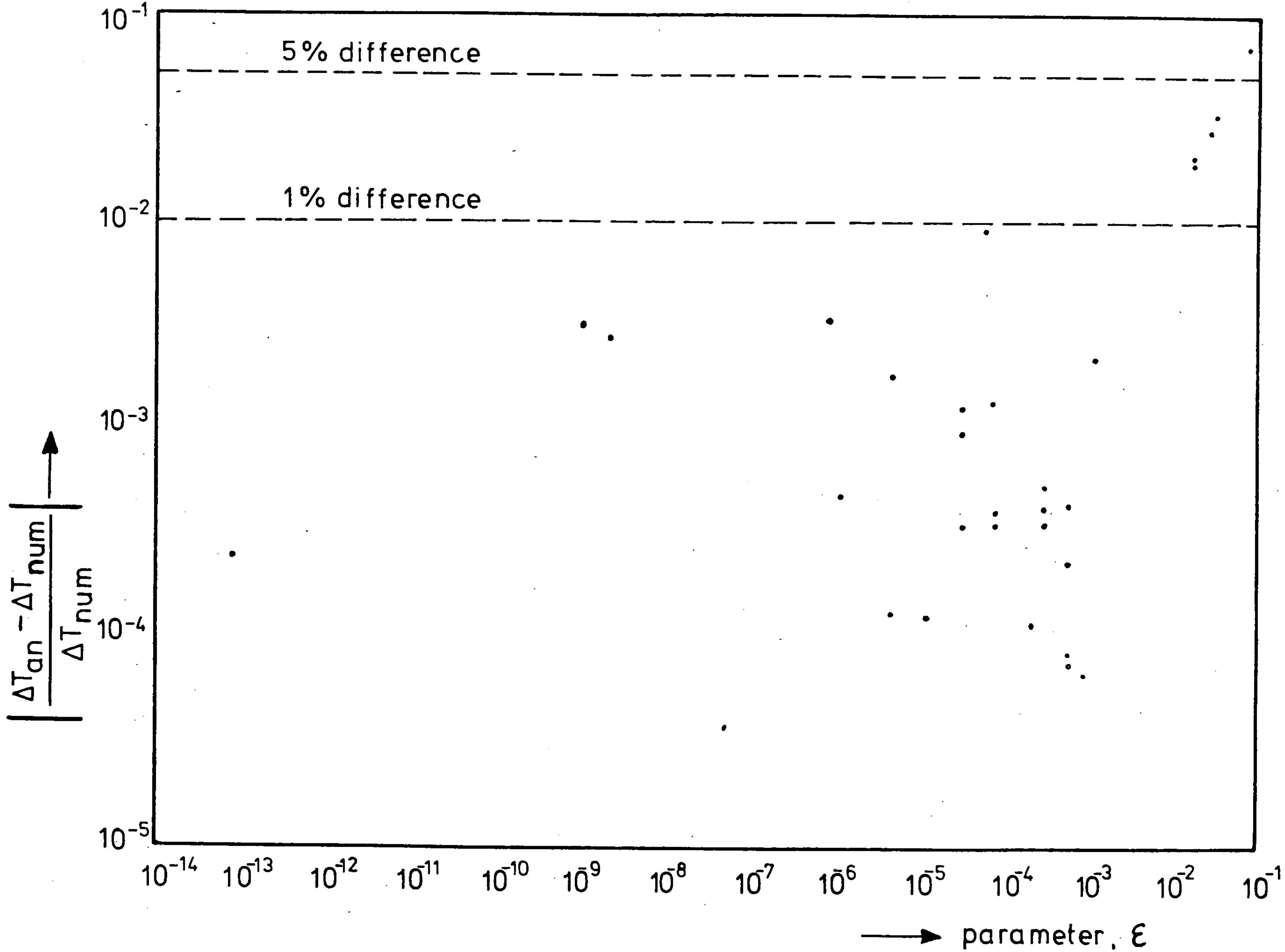


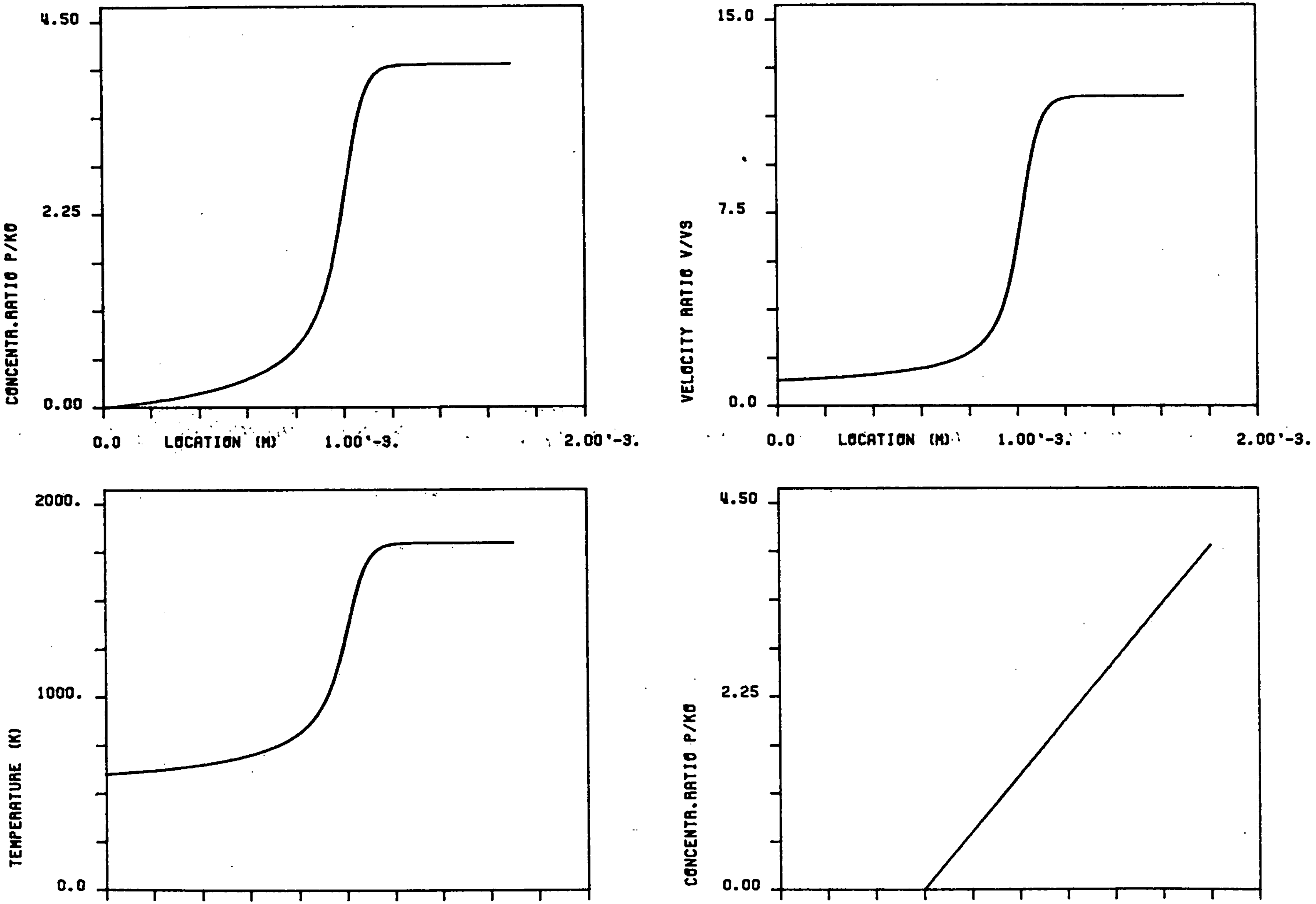
Fig. 6.1. The difference between analytically determined temperature rise, ΔT_{AN}, and the numerically determined temperature rise, ΔT_{NUM}, versus the parameter ε.

Fig. 6.2. Temperature-, concentration ratio- and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_s = 10$ $(kg/(m^2.S))$
$\varepsilon = 2,99.10^{-4}$



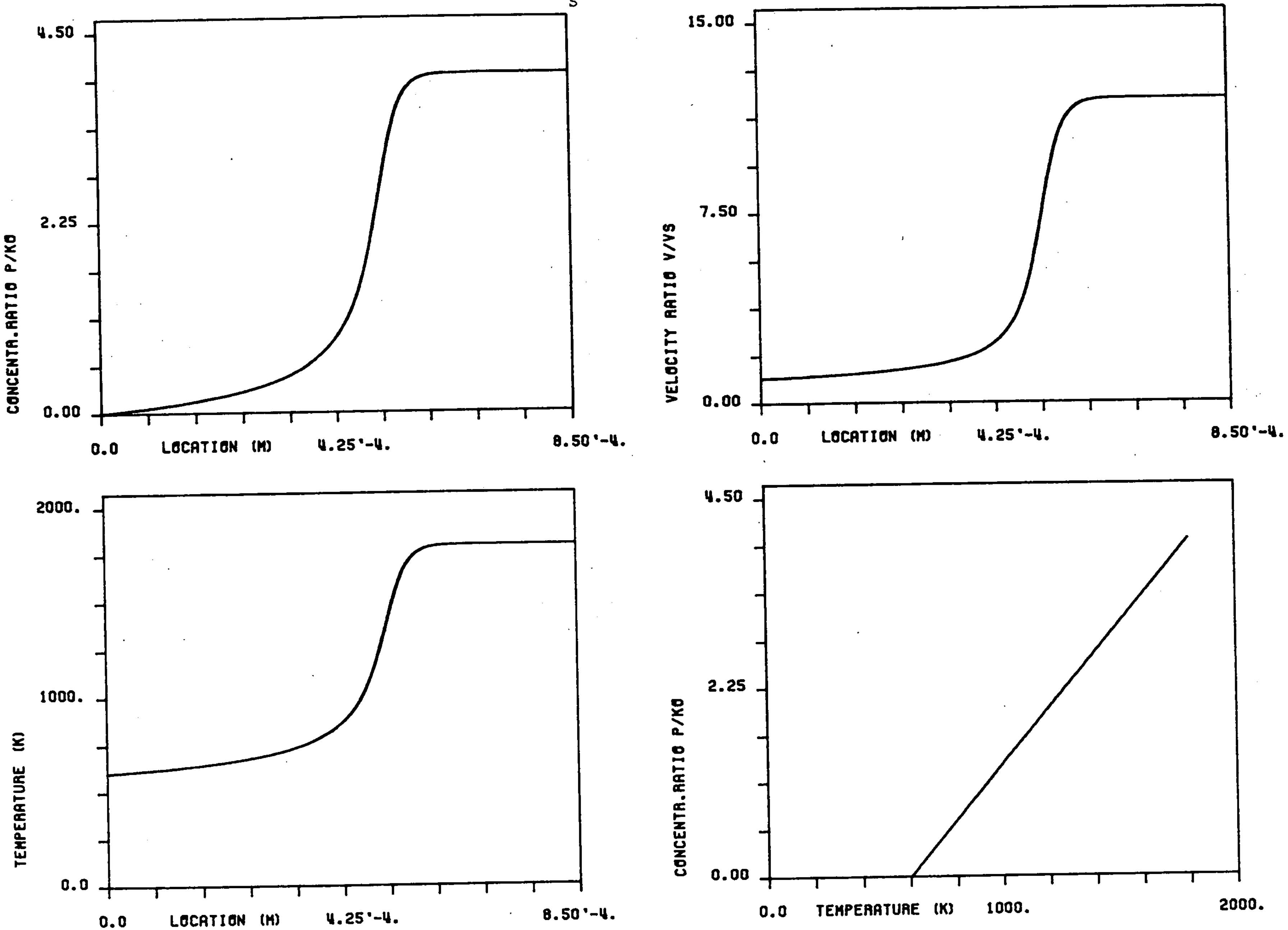


Fig. 6.3. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 4.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)
$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)
$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 5,97.10^{-4}$

Fig. 6.4. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 6.10^8$ (S^{-1})
$\nu = 0{,}25$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 8{,}96.10^{-4}$

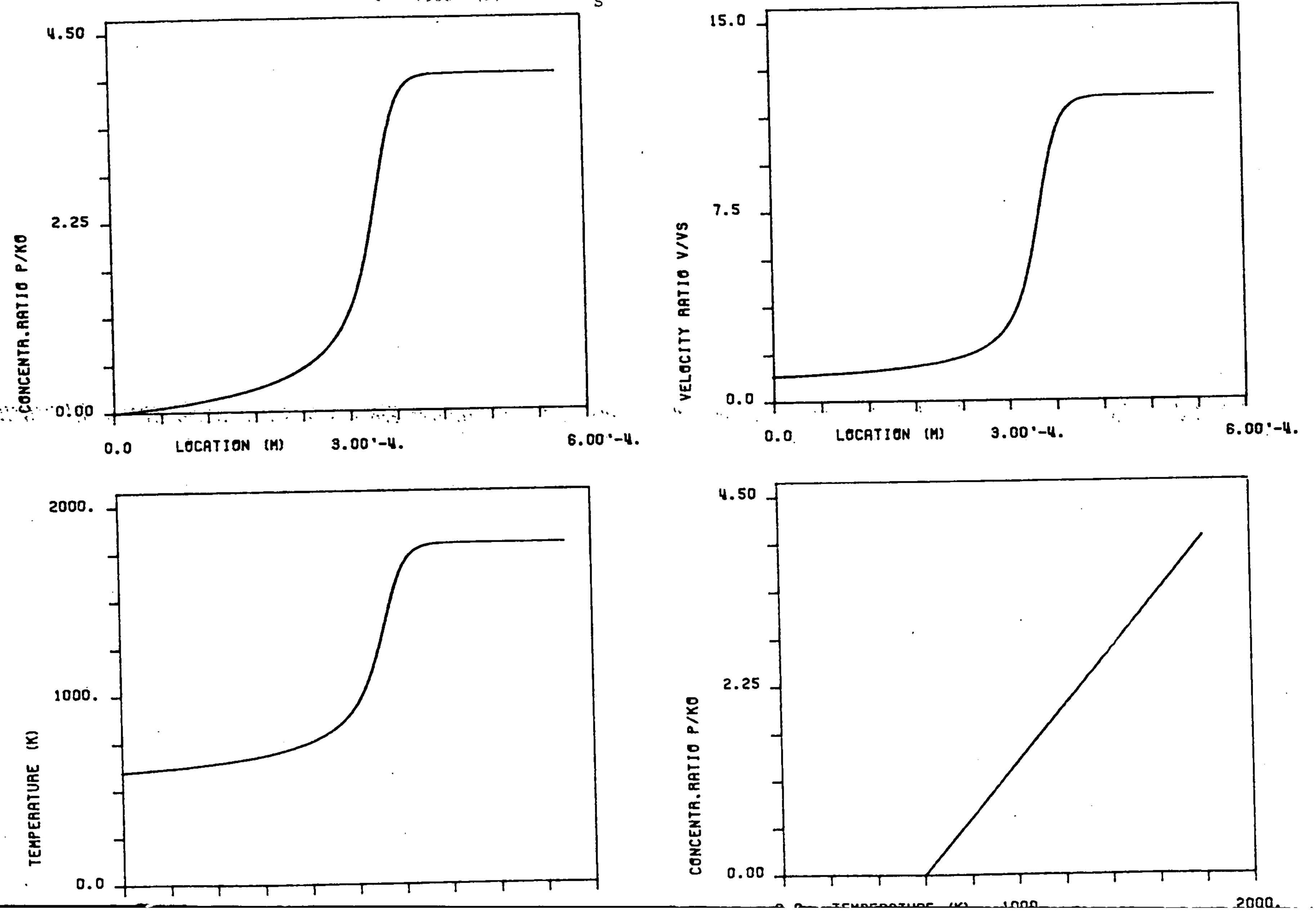


Table 6.2. The effect of the pre-exponential factor.

Pre-exponential Factor, A, (S^{-1})	Flame Temperature, T_F, (K)	Reference Temperature T^* (K)	Location X*		Product A.X*		Temperature Gradient at surface, $(dT/dx)_s$ (K/m)
			Analytic (m)	Numerical (m)	Analytic (m/s)	Numerical (m/s)	
2.10^8	1799,64	1796	$1,215.10^{-3}$	$1,225.10^{-3}$	$2,43.10^5$	$2,45.10^5$	$8,96.10^4$
4.10^8	1799,28	1796	$6,097.10^{-4}$	$6,125.10^{-4}$	$2,44.10^5$	$2,45.10^5$	$1,79.10^5$
6.10^8	1798,93	1796	$4,080.10^{-4}$	$4,080.10^{-4}$	$2,45.10^5$	$2,45.10^5$	$2,69.10^5$

Table 6.3. The effect of Heat of Formation, ΔH_f^o.

Heat of formation ΔH_f^o ($kg.m^2/(kMol.S^2)$)	Flame Temperature, T_F (K)	Reference Temperature, T^* (K)	Location X*		Temperature gradient at surface $(dT/dx)_s$, (K/m)	Flame Velocity, V_F, (m/S)
			Analytic (m)	Numerical (m)		
-6.10^7	1799,64	1797	$1,236.10^{-3}$	$1,250.10^{-3}$	$8,96.10^4$	29,92
$-1,2.10^8$	2999,28	2995	$5,125.10^{-4}$	$5,155.10^{-4}$	$1,79.10^5$	49,86

X* is the location where the temperature T* is achieved.

Pre-exponential factor, A.

The major effect of the pre-exponential factor is felt in the length scale. According to Eq. (3.32) the product A.X, where X is the length scale is the primary variable i.e. if A is doubled this will result in a reduction by two for the location X* where a temperature T* is achieved. Flames for three different values of A have been calculated. The results are shown in the Figs.6.2 through 6.4.
A second effect of the variation of A is that the temperature gradients, and hence heat transfer also changes. As a result the flame temperature will slightly change.
Table 6.2 shows some of the results. A compilation of all major parameters is given in Table 6.1.

It is seen that indeed the product A.X* for a reference temperature T* remains constant. Moreover the differences between the analytic and numerical solutions are negligible.

Heat of formation ΔH_f^o.

The main effect of varying the heat of formation is to change the flame temperature. As a result also the flame velocity and the temperature gradient change. The effect of a variation of the heat of formation may be seen by comparing the Figs. 6.2 and 6.5. The main resulting differences are compiled in Table 6.3, while a compilation of all relevant parameters may be found in Table 6.1.

Again it is seen that there is a good correspondence between the numerically and analytically obtained values.

Order of reaction, m.

The order of the reaction strongly affects the shape of the temperature and concentration profile. This is easily seen by comparing the Figs. 6.1 and 6.6 (m = 1 and m = 2) and the Figs. 6.7 and 6.8 (m = 1 and m = 1,5). As may be seen from Eq. (3.32) the effect of a variation of the order of reaction is rather complicated. The flame temperature and flame velocity are not affected by the order of reaction but the temperature gradient at the burning surface is severely affected. Table 6.4 shows the main resulting differences, while table 6.1 again lists all relevant parameters.

Table 6.4. The effect of the Order of Reaction, m.

Order of Reaction m (-)	Reference Temperature T* (K)	Location X*		Temperature Gradient at Surface $(dT/dx)_s$ (K/m)
		Analytic (m)	numerical (m)	
1	1791,1	$1,185.10^{-3}$	$1,194.10^{-3}$	$8.96.10^{4}$
2	1791,1	1,634	1,321	$3,59.10^{3}$
1	2995	$1,306.10^{-3}$	$1,320.10^{-3}$	$7,00\ 10^{4}$
1,5	2995	$7,315.10^{-3}$	$6,499.10^{-3}$	$7,01\ 10^{4}$

X* is the location where the temperature T* is reached.

and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)

$\Delta H_f^o = -1,210^8$ $(kg.m^2/(kMol.S^2)$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 2,99.10^{-4}$

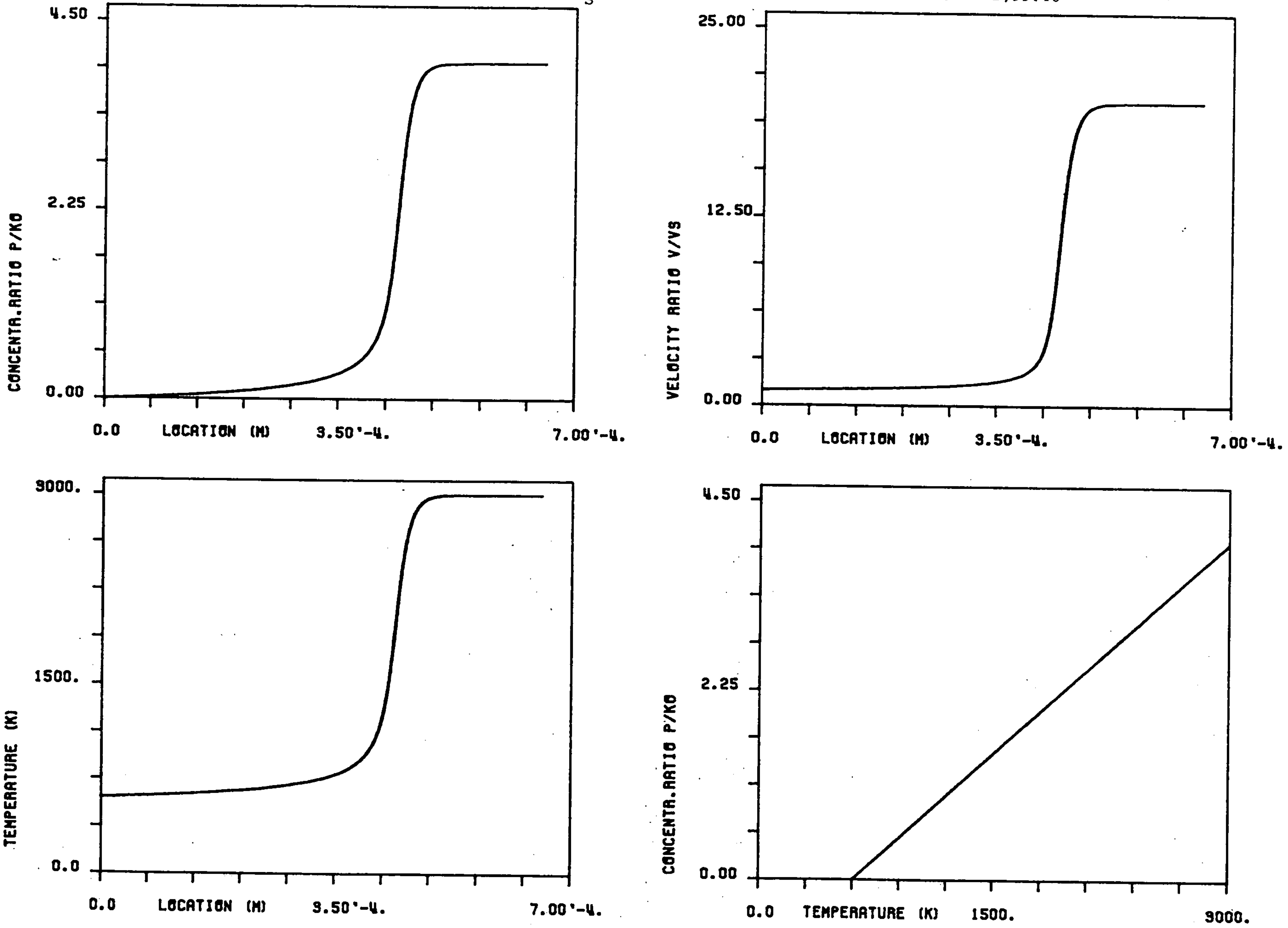


Fig. 6.6. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)
$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)
$m = 2$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 1,20.10^{-5}$

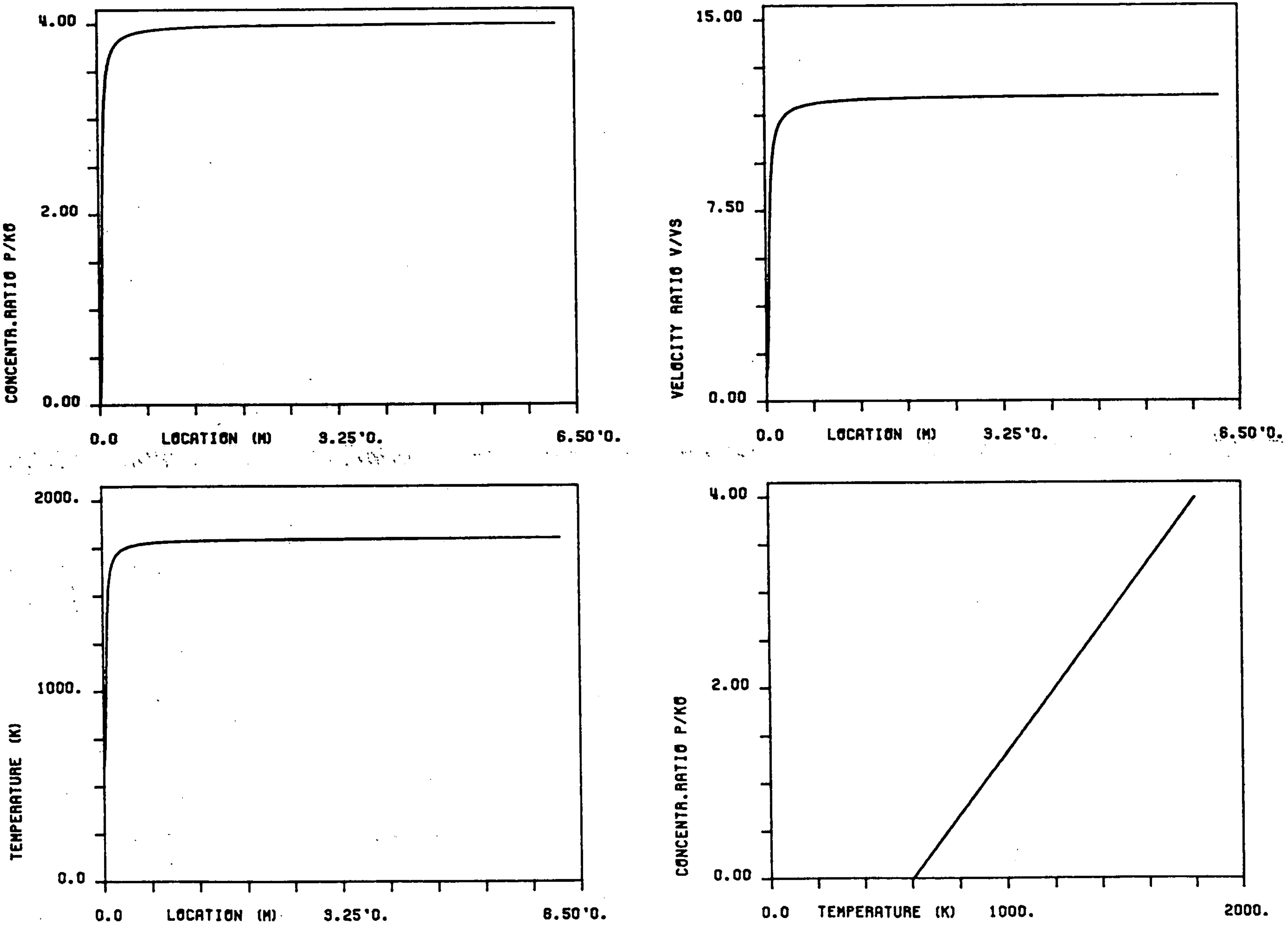


Fig. 6.7. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 5.10^6$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)
$\Delta H_f^o = -1,2.10^8$ $(kg.m^2/(kMol.S^2)$
$P = 5.10^6$ (N/m^2)
$T_S = 600$ (K)
$m = 1$
$m_S = 16$ $(kg/(m^2.S))$
$\varepsilon = 7,29.10^{-5}$

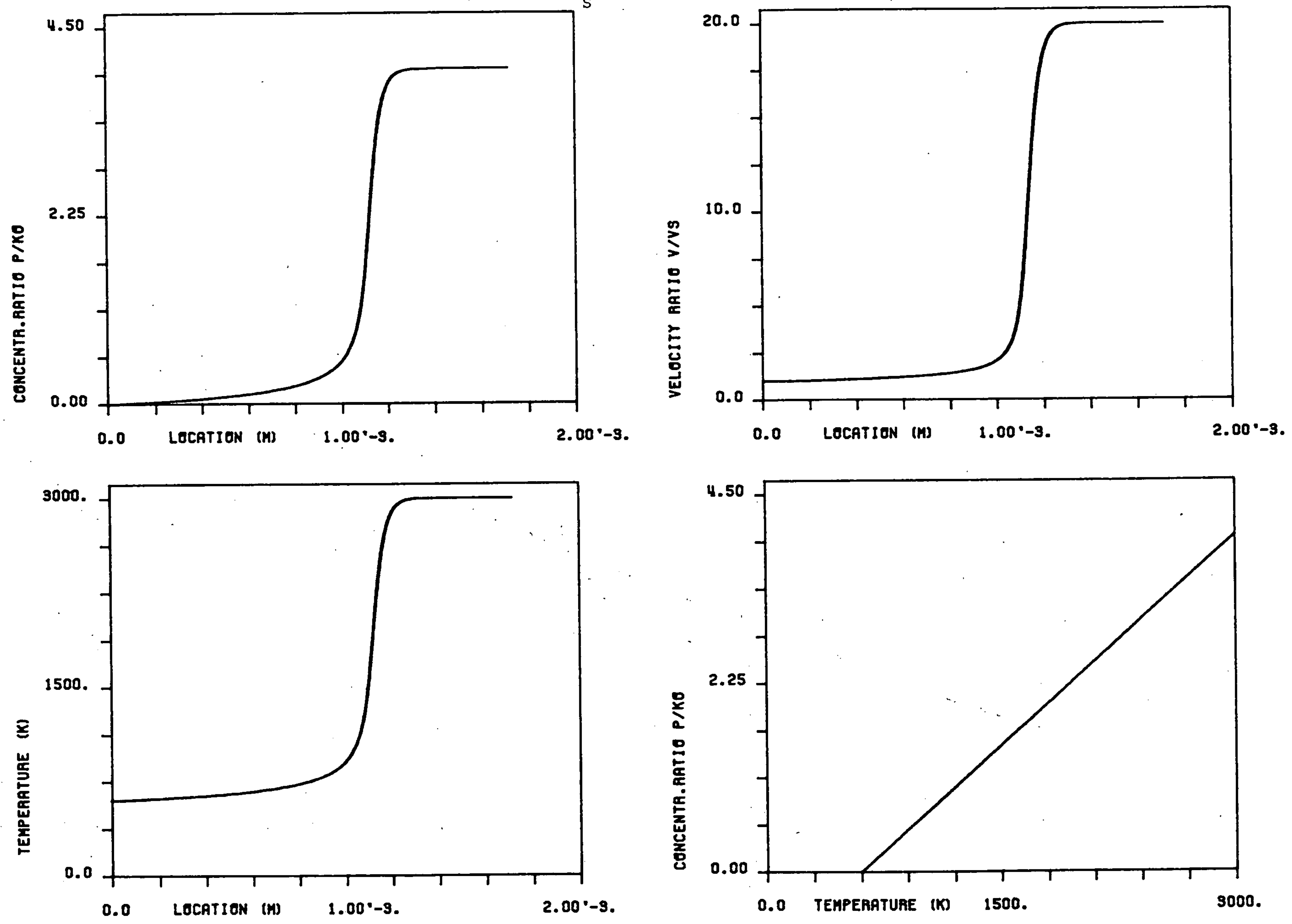


Fig. 6.8. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 5.10^6$ (S^{-1})
$\nu = 0{,}25$
$\theta = 7500$ (K)

$\Delta H_f^o = -1{,}2.10^8$ $(kg.m^2/(kMol.S^2))$
$P = 5.10^6$ (N/m^2)
$T_S = 600$ (K)

$m = 1{,}5$
$m_S = 16$ $(kg/(m^2.S))$
$\varepsilon = 7{,}30.10^{-5}$

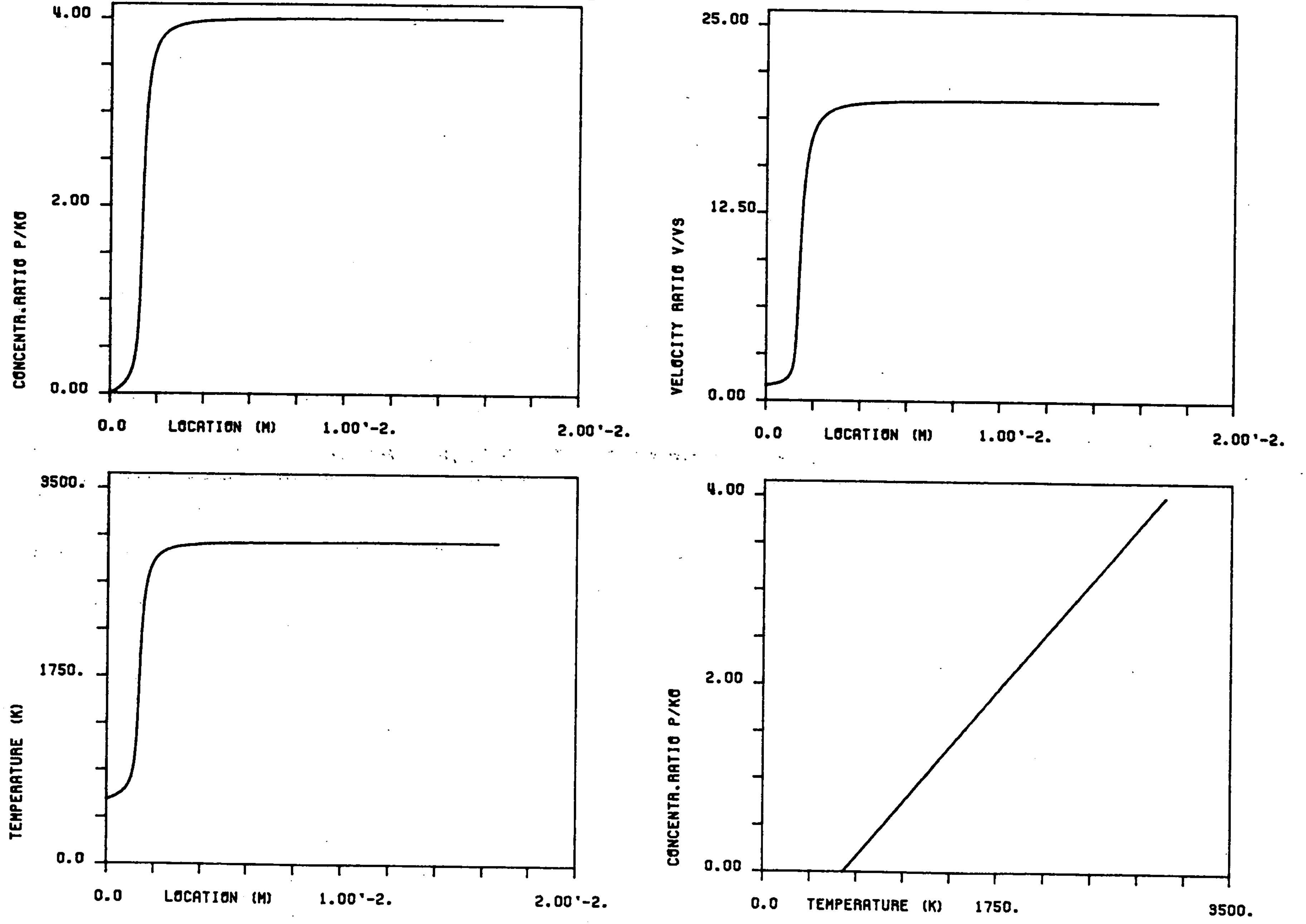
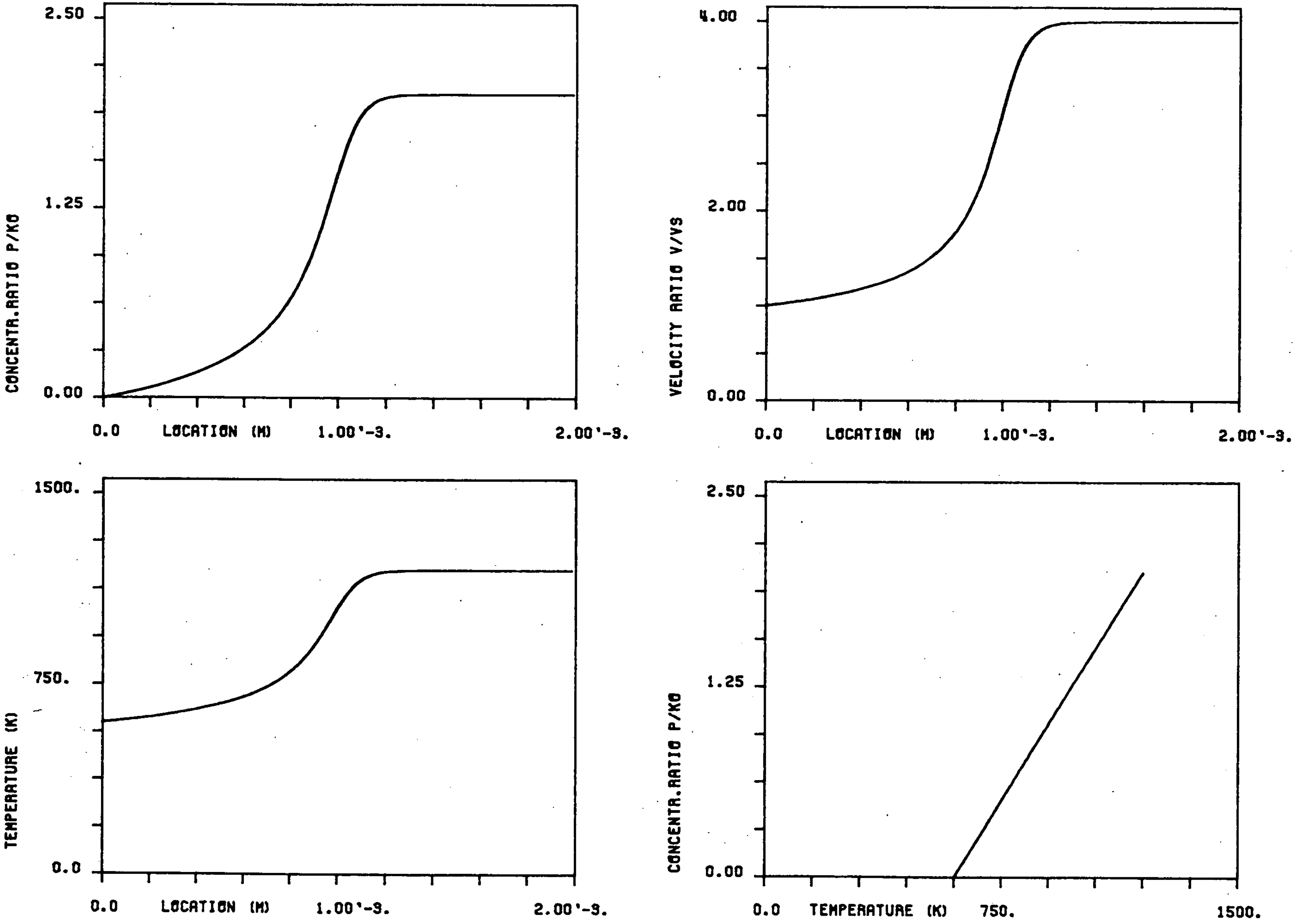


Fig. 6.9. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,50$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 5,97.10^{-4}$



The differences in the numerically and analytically determined locations X* at a reference temperature T* are mainly large, due to the fact that near the flame temperature, $\frac{dT}{dx} \to 0$ and $\frac{dx}{dT} \to \sim$. In other words, very large differences in location are accompanied by extremely small differences in temperature. This is also illustrated by the Figs. 6.6 through 6.8 where the temperature-location curves for the analytic and numerical calculation complete cover each other.

Stoichiometric Coefficient, ν.

A variation in the stoichiometric coefficient implies that one mol of reactants will produce a different number of mols of products. Hence, the amount of gas that is produced will vary with the variation of the stoichiometric coefficient. Due to the definition of the heat of formation also the flame temperature will be affected which on its turn again affects the flame velocity. While a compilation of all parameters for the flame is given in Table 6.1, Table 6.5 lists the major differences that occur when the stoichiometric coefficient is doubled. It is seen that the concentration ratio P/K_O is strongly affected, as also appears from Fig. 6.9, which should be compared with Fig. 6.2. The temperature gradient at the burning surface, $(dT/dx)_S$ is not affected. The location where the flame temperature is about achieved is somewhat larger for $\nu = 0,5$ then for $\nu = 0,25$ although for the latter case the flame temperature is higher.

Table 6.5. The effect of the Stoichiometric Coefficient, ν.

Stoichiometric Coefficient, ν (-)	Flame Temperature, T_F (K)	Reference Temperature T* (K)	Location X*		Concentration ratio $(P/K_O)_F$ (-)	Flame Velocity V_F (m/S)
			Analytic (m)	Numerical (m)		
0,25	1799,64	1797	$1,236.10^{-3}$	$1,250.10^{-3}$	4	29,92
0,50	1198,28	1197	$1,244.10^{-3}$	$1,255.10^{-3}$	2	9,97

X* is the location where the temperature T* is reached.

Again it is seen by comparing the numerically and analytically calculated values of X*, that there is a good agreement between the two methods for flame calculation.

Combustion pressure, p.

The combustion pressure directly affects the concentration of reactants and products and hence the reaction rate. According to Eq. (3.32) $p^m.x$ should be about constant i.e. by increasing the combustion pressure, the flame thickness is reduced, except for zeroth order reactions. A second aspect is that, because of a higher pressure and hence higher density the flame velocity is reduced.
Again the various parameter values may be found in table 6.1, while the effects, resulting from a change in the combustion pressure are listed in Table 6.6, and are also illustrated by comparing the Figs. 6.10 and 6.1.

Fig. 6.10. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 4.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 5,97.10^{-4}$

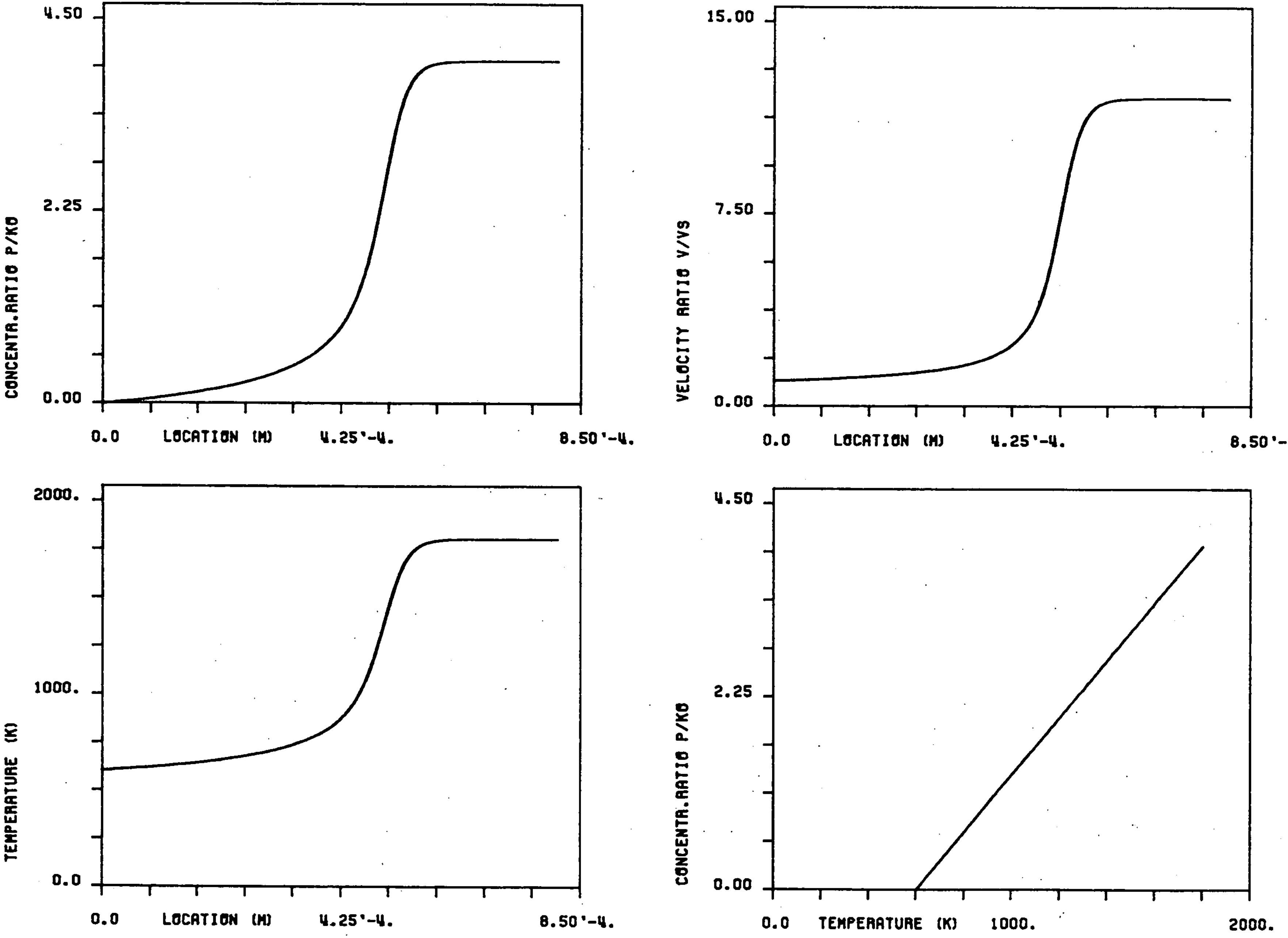


Table 6.6. The effect of the combustion pressure, p.

Pressure, p. (N/m^2)	Reference temperature, T^*. (K)	Location X^* Analytic (m)	Location X^* Numerical (m)	Temperature Gradient at surface $(dT/dx)_s$ (K/m)	$p.X^*$ (N/m)	Flame Velocity V_F. (m/s)
2.10^5	1796,78	$1,231.10^{-3}$	$1,244.10^{-3}$	$8,96.10^4$	$2,46.10^2$	29,92
4.10^5	1796,78	$6,164.10^{-4}$	$6,193.10^{-4}$	$1,79.10^5$	$2,47.10^2$	14,96

X^* is the location where the temperature T^* is reached.

For the product pX^*, the analytic values have been taken, but the numerical values yield similar results.

Mass flow rate, m_s.

The main effect of the mass flow rate is felt on the flame velocity V_F. The flame velocity increases with increasing mass flow rates; in some cases to such an extent that there is a noticeable difference between the analytic and numerically calculated flame temperature and the temperature profiles. It should be recalled that for the analytic calculation the kinetic energy has been neglected. In total eleven different cases have been calculated. In these examples also the preexponential factor, the heat of formation, the stoichiometric coefficient, the pressure, the activation temperature and the surface temperature have been changed. It is always possible, however, to consider groups in which only the mass flow rate has been varied.

The first group consists of the cases that have been plotted in the Figs. 6.2 and 6.11.
The second group consists of the cases that have been plotted in the Figs. 6.12 and 6.13.
The third group encompasses the cases plotted in the Figs. 6.14 and 6.15, and the fourth group consists of the cases that have been plotted in the Figs. 6.7, 6.16 and 6.17, while finally the fifth group consists of the cases that have been plotted in the Figs. 6.18 and 6.19.

The values of the various parameters that have been used may be found in Table 6.1. Table 6.7 shows the effect of the mass flow rate on the flame properties.

Table 6.7. The effect of the mass flow rate, m_s.

Mass flow rate, m_S (kg/(m^2.S))	Flame-Temperature, T_F, Analytic (K)	Numerical (K)	Flame Velocity V_F (m/s)	Temperature gradient at Surface $\left(\frac{dT}{dx}\right)_s$ (K/m)	Reference Temperature T^* (K)	Location X* Analytic (m)	Numerical (m)
10	1799,64	1799,01	29,92	$8{,}96.10^4$	1795,6	$1{,}215.10^{-3}$	$1{,}225.10^{-3}$
20	1799,91	1798,26	59,83	$4{,}48.10^4$	1795,7	$2{,}446.10^{-3}$	$2{,}478.10^{-3}$
16	1479,07	1503,13	78,62	$8{,}36.10^6$	1410,6	$1{,}396.10^{-3}$	$1{,}203.10^{-3}$
64	1498,67	1475,87	313,77	$2{,}08.10^6$	1412,5	$6{,}608.10^{-3}$	$6{,}658.10^{-3}$
128	600,00	597,92	63,77	$7{,}81.10^2$	596,4	$1{,}865.10^{-2}$	$1{,}876.10^{-2}$
16	599,98	598,67	7,98	$6{,}26.10^3$	596,3	$2{,}323.10^{-3}$	$2{,}335.10^{-3}$
16	2999,82	2998,98	3,19	7.10^4	2995,8	$1{,}306.10^{-3}$	$1{,}320.10^{-3}$
64	2999,99	2998,95	12,77	$1{,}75.10^4$	2995,1	$5{,}200.10^{-3}$	$5{,}253.10^{-3}$
128	2999,99	2998,78	25,54	$8{,}75.10^3$	2995,5	$1{,}043.10^{-2}$	$1{,}055.10^{-2}$
0.16	2936,57	2997,01	$3{,}13.10^{-2}$	$2{,}54.10^5$	2927,49	$1.966.10^{-4}$	$1{,}916.10^{-4}$
1.6	2999,35	2997,41	0,32	$2{,}61.10^4$	2929,43	$1{,}903.10^{-3}$	$1{,}912.10^{-3}$

X* is the location where T* is achieved.

Fig. 6.11. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature:

$A = 2.10^8$ (S^{-1}) $\Delta H_f^o = -6.10^7$ ($kg.m^2/(kMol.S^2)$) $m = 1$

$\nu = 0,25$ $P = 2.10^5$ (N/m^2) $m_S = 20$ ($kg/(m^2.S)$)

$\theta = 7500$ (K) $T_S = 600$ (K) $\varepsilon = 7,47.10^{-5}$

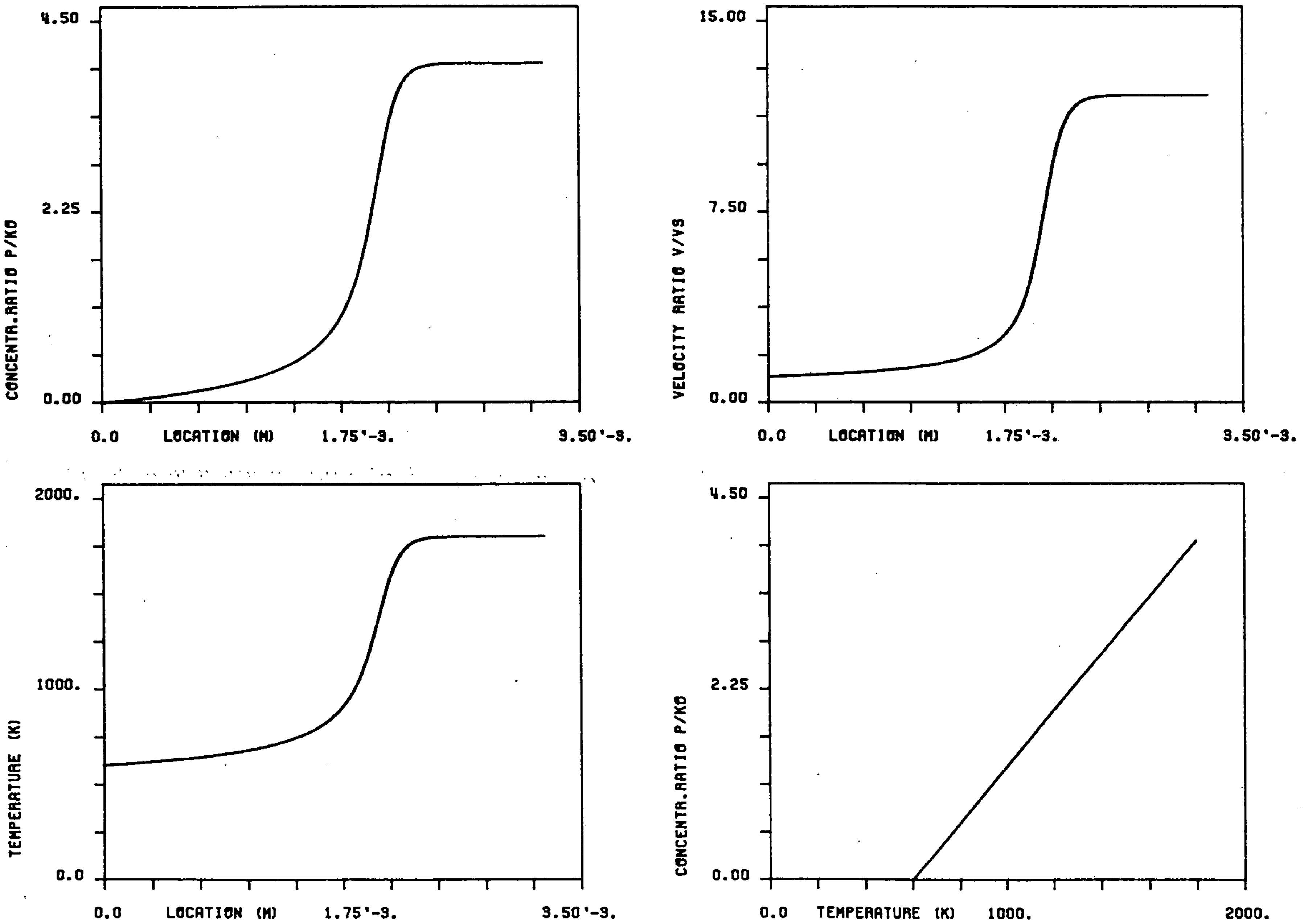


Fig. 6.12. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 6.10^5$ (S^{-1})
$\nu = 0{,}25$
$\theta = 500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 10^5$ (N/m^2)
$T_S = 300$ (K)

$m = 1$
$m_S = 16$ $(kg/(m^2.S))$
$\varepsilon = 1{,}74.10^{-2}$

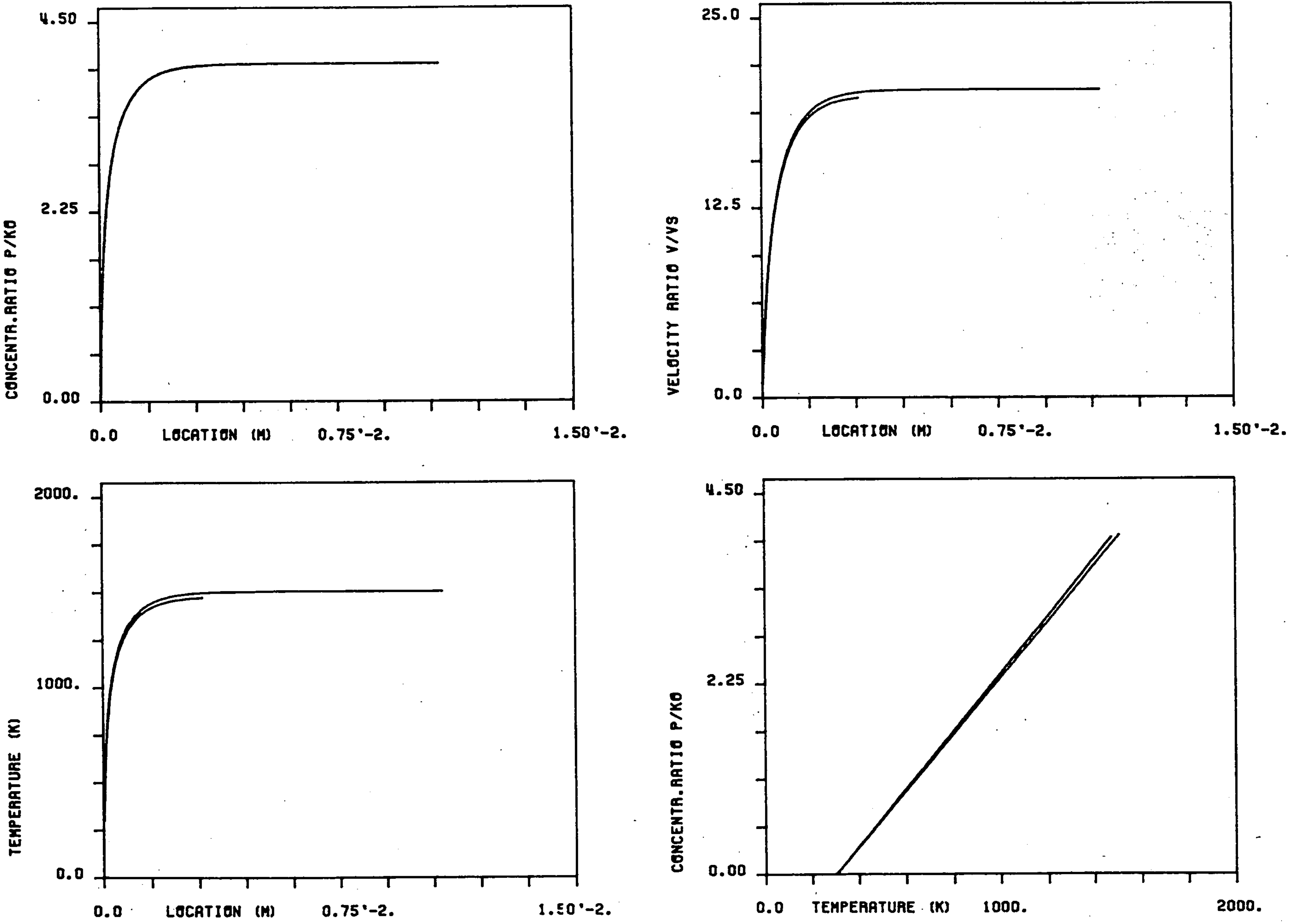


Fig. 6.13. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 6.10^5$ (S^{-1})
$\nu = 0,25$
$\theta = 500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 10^5$ (N/m^2)
$T_S = 300$ (K)

$m = 1$
$m_S = 64$ $(kg/(m^2.S))$
$\varepsilon = 1,11.10^{-3}$

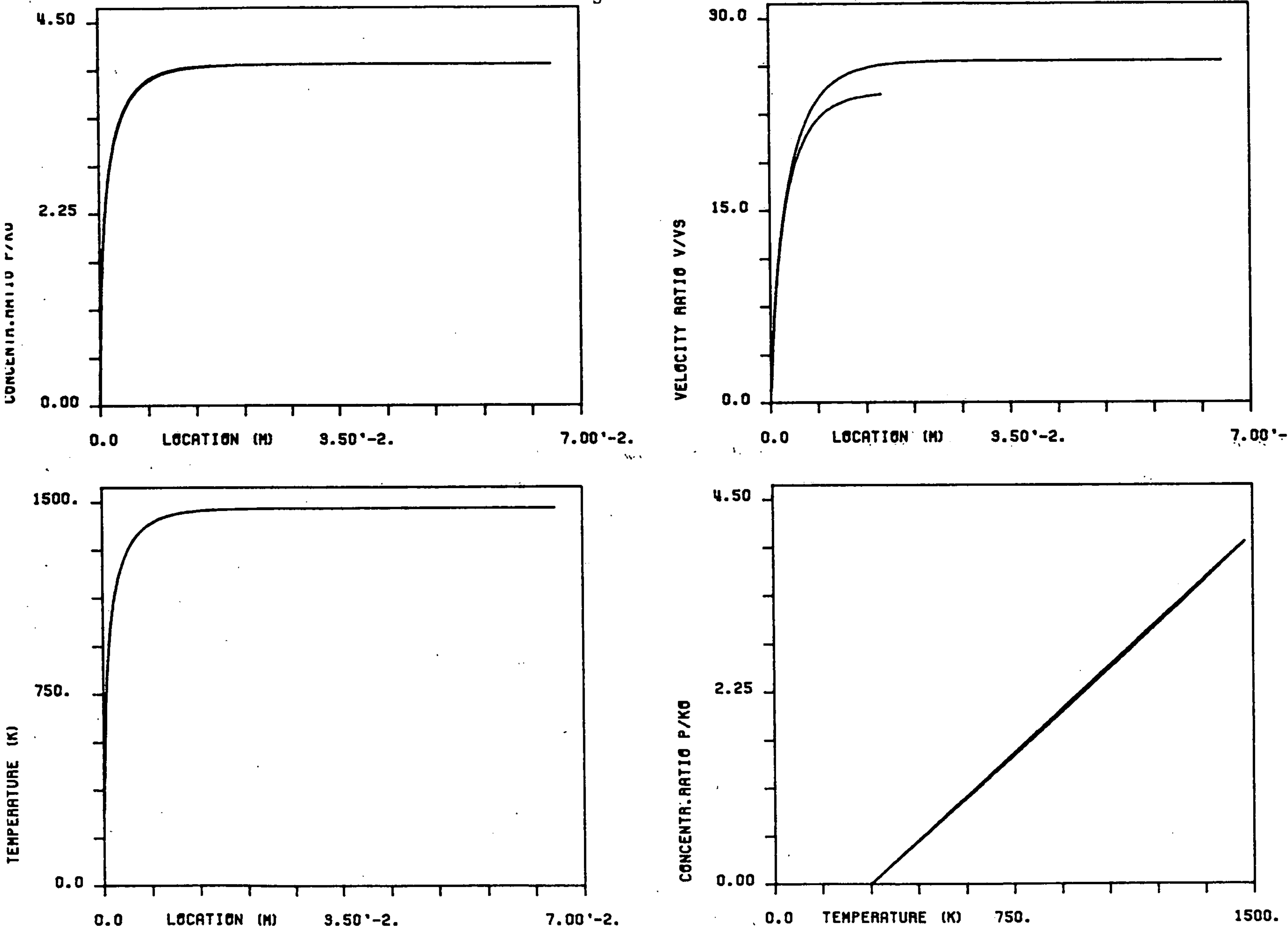


Fig. 6.14. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 6.10^{12}$ (S^{-1})
$\nu = 1$
$\theta = 7500$ (K)
$\Delta H_f^{\,o} = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 10^5$ (N/m^2)
$T_S = 300$ (K)
$m = 1$
$m_S = 128$ $(kg/(m^2.S))$
$\varepsilon = 8{,}16.10^{-7}$

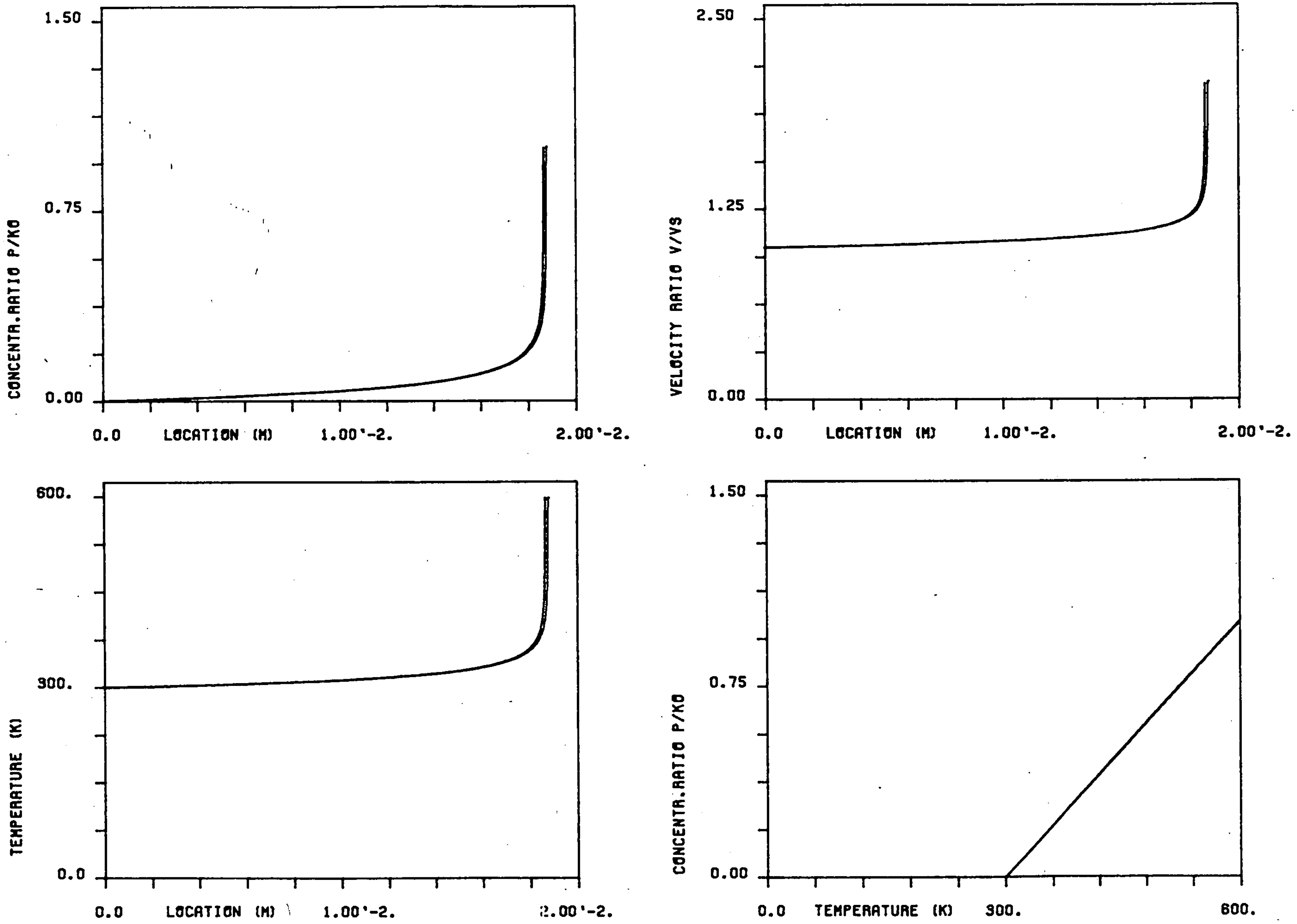


Fig. 6.15. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 6.10^{12}$ (S^{-1}) $\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$ $m = 1$
$\nu = 1$ $P = 10^5$ (N/m^2) $m_S = 16$ $(kg/(m^2.S))$
$\theta = 7500$ (K) $T_S = 300$ (K) $\varepsilon = 5{,}22.10^{-5}$

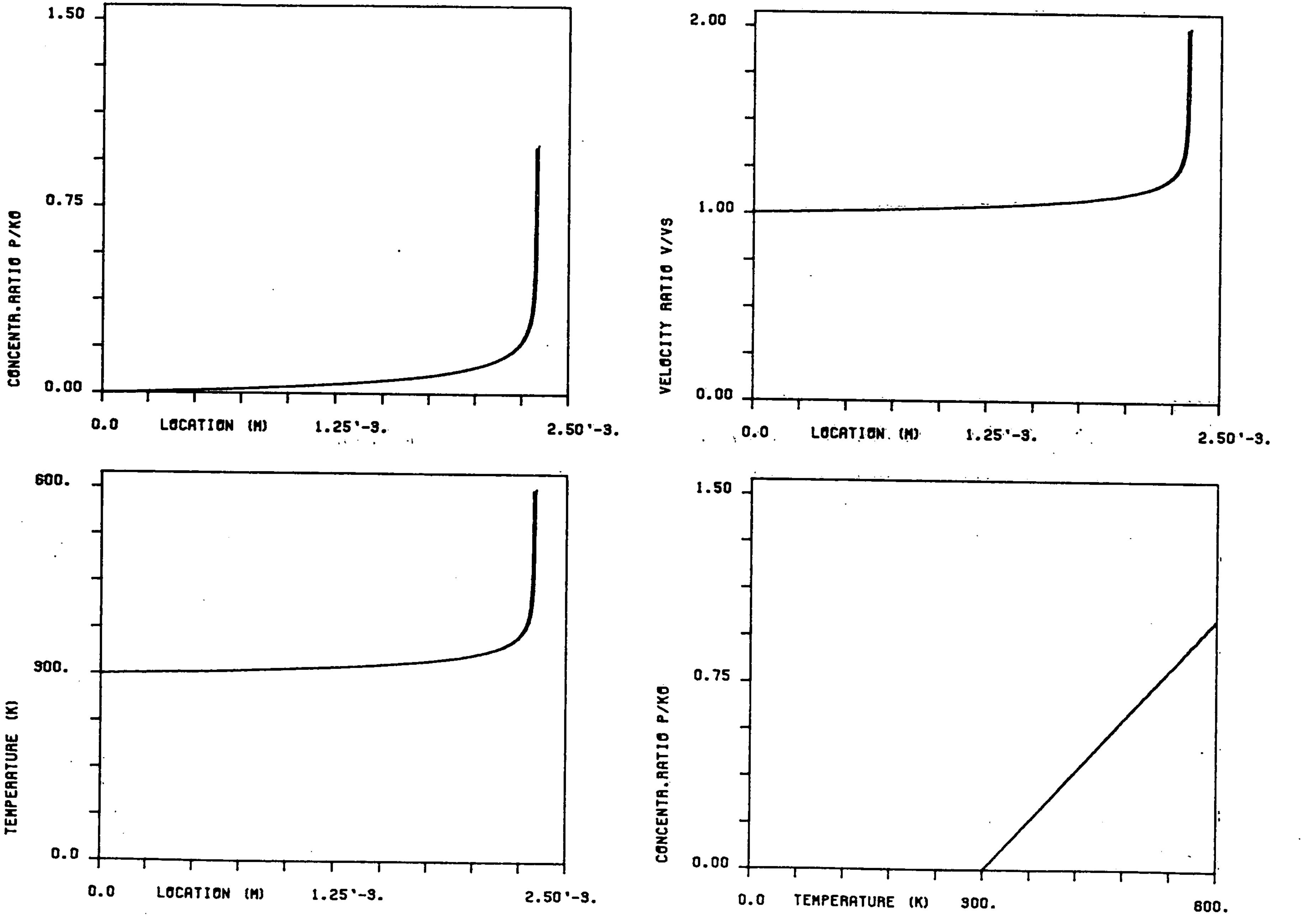


Fig. 6.16. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 5.10^6$ (S^{-1}) $\Delta H_f{}^o = -1{,}2.10^8$ $(kg.m^2/(kMol.S^2))$ $m = 1$

$\nu = 0{,}25$ $P = 5.10^6$ (N/m^2) $m_S = 64$ $(kg/(m^2.S))$

$\theta = 7500$ (K) $T_S = 600$ (K) $\varepsilon = 4{,}56.10^{-6}$

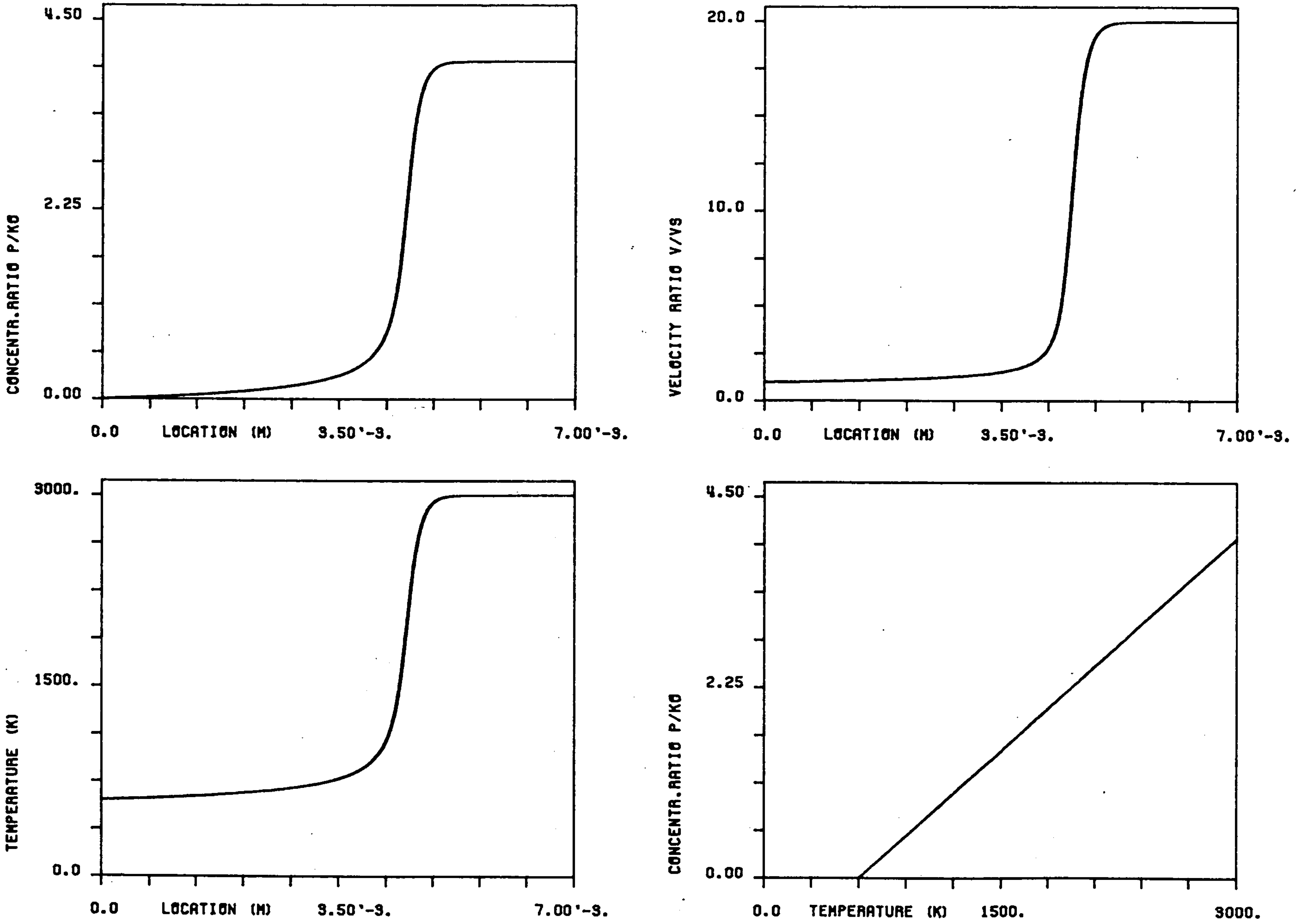


Fig. 6.17. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 5.10^6$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)
$\Delta H_f^o = -1,2.10^8$ $(kg.m^2/(kMol.S^2))$
$P = 5.10^6$ (N/m^2)
$T_S = 600$ (K)
$m = 1$
$m_S = 128$ $(kg/(m^2.S))$
$\varepsilon = 1,14.10^{-6}$

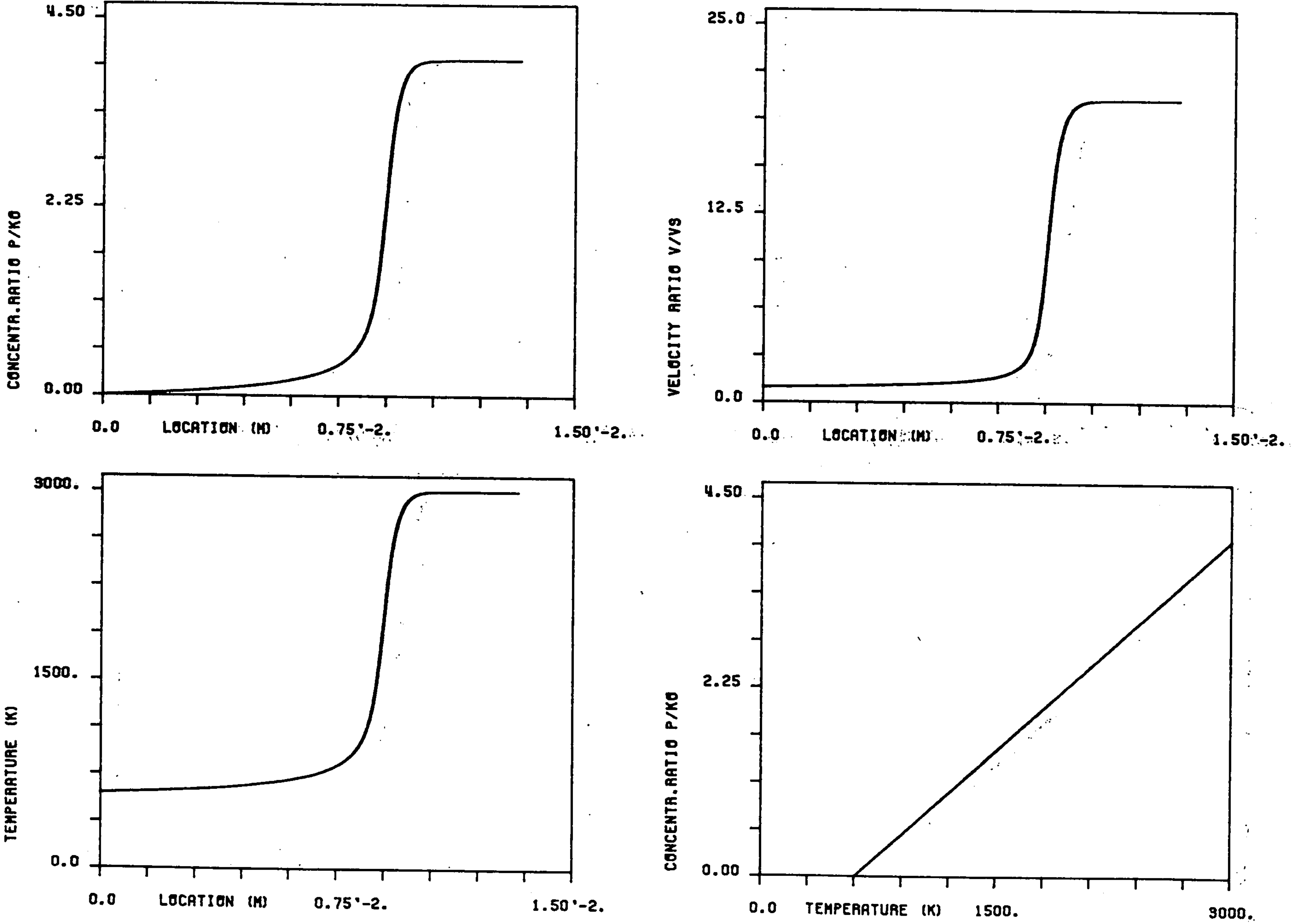


Fig. 6.18. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 1,2.10^7$ (S^{-1}) $\Delta H_f^o = -1,2.10^8$ $(kg.m^2/(kMol.S^2))$ $m = 1$

$\nu = 0,25$ $P = 5.10^6$ (N/m^2) $m_S = 0,16$ $(kg/(m^2.S))$

$\theta = 10.000$ (K) $T_S = 600$ (K) $\varepsilon = 2,64.10^{-2}$

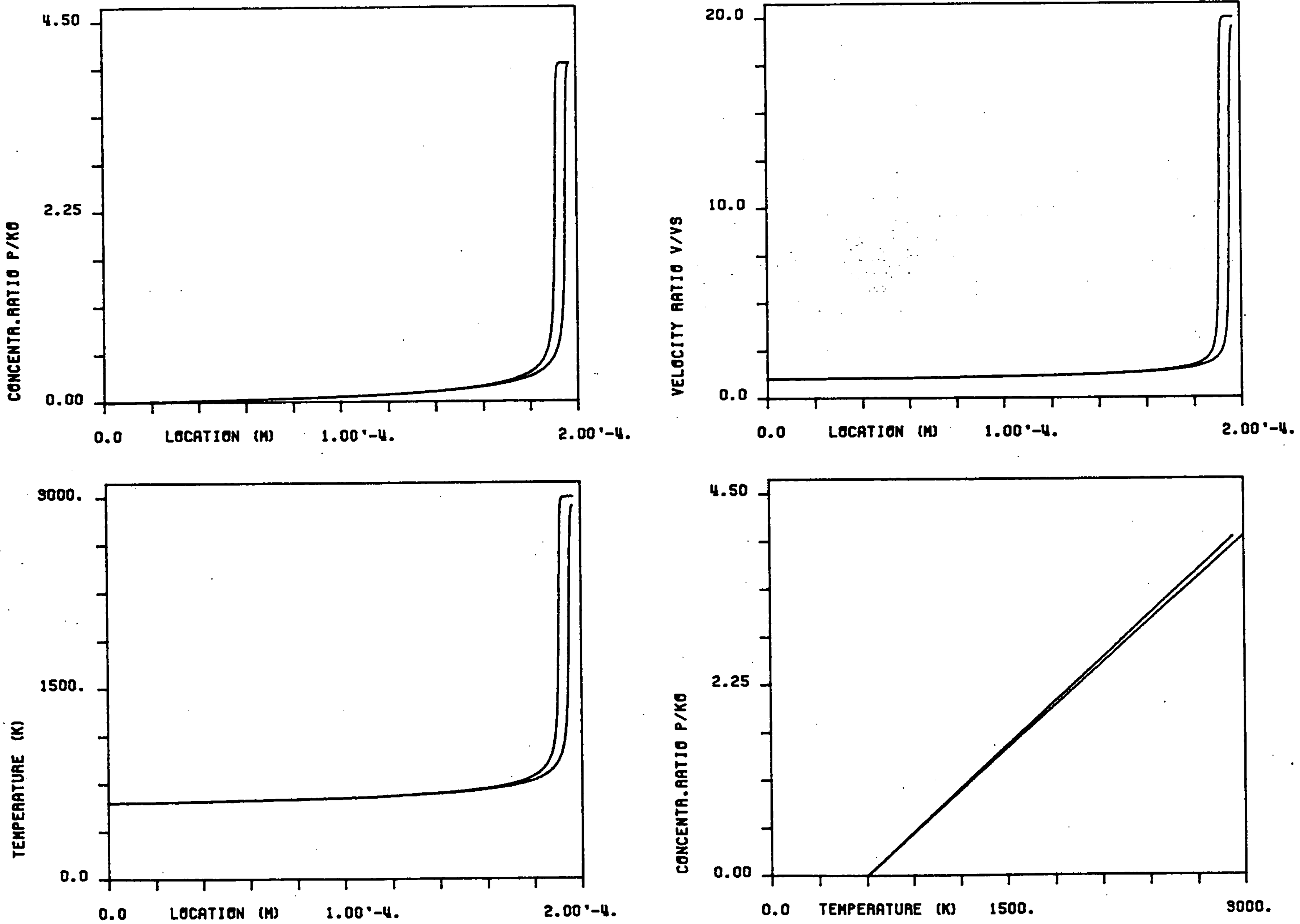


Fig. 6.19. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 1{,}2.10^7$ (S^{-1}) $\Delta H_f^o = -1{,}2.10^8$ $(kg.m^2/(kMol.S^2))$ $m = 1$
$\nu = 0{,}25$ $P = 5.10^6$ (N/m^2) $m_S = 1{,}6$ $(kg/(m^2.S))$
$\theta = 10.000$ (K) $T_S = 600$ (K) $\varepsilon = 2{,}71.10^{-4}$

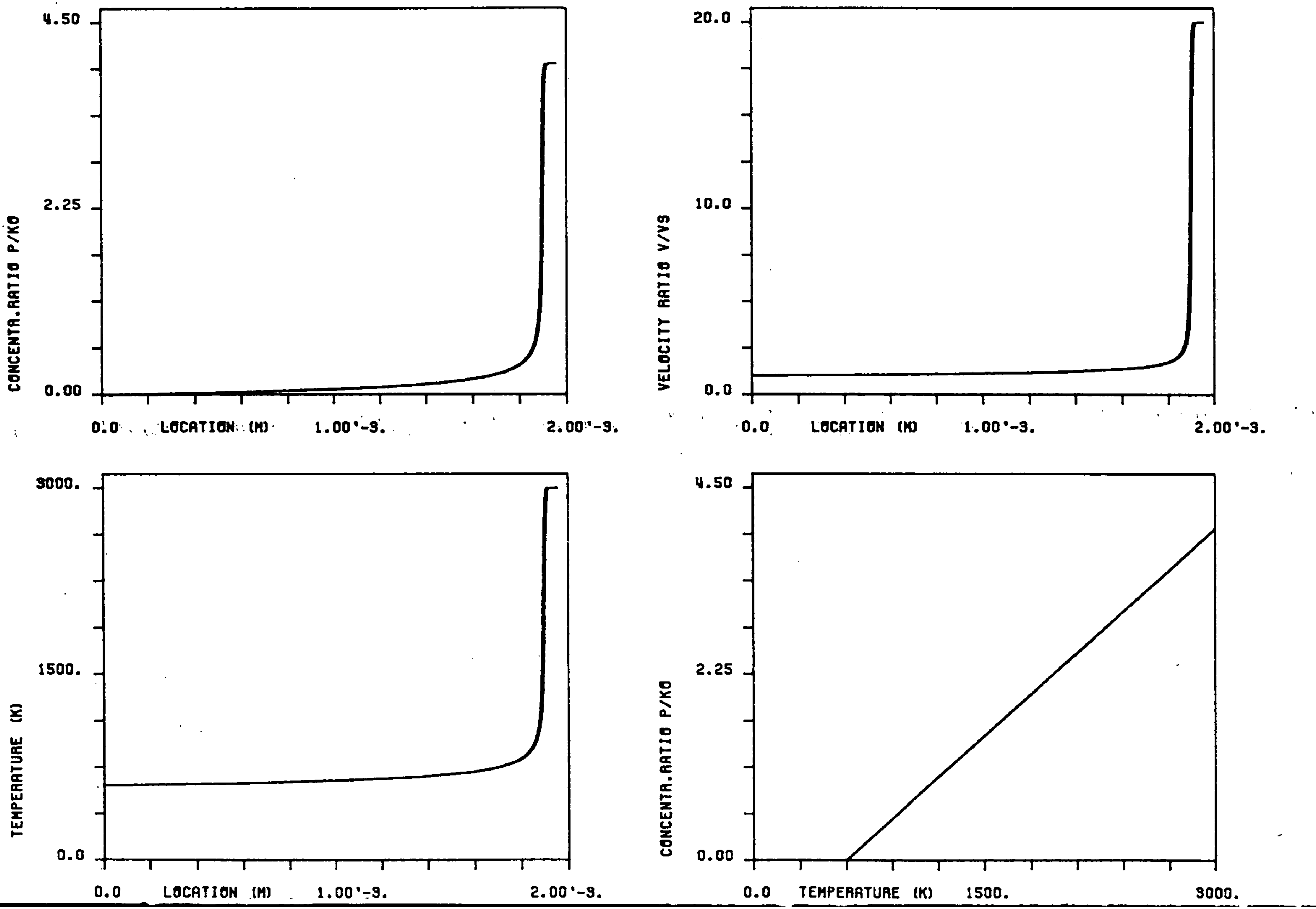


Fig. 6.20. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^{8}\ (S^{-1})$
$\nu = 0{,}25$
$\theta = 3750\ (K)$
$\Delta H_f^{o} = -6.10^{7}\ (kg.m^{2}/(kMol.S^{2}))$
$P = 2.10^{5}\ (N/m^{2})$
$T_S = 600\ (K)$
$m = 1$
$m_S = 10\ (kg/(m^{2}.S))$
$\varepsilon = 1{,}34.10^{-1}$

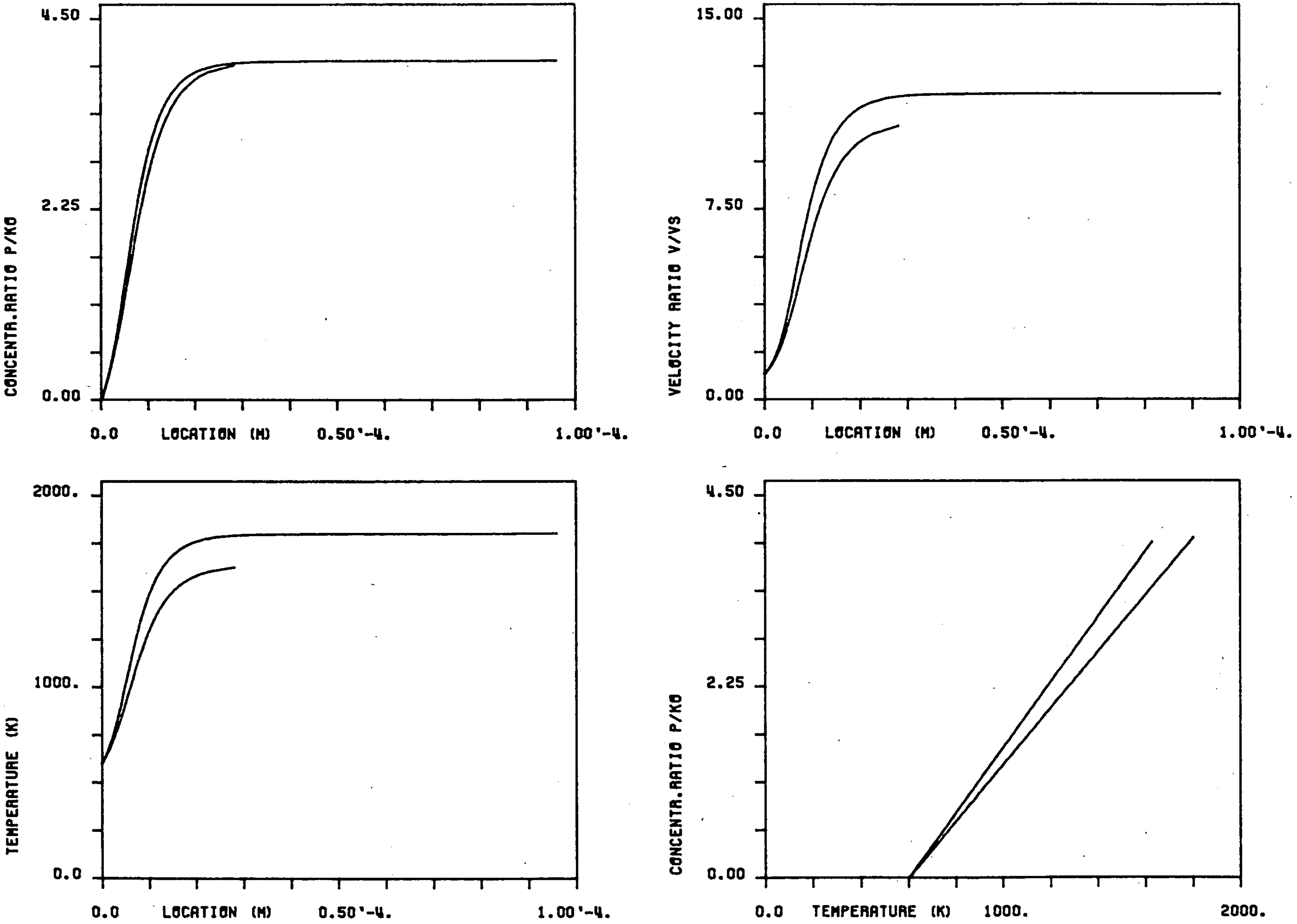
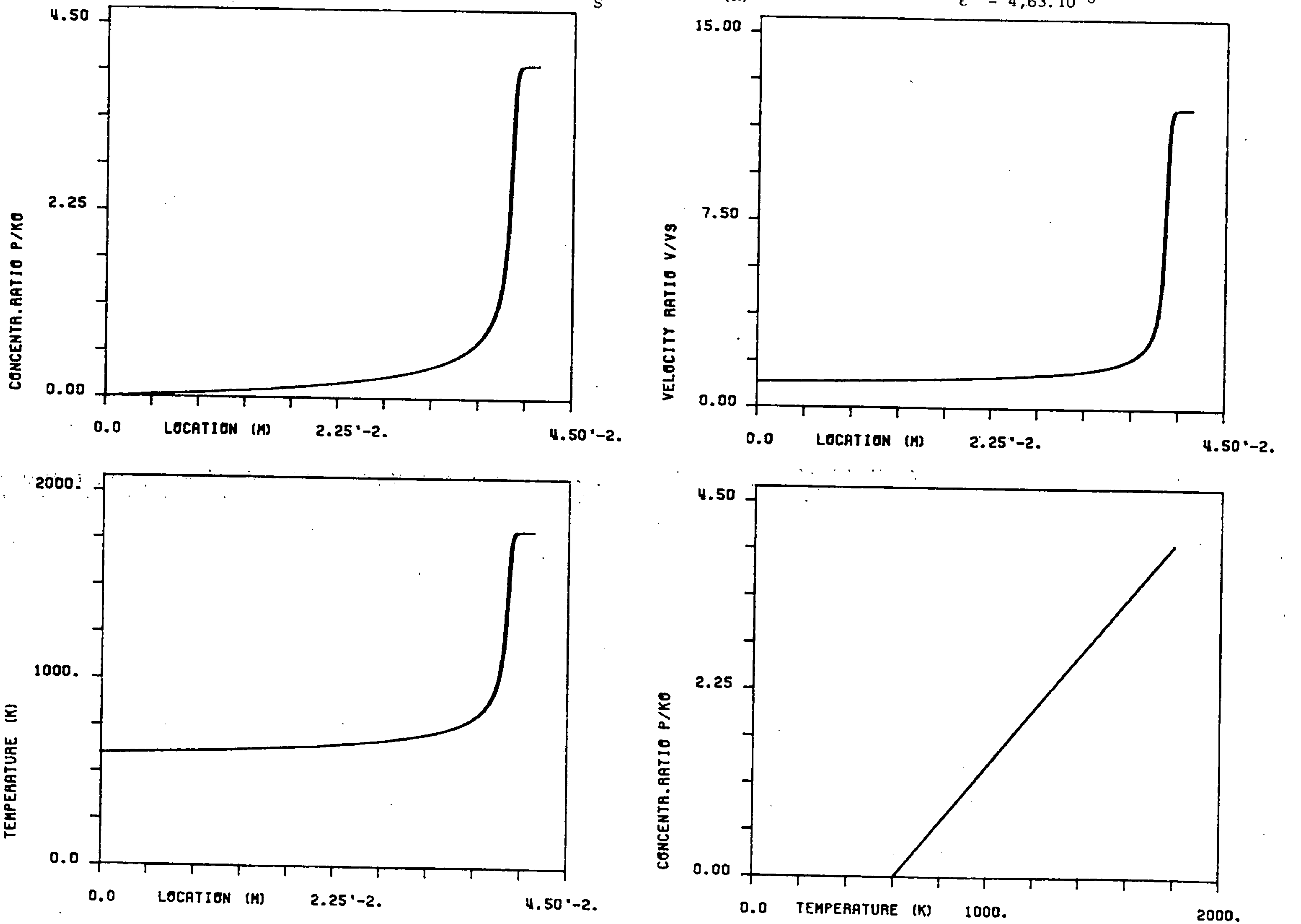


Fig. 6.21. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^{8}\ (S^{-1})$
$\nu = 0{,}25$
$\theta = 10.000\ (K)$
$\Delta H_f^{o} = -6.10^{7}\ (kg.m^{2}/(kMol.S^{2}))$
$P = 2.10^{5}\ (N/m^{2})$
$T_S = 600\ (K)$
$m = 1$
$m_S = 10\ (kg/(m^{2}.S))$
$\varepsilon = 4{,}63.10^{-6}$



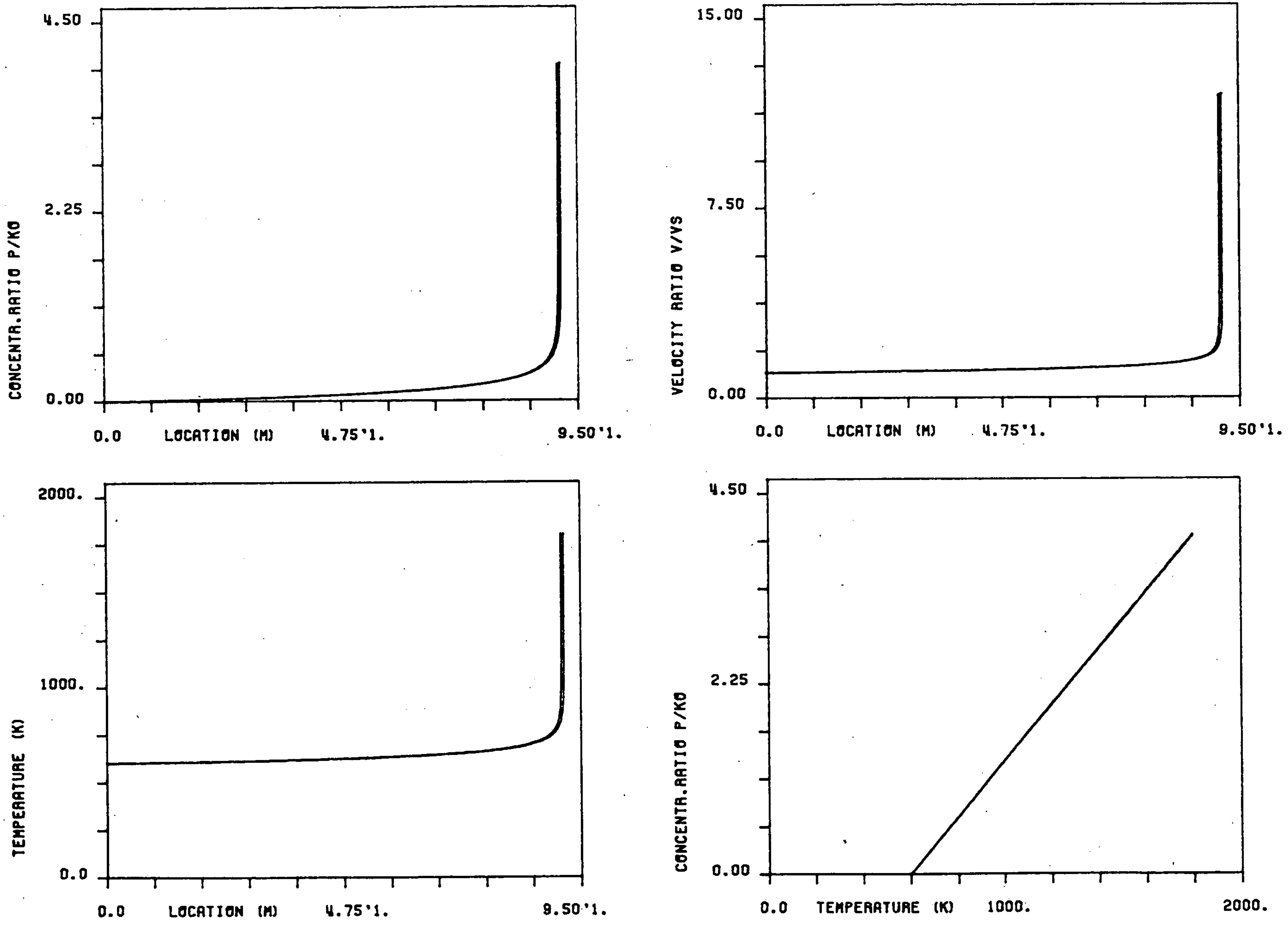


Fig. 6.22. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 15000$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 1,11.10^{-9}$

It is seen that for the second group some large discrepancies arise between the numerical and analytic values. As can be seen from Table 6.1, the parameter ε, which should be small is already relatively large for these cases ($1,74.10^{-2}$ and $1,11.10^{-3}$) which yields errors in the analytic approximation, as may also be seen from Fig. 6.1.
In addition to varying the length scale of the flame, it is seen from Table 6.7 that also the temperature gradient at the burning surface is severely affected by variations in the mass flow rate.

Activation temperature, θ.

The activation temperature θ directly affects the reaction rate. Therefore its effect is directly visible in the length scale of the flame and the temperature gradient at the surface. In those cases that the parameter ε becomes too large errors may be introduced. Four different cases have been calculated, they have been plotted in the Figs. 6.2 and 6.20 through 6.22. The case that has been plotted in Fig. 6.20 suffers from a high value of ε, as is clearly visible. Again the governing parameters for all four cases are listed in Table 6.1 while the specific effects may be found in Table 6.8.

Table 6.8. The effect of the activation temperature, θ.

Activation Temperature, θ. (K)	Reference Temperature, T^* (K)	Location X^* Analytic	Location X^* Numerical	Temperature Gradient at Surface $(dT/dx)_s$ (K/m)
3750	1626,6	$2,816.10^{-5}$	$1,294.10^{-5}$	$4,02.10^{7}$
7500	1795,6	$1,215.10^{-3}$	$1,225.10^{-3}$	$8,96.10^{4}$
10.000	1795,9	$3,997.10^{-2}$	$4,029.10^{-2}$	$1,39.10^{-3}$
15.000	1795,3	$9,123.10^{1}$	$9,172.10^{1}$	0,33

X^* is the location where T^* is achieved.

It is seen that for $\theta = 3750$ K, there are severe discrepancies between the numerical and analytic solutions. This is due to the large value of ε ($\varepsilon = 0,134$).

Surface temperature, T_s.

The surface temperature primarily, like the activation temperature, affects the reaction rate. As at higher temperatures, the densities are lower, velocities generally increase with increasing surface temperatures. Although the flame temperature also increases with surface temperature, the temperature rise over the flame is hardly affected. The temperature gradient severely increases with the surface temperature while the length scale of the flame decreases with increasing flame temperatures. Again the relevant parameters are given in Table 6.1, while the effects of surface temperature have been presented in Table 6.9. The results of the calculation have been plotted in the Figs. 6.2, 6.23 and 6.24. The case of Fig. 6.24 suffers from a high value of ε ($\varepsilon = 0,0718$) which results in too low a prediction of the flame temperature.

Fig. 6.23. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^{8}$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)
$\Delta H_f^{o} = -6.10^{7}$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^{5}$ (N/m^2)
$T_S = 300$ (K)
$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 2,23.10^{-9}$

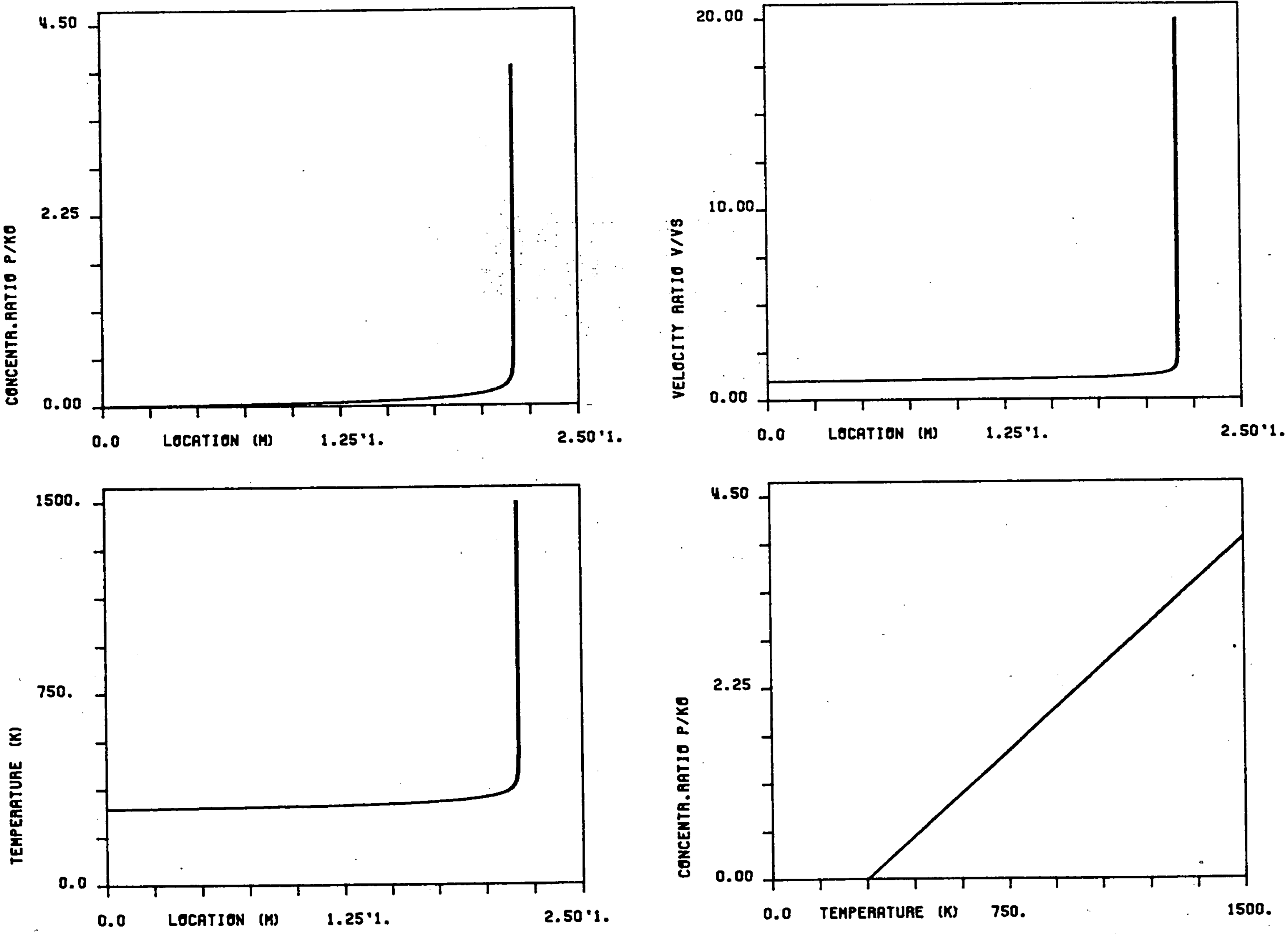


Fig. 6.24. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 1200$ (K)

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 7,18.10^{-2}$

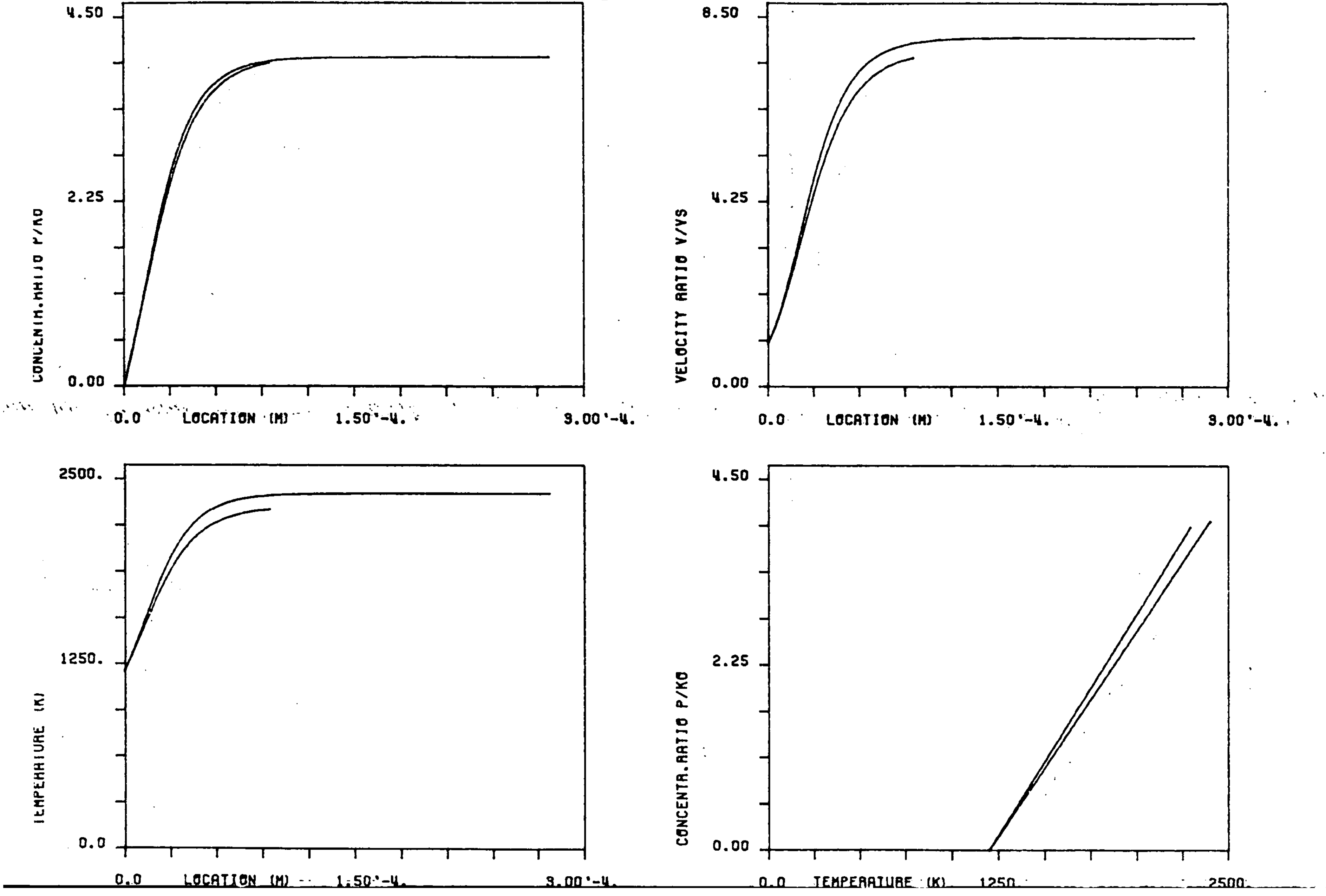


Table 6.9. The effect of the surface temperature, T_s.

Surface Temperature, T_s (K)	Reference Temperature, T* (K)	Location X* Analytic (m)	Location X* Numerical (m)	Temperature Gradient at the Surface $(dT/dx)_s$ (K/m)	Initial Velocity V_s (m/s)	Flame Velocity V_F (m/s)
300	1496,7	21,642	21,738	0,668	1,25	24,94
600	1797,2	$1,215.10^{-3}$	$1,225.10^{-3}$	$8,96.10^{4}$	2,49	29,92
1200	2294,7	$9,521.10^{-5}$	$5,784.10^{-5}$	$2,16.10^{7}$	4,99	38,47

Heat conduction coefficient, λ.

All cases that have been discussed until now had a heat conduction coefficient, $\lambda = 0,08$ kg.m/(S^3.K). Fig. 6.25 shows the results of a flame calculation with $\lambda = 0,008$ kg.m/(S^3.K), while Fig. 6.26 shows the results of a calculation with the gas heat conduction coefficient $\lambda = 0,16$ kg.m/(S^3.K). These figures may be compared with the reference figure, Fig. 6.2.
The differences between these three cases are hardly distinguishable, as is also evident from Table 6.10.

Table 6.10. The effect of the gas heat conduction coefficient, λ.

Gas heat Conduction Coefficient, λ (kg.m/(S^3.K))	Flame Temperature Analytic (K)	Flame Temperature Numerical (K)	Temperature Gradient at Surface $(dT/dx)_s$ (K/m)
0,008	1799,96	1798,64	$8,96.10^{4}$
0,08	1799,64	1799,01	$8,96.10^{4}$
0,16	1799,28	1799,18	$8,96.10^{4}$

It is remarkable that the effect of the heat conduction coefficient is opposite for the analytically calculated flame temperature and the numerically calculated one. This is believed to be due to rounding off errors in the numerical calculation. For example the respective reactant concentrations for the three successive cases are: $3,2.10^{-7}$, $8,5.10^{-9}$ and $7,9.10^{-10}$ kMol/m^3, therefore the numerical integration procedure ends for the three cases at slightly different amounts of reactant concentrations, which will result in slight temperature differences

Fig. 6.25. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0,25$
$\theta = 7500$ (K)

$\Delta H_f^o = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)
$\lambda^S = 0,008$ $kg.m/(S^3.K)$

$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 2,99.10^{-5}$

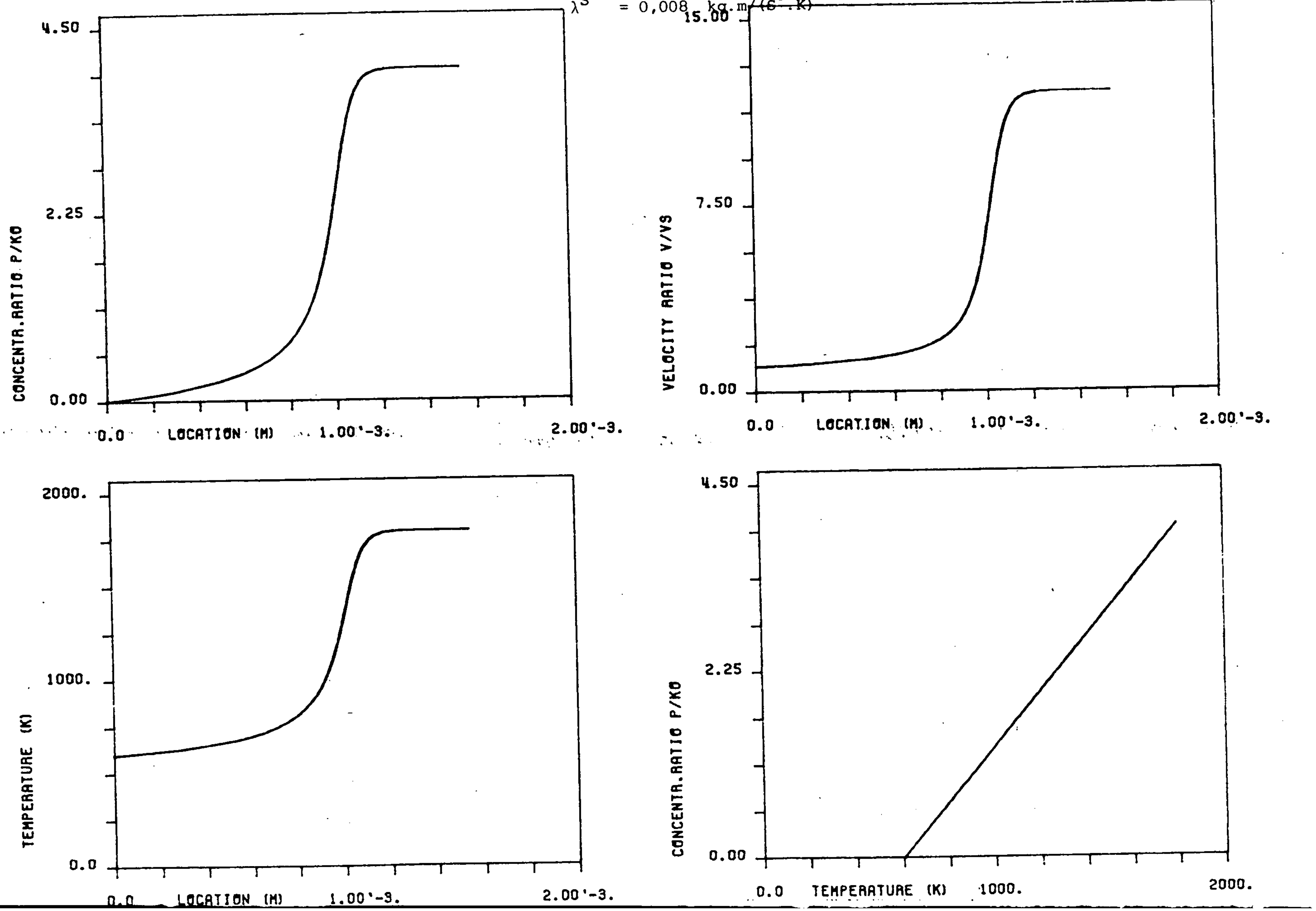
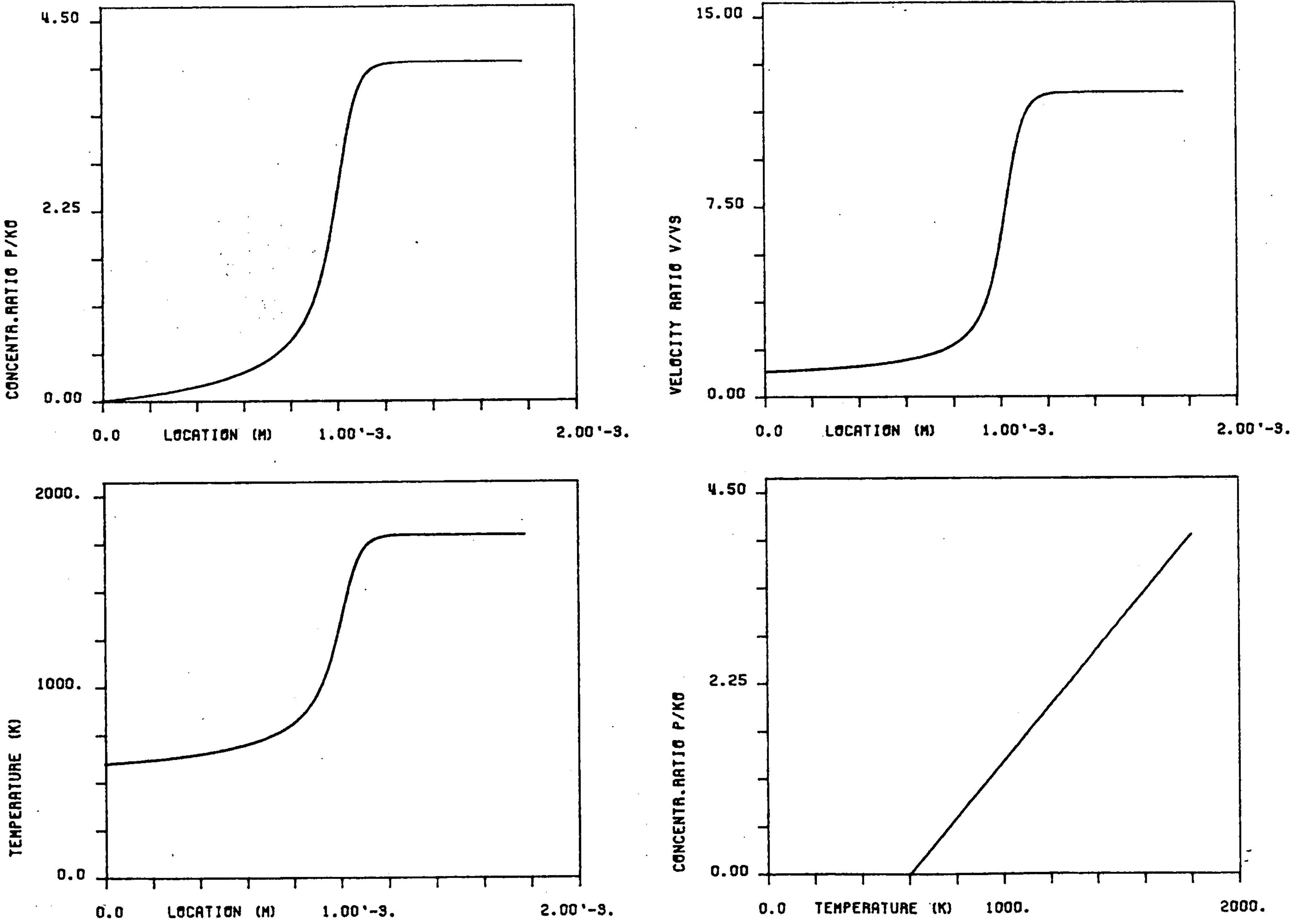


Fig. 6.26. Temperature -, concentration ratio - and velocity ratio versus location. Concentration ratio versus temperature.

$A = 2.10^8$ (S^{-1})
$\nu = 0{,}25$
$\theta = 7500$ (K)
$\Delta H_f^{\,o} = -6.10^7$ $(kg.m^2/(kMol.S^2))$
$P = 2.10^5$ (N/m^2)
$T_S = 600$ (K)
$\lambda = 0{,}16$ $kg.m/(S^3.K)$
$m = 1$
$m_S = 10$ $(kg/(m^2.S))$
$\varepsilon = 5{,}97.10^{-4}$



7. CONCLUSIONS

A new method has been develloped for the approximate analytic calculation of premixed flames. The result is a simple quadrature for the temperature in the flame in relation to the location. The method is applicable to any order of reaction, and any value of the stoichiometric coefficient. There are no restrictions on the activation temperature (or activation energy). The only requirement is that the combustion reaction may be described by an overall reaction equation of the type:

$$\nu K \overset{k}{\rightarrow} P \quad , \tag{7.1}$$

while the rateconstant, k, is described by an Arrhenius expression

$$k = A.\exp\left\{\frac{-\theta}{T}\right\} \quad . \tag{7.2}$$

Comparison of the analytic results with numerical integration of the differential equations, shows that in most cases the results of the two calculations are hardly distinguishable.
In how far a real flame is well described by the method depends mainly on how good the assumptions are that this flame may be described by an overall reaction of the type of Eq. (7.1) and on how good the estimates of the overall frequency factor, A, and overall activation temperature, θ, in Eq. (7.2) are.

The assumption that the temperature rise in the flame is linear with the relative product concentration, P/K_o, turns out to be valid, also in those cases that discrepancies between the analytic and numerical results occur. It is found that in those cases $d(P/K_o)/dT$ is somewhat larger for the analytic method than for the numerical integration, but the assumption of linearity is not violated.

Accurate results, i.e. results where there is hardly any appreciable difference between the numerical and analytic solution, will be obtained for values of the parameter, ε, satisfying

$$\varepsilon < 10^{-3} \quad . \tag{7.3}$$

This allows for very large ranges of parameters which usually lie within the range of physically realistic values.

Due to the analytic solution, the effects of varying parameters on the flame structure become very tractable. This may be of help when tracing such effects.

From the analytic solution, also some conclusions may be drawn with respect to some longlived concepts in flame calculations.
First of all, it is seen that by an appropriate choice of, physically realistic, mathematical boundary conditions, there is no "cold boundary" or "cold wall" difficulty. In fact Hirschfelders'(3) concept of a flameholder seems to be the most realistic approach to the boundary conditions. In this way one may discard artificiallities like "ignition temperature" (2) or "modified Arrhenius kinetics"(5). In itself these conclusions are not new; they have already been expressed by others, amongst whom Kassoy et al(7). Finally the analysis shows that it is at least difficult, if not impossible to speak of a flame thickness or flame front.

Although in a real flame, where there is a heat loss to the surroundings, somewhere a maximum temperature may be reached, this does not imply that one can speak of a "flame front" or "flame thickness" which is an inherent flame property, because this property depends on the surroundings and not primarily to the flame. For a purely one-dimensional flame, where there will be no heat transfer normal to the flow velocity, the concept of a "flame thickness" becomes artificial as the flame becomes infinitely thick.

Although the present report only concerns itself with steady state solutions for the premixed flames, the authors are convinced that the same technique can succesfully be applied to timedependent problems.

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