NUMERICAL METHOD FOR SOLVING A PREMIXED LAMINAR FLAME*

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Abstract

A splitting-up method, which splits the chemical kinetic terms from the flow terms, is presented to solve time-dependent, one-dimensional, laminar, premixed flame problems. An example for studying the development of an ozone decomposition flame is calculated. A movable boundary technique is adopted, so that the number of grid points can be significantly reduced. Special care is taken to maintain the accuracy of the solution. The results are checked in many ways. All checks show that the present method is satisfactory.

Nomenclature

x space coordinate
t time coordinate
p pressure
ρ density of fluid mixture
T temperature
y_i mass fraction of the i-th species
v velocity of fluid mixture
R universal gas constant
C_p specific heat capacity at constant pressure of the fluid mixture
C_{p_i} specific heat capacity at constant pressure of the i-th species
ω_i rate of production of i-th species
M_i molecular weight of i-th species
D_i binary diffusion coefficient for the i-th species
λ thermal conductivity
h_i enthalpy of i-th species
h_0^i standard enthalpy of formation of i-th species

1. Introduction

More and more attention is paid to combustion problems not only by engineers but also by mathematicians, because a number of interesting and difficult problems occur. For example, a premixed flame problem will reduce to a typical reaction-diffusion equation.

It is well known that in a premixed combustible fluid mixture a steady flame

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will be developed when it is ignited. This fact has been proved theoretically for a simple chemical reaction model. There have been many works on studying the configuration of a laminar, premixed flame. These works have essentially followed two different approaches. One is the steady-state approach in which the problem to be solved is reduced to a two-point boundary value problem of ordinary differential equations. The other is the time-dependent approach in which the full time-dependent equations with proper boundary and initial conditions are treated. In this paper our attention is focused on the latter approach.

Since the combustion processes are highly exothermic, chemical reaction processes and there exist a number of vastly differing time scales, numerical solutions will suffer from a number of difficulties. One is stiffness. With this in mind a splitting-up method is presented, which splits the chemical kinetic terms from the fluid mechanical terms. We think it might ameliorate some of the difficulties.

Generally speaking, the region of calculation must be taken large enough, therefore a large amount of grid points must be taken. Obviously it is costly. In order to reduce grid points a movable boundary technique is adopted.

Special care of error control is taken to maintain the accuracy of the solutions.

For comparison of the results obtained by the present methods with published results an example for an ozone decomposition flame is calculated. The results are also checked in many ways. The comparison and check show that the present methods are satisfactory.

2. Formulation of the Problem

2.1 *Governing Equations*

We consider one-dimensional flow and neglect the effects of radiative heat transfer and thermal and pressure diffusion. The governing equations are as follows.

Continuity

$$\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0. \tag{2.1}$$

Conservation of momentum

$$\rho\frac{\partial u}{\partial t}+\rho u\frac{\partial u}{\partial x}=-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left[\left(\mu+\frac{4}{3}\varkappa\right)\frac{\partial u}{\partial x}\right]. \tag{2.2}$$

Conservation of species

$$\rho\frac{\partial y_i}{\partial t}+\rho u\frac{\partial y_i}{\partial x}=\frac{\partial}{\partial x}\left(\rho D_i\frac{\partial y_i}{\partial x}\right)+\omega_i. \tag{2.3}$$

Conservation of energy

$$\rho C_p\frac{\partial T}{\partial t}+\rho C_p u\frac{\partial T}{\partial x}=\frac{\partial p}{\partial t}+u\frac{\partial p}{\partial x}+\left(\mu+\frac{4}{3}\varkappa\right)\left(\frac{\partial u}{\partial x}\right)^2+\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)$$

$$-\sum_{i=1}^{N}\omega_i h_i-\sum_{i=1}^{N}\rho D_i C_{p_i}\frac{\partial y_i}{\partial x}\frac{\partial T}{\partial x}, \tag{2.4}$$

and equation of state