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**Development of a Computer Code for a Solid Fuel Ramjet
Combustor**

by

Zhenlong Xu

B. ENG. (Mechanical), Tong Ji University

*A thesis submitted to
the Faculty of Graduate Studies and Research
in partial fulfilment of
the requirements for the degree of*

Master of Engineering

Department of Mechanical and Aerospace Engineering

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Ottawa, Ontario K1S 5B6

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Thesis Supervisor

A handwritten signature in cursive script, appearing to read 'M. ...', written over a horizontal line.

Chairman

Department of Mechanical
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Abstract

In the present thesis, the computer code DRAGON was developed for the prediction of the reacting flowfield in a solid fuel ramjet combustor. In the program, a one-step, irreversible chemical reaction between fuel and oxidizer (air) is considered. Two combustion models are selected to calculate the mixture composition using the diffusion flame model, which is based on infinitely fast reaction rate. In the first model, the diffusion flame model, the influence of turbulence on combustion is neglected, while in the second model, the turbulent diffusion flame model, this influence is included by weighting the mass fractions of the species involved in the chemical reaction by means of the beta Probability Density Function. In addition, solid fuel ignition and depletion events are ignored since a steady state is assumed. Radiation effects due to combustion are also neglected. The $k - \epsilon$ turbulence closure model is used. The resulting nonlinear differential equations that describe the turbulent, reacting flow are solved by using a finite volume method.

From calculations, it can be concluded that both combustion models work satisfactorily, but the turbulent diffusion flame model yields more realistic results than the diffusion flame model. However, because the diffusion flame concept does not take into account dissociation of atoms and molecules, temperatures in the combustion zone are overpredicted. A comparison between the numerical results with experimental data shows that the general trend of the local regression rate along the fuel wall is reproduced to satisfactory tolerance, but the reattachment length is underpredicted, which may be attributed to shortcomings of the $k - \epsilon$ turbulence model.

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Nomenclature

a	– Coefficient used in the beta probability density function
a	– Total convective and diffusive flux coefficients in the finite difference equations
A	– Area of cell boundary
b	– Coefficient used in the beta probability density function
c_p	– Specific heat at constant pressure
C	– Convective flux
C_1, C_2	– Empirical constants in the equation for the dissipation rate, ϵ
C_μ	– Empirical constant in the equation for the turbulent viscosity
C_{g_1}, C_{g_2}	– Empirical constants in the equation for the mass fraction variance
D	– Diffusion flux
D	– Diameter of the combustion chamber
E	– Von Kármán constant in the “law of the wall”
f	– Mixture fraction
$FACTKE$	– Turbulence intensity factor
$FACTED$	– Turbulence length scale factor
g	– Variance of the mixture fraction
G	– Generation term in the equations of the turbulence kinetic energy and turbulence energy dissipation rate

h	- Step height
$\tilde{h}$	- Total (stagnation) enthalpy
h^0	- Heat of formation at reference temperature
h_v	- Effective heat of gasification (heat of vaporization)
k	- Turbulence kinetic energy
L	- length of the combustion chamber
m	- Mass fraction
M	- Molecular weight
p	- Static pressure
p'	- Pressure correction
$P(f)$	- Probability density function
$P(\cdot)$	- Jayatilleke function
PV	- Pressure-velocity term in the equations for the turbulence
	- kinetic energy and turbulence energy dissipation rate
q	- Heat flux
r	- Radial coordinate
r	- Radius
r_{st}	- Stoichiometric ratio
R	- Reaction rate per unit volume
R_u	- Universal gas constant
S_ϕ	- Source term for variable ϕ
S_p	- Implicit source term
S_u	- Explicit source term

T	– Temperature
T_0	– Reference temperature
T^+	– Dimensionless temperature in a boundary layer, Eq.(2.31)
u	– Axial velocity
u_τ	– Friction velocity
v	– Radial velocity
$\vec{V}$	– Velocity vector
Vol	– Volume of cell
x	– Coordinate
Y	– Normal distance from a wall
Y^+	– Dimensionless distance from a wall in a boundary layer, Eq. (2.17)
β	– Beta function
Γ	– Exchange coefficient
$\Gamma()$	– Gamma function
ϵ	– Dissipation rate of turbulence kinetic energy
κ	– Von Kármán constant
μ	– Laminar viscosity coefficient
μ_t	– Turbulent viscosity coefficient
μ_{lam}	– Laminar viscosity coefficient
ρ	– Density
$\sigma_f, \sigma_g, \sigma_{N_2}$	– Schmidt numbers
σ_l	– Laminar Prandtl number

σ_t	-	Turbulent Prandtl number
$\sigma_k, \sigma_\epsilon$	-	Empirical constants in the $k - \epsilon$ turbulence model
τ	-	Shear stress
ϕ	-	Arbitrary independent variable such as u, v, k, ϵ , etc.
$\phi_{fo}, \phi_{fp}, \phi_{op}$	-	Conserved scalars

Subscripts

CO_2	-	Carbon dioxide, product of the reaction
eff	-	Effective
f	-	Mixture fraction
fu	-	Fuel
g	-	Variance of mixture fraction
H_2O	-	Water, product of the reaction
in	-	Inlet
n, N_2	-	Nitrogen
n, s, e, w	-	Points of the compass for cell boundaries
N, S, E, W	-	Points of the compass for grid points
ox	-	Oxygen
P	-	Grid point
pr	-	Products of the chemical reaction
st	-	Stoichiometric
t	-	Turbulent
v	-	Vaporization

- v - Viscous sublayer
- w - Solid wall
- ϕ - Pertaining to variable
- 1 - Fuel stream
- 2 - Oxidizer stream

Superscripts

- $()''$ - Favre fluctuation
- $(\tilde{ })$ - Favre mean
- $(\bar{ })$ - Mean
- $()'$ - Fluctuation
- $()^0$ - Reference state

Chapter 1

Introduction

The solid fuel ramjet (SFRJ) is perhaps the simplest form of airbreathing propulsion. It consists of an intake and diffuser, a combustion chamber with a case bonded solid fuel grain, an aft mixing and combustion chamber and a nozzle. One advantage of the SFRJ over a conventional solid propellant rocket motor is that it uses atmospheric air to oxidize the fuel and thereby achieves much higher specific impulse [1].

The high specific impulse inherent in ramjet propulsion systems has attracted designers whose missiles are required to combine long range with high speed. The simple design and operation, especially of solid fuel ramjets, adds to the attractiveness of this propulsion option. The one major disadvantage of ramjet propulsion, the lack of zero velocity start capability, is overcome by combining with another engine type (such as a rocket motor [2]) to produce that initial boost. Figure 1.1 is a schematic representation of a SFRJ, illustrating the inherent simplicity of the concept.

Solid-fuel ramjets also pose several advantages over liquid fuel systems. They do not require fuel tanks, fuel pumping devices or fuel controls to operate [3]. The self-throttling characteristics of the SFRJ permits operation from sea level to high altitude conditions. In addition, the basic diffusion-controlled SFRJ combustion process results in a high degree of uniformity in the energy release in the combustion region, resulting in no combustion instability problems in over 2500 test firings with numerous combustion configurations [3].

Because of all these merits as the propulsion device, solid fuel ramjet technology is currently of high interest not only in the military but also in commercial circles. It has been chosen for the future European spaceplane HOTOL and SANGER [4]. Nevertheless, many fundamental issues must still be resolved in order to properly exploit this emerging technology. They include the following [3]:

- Selection of a fuel type
- Flameholding requirements that limit maximum fuel loading
- Fuel regression rate behaviour as a function of flight speed and altitude
- Diffusion controlled combustion process that requires special mixing section
- Inlet/combustor matching

As the use of this propulsion device receives increased attention, it becomes more important that the operation of each of these components be well understood and their designs be properly integrated. A computer code which appropriately models each of these component parts and operates in such a manner that the components

interact correctly according to fluid dynamic and combustion principles, would be a very useful tool in the design of missile systems using an SFRJ propulsion system.

1.1 Objectives of the Thesis

The objective of this research is to develop an appropriate computer code for the prediction of turbulent, reacting, recirculating flowfields in the combustion chamber of subsonic combustion solid fuel ramjets. This code, as a part of overall computer modelling of SFRJ, would allow the computation of the two-dimensional velocity field, pressure, temperature, and the regression rate of the fuel grain, as a function of distance along the combustor axis.

1.2 Global View of the SFRJ Combustor

A schematic of a common-configuration SFRJ combustor shown in Figure 1.2 illustrates some of flowfield characteristics and combustion features. As noted in the sketch, the combustor may, in fact, be considered in terms of two parts, the fuel section and an aft mixing/combustion chamber. Studies [3] show that only about 50% of the fuel had mixed sufficiently with the air to burn by the time the flow reached the end of chamber containing the fuel. Consequently, the aft mixing and combustion zone is quite essential to good fuel utilization.

The sketch shown as Figure 1.3 illustrates some of the major features involved in the forward region of an SFRJ combustor. The sudden dump at the combustor entrance leads to a vortex and a recirculation region, which causes intense mixing of

fuel, air and hot combustion products. Thus, the stabilized flame in the recirculation zone can propagate throughout the combustor and provide a continuous ignition source for fuel further downstream. It is, therefore, important to have this modelled correctly, with the appropriate emphasis on the mixing of fuel and oxidizer as well as the determination of the region of combustion, whether controlled by reaction kinetics or by the availability of oxidizer where the fuel is available (transport controlled). Heterogeneous surface reactions may be considered less important because it is generally conceded that the combustion in a solid fuel ramjet is predominantly a gas phase diffusion flame, not of a surface reaction type, at least for the hydrocarbon components in the fuel [5].

Figure 1.3 also shows the point at the downstream end of the recirculation region where the flow attaches and begins a boundary layer flow. Heat is transferred from the main stream through the boundary layer to the solid fuel surface. The fuel is vapourized at a rate determined by the energy supplied to the surface. This fuel vapour diffuses away from the surface toward the freestream, reacting with oxygen as it forms a combustible mixture. For the basic case with no metal included in the fuel, it is a classical case of a reacting boundary layer flow, in which mass, momentum and energy conservation principles are combined with the reaction relations which account for the species reacting with each other to form other species and release energy [5].

Downstream of the main combustor is the aft mixing chamber which is added to permit any previously unreacted fuel to burn to completion. A step change in flow area entering the aft mixing chamber is used to create another recirculation zone to

stabilize a reaction zone in this compartment. In this chamber, the major change from the previous chamber is that no new fuel is added at the boundary, so the reactions are only with those reactive species carried from the previous chamber. The model used in the main combustor will therefore need to contain a sufficient number of species to simulate the species which are completely oxidized in the main combustor, but also to permit the remaining oxidizable species to be represented as they enter the aft chamber. It may be expected that a large portion of the reactions in this aft chamber will occur in the recirculation region at the entrance. If any reactable species remain beyond the recirculation, they would need to be permitted to react as the flow proceeds through this chamber [5].

1.3 Outline of the Thesis

To describe the flow and combustion processes in an SFRJ, a computer program, DRAGON, was developed. This program calculates two-dimensional steady-state turbulent reacting flows through pipes with or without a sudden expansion or through an axisymmetric sudden expansion configuration.

For simplicity, the two-dimensional approach was adopted in the program. The flows in the cylindrically shaped combustor are assumed to be axisymmetrical. The assumption is considered to be very good if an air mixing manifold is used between the diffuser and combustion chamber inlet, causing mixing and a more uniform flow to the combustor than that entering at the inlet [3]. However, it could not be used to model two other SFRJ geometries, side-dump and bypass. The side-dump

configuration has air injected through the side of the fuel grain and the dome region also contains fuel. The bypass configuration ducts a portion (typically 50%) of the total airflow into an aft mixing chamber. A full three-dimensional model is needed to predict the flowfield in these configurations.

Owing to the very large Reynolds number in the combustion chamber (usually of the order of millions) the flow is definitely turbulent. When trying to numerically predict such flows, we are faced with some of the hardest stumbling blocks in the field of CFD, namely turbulence, combustion (interacting with turbulence) and recirculation. Accordingly the modelling and numerical simulation of such flows need special tools for the three main building blocks of a devoted numerical code, i.e. the turbulence model, the turbulent combustion model, and the numerical algorithm to solve for the resulting equations.

First in Chapter 2, the DRAGON computer program, before implementation of a combustion model, will be described, which includes a discussion of turbulence models and the incorporation of numerical schemes to solve the resulting equations.

In the program, turbulence is accounted for by Favre-averaging of the conservation equations and by modelling terms containing products of fluctuating variables with the high Reynolds number version of the $k - \epsilon$ turbulence closure model [6, 7]. The influence of combustion on turbulence fields by means of density gradients is taken into account by a special pressure-velocity correlation term occurring in the equations for k and ϵ [8, 9, 10, 11].

The finite volume integration method is employed to reduce the system of partial differential equations describing the flow to a system of algebraic difference equations

which can be solved numerically. The combined convective-diffusive flux at the cell interfaces are approximated with a hybrid scheme [12]. The solution is done in a segregated approach, in which an iteration procedure takes into account the non-linear coupling between the equations. The strong coupling between pressure and the velocity field is handled by the SIMPLE algorithm [12, 13, 14], together with a line continuity and a block correction procedure.

The two combustion models have been implemented in the program based on the assumption that the combustion process can be described by one irreversible, infinitely fast chemical reaction.

One of these models, the diffusion flame model, is described in Chapter 3. The main assumption involved in this model is that fuel and oxidizer cannot exist together at the same place and at the same time. In the combustion chamber there will be a thin flame sheet where combustion takes place. At this stage the influence of turbulence on combustion is neglected.

In Chapter 3 the turbulent diffusion flame model is also presented in which the influence of turbulence on combustion is taken into account by weighting the mass fractions of fuel, oxidizer and products with a Probability Density Function. Here fuel and oxidizer can exist at the same place, their mass fractions being a time-average of the instantaneous situation. In this case, combustion takes place in a flame zone which is thicker than the flame sheet of the diffusion flame model.

Finally, the description of the code and the results of calculations using both models are discussed in Chapter 4 and Chapter 5, respectively. Conclusions and recommendations for further work are made in Chapter 6.

1.4 Literature Survey

1.4.1 Combustion Models

Several papers examined in the literature survey contained a discussion of the solid fuel combustion model, e.g. Nusca, et al [16], Netzer, et al [17, 18, 19, 20, 21, 22], based on work in the U.S., Lentini, et al [4], based on work in Italy and England, as well as Vos [8] and Elands et al [9, 23, 11], based on their work in the Netherlands. Nusca [16], Netzer et al [17, 18, 19, 20, 21, 22], Elands et al [9, 23, 11] and Lentini et al [4] all resort to a diffusion-controlled reaction model in which the fuel is vaporized at the wall and diffuses into the gas stream until it encounters sufficient oxidizer to completely convert it to products in one step. This approach shifts attention away from the chemical kinetics and more fully onto the transfer processes which are strongly affected by turbulence. Consequently, much of the attention focuses on the turbulence model. Elands et al [9, 23, 11] conclude that the major difficulty with this simple one-step model is that it does not account for dissociation of species, resulting in temperatures which are too high. They, in turn, referred to a model of Vos [8], containing more chemistry, as worth considering. But the model referred to does not involve an actual solid fuel, but a simulated reaction involving hydrogen injection at the wall. The difference in chemistry between simple hydrogen diffusing and reacting in the presence of oxygen as opposed to a solid fuel vaporizing and these products reacting with oxygen is immense [5]. Nusca [16] noted that the true chemistry of solid fuel combustion may be far more complex than our knowledge can encompass. Even if it was technically desirable and computationally possible to

include all species and reactions within the framework of a calculation, to attempt to do so would be defeated by an ignorance of the thermodynamic, transport, and chemical-kinetic properties of the great majority of the species.

In the work of Elands [10, 11], two combustion models based on the diffusion flame concept were implemented in a 2 - D computer code COPPEF describing turbulent flows through channels with and without a sudden expansion. The results were compared with results of a finite chemical kinetics model, obtained by Vos [8] in the same computer code.

In the diffusion flame representation, one model does not account for the effect of turbulence on combustion whereas the other does, by weighting the mass fractions with a beta Probability Density Function. The latter also takes into account the influence of combustion on turbulence by means of a pressure velocity correlation term in the Favre-average equations for k and ϵ . The model in which turbulence interacted with the combustion process provided a more realistic representation of the real combustion process than the one in which they did not interact. It was found that the diffusion flame model can be run in about 5% of the time taken for the chemical kinetics computation. However, the simple diffusion flame model used cannot account for dissociation. Consequently, temperatures predicted are too high, and formation of pollutants cannot be predicted. It is, however, an efficient and fast tool for preliminary calculations.

As it has been mentioned above, Vos [8] implemented a finite kinetics combustion model in the computer code COPPEF. But the calculations did not represent real combustion processes in SFRJ combustors. It merely simulated hydrogen injec-

tion at the wall with oxygen and nitrogen in the inlet flow. The number of reactions considered was equal to 24 for the combustion of N_2/O_2 with H_2 , and 46 for the combustion of air with H_2 . In the latter case, the formation of nitrogen oxides was taken into account. The solution was achieved by splitting the transport equation of mass fractions into a convection/diffusion part, and a chemical production/destruction part, and solving these two parts separately with different techniques, giving good results. Calculations were carried out with a range of blowing of hydrogen and expansion ratios in the core. These variations caused a variation in the location of the reattachment point. Allowing for the formation of species such as NO_x resulted in reduced temperatures by approximately $100K$.

Two very similar diffusion combustion models were developed by Nusca, et al [16] and Netzer, et al [17, 18, 19, 20, 21, 22], respectively. In their models, a one-step, irreversible, mass-controlled reaction is considered for which the reactant species are fully consumed. The reaction maintains a fixed stoichiometric ratio, and the reaction rate is much faster than the rate of diffusion so that the reaction is diffusion controlled. Thus, the models they used are essentially the same as the diffusion flame model developed by Elands [10, 11]. The only difference is a conserved scalar they adopt for solving the mass conservation equation. Elands employs the one called mixture fraction which he believes gives a good physical interpretation of the mixing of the two feeds, and Netzer, et al and Nusca, et al use a somehow different but simple variable defined as $Y_F - Y_O/r$.

Lentini, et al, in his recent work [4], also adopted a turbulent combustion model which is virtually the same as the one of Elands [10, 11]. The comparisons with

experimental data reported in his work indicate that this approach, while giving reasonably accurate predictions of the velocity field all over and of the temperature field in the directed flow region, results in largely overpredicted temperatures in the recirculation region. They ascribed this to a poor prediction of the conserved scalar field.

1.4.2 Turbulence Models

In fact, all of the papers dealing with modeling of ramjets had some comments about turbulence models, since it is such an intrinsic part of the problem. Besides, many of the papers discussed here have direct connection to some aspect of ramjet combustion. The work of Elands [10, 11] is an example of this, in which interactions between turbulence and combustion are accounted for through the $k - \epsilon$ turbulence model and turbulent combustion model. The literature survey in this matter indicates that the $k - \epsilon$ turbulence model has been the most popular one used so far for the calculation of flowfields in SFRJ combustors in spite of the well-known inaccurate prediction of the flowfield in the recirculation region.

Abujela and Lilley [24] assessed shortcomings and recommended corrections to the standard two equation $k - \epsilon$ turbulence model, based on its applicability to turbulent swirling recirculating flow. Experimental data on swirling confined flow obtained with a five-hole probe and a six-orientation hot-wire probe are used to obtain the constants used in the model. It is found that when these parameters are used, predictions with the model agree more closely with observations than when other standard or simple extensions of the $k - \epsilon$ turbulence models are used. The

extensions used by various investigators are reviewed.

It may be fair to say that other investigators also saw improvements in their correlations when they adjusted the parameters in the $k - \epsilon$ model to suit their geometry. Therefore, just because these authors have seen better agreement with data available to them does not guarantee that their method will be as good as another in another configuration. That is, although the $k - \epsilon$ is supposed to be a universal model with the same constants applicable to all cases, various examples have shown that the universality of the model is limited [5].

In the work of Ha and Lilley [25], the $k - \epsilon$ turbulence model and a three component combustion model are used. Solutions are obtained with axisymmetric flows in channels with irregularly shaped external boundaries. The $k - \epsilon$ turbulence model is found to give good predictions with non-swirling flows, but not such good results with swirling flows.

Jones and Launder [26] contributed one of the early papers relating to the use of the $k - \epsilon$ model of turbulence in some specialized cases, and how the constants can be tailored to the particular case. This tailoring of the constants is criticized by others (ref. [27], for example) since it takes away the universality of the method, if it was ever intended to be a universal method. The major component of this work is the development of a suitable method for regions where the turbulence Reynolds number is low. This would certainly be the case in the vicinity of the reattachment point in a concentric SFRJ. A distinction is drawn between the form of the equations for computing the k and ϵ in high Reynolds number flows compared with low Reynolds number flows. The low Reynolds number flows allow that as the turbulent

viscosity gets small, it is complemented by the laminar viscosity coefficient in the gradient term, and another term is included in the turbulence energy conservation equation (for k). In addition, in the energy dissipation calculation (for ϵ), some multipliers, f_1 and f_2 , etc., are used in two terms of the equation, as well as in auxiliary equations. Although the first of these is constant at a value of unity, others have a Reynolds number dependence. The resulting form appears to give good results in an accelerating region of the boundary-layer flow.

The $k - \epsilon$ model used for the calculation of SFRJs is only valid for high Reynolds number flows. To account for viscous or low-Reynolds number effects near solid walls, the production and dissipation terms in the equations for k and ϵ are replaced by expressions obtained from wall-functions. A distinction has to be made between walls with and without blowing or suction. In principle, wall-functions cannot be used in flows with blowing or suction. As the regression rates of most solid fuels are very small ($< 0.1\text{m/s}$), the boundary layer will only be slightly affected [8]. Thus, Vos [8], in his work proposed an adapted version of the wall-function method of Chieng and Launder [28] to take into account the contribution of a non-zero normal velocity at the wall to the production rate, dissipation of turbulent kinetic energy and heat flux to the wall. He also concluded that the Von Kármán constant E was not a constant anymore, but depended on the local flow and boundary layer structure and had to be calculated from a set of three equations. The computed results showed that for relatively small blowing velocities, the adapted wall-function method worked satisfactorily.

As mentioned above, a wall function is needed to transfer wall boundary condi-

tions to computational points removed from the wall, where R_t is large enough to render the $k - \epsilon$ equations valid. There are, however, no universal wall functions and all existing ones are based on the law of the wall, which is invalid under detached flow conditions [29]. To avoid this limitation, Goldberg, et al [29] introduced a near-wall formulation for the $k - \epsilon$ turbulence model. In their work, the original $k - \epsilon$ equations were modified in a way to extend their validity to the viscous sublayer. The main features of this formulation are: (1) an analytically derived expression for the function f_μ appearing in the formula for ν_t ; and (2) a treatment designed to avoid the abnormally high values of heat transfer that many low Reynolds number $k - \epsilon$ models tend to predict in flow reattachment regions. The new approach was claimed to be very encouraging after being tested against a number of cases for which experimental data are available.

Another research work on near-wall turbulence models was conducted by Djilali, et al [30], in which the performances of seven near-wall turbulence models were examined. The first two models were one-equation low Reynolds number (Re) models requiring a fine grid near-wall treatment. The other near-wall turbulence models considered were based on wall functions that bridge the thermally important near-wall region with a single cell. Standard wall functions based on the local equilibrium assumption, wall functions using a two- and three-layer approach to evaluate local variations of turbulence quantities in the k equation, and extension of the two- and three-layer treatments to the ϵ equation were considered. The numerical predictions were obtained using a variant of the $k - \epsilon$ model incorporating a curvature correction. The solutions were obtained using a two-pass procedure, devised to allow for

the correct use of the wall functions. The various near-wall models were assessed by comparing resulting Nusselt number distributions and selected fluid dynamic results with available experimental data for the turbulent flow about a two-dimensional blunt rectangular section. The final conclusion was that a three-layer model of the wall region, applied to the k and ϵ equations, gave good agreement with the data; the standard wall function treatment was not satisfactory at all for this flow.

Many separated flows often involve regions where the flow detaches from a solid surface and reattaches further downstream, thereby forming a separation bubble. Goldberg [31] thinks that most existing turbulence models either do not treat such bubbles or do so in an ad hoc fashion, which is frequently inadequate. Thus, in 1986 he developed an algebraic $k - \epsilon$ formulation for turbulence modeling within wall-bounded two-dimensional separation bubbles. The model is based on experimental observations. Two basic features of the model are: (1) turbulence kinetic energy within the backflow region is a Gaussian function of the distance from the wall; (2) the length scale of turbulence within the bubble is proportional to the local distance from the wall to the edge of the viscous sublayer located outside the backflow region. The formulation enables unified $k - \epsilon$ modeling between the wall and the viscous sublayer edge.

Subsequently in 1988, Goldberg, et al [32] incorporated this algebraic backflow model into a Reynolds-averaged Navier-Stokes solver that used the Baldwin-Lomax algebraic turbulence model [33] outside of separation bubbles. This code has been applied to calculate the reattaching flow over a backward-facing step and the shock-induced separated flow over an axisymmetric bump. Comparisons with data show

improvement in predictive capability as compared to that resulting from using the $k - \epsilon$ model and a similar performance to that of the Johnson-King model [34]. The new model enables good prediction of time-averaged flow quantities as well as skin friction but falls short of adequately predicting Reynolds stresses, although the qualitative prediction of these stresses is good.

In addition, Goldberg, et al [35] applied the computer code to calculate internal and external flows for a ramjet projectile under turbulent, supersonic conditions, in which two turbulence modeling approaches were tried: (1) The Baldwin-Lomax model [33] applied throughout the flow field; (2) The Baldwin-Lomax model applied outside of backflow regions and this backflow model applied within these regions. Comparison with experimental data shows a significant improvement in the code's predictional capability when the latter approach is used.

1.4.3 Experimental Investigations

Plett [5], in his report to DND, made an excellent and comprehensive review on experimental studies toward SFRJ combustors. Some of the papers cited before also have a substantial component of experimentally obtained information which can be used for model verification. Others which are cited in this section have their major contribution to the experimental results.

Hewett and Netzer [36] used light transmission to attempt to characterize the solid particle sizes in the gaseous flow – partially because earlier measurements by Mady et al [37] had produced some unexpected trends when bypass air was introduced. It was thought that unburned carbon may not burn when the cooler

bypass air impinges on it, whereas the results of this study indicate that the large amount of unburned hydrocarbons in the boundary layer are the cause for low combustion efficiencies. It was also learned that the fuel batch can make a difference – the batch used by Mady had quite different combustion characteristics than the batch used in this work [36], although both were nominally PMM (fuel).

Nabity and Walls [38] showed, by experiments, that the side-dump SFRJ can provide a significant performance increase over the center-dump configuration in a volume limited application. This occurs because the side-dump configuration can achieve improved fuel loading, and more uniform regression along the fuel grain, if the side-dump geometry is optimally chosen. Fuel utilization was best for configurations with a 60-degree dump angle and 4.5 inch dome length in a 4 inch diameter test combustor.

Duesterhaus and Hogl [39] conducted experiments with a directly connected solid fuel ramjet combustor with and without inlet flow swirl. The use of swirl increased fuel regression of PE (polyethylene) and UTX (a modified hydroxyl terminated polybutadiene (HTPB) mixture, containing carbon black and styrene) fuels in a solid fuel ramjet combustor by as much as 60% and 28%, respectively. (i.e. there is some variation with fuel type) The swirl also caused an increase in pressure loss in the combustor.

It has been shown [39] that an increased step height is needed when using swirl in a dump type ramjet combustor to allow for an adequate recirculation zone. Ignition stability is altered when using swirl – higher temperatures may be required as the swirl is increased. Temperature and gas concentration measurements in their

investigation confirm that mixing is poorer at the center of the combustor with swirl. No change is noted at the wall, in terms of oxygen concentration, but mixing appeared to be much improved in the afterburner region with swirl. Attempts were made to stop the swirl before the flow entered the nozzle, since the swirl causes a thrust reduction. The swirl reverse attempts did produce slightly higher thrust, but pressure loss ratio was essentially unchanged, and combustion efficiency was reduced by about 1% [39].

Netzer and Gany [40] studied the combustion and flameholding limits of solid fuels in ramjet combustor configurations, in very small scale. The combustor size was 10 mm inside diameter, 70 mm long, with a 14 mm I.D., 40 mm long aft-mixing chamber. Several port (diameter of the solid fuel) to throat (of the nozzle) diameter ratios were studied to investigate their effect on flameholding, in addition to the variation of inlet diameter to port diameter (step height). The general features noted in larger motors were observed, but quantitatively, there was a strong effect of motor size. The smaller motor generally had narrower flame holding regions than did the larger ones - as was noted in the scaling - that the smaller diameter combustors had lower heat capacity to heat loss areas than did the larger ones.

Using the same combustor as their predecessors [40], and a PMMA fuel, Zvuloni, Levy and Gany [41], sought a relationship between the fuel regression rate and flow and geometric parameters. Fuel regression rate vs. axial distance along the combustor was measured and compared with thermochemical equilibrium calculations, with good agreement, indicating that the reactions are completed and equilibrium is being attained. This was first done with various fuel/air ratios (vary fuel length

and air inlet flow rates), or by holding fuel length constant and varying air flow rate. The exponent on the air flow rate was higher (nearly unity), compared with typical values of the order of 0.4 to 0.6. It seems that the fuel regression causes a significant change in port diameter in this small burner, even with very short duration burns. A correction for the size of the burner was sought. Since, it is concluded, the fuel regression rate is very strongly dependent on the convective heat transfer, it is to be expected that the regression rate would similarly be strongly dependent on the geometric dimensions of the combustor.

Another paper by Zvuloni, Gany and Levy [42] published just prior to [41], although the work was done somewhat earlier, provides further insight into the relationship between solid fuel regression rate, air flow rate and port diameter. In using the expression for burning rate, r

$$r = aG^n$$

Where G is the air mass flux (per unit area), it is pointed out that as the combustor port diameter changes, the air mass flux changes in a non-linear way such that taking the average mass flux and raising it to an exponent gives different results than raising the local time mass flux to the same exponent before averaging.

Another approach is to add a diameter term to the equation as suggested by work from United Technologies Chemical Systems [43] so that it appears as

$$r = aG^n d^{n-1}$$

This allows the port diameter effect to be more directly accounted for, and appears to be a better representation of the real effect, which is dependent on heat transfer

to the solid fuel surface to vapourize the fuel before it burns. This expression, with $n = 0.6$, correlates data from several sizes of combustor.

It is further noted that short burn-time tests will not usually show this effect if the diameter does not change appreciably during the test.

Schulte [44] described an experimental study to simulate the effect of varying the flight speed (hence the shock strength at the inlet, which would affect the pressure and temperature of the air coming in) and altitude, chamber pressures, air mass flow rates and temperatures. The effect of relative sizes of nozzle, port and inlet on flame holding were also investigated. Polyethylene (PE) was used for most of the tests, with some done with hydroxyl terminated polybutadiene (HTPB).

The reattachment distance was found to correlate with step height (with some scatter in observed results). It was found that increasing the inlet pressure or temperature had a similar effect on the fuel regression rate (probably because it affected the heat transfer to the solid fuel surface in much the same way, which is found in other papers to correlate well with fuel regression rate and therefore, combustion rate). The effect of temperature is stronger than the effect of pressure or air mass flow rate. It was also observed that increased port diameter resulted in decreased regression rate. This too has been noted in the work of others.

Combustion of solid fuels were studied in a small ramjet type combustor by Schulte, Pein and Hogl [45]. Polyethylene (PE) and HTPB were used, with mostly PE. The air was preheated, to simulate high temperature intake. Measurements of fuel regression rate, temperature and concentration profiles were used to arrive at the following conclusions:

1. In the recirculation zone, combustion takes place primarily in the shear layer of the incoming air, leading to maximum temperatures in the shear layer.
2. The recirculation zone is fuel rich, and not well stirred, consequently, well stirred reactor models should not be used here.
3. The fuel is not immediately consumed when it encounters some oxygen, since some oxygen is detected at the wall.

They also observed that:

4. The flame position in the redeveloping boundary layer is dependent on the air mass flux and on the type of fuel regression behaviour and is slightly dependent on inlet temperature.
5. The flow in the combustor can be separated into two zones, a colder zone in the core, which is air rich, and a zone of combustion products closer to the wall, with the two zones mixing incompletely along the combustion chamber.

Korting, Van der Geld, Vos, Wijchers, Nina and Schoyer [46], combined on a piece of work which was primarily based on experiments, although some cold flow $(2 - D)$ computer calculations were performed and showed good agreement with experimentally obtained results.

In the experiments, PMMA was burned in a connected pipe test facility, using a rearward facing step for flame stabilization. Below 0.6 MPa, there was no evidence of pressure dependence on burning rate, and no noticeable soot was formed. At higher pressures, regression rate was strongly dependent on pressure. They conclude that

heat transfer is predominantly by convection at pressure below 0.6 MPa, whereas radiation becomes an important mode of heat transfer at pressures above 0.6 MPa. Regression rates are observed to increase with:

- increasing expansion ratio,
- increasing inlet temperature,
- increasing oxygen content.

all of which might cause an increase in convective heat transfer, thereby increasing the regression rate.

Reaction kinetics were believed to have some role in the processes, in some regions, since it was observed that increasing the fuel length and increasing the size of the aft mixing chamber resulted in increased combustion efficiency.

Chapter 2

Mathematical Background

In this Chapter, the Dragon code, for calculating two-dimensional parabolic and elliptic flows without combustion, is described.

First the partial differential equations describing a two-dimensional turbulent flow are discussed. In the second section the boundary conditions needed to solve these equations are given. The discretization method used to reduce the partial differential equations to algebraic difference equations is described in Section 2.3. Finally the procedure to solve these algebraic difference equations is also discussed in this section.

2.1 Governing Equations

The equations describing a two-dimensional steady turbulent flow of a non-reacting mixture are given in references [18, 15]. In order to include turbulence, Favre or mass-weighted averaging of the conservation equations is applied and the terms containing fluctuating quantities are modeled with the $k-\epsilon$ turbulence closure model

[6, 7]. It uses five empirical constants (Table 2.1) and requires that two additional variables [turbulence kinetic energy (k) and turbulence energy dissipation rate (ϵ)] be evaluated. Effective viscosity is calculated using the formulas

$$\mu_{eff} = \mu_{lam} + \mu_t \quad (2.1)$$

where the turbulent viscosity, μ_t , is defined in terms of a characteristic turbulent length scale, $C_\mu k^{3/2}/\epsilon$, and a velocity scale, $k^{1/2}$, as follows:

$$\mu_t = C_\mu \rho k^2 / \epsilon \quad (2.2)$$

For simplicity, the value of specific heat (c_p) is assumed to be constant although its dependence on temperature and/or composition could easily be included. The turbulent and laminar Prandtl numbers are taken to be unity.

The conservation equations for axisymmetrical flows with no tangential variations can be put into the general form [15, 18]

$$\frac{\partial}{\partial x}(\rho u \phi) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v \phi) - \frac{\partial}{\partial x}(\Gamma_\phi \frac{\partial \phi}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_\phi \frac{\partial \phi}{\partial r}) = S_\phi \quad (2.3)$$

convective terms

diffusion terms

source terms

where ϕ stands for the dependent variables (u, v, k, ϵ, h , etc ...) being considered ($\phi = 1$ for the continuity equation), Γ_ϕ is the appropriate effective exchange coefficient for turbulent flow, and S_ϕ is the source term (Table 2.2). For simplicity, the Schmidt number in the energy equation is taken equal to the Prandtl number (unity), so source term of the energy equation in terms of stagnation enthalpy can be reduced to zero. Radiative transport was neglected at this stage.

The stagnation enthalpy for a flow at temperature, T , and with velocity components u and v , is defined as

$$\tilde{h} = (T - T_0) \sum_j c_{p,j} m_j + \sum_j h_j^0 m_j + \frac{u^2 + v^2}{2} + k \quad (2.4)$$

where m_j is the mass fraction of species j , and h_j^0 is the heat of formation of species j at reference temperature T_0 . The calculation of temperature is made using Eqs.(2.4) and shown below:

$$T = \frac{\tilde{h} - \sum_j h_j^0 m_j - \frac{u^2 + v^2}{2} - k}{\sum_j c_{p,j} m_j} + T_0 \quad (2.5)$$

The equation of state is used to calculate density and is written as:

$$\rho = \frac{p/(R_u T)}{\sum_j \frac{m_j}{M_j}} = \frac{p/R_u}{\tilde{h} - \frac{u^2 + v^2}{2} - k - \sum_j h_j^0 m_j + T_0 \cdot \sum_j c_{p,j} m_j} \cdot \frac{\sum_j c_{p,j} m_j}{\sum_j \frac{m_j}{M_j}} \quad (2.6)$$

The influence of density gradients on the turbulence field is taken into account by the pressure-velocity correlation term (PV)[11, 8, 9, 10]. This term (PV) occurs in the Favre-averaged equations for k and ϵ (Table 2.2) [51] and is written as:

$$PV = -\overline{V_j'' \frac{\partial p}{\partial x_j}} \approx -\overline{V_j''} \frac{\partial \bar{p}}{\partial x_j} \quad (2.7)$$

where j denotes x and r in cylindrical coordinate system (see Table 2.2). For constant-density flows, the PV term can be neglected, but for turbulent reacting flows, density varies significantly in flowfield, and this pressure-velocity correlation becomes very important, representing how combustion affects turbulence through the variation of density. It must be retained in the equations for k and ϵ . The mean velocity fluctuation in the PV term, which is not zero when Favre-averaging is applied, can be then modeled as follows. From the definition of Favre-averaging,

it follows that:

$$\tilde{V}_j = \frac{\overline{\rho V_j}}{\bar{\rho}} \quad (2.8)$$

The velocity may be written as

$$V_j = \tilde{V}_j + V_j'' \quad (2.9)$$

where V'' is the superimposed velocity fluctuation. Multiplying the equation above by ρ and decomposing the velocity into two parts, we have

$$\rho V_j = \rho(\tilde{V}_j + V_j'') = \rho \tilde{V}_j + \rho V_j'' \quad (2.10)$$

by time-averaging the above equation, we get

$$\overline{\rho V_j} = \bar{\rho} \tilde{V}_j + \overline{\rho V_j''} \quad (2.11)$$

From the definition of Favre-averaging of the velocity (Eq. (2.8)), it follows that

$$\overline{\rho V_j''} = 0 \quad (2.12)$$

Decomposing the density into two parts, we yield

$$\overline{\rho V_j''} = \overline{(\bar{\rho} + \rho') V_j''} = 0 \quad (2.13)$$

After arranging the equation, we have

$$\overline{V_j''} = -\frac{\overline{\rho' V_j''}}{\bar{\rho}} \quad (2.14)$$

and the right hand side of this equation can be modeled using an eddy-diffusivity concept:

$$\overline{\rho' V_j''} = -\frac{\mu_t}{\sigma_t} \frac{\partial \bar{\rho}}{\partial x_j} \quad (2.15)$$

Substituting Eqs. (2.14) and (2.15) into Eq. (2.7), the pressure-velocity correlation finally yields:

$$PV = -\frac{\mu_t}{\sigma_t} \frac{1}{\bar{\rho}^2} \frac{\partial \bar{p}}{\partial x_j} \frac{\partial \bar{\rho}}{\partial x_j} \quad (2.16)$$

As can be seen from this equation, density gradients can generate turbulence, but they can also suppress it.

2.2 Boundary Conditions & Wall Function Method

Boundary Conditions

The system of partial differential equations can be solved if all the inlet and boundary conditions are specified. The inlet conditions are specified as follows:

$$\begin{aligned} u &= u_{in} \\ v &= 0 \\ k &= \frac{1}{2}(\text{FACTKE} \cdot u_{in})^2 \\ \epsilon &= C_D \frac{k^{\frac{3}{2}}}{\text{FACTED} \cdot r} \\ p &= p_{in} \\ m_j &= m_{j,in} \\ \hat{h} &= (T_{in} - T_0) \sum_j c_{p,j} m_{j,in} + \sum_j h_j^0 m_{j,in} + \frac{u_{in}^2}{2} + k_{in} \end{aligned}$$

where FACTKE, FACTED are defined as turbulence intensity factor and turbulence length scale factor, respectively. Their values can be found in Table 5.1.

At the outlet and at the centreline of the channel, a non-gradient condition is used for all equations, except the r -momentum equation for which a zero velocity is

specified.

$$\begin{array}{lll} \text{outlet:} & \frac{\partial \phi}{\partial x} = 0 & v = 0 \\ \text{centreline:} & \frac{\partial \phi}{\partial r} = 0 & v = 0 \end{array}$$

At solid fuel walls, fuel could be blown into the combustion chamber. The following boundary conditions can be prescribed:

$$\begin{array}{ll} u & = 0 \\ v & = 0 \quad \text{or} \quad v = v_w \\ T & = T_{wall} \\ m_j & = m_{j,wall} \end{array}$$

The fuel injection rate may not be constant in reality. It should be coupled to the heat flux to the wall in order to fully simulate a pyrolyzing fuel at wall. The detailed discussion will be given in Chapter 3.

The values of k and ϵ are not specified at the wall, but are calculated just near the wall using the wall function method [6, 7].

Wall Function Method

The $k-\epsilon$ turbulence model that has been described is restricted to high Reynolds numbers, where the turbulent structure can be assumed to be independent of molecular viscosity. The prominent influence of laminar viscosity and strong variations of the flow and turbulence properties near a solid boundary necessitates modification of the turbulence model and use of very fine, economically nonviable computational grids in this region. The approach adopted here is to define a wall-layer and to link the flow conditions in the interior, fully turbulent region to the values of variables at the wall through special wall functions. These wall-functions are derived from a one-dimensional steady Couette flow analysis of the wall region and they define the flow conditions across the wall-layer as functions of the local Reynolds number Y^+ [6], defined as

$$Y^+ = \rho u_\tau Y / \mu \quad (2.17)$$

where Y is the normal distance from the wall and u_τ is the friction velocity, defined in terms of the wall shear stress τ_w as:

$$u_\tau = \sqrt{\tau_w / \rho} \quad (2.18)$$

From observation of the experimental data used to determine the law of the wall, it is known that the wall flow region is made up of three zones: the viscous sublayer ($0 < Y^+ < 5$), where viscous effects dominate, the inertial sublayer ($30 < Y^+ < 400$), where the flow is assumed to be completely turbulent but $\tau = \tau_w$, and the transition (or buffer) layer ($5 < Y^+ < 30$) of vigorous turbulence dynamics, where the flow is neither completely turbulent nor completely dominated by viscous

effects. Following the normal practice [13], as is indeed done in many engineering calculations, the buffer layer is dispensed with by extending the viscous and inertial sublayers to a common boundary at $Y^+ = 11.5$. Above this common boundary, the flow is assumed to be purely turbulent and the velocity variation may be described by a logarithmic relationship. In the viscous sublayer, the flow is purely viscous and velocity profile is linear. The profiles of velocity across the wall layer may be represented as follows:

$$\frac{u}{u_\tau} = \begin{cases} Y^+ & \text{for } Y^+ \leq 11.5 \\ \ln(EY^+)/\kappa & \text{for } Y^+ > 11.5 \end{cases} \quad (2.19)$$

where κ and E are the Von Kármán constants. Both values, given in Table 2.1, are known from experiment for smooth and impermeable walls with constant shear stresses. For SFRJ combustors, as the regression rates of most solid fuels are very small, blowing velocities are very small ($< 0.1\text{m/s}$) and boundary layer will only be slightly affected. Thus for simplicity, the Von Kármán constants are still assumed to be the same as the ones at impermeable walls.

In the near-wall region of a Couette flow, the turbulence is in local equilibrium [7] and in these circumstances, the algebraic expressions for the wall shear stress and the dissipation rate ϵ within the fully turbulent sublayer ($Y^+ > 11.5$) [13] can be derived, as follows:

The shear stress is assumed uniform from the wall to the near-wall grid point, and is calculated from

$$\tau_w \approx \tau = \mu_t \frac{\partial u}{\partial y} \quad (2.20)$$

Near a wall, the transport equation for the turbulence kinetic energy (see Table 2.2)

reduces to a balance between the local production and dissipation of k [7]

$$\mu_t \left(\frac{\partial u}{\partial y} \right)^2 = \rho \epsilon \quad (2.21)$$

The velocity gradient and dissipation rate are replaced from Eqs. (2.2) and (2.20) to give

$$\tau_w = C_\mu^{\frac{1}{2}} \rho k = \rho u_\tau^2 \quad (2.22)$$

Substituting Eq. (2.22) into Eq. (2.19), we yield

$$\tau_w = \frac{\rho C_\mu^{\frac{1}{2}} k^{\frac{1}{2}} u \kappa}{\ln(EY^+)} \quad (2.23)$$

where the local Reynolds number is evaluated from

$$Y^+ = \rho \sqrt{\frac{\tau_w}{\rho}} Y / \mu = \rho C_\mu^{\frac{1}{2}} k^{\frac{1}{2}} Y / \mu \quad (2.24)$$

Within the viscous sublayer ($Y^+ \leq 11.5$), the wall shear stress is derived from Eq. (2.19)

$$\frac{u}{u_\tau} = \frac{\rho u_\tau Y}{\mu} \quad (2.25)$$

$$\tau_w = \rho u_\tau^2 = \mu u / Y \quad (2.26)$$

For the derivation of the boundary condition for the dissipation rate, the turbulent viscosity in Eq. (2.21) is replaced by the value from Eq. (2.2) to give

$$C_\mu k^2 \left(\frac{\partial u}{\partial y} \right)^2 = \epsilon^2 \quad (2.27)$$

Differentiating Eq. (2.19) gives

$$\frac{\partial u}{\partial y} = \frac{u_\tau}{\kappa Y} \quad (2.28)$$

So

$$\epsilon = \frac{C_\mu^{\frac{3}{4}} k^{\frac{3}{2}}}{\kappa Y} \quad (2.29)$$

Due to the steep gradients of properties in turbulent flows near solid boundaries, the source terms for k and ϵ at near wall nodes are best expressed in terms of the wall shear stress. For the boundary condition for the equation k , the generation rate G and viscous dissipation term are evaluated using the calculated shear stress, such that

$$\begin{aligned} S_k &= G_k - \rho \epsilon \\ &= \tau_w \frac{\partial u}{\partial y} - \frac{C_\mu \rho^2 k^2}{\mu_t} \\ &= \tau_w \frac{\partial u}{\partial y} - \frac{C_\mu \rho^2 k^2}{\tau_w} \frac{\partial u}{\partial y} \end{aligned} \quad (2.30)$$

τ_w also provides the boundary condition for the u and v equations.

For the calculation of wall heat flux, the following practice [28] is used. The layer close to the wall is assumed to be of constant heat flux. The link between the near wall variation of temperature and the heat flux to the wall is given by

$$T^+ = [\ln(EY^+)/\kappa + P + \left(\frac{\sigma}{\sigma_t}\right)] \sigma_t \quad (2.31)$$

where T^+ is defined as

$$T^+ = \frac{\rho c_p k^{\frac{1}{2}} C_\mu^{\frac{1}{4}} (T_w - T)}{q_w} \quad (2.32)$$

and $P + \left(\frac{\sigma}{\sigma_t}\right)$ is the Jayatilke function [28] given by

$$P + \left(\frac{\sigma}{\sigma_t}\right) = 9.24 \left[\left(\frac{\sigma}{\sigma_t}\right)^{0.75} - 1 \right] [1 + 0.28 \exp(-0.007 \frac{\sigma}{\sigma_t})] \quad (2.33)$$

Thus, the wall heat flux, required for incorporation into the energy conservation equation through source terms, is now given by

$$q_w = \frac{\rho c_p k^{\frac{1}{2}} C_\mu^{\frac{1}{4}}}{\sigma_t} (T_w - T) [\ln(EY^+)/\kappa + P + \left(\frac{\sigma}{\sigma_t}\right)]^{-1} \quad (2.34)$$

2.3 Method of Solution

2.3.1 Finite Difference Equations

The general partial differential equation (Eq. 2.3) is integrated over a small control volume to obtain an algebraic difference equation, which can be solved numerically. This method ensures that over the control volume the conservation equations are always satisfied. Moreover, it is possible to use arbitrarily small or large control volumes. In regions with large gradients, small control volumes can be used while in other regions, larger control volumes are sufficient for an accurate approximation of the variables. A staggered grid system is used in which the u and v velocities are stored at the boundaries of the control volume for the other variables, shown in Figure 2.1. When calculating the convective fluxes across the control volume boundaries it is not necessary to approximate the velocity at the boundaries. Furthermore, when solving the momentum equations, the pressure difference between two grid points acting on the velocity in between is directly available.

Integrating Eq. (2.3) over the control volume drawn in Figure 2.2 yields, for axisymmetric flows:

$$\int_0^{2\pi} \int_{x_w}^{x_e} \int_{r_s}^{r_n} \frac{\partial}{\partial x} (\rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x}) r d\theta dx dr + \int_0^{2\pi} \int_{x_w}^{x_e} \int_{r_s}^{r_n} \frac{\partial}{\partial r} (\rho v \phi - \Gamma_\phi \frac{\partial \phi}{\partial r}) r d\theta dx dr = \int_0^{2\pi} \int_{x_w}^{x_e} \int_{r_s}^{r_n} S_\phi r d\theta dx dr \quad (2.35)$$

Integration of Eq. (2.35) yields:

$$\int_{r_s}^{r_n} \{ \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \}_w^e r dr + \int_{x_w}^{x_e} \{ \rho v \phi - \Gamma_\phi \frac{\partial \phi}{\partial r} \}_s^n r dx = \int_{x_w}^{x_e} \int_{r_s}^{r_n} S_\phi r dr dx \quad (2.36)$$

where the factor 2π , appearing from integration over $d\theta$ is cancelled out in the above equation.

The first term at the left hand side of this equation may, at location x_e , be approximated by:

$$\begin{aligned} \int_{r_s}^{r_n} \left\{ \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right\}_e r dr &\approx \left\{ \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right\}_e \int_{r_s}^{r_n} r dr \\ &= \left\{ \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right\}_e A_e = J_e \end{aligned} \quad (2.37)$$

where A_e is the area of the eastern face of the control volume. At the other three cell faces the combined convective and diffusive fluxes are approximated in an analogous way. Integrating the source term in Eq. (2.35) yields:

$$\int_{x_w}^{x_e} \int_{r_s}^{r_n} r S_\phi dx dr = (S_U - S_P \phi_P) Vol. \quad (2.38)$$

Here S_ϕ is incorporated in a linearized form and is assumed to be constant inside the control volume. S_U and S_P are positive definite quantities. This formulation eventually increases the diagonal dominance of the finite volume coefficient matrix and thereby enhances numerical stability [12].

The total flux (convective plus diffusive) across the interface e , J_e , is approximated by the hybrid differencing [12], where a hybrid of ‘central difference’ scheme for low Peclet numbers (defined below) and ‘upwind difference’ scheme for high Peclet number is employed. The main advantage of this scheme is to enhance the numerical stability of the solution, and to give the correct limiting behaviour as Pe becomes large or small, at least when the flow is parallel to the mesh. It is described

as follows:

$$J_e = \begin{cases} C_e \phi_E & Pe_e < -2 \\ (D_e + \frac{1}{2}C_e)\phi_P - (D_e - \frac{1}{2}C_e)\phi_E & -2 \leq Pe_e \leq 2 \\ C_e \phi_P & Pe_e > 2 \end{cases} \quad (2.39)$$

where $C_e = (\rho u A)_e$ is the convective flux across interface e , $D_e = \Gamma_\phi A_e / (x_E - x_P)$ is the diffusive flux across interface e , and $Pe_e = C_e / D_e$ is the cell Peclet number at interface e .

Equation (2.39) may be rewritten as

$$J_e = a_{PE} \phi_P - a_E \phi_E \quad (2.40)$$

where

$$a_E = \max[-C_e, D_e - C_e/2, 0] \quad (2.41)$$

$$a_{PE} = a_E + C_e$$

The convective and diffusive fluxes across the other walls of the control volume are approximated analogously, and Eq. (2.36) may be rearranged as follows:

$$a_P \phi = a_E \phi_E + a_S \phi_S + a_W \phi_W + a_N \phi_N + \dot{S}_U \cdot Vol \quad (2.42)$$

where

$$a_P = a_E + a_S + a_W + a_N + C_e + C_s - C_w - C_n + \dot{S}_P \cdot Vol \quad (2.43)$$

Integration of the continuity equation ($\phi = 1$ in Eq. (2.3)) over the control volume yields:

$$C_e - C_w + C_s - C_n = 0 \quad (2.44)$$

and Eq. (2.43) may finally be written as

$$a_P = \sum_i a_i + S_P \cdot Vol \quad (2.45)$$

where i denotes the four neighbours of point P, namely, E, S, W, N.

The difference equations for the u and v velocity are obtained in a similar way as the ones for the scalar variable, except that the source term, S_U , contains the pressure difference between two grid points, and that the velocities in the convection terms are obtained by weighted averaging.

The difference equations for the u and v velocity are written as:

$$a_e u_e = \sum_i a_i u_i + S_U^u \cdot Vol + A_e (p_P - p_E) \quad (2.46)$$

where i denotes the neighbour points surrounding e , and

$$a_n v_n = \sum_i a_i v_i + S_U^v \cdot Vol + \frac{1}{2} (A_P + A_N) (p_P - p_N) \quad (2.47)$$

where i denotes the neighbours of n .

At the boundaries of the calculation domain, the general finite difference equations are not applicable. Hence, special measures are required for the cells next to the boundaries. In the present program, specified gradient boundary conditions are handled by setting the appropriate convection/diffusion coefficient to zero in the finite-difference equation ("breaking the link", e.g. $A_N = 0$, for cells adjacent to a north boundary; $A_S = 0$, for cells next to a south boundary), and then entering the appropriate gradient through the linearized "false" source term (Eq. (2.38)).

2.3.2 Solution Procedure

The system of algebraic difference equations, derived in Section 2.3.1, is solved in a segregated approach, i.e. each dependent variable is solved from an algebraic difference equation. The strong non-linear coupling of the equations, prohibiting simultaneous solutions, is taken into account by means of an iteration procedure.

The general finite volume equation (2.42) can be recast into the following form (see Figure 2.3)

$$a_P \phi_{i,j} = a_N \phi_{i,j+1} + a_E \phi_{i+1,j} + a_S \phi_{i,j-1} + a_W \phi_{i-1,j} + S_U \cdot Vol \quad (2.48)$$

This equation is solved by marching in the flow direction through the grid. In this sequence, the equations for the grid nodes on each grid line are assembled into a tri-diagonal matrix by temporarily assuming that values on neighbouring lines are known, as in the Gauss-Seidel method. The temporarily known values are taken from the most recently calculated values. Then Eq. (2.48) reduces to

$$\phi_j = A_j \phi_{j+1} + B_j \phi_{j-1} + C_j \quad (2.49)$$

where

$$A_j = a_N / a_P$$

$$B_j = a_S / a_P$$

$$C_j = (a_E \phi_{i+1,j} + a_W \phi_{i-1,j} + S_U \cdot Vol) / a_P$$

and the i subscript has been dropped in Eq. (2.49). If the ϕ values at the boundaries $j = 1$ and $j = M$ are known, then, for example:

$$A_1 = B_1 = 0, \quad C_1 = \phi_1 \quad (2.50)$$

Thus, Eq. (2.49) represents $(M - 2)$ equations, for which the coefficient matrix is tri-diagonal. The method of solution used here, is sometimes referred to as the Thomas algorithm [47, 48, 49] but is merely a special adaptation of the Gaussian elimination procedure, as described below.

If ϕ_j is expressed in terms of ϕ_{j+1} only,

$$\phi_j = A'_j \phi_{j+1} + C'_j \quad (2.51)$$

then Eq. (2.49) may be written as:

$$\phi_j = A_j \phi_{j+1} + B_j A'_{j-1} \phi_j + B_j C'_{j-1} + C_j \quad (2.52)$$

which after rearrangement, becomes:

$$\phi_j = \left(\frac{A_j}{1 - B_j A'_{j-1}} \right) \phi_{j+1} + \frac{B_j C'_{j-1} + C_j}{1 - B_j A'_{j-1}} \quad (2.53)$$

Comparison of the coefficients in Eqs. (2.51) and (2.53) gives the recurrence relations:

$$A'_j = \frac{A_j}{1 - B_j A'_{j-1}}, \quad C'_j = \frac{B_j C'_{j-1} + C_j}{1 - B_j A'_{j-1}} \quad (2.54)$$

Using the values for A_1, B_1 and C_1 given by Eqs. (2.50), the recurrence process is started by the values:

$$A'_1 = 0 \quad C'_1 = \phi_1 \quad (2.55)$$

and proceeds from $j = 2$ to $M - 1$

When the coefficients A'_j and C'_j are known for the line, the values of ϕ_j are determined from Eq. (2.51).

This process is carried out for each value of i in turn by starting at the line adjacent to one boundary ($i = 2$) and marching through the field to the line adjacent to the opposite boundary ($i = N - 1$).

Since the pressure field is not known a priori, it must be computed by an iterative 'guess and correct' procedure. Because the momentum equations are solved for a guessed pressure field, the calculated velocity components satisfy these, but do not, in general, satisfy the local mass balance. To overcome this difficulty, the SIMPLE algorithm developed by Patankar [12] is adopted, in which mass conservation is ensured through the solution of a special 'pressure correction' equation. Its main features are given below.

First, the pressure field p^* is guessed, and the momentum equations may then be solved by the solution procedure discussed earlier to yield corresponding values of u^* and v^* . The resulting set of 'incorrect' values (p^* , u^* and v^*) requires the imposition of some corrections (primed values: p' , u' and v'), as defined in the following:

$$p = p^* + p' \quad (2.56)$$

Then, the velocity corrections are assumed to depend upon pressure correction changes and are given, for example, by

$$u_e = u_e^* + u_e' \quad u_e' = D_e(p_P' - p_E') \quad (2.57)$$

where D_e is determined from the u -momentum equation (2.46) and its associated source terms to give

$$D_e = \frac{\partial u_p}{\partial (p_P - p_E)} \approx \frac{A_e}{a_p^u} \quad (2.58)$$

Substitution of ρ , u_e , etc. into the finite volume mass conservation equation (2.42) yields

$$a_P p_P' = \sum_i a_i p_i' + S_U^p \quad (2.59)$$

where the summation convection $\sum_i$ is over the four neighbours N, W, S, E; S_U^p is the mass imbalance over the cell.

$$S_U^p = m_w^* - m_e^* + m_s^* - m_n^* \quad (2.60)$$

$$a_P = \sum_i a_i \quad (2.61)$$

$$a_E = (\rho A)_e D_e \text{ etc.} \quad (2.62)$$

Besides the SIMPLE algorithm, a line continuity correction method [15] is incorporated in the program. This procedure adjusts the u velocity and pressure field to ensure that at every grid line overall continuity is satisfied.

The solution procedure can be summarized as:

1. initialize or guess the fields of all variables (scalar, velocity)
2. solve the momentum equations to obtain velocities u^*, v^* .
3. correct u and p to satisfy overall continuity by means of the line continuity method.
4. solve the p' equation and adjust p from the equation $p = p^* + \alpha_p p'$, where α_p is a relaxation factor which is usually assigned a value between 0.5 and 0.8.
5. correct u and v to satisfy cell-continuity using the Eqs. (2.57).
6. calculate other variables (h, k, c , etc.)
7. treat the corrected pressure, p , as a new guessed pressure p^* , return to step 2, and repeat the whole procedure until a converged solution is obtained.

During the above iterative process, convergence is assessed at the end of each outer iteration on the basis of the 'Residual-Source' criterion, which compares the residual sources of each finite difference equation with a reference value $R_{\phi,ref}$, which is typically the flux of the dependent variable ϕ applied at the boundary of the domain of calculation, e.g. the total inlet mass flow and momentum.

Referring to the general finite difference equation (Eq. 2.42), the local residual of the ϕ -equation at the j' th iteration is defined as

$$R_{\phi} = \sum_i a_i \phi_i + S_U^{\phi} \cdot Vol - a_P \phi_P \quad (2.63)$$

The solution is assumed to have converged when the sum of the normalized absolute residuals has fallen below a specified level λ , typically 10^{-3} , i.e.

$$\sum_{field} |R_{\phi}| < \lambda R_{\phi,ref} \quad (2.64)$$

The advantage of this practice is to ensure the finite difference equations are properly solved.

Since the equations involved are strongly non-linear, under-relaxation is necessary to control stability and convergence. This process is introduced into the iterative solution of the general finite difference equation (Eq. 2.42) as follows:

$$\phi_P^R = f \phi_P^j + (1 - f) \phi_P^{j-1} \quad (2.65)$$

where the superscript j denotes the j' th iteration and f is the under-relaxation factor in the range $0 < f \leq 1$. On substitution of Eq. (2.65) into Eq. (2.42), we obtain

$$\frac{a_P}{f} [\phi_P^R - (1 - f) \phi_P^{j-1}] = \sum_i a_i \phi_i + S_U^{\phi} \cdot Vol \quad (2.66)$$

There are no general rules for choosing the best values of f . The optimum value depends upon a number of factors, such as the nature of the problem, the number of grid points, the grid spacing, and the iterative procedure used. In this program, the values are found by experience and from exploratory computations of the given problem.

Chapter 3

Combustion Modeling

3.1 Introduction

The modeling of turbulent flows with combustion is a difficult task. First of all the number of species and reactions involved in even a simple combustion process, as for instance the formation of water, is large. This may be due to the occurrence of all sorts of intermediate species such as radicals which play a crucial role in the formation of water. At every grid point in the flow field a large system of strongly coupled equations has to be solved to describe the formation of water in detail. When the species include complex hydrocarbons, the number of species and reactions involved becomes tremendously large requiring an excessive amount of computing time. Secondly, in turbulent reacting flows, turbulent fluctuations influence the combustion process, and vice-versa. This strong turbulence-chemistry interaction is often extremely complicated and not well understood.

In addition, the chemical production/destruction rate R_k , in general, is a highly

nonlinear function of temperature and species concentrations, but knowledge of the values of these latter quantities is insufficient to allow the evaluation of R_k . Also the importance of fluctuations of these quantities in turbulent flows must be represented in the evaluation of R_k , which requires the modeling of a large number of terms containing products of fluctuating variables. For hydrocarbon fuels, the evaluation of R_k becomes even more difficult because knowledge of the detailed kinetics is very limited.

For the above reasons, obtaining a complete and detailed description of the flow and combustion processes is impossible. Even if it were technically desirable and computationally possible to include all these species and reactions within the framework of a calculation, such a prediction procedure, without care, would very quickly become too expensive for engineering use. In order to achieve an acceptable balance between economy and accuracy, one has to make some carefully chosen assumptions and simplifications. Before discussing these assumptions and simplifications it is perhaps a good thing first to look at some physics of turbulent combustion.

Turbulent flows usually contain a spectrum of vortex (eddy) sizes: the largest is of the order of a characteristic flow dimension, the smallest is only two or three orders of magnitude larger than the molecular free path length. The large vortices are the 'youngest' and their energy is primarily derived from the mean rate of strain in the main flow. Later the vortices are stretched by viscous interaction between them in the following way. As turbulence is three-dimensional, there is a tendency for vortices to be stretched along their axes by the relative motion of neighbouring vortices, whose axes are not parallel to that of the one being stretched. The stretching

process is repetitive and is continuously producing new generations of smaller and faster eddies; their rotational speeds increase because of the conservation of angular momentum. Eventually, vortices become so small that their identities are destroyed by molecular diffusion. This 'cascade' process is controlled by the large time scales of the large motions [50].

For the turbulence-chemistry interaction, molecular mixing occurs across the interface of the smallest eddies, because the eddies have the greatest specific surface area and the stretching process augments the concentration gradients. Therefore, species mix at the microscale level to allow combustion [50].

Since the smallest eddies are in equilibrium, being eliminated as rapidly as they are formed from larger vortices, the eddy decay time can be characterized by the time scale of large vortices. For non-premixed combustion, fuel and oxidant are initially contained in separate eddies and mixing can occur only after a period equal to the eddy lifetime. For typical engineering application, eddy lifetimes are long and might be equal to 0.1 s. However, the time scale for overall chemical reaction is of the order of a millisecond at most. Therefore most turbulent combustion processes are controlled by mixing, rather than by chemical kinetics [50].

Because of the above considerations, two combustion models were selected to be incorporated in the computer program. Both models are based on the assumption of fast chemistry (or infinite reaction rate chemistry), where chemical kinetic rate is considered to be much faster than rate of mixing. The approaches used here take no explicit account of chemical kinetics and only relate to combustion situations that are entirely mixing controlled. But it allows for a reasonably accurate descrip-

tion of many other combustion features, including field of species concentration and flame position. However, the assumption is not appropriate for the prediction of the formation and emission of pollutants such as carbon monoxide (CO) and nitrogen oxides (NO_x). Because of the single-step irreversible reaction assumption, the models do not take dissociation into account, and temperatures in the high temperature region will be overpredicted. Another disadvantage of the diffusion flame model compared to the finite chemical kinetics model is that due to the infinite reaction rate assumption, phenomena such as ignition or extinction cannot be investigated. However, the diffusion flame models have their own advantage, i.e. simplicity.

The first model, the diffusion flame model, does not take into account the effect of turbulence on combustion, while with the second model, the turbulent diffusion flame model, this effect is included by weighting the mass fractions with a beta Probability Density Function. The aim of investigating two combustion models is to be able to compare the results of both models, their accuracy and required computing time, and thus make the DRAGON code more flexible.

3.2 The Diffusion Flame Model

As mentioned above, the main assumption of the diffusion flame concept is that the chemical reaction between fuel and oxidizer is a single-step, irreversible and infinitely fast reaction. This implies that fuel and oxidizer cannot exist together at the same time and at the same place. As soon as the fuel and the oxidizer get together in the combustion chamber, reactions will occur. Since fuel and oxidizer are fed separately

into the combustion chamber, combustion will take place only at the interface of the two streams, and thus the reaction flame is considered to be nonpremixed, steady, and of zero thickness, i.e. a diffusion flame. The reacting solid surface is assumed energetically homogeneous (i.e. gas-solid interface effects are neglected). The whole reaction is diffusion controlled.

Since the diffusion is the controlling mechanism, the need to evaluate the mean chemical production or destruction rate of the species is thereby removed. With reasonable accuracy, the reacting fluid is treated as a continuum with equal mass diffusivity (Γ_j) properties for species. The species concentration and thermochemical variables, such as the density and temperature, can be related to one conserved scalar if the combustion process is adiabatic, as will be discussed below.

Consider the one-step irreversible reaction in which 1 kg of fuel combines with r kg of oxidant to form $(1 + r)$ kg of product without intermediaries.

where r is the fixed stoichiometric ratio, defined as the mass ratio of oxidant to fuel. Here the products of combustion are treated as a single species.

Conservation of chemical species can be written for each specie in the above reaction. In particular, the mass conservation of fuel and oxidizer are expressed as:

$$\frac{\partial}{\partial x}(\rho u m_{fu}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v m_{fu}) - \frac{\partial}{\partial x}(\Gamma_{fu} \frac{\partial m_{fu}}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_{fu} \frac{\partial m_{fu}}{\partial r}) = R_{fu} \quad (3.2)$$

$$\frac{\partial}{\partial x}(\rho u m_{ox}) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v m_{ox}) - \frac{\partial}{\partial x}(\Gamma_{ox} \frac{\partial m_{ox}}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_{ox} \frac{\partial m_{ox}}{\partial r}) = R_{ox} \quad (3.3)$$

where R_{fu} and R_{ox} are the reaction rates per unit volumes and m is a mass fraction. For the one-step reaction described above, the reaction rates of fuel (R_{fu}) and

oxidizer (R_{ox}) are related by:

$$R_{fu} = R_{ox}/r$$

The R terms can be eliminated from Eqs. (3.2) and (3.3) by dividing Eq. (3.3) by r and subtracting the resultant equation from Eq. (3.2):

$$\begin{aligned} \frac{\partial}{\partial x} [\rho u (m_{fu} - m_{ox}/r)] + \frac{1}{r} \frac{\partial}{\partial r} [\rho r v (m_{fu} - m_{ox}/r)] - \frac{\partial}{\partial x} [\Gamma_{eff} \frac{\partial}{\partial x} (m_{fu} - m_{ox}/r)] \\ - \frac{1}{r} \frac{\partial}{\partial r} [r \Gamma_{eff} \frac{\partial}{\partial r} (m_{fu} - m_{ox}/r)] = 0 \end{aligned} \quad (3.4)$$

where $\Gamma_{eff} = \Gamma_{fu} = \Gamma_{ox}$.

In this equation no source term is present anymore and therefore

$$\phi_{fo} = m_{fu} - m_{ox}/r \quad (3.5)$$

is a conserved scalar. Analogously, other conserved scalars may be constructed, for instance

$$\phi_{fp} = m_{fu} + m_{pr}/(1+r) \quad (3.6)$$

$$\phi_{op} = m_{ox}/r + m_{pr}/(1+r) \quad (3.7)$$

These are conserved scalars of the Shvab-Zeldovich type [51]. Using the assumption that fuel and oxidizer cannot exist together, one can distinguish three different situations in the flow field, depending on the value of ϕ_{fo} :

1.	$\phi_{fo} > 0,$	$m_{ox} = 0,$	$m_{fu} = \phi_{fo}$	
2.	$\phi_{fo} < 0,$	$m_{ox} = -r \phi_{fo},$	$m_{fu} = 0$	(3.8)
3.	$\phi_{fo} = 0,$	$m_{ox} = 0,$	$m_{fu} = 0$	

Situation 1 is called a fuel-rich mixture, situation 2 a fuel-lean mixture and situation 3 stoichiometric condition. The last situation occurs at the location of

the flame sheet, where the combustion is complete and only reaction products are present.

If fuel and oxidizer are fed separately into the combustion chamber, and if only two feeds are present, it is more convenient to use the dimensionless mixture f as a conserved scalar, because it gives a good physical interpretation of the mixing of the two feeds. This mixture fraction is defined as

$$f = \frac{\phi_{fo} - \phi_{fo,2}}{\phi_{fo,1} - \phi_{fo,2}} \quad (3.9)$$

where $\phi_{fo,1}$ and $\phi_{fo,2}$ are the values of ϕ_{fo} in fuel and oxidizer feeds respectively, see Figure 3.1. Since the mixture fraction is formed from a linear combination of the conserved variables, it is a conserved variable as well.

In feed 1, ϕ_{fo} equals $\phi_{fo,1}$ and f equals one, while in feed 2, ϕ_{fo} equals $\phi_{fo,2}$, yielding f equal to zero. Therefore f may be interpreted as a measure of mixing of the two different feeds. Substitution of Eq. (3.5) into the f equation, Eq. (3.9), yields

$$f = \frac{(r m_{fu} - m_{ox}) + m_{ox,2}}{r m_{fu,1} + m_{ox,2}} \quad (3.10)$$

At stoichiometric conditions ($r m_{fu} - m_{ox} = 0$) the mixture fraction becomes

$$f_{st} = \frac{m_{ox,2}}{r m_{fu,1} + m_{ox,2}} \quad (3.11)$$

As it has been mentioned before, the location where $f = f_{st}$ corresponds with the location of the flame sheet. At this location neither fuel nor oxidizer are present and combustion is complete. Besides, both the maximum flow temperature and a reduction in local flow density can occur. From Eq. (3.11) it can be seen that the

stoichiometric mixture fraction is fixed for a given reaction, only depending upon the values of m_{fu} and m_{ox} in the fuel and oxidizer streams.

The differential equation for conservation of species can be expressed in terms of f

$$\frac{\partial}{\partial x}(\rho u f) + \frac{1}{r} \frac{\partial}{\partial r}(\rho r v f) - \frac{\partial}{\partial x}\left(\frac{\mu}{\sigma_l} \frac{\partial f}{\partial x}\right) - \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\mu}{\sigma_l} \frac{\partial f}{\partial r}\right) = 0 \quad (3.12)$$

After Favre-averaging, the equation is written as

$$\frac{\partial}{\partial x}(\bar{\rho} \tilde{u} \tilde{f}) + \frac{1}{r} \frac{\partial}{\partial r}(\bar{\rho} r \tilde{v} \tilde{f}) - \frac{\partial}{\partial x}(\Gamma_f \frac{\partial \tilde{f}}{\partial x}) - \frac{1}{r} \frac{\partial}{\partial r}(r \Gamma_f \frac{\partial \tilde{f}}{\partial r}) = 0 \quad (3.13)$$

where Γ_f is taken as

$$\Gamma_f = \frac{\mu}{\sigma_l} + \frac{\mu_t}{\sigma_t} \quad (3.14)$$

and $\sigma_t = \sigma_l = 0.7$. This equation will be solved numerically to obtain the value of the mixture fraction at each point in the flow field. From the mixture fraction it is possible to determine the mixture composition and thermochemical states as follows.

From Eq. (3.11) the value of f_{st} is calculated. If the local value of f at a grid point is less than the stoichiometric value of f , it is a fuel-lean mixture and $m_{fu} = 0$; and if it is larger than f_{st} , then it is a fuel-rich mixture and $m_{ox} = 0$, see Figure 3.2.

The relations between the mixture fractions and mass fractions can be deduced from Eq. (3.10) and given as follows:

$$\begin{aligned} 0 \leq f \leq f_{st} : \quad & m_{fu} = 0, \quad m_{ox} = r m_c (f_{st} - f) \\ f_{st} < f \leq 1 : \quad & m_{ox} = 0, \quad m_{fu} = m_c (f - f_{st}) \end{aligned} \quad (3.15)$$

where $m_c = m_{fu,1} + m_{ox,2}/r$.

In many practical situation, inert or non-reacting species are present in either the fuel stream or the oxidizer stream or both. Because these species do not react, the mass fractions of these species are also conserved scalars. In this program, nitrogen is selected as the non-reacting specie for the calculation. From the definition of the mixture fraction,

$$f = \frac{m_n - m_{n,2}}{m_{n,1} - m_{n,2}} \quad (3.16)$$

then the mass fraction of nitrogen can be calculated from

$$m_n = f m_{n,1} + (1 - f) m_{n,2} \quad (3.17)$$

where $m_{n,1}$ is the mass fraction of nitrogen in the fuel stream and $m_{n,2}$ is the mass fraction of nitrogen in the oxidizer stream.

Finally, since the sum of the mass fractions in the flow field must be equal to unity, the mass fraction of the product can be obtained from the equation below.

$$m_{pr} = 1 - m_{ox} - m_{fu} - m_n \quad (3.18)$$

In this program, the chemical reaction between ethylene and oxygen is chosen for the simulation of the combustion process in the SFRJ.

The mass fractions of CO_2 and H_2O may be determined from the product mass fraction m_{pr} .

$$m_{CO_2} = \frac{M_{CO_2}}{M_{CO_2} + M_{H_2O}} m_{pr} = \frac{44}{44 + 18} m_{pr} = 0.7097 m_{pr} \quad (3.20)$$

$$m_{H_2O} = \frac{M_{H_2O}}{M_{CO_2} + M_{H_2O}} m_{pr} = \frac{18}{44 + 18} m_{pr} = 0.2903 m_{pr} \quad (3.21)$$

where M_{CO_2} and M_{H_2O} are the molecular weights of CO_2 and H_2O .

The boundary conditions for the partial differential equation for the mixture fraction, Eq. (3.14), are given in the following. At the inlet only the oxidizer stream is present and $f = 0$. The mass fractions of oxygen and nitrogen are prescribed to be 0.231, 0.769, respectively. At the solid wall $f = 1$ since only fuel is present, and no oxygen and nitrogen exist ($m_{ox} = m_n = 0$). At the centreline and outlet a non-gradient condition is applied.

The regression rate on the fuel wall varies as a function of position along the wall and is modeled as follows

$$r = \frac{q_{wall}}{\rho_{wall} h_v} \quad (3.22)$$

where q_{wall} is the local heat flux from the main flow to the wall and h_v is the effective heat of gasification, which is defined as the amount of heat required to pyrolyze 1 kg of fuel. Values found for h_v in the literature range from 1.7 to 6.0 MJ/kg and depend on the heat transfer mechanism. For convective heat transfer, values between 4.0 and 5.5 MJ/kg are often found for PE [52]. The density ρ_{wall} is taken to be 950 kg/m³ for PE.

In order to simulate the blowing fuel at the solid wall, the injection velocity must be properly modeled. This injection generates a flux of enthalpy and a flux of mass from the wall to the flow, and thus indirectly a flux of mixture fraction. From the wall to the near wall cell only convective flux is changed because only convection of fuel is taken into account. The diffusive flux at the wall remains zero, because if there would be a diffusive flux of mass fraction of a certain species from the wall to the flow, inherently there should also be a diffusive flux of mass fraction of another

species from the flow into the wall, the latter being impossible. Based on the above consideration and the mass balance at the interface (see Figure 3.3), the injection velocity can be calculated below.

$$v_w = \frac{\rho_w r}{\rho_f} \quad (3.23)$$

where r is the regression rate and ρ_w the density of solid fuel (PE). ρ_f is the density of the flow immediately adjacent to the wall.

Because there is only a convective flux at the wall in the near wall cell, which can be added to the coefficient of the differential equation, no source term is necessarily added to the equation. Thus f remains a conserved scalar. The differential equation for the mixture fraction is solved in a way analogous to the method described in Chapter 2.

3.3 Turbulent Diffusion Flame Model

A great disadvantage of the diffusion flame combustion model, as discussed in Section 3.2, is the fact that the influence of turbulence on combustion is neglected. Thus in the model, mass fractions are directly related to the mean value of the mixture fraction and turbulence does not affect the mass fraction directly, which is not true in turbulent flows, realistically. But in the turbulent diffusion flame model the effect of turbulence on the mass fraction distributions of fuel, oxidizer and products is taken into account by relating the fluctuation in mixture fraction to fluctuations in mass fractions. Since time-averaged mass fraction distributions of fuel, oxidizer and products are now used, instead of the instantaneous distributions, fuel and oxidizer

can exist together at the same location (but not at the same time). This results in a thicker flame zone compared to the non-averaged situation. The distribution of mass fraction will be like the profiles in Figure 3.4. As it is clearly shown in the figure, at stoichiometric conditions the amount of products formed with the turbulent diffusion flame model will be less than that with the diffusion flame model. So less heat is released from the reaction, resulting in a lower temperature.

The most convenient way of coupling turbulence to combustion to include the influence of turbulence on combustion is by means of a Probability Density Function (P.D.F) for the mixture fraction, which is explained as follows.

For instance, there is a variable $\phi(t, x)$ fluctuating with time at a fixed point x . The probability that the value of $\phi(t, x)$ at that point lies in the range from $\phi(x)$ to $\phi(x) + d\phi$ is given by $P(\phi)d\phi$, where $P(\phi)$ is called the Probability Density Function. It is obvious that the probability that ϕ lies between $-\infty$ and $+\infty$ is 1. To weight an arbitrary variable $\phi(f)$, which is a function of the mixture fraction f , a Probability Density Function $P(f)$ will be used

$$\phi = \int_0^1 \phi(f)P(f)df \quad (3.24)$$

Because of $0 \leq f \leq 1$, it follows that $P(f)$ must satisfy the following constraints:

$$P(f) = 0 \quad f < 0, f > 1 \quad (3.25)$$

$$P(f) \geq 0 \quad 0 \leq f \leq 1 \quad (3.26)$$

About the simplest and the most popular approach is to specify a two-parameter form of the Probability Density Function in terms of the mean and the variance of

the mixture fraction f . This variance g is defined as

$$g = \overline{f'^2} = \overline{(f - \bar{f})^2} \quad (3.27)$$

and is obtained by solving a transport equation for g [10, 11].

$$\begin{aligned} \frac{\partial}{\partial x}(\bar{\rho} \bar{u} g) + \frac{1}{r} \frac{\partial}{\partial r}(r \bar{\rho} \bar{v} g) - \frac{\partial}{\partial x} \left(\frac{\mu_{eff}}{\sigma_g} \frac{\partial g}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \mu_{eff}}{\sigma_g} \frac{\partial g}{\partial r} \right) = \\ C_{g1} \mu_t \frac{\partial \bar{f}}{\partial x} \frac{\partial \bar{f}}{\partial x} + C_{g1} \mu_t \frac{\partial \bar{f}}{\partial r} \frac{\partial \bar{f}}{\partial r} - C_{g2} \bar{\rho} \frac{\epsilon}{\bar{k}} g \end{aligned} \quad (3.28)$$

where $\sigma_g (= 1.0)$ is the Schmidt number; $C_{g1} (= 2.8)$ is the production constant; $C_{g2} (= 2.0)$ is the dissipation constant; $\bar{k}$ is the turbulence kinetic energy, and ϵ is the dissipation rate of turbulence kinetic energy. Eq. (3.28) is obtained by multiplying the equation for the instantaneous mixture fraction with f , followed by Favre-decomposition and averaging of the resulting equation. The last three terms in the right hand side of the equation represent production and dissipation of g , respectively.

As mentioned before, the mass fractions of oxidizer, fuel and products will be weighted with a Probability Density Function to include the influence of turbulence on combustion. Usually, there are two ways that can be used to obtain a P.D.F. The first is to solve a transport equation for it. However, the Favre-averaged form of such equation contains a lot of terms of correlations of fluctuating variables which are hard to model, and a lot of assumptions have to be made to allow for the solution of this equation. Therefore solving a transport equation for the Probability Density Function is not used here. The second method to obtain a P.D.F. for the mixture fraction is to prescribe its shape. The exact value of the probability

of mass fraction at a certain location in the flow field only depends on the mean mixture fraction f and its variance g . Elands in his report [11] discussed three shapes of Probability Density Functions often used in the calculation of reacting turbulent flows, i.e. two delta function, clipped Gaussian PDF, and β Probability Density Function. He concluded that the beta Probability Density Function has a continuous distribution, without delta functions at $f = 0$ and at $f = 1$, and is believed to be realistic, compared to the results of the experiments [61]. Jones [61] presented results of the calculation of a turbulent diffusion flame, using the those shapes described above. He concluded that the double delta function approach was unsuitable because it generated temperature profiles with two maxima. For flows with non-premixed reactants, only one temperature maximum occurs at the location where fuel and oxidizer are burnt in their stoichiometric ratio. The double delta function, therefore, produced unphysical results. The calculations using the clipped Gaussian and β Probability Density Function did not show large differences, and Jones recommends the latter to be used in calculations. Based on the discussion, the beta PDF approach is adopted in the current combustion model.

The beta Probability Density Function is defined as

$$P(f) = \frac{f^{a-1}(1-f)^{b-1}}{\int_0^1 f^{a-1}(1-f)^{b-1} df} \quad 0 \leq f \leq 1 \quad (3.29)$$

where

$$a = \hat{f} \left(\frac{\hat{f}(1-\hat{f})}{g} - 1 \right) \quad (3.30)$$

$$b = (1-\hat{f}) \left(\frac{\hat{f}(1-\hat{f})}{g} - 1 \right) \quad (3.31)$$

The shape of this Probability Density Function is shown in Figure 3.5. The denominator of the beta P.D.F. is a normalization factor to satisfy the constraint that

$$\int_0^1 P(f)df = 1 \quad (3.32)$$

and it can be calculated separately.

The mass fractions of oxidizer, fuel and products are weighted with the P.D.F. This yields for the mass fraction of fuel

$$\dot{m}_{fu} = \int_0^1 m_{fu}(f) P(f) df \quad (3.33)$$

where $m_{fu}(f)$ is given by Eq. (3.15)

$$\begin{aligned} m_{fu}(f) &= m_c(f - f_{st}) & f_{st} < f \leq 1 \\ m_{fu}(f) &= 0 & 0 \leq f \leq f_{st} \end{aligned} \quad (3.34)$$

and $m_c = m_{fu,1} + m_{ox,2}/r$. Substitution of Eq. (3.34) into Eq. (3.33) yields

$$\dot{m}_{fu} = \int_{f_{st}}^1 m_c(f - f_{st})P(f)df \quad (3.35)$$

For oxidizer it follows analogously

$$\dot{m}_{ox} = r m_c \int_0^{f_{st}} (f_{st} - f)P(f)df \quad (3.36)$$

Inert species are conserved scalars so the distribution of inert species is analogous to that of the mixture fraction f . So the mass fraction of nitrogen is found from

$$\dot{m}_n = m_{n,1}\tilde{f} + m_{n,2}(1 - \tilde{f}) \quad (3.37)$$

and the mass fraction of the product is obtained below

$$\dot{m}_{pr} = 1 - \dot{m}_{ox} - \dot{m}_{fu} - \dot{m}_n \quad (3.38)$$

After substituting the beta Probability Density Function into the Eq. (3.35), Eq. (3.35) can be rewritten as

$$\dot{m}_{fu} = m_c(\tilde{f} - f_{st}) + m_c \cdot \frac{c}{a} (1 - f_{st})^{b-1} f_{st}^{a+1} - m_c \cdot c \int_0^{f_{st}} [f^a (1 - f)^{b-1} - f_{st} \frac{(b-1)}{a} f^a (1 - f)^{b-2}] df \quad (3.39)$$

where

$$c = \frac{1}{\int_0^1 f^{a-1} (1 - f)^{b-1} df} \quad (3.40)$$

Analogously, the mass fraction of oxidizer is found from

$$\dot{m}_{ox} = r \cdot m_c \cdot \frac{c}{a} (1 - f_{st})^{b-1} f_{st}^{a+1} - r \cdot m_c \cdot c \int_0^{f_{st}} [f^a (1 - f)^{b-1} - f_{st} \frac{(b-1)}{a} f^a (1 - f)^{b-2}] df \quad (3.41)$$

The integral in Eqs. (3.39) and (3.41)

$$\int_0^{f_{st}} [f^a (1 - f)^{b-1} - f_{st} \frac{(b-1)}{a} f^a (1 - f)^{b-2}] df \quad (3.42)$$

can only be solved if $a > 0$. From Eq. (3.30) it follows the constraint that

$$\tilde{f}(1 - \tilde{f}) \geq g \quad (3.43)$$

This also implies $b \geq 0$. In the program, the integral is solved with a Simpson approach.

Eq. (3.42) cannot be solved analytically and is therefore solved numerically. The constant ‘c’, Eq. (3.40), whose inverse is the so called beta function, is calculated using gamma functions. By definition, a beta function can be written as a product of gamma function

$$\int_0^1 t^{x-1} (1 - t)^{y-1} dt = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x + y)} \quad (3.44)$$

In the present code, it is solved by a couple of special function routines developed by Fullerton in LOS ALAMOS scientific laboratory, and which are resident in the SLATEC mathematical library of the APOLLO system of the Department of Mechanical & Aerospace Engineering at Carleton University.

The boundary conditions for the variance of the mixture fraction are $g = 1 \times 10^{-4}$ at the inlet, while at the centreline and at the outlet a non-gradient condition is specified. At the solid fuel wall g is zero because $f = 1$ by definition.

At the solid wall another boundary condition is specified for the gradient of f in radial direction. In the production term of the variance equation

$$C_{g1} \cdot \mu_{eff} \cdot \left(\frac{\partial f}{\partial x} \frac{\partial f}{\partial x} + \frac{\partial f}{\partial r} \frac{\partial f}{\partial r} \right) \quad (3.45)$$

the gradient of f in the axial direction will be relatively small but the gradient of f in radial direction will be very large, due to the fact that at the south wall $f = 1$ by definition. This results in unrealistically large values of g near solid walls [10, 11]. To obtain a more realistic value for $\frac{\partial f}{\partial r}$ in the near wall cell, the gradient $\frac{\partial f}{\partial r}$ is approximated by using f at the near wall cell southern boundary and f at the near wall cell centre instead of f at the near wall cell northern boundary, see Figure 3.6.

The other differential equations and boundary conditions are the same as those in the diffusion flame model. The calculations will be described in more detail in the following chapters.

Chapter 4

Description of the Code

The purpose of this chapter is to describe the capabilities, principles of organization and structure of the DRAGON code. Also included is a description of the structure and function of the individual subroutines.

4.1 Range of Applicability

The base of the DRAGON code is the CHAMPION code, which was first developed along with PHOENICS in 1975 by Spalding et al [53]. Compared with early TEACH code series [13] then, the PHOENICS/CHAMPION series are more economical and require less computer storage and time, especially when the flow pattern is a simple one [15]. The PHOENICS/CHAMPION codes series are similar in structure, but the PHOENICS codes are oriented towards particular industrial applications, often complex ones, embodying commercially classified information; whereas the CHAMPION codes are intended for simpler, educational uses. The present code is an adaptation of CHAMPION 2/E/FIX [15].

The DRAGON code is a general program for calculating two dimensional, steady, turbulent, combusting, compressible and recirculating flows inside complex domains in either Cartesian or Cylindrical coordinates. The spacing of the computation grid may be arbitrarily specified as uniform or non-uniform. The standard version of the DRAGON code embodies subroutines for solving the Navier-Stokes equations and the $k - \epsilon$ equations, and for combusting flows, additional equations of chemical species and energy are added. The modular structure allows further variables to be added with ease. In the same vein, variables may be suppressed with similar ease. The programming language used is Fortran 77, and the code may be run on various computers including APOLLO-4000 and SUN workstations. (There are a few machine-dependent constants which may need to be chosen for solving turbulent combusting flows. These are identified in the code.)

4.2 Organization of the Computer Code

4.2.1 Overall Organization

Figure 4.1 illustrates the organization of the code by means of a flow chart. It shows how the code is structured in four main blocks of subroutines or subroutine fragments: PRBLM, MAIN, COMP and PHYS, which is also the standard PHOENICS pattern. Overall control of the program is exerted by the main routine MAIN which performs the initial and final operations, and also controls the iteration. Within the MAIN, twelve chapters with prescribed functions are divided. The first five are preliminary chapters, concerned with setting the code up for the particular problem;

the remainder are concerned with controlling the making of a forward step of the marching integration. In detail, a forward step is handled by the following chapters in MAIN:

- 6, which determines the step size;
- 7, which handles boundary conditions;
- 8, which makes the step;
- 9, which completes it, with the supply of auxiliary information; and
- 10, which makes such adjustments as are needed to satisfy continuity and other considerations.

Each chapter may call upon other subroutines to assist in the performance of its function. Subroutines on the left-hand side of the flow chart (under PRBLM) are invoked for the supply of problem-dependent information; those on the right of MAIN in the diagram (under COMP) are concerned with performing computational function, for example, setting up coefficients of finite-difference equations, and solving these equations. The COMP group of subroutines may, in general, call upon the PHYS group, to its right, for assistance with material of a physical model character; for example, the source terms in the turbulence model equations are grouped under PHYS.

4.2.2 The Computational Grid System

As stated in the earlier chapter, a staggered grid is used in the present code. Figure 4.2 illustrates the grid system. The domain of calculation is the entire rectangular region (or cylindrical sector region) bounded by

$$1 \leq IX \leq NX, \quad 1 \leq IY \leq NY$$

where NX , NY are the total number of lines of respectively constant x , y , in Cartesian coordinates, or of respectively constant x , r in cylindrical coordinates. In Figure 4.2, grid lines are drawn as solid lines. Grid nodes are the intersections of grid lines, and denoted by dots. These are stored values of all variables other than U and V , for example: p , h , concentrations, k , ϵ , ρ , μ , etc. U -nodes are indicated by arrows pointing in the x -direction; V -nodes are indicated by arrows pointing in the y -direction. All nodes within the L-shaped envelope have the same IX and IY values. The three types of cells (U -, V - and grid node-cells) are also shown in Figure 4.3. Dashed lines, drawn midway between grid lines except at grid edges, indicate control volume boundaries for variables other than U and V . A few of these control volumes are shaded by inclined lines. Control volumes for U -nodes, the U -cells, are formed by vertical grid-lines and horizontal dashed lines, as shown shaded by horizontal lines. Control volumes for V -nodes, the V -cells, are formed by horizontal grid-lines and vertical dashed lines, as shown shaded by vertical lines. U -cells touching the vertical grid edges have three grid lines passing through them, while V -cells touching the horizontal grid edges have one grid line and two vertical dashed lines surrounding them.

Since the general transport equation (Eq. 2.3) in cylindrical coordinates is similar to the one in Cartesian coordinates, the code DRAGON is made valid for either coordinate system. The coordinate system can be easily chosen by setting a flag, namely KRAD (=1 for Cartesian, =2 for cylindrical).

4.2.3 Description of Subroutines

The purpose of this section is to give a brief description of the functions of the various subroutines.

MAIN Routine

Chapter 1 — Preliminaries

This is a problem-dependent chapter.

Chapter 2 — Grid

This chapter is traversed once only. The size of the grid is specified by NX and NY in BLOCK DATA. Quantities related to NX and NY are computed by CONST2. The grid coordinates can be either specified in BLOCK DATA or computed in this chapter. From the grid size and grid-line coordinates, other geometrical data are generated by GEOM. The grid-specification section is highly problem-dependent.

Chapter 3 — Variables

This is a problem-dependent chapter, and it is traversed once only. Its function is to provide variable-related information. All variables are stored in a one-dimensional array F() in order to save storage. The block position of all the variables in the F-array has been decided through the assigning of values to JU, JV, etc in BLOCK

DATA. Here this information is used to generate, by calling CONST3, the arrays IEW(JPHI), IZERO(JPHI), ILAST(JPHI), etc. All the storage of the TITLE array has been dimensioned in BLOCK DATA. Those, which are to be used later, are reassigned in CONST3.

Chapter 4 — Property Data

This is a problem-dependent chapter and is traversed once only. The function of the chapter is to supply all initial property data not available from BLOCK DATA. In the present arrangement, the effective Prandtl/Schmidt numbers are appropriately expressed in terms of the laminar and turbulent values in the first section; the reference values are put into the main-property arrays in the second section, and the cell-wall-value arrays in the third. Updating of the property values during the iteration is carried out in Chapter 9.

Chapter 5 — Starting Preparations

This is a problem-dependent chapter. The part (before statement 50) is traversed once only. Its function is to put starting values, where suitable, into the variable storages. The RSREF array (reference residual-source values used to normalize the residual sources for variable J) is also filled here. The rest of the chapter is concerned with preparations at the start of a new iteration sweep, and at the beginning of a new line.

Chapter 6 — Step Control

This chapter is traversed once for each line. It provides information about the line to be considered, including the IX value of the line, the limits of traverse, etc. Also calculated are quantities related to IX needed elsewhere.

Chapter 7 -- Boundary Conditions

This chapter is highly problem-dependent. It supplies, for each line for all variables, boundary conditions not requiring updating during iteration. It is activated each time a new line is considered during the first iteration. Boundary values requiring updating during iteration are handled in BOUND1.

Chapter 8 -- Advance

This updates all dependent variables except pressure, on a line. The solution of each dependent variable (if needed) is controlled by the DO-loop. The calculation of the finite-difference coefficients, the introduction of the boundary conditions and the solution of the equations are performed in that order.

Chapter 9 -- Complete

At present, this only completes preparations before moving to a new line or before starting a new iteration sweep.

Chapter 10 -- Adjust

This is a problem-dependent chapter. It provides two adjustments for mass continuity. The one is for the overall mass continuity, accomplished through subroutine OVACON. This can be carried out more than once. The other is for the cell-wise continuity, solving the pressure correction equations along the line, with the help of subroutine CELCON and other subroutines. Also included are calculations of concentrations of fuel, oxygen and products. Two chemical submodels are assembled here. For turbulent diffusion model, a group of special function-routines (BETA) are called to solve beta function. The subroutine INTEGRAL is also called here to compute the integral appearing in Eqs. (3.39) and (3.41). Fluid properties, including

density and temperature, etc, are also updated.

Chapter 11 -- Print

This chapter contains special preparations for print-out purposes. BOUND1 is called to update variable values at boundaries.

Chapter 12 -- Decide

All the decisions that have to be made at the end of a line traverse or of sweep are grouped here. They include whether to move to the next line, whether to start a new sweep, whether to print out values in field and whether to terminate the computation, etc.

Subroutine ADJUST

The subroutine ADJUST effects various adjustments to the different variables in order to enhance the rate of convergence. In the present set-up, there are two sections. Each section is defined and called by an entry name and terminated by a return statement.

ENTRY OVACON

This section adjusts the mean pressure. Its effect is to alter the relevant velocities along a line IXU to ensure the satisfaction of the overall mass continuity. But such an adjustment is only meaningful when the problem is of the fixed-flow-rate type. The mathematical basis of this procedure is as follows:

- Each U is corrected by addition of DELU.

- DELU results from the overall continuity:

$$\text{DELU} = (\text{FLOWIN} - \text{FLOWST}) / \text{SUMTRA} .$$

Where FLOWIN is the correct mass flow rate, FLOWST that from prevailing U-values and SUMTRA the summation of (DENSITY * CELL AREA).

- The pressures at locations to the right of U-values under consideration are increased by a constant value of DP, which is deduced from consideration of the momentum change:

$$\text{DP} = -\text{DELU} * (\text{FLOWIN} + \text{FLOWST}) / (\text{SECTION AREA}) .$$

- New U = OLD U + DELU.

ENTRY CELCON

The function of this section is to apply the cell-wise continuity correction (SIMPLE algorithm), through the use of P' values calculated in Chapter 10 of MAIN. Such a correction is applied after the overall-continuity correction.

BLOCK DATA

All the numerical data are specified here so as to facilitate the change of problem parameters.

Subroutine BOUND

This is a problem-dependent subroutine. It is divided into two sections by entry names.

ENTRY BOUND1

This updates the values on boundaries of the flow domain.

ENTRY BOUND2

It modifies the source terms to apply boundary conditions. It is called from various points in chapters 8, 10 and 11 of MAIN, after the dependent-variable values on a line have been updated and appropriately adjusted.

Subroutine CELPHI

This is a core subroutine. It provides cell-wall densities and viscosities for U-, V- and other cells. Cell-wall values of other quantities can also be generated if required. The whole subroutine is divided into three sections defined by entry names, one for each of the three types of cells.

ENTRY CELU

This generates cell-wall values for a column of U-cells.

ENTRY CELV

This generates cell-wall values for a column of V-cells.

ENTRY CELG

This generates cell-wall values for a column of cells around grid nodes for variables other than U and V.

Subroutine COEFF

All finite-difference coefficients are calculated here. The subroutine is divided into:

Chapter 2 For U-equations

Chapter 3 For V-equations

Chapter 4 For P' -equations

Chapter 5 For equations of other variables

Chapter 1 provides the density and viscosity values at all the cell boundaries with the help of subroutines CELU, CELV and CELG, and it also provides convective fluxes and diffusional terms for cells around grid nodes, once only for use with all variables other than U, V and P' . Use is made of the reciprocity of the fluxes through cell walls common to adjacent cells. All source terms for the equations are to be specified in the SOURCE subroutine, which is called from this subroutine.

Subroutine CONST

The subroutine is divided into three sections by entry names.

ENTRY CONST2

This calculates quantities related to NX and NY.

ENTRY CONST3

This section calculates all constants related to the variables.

ENTRY CONST5

This provides constants for Chapter 5, i.e. for starting preparations. At present, only the reference-pressure-location and the monitoring-location indices are specified here.

Subroutine GEOM

This is a core subroutine called once from Chapter 2 of MAIN. It evaluates all geometrical quantities related to the grid.

Subroutine OUTPUT

The subroutine is problem-dependent. It organizes the bulk of the print-out results. It is divided into a number of sections by entry names.

ENTRY OUTPH

This prints out headings like problem title, flow Reynolds number, pipe length, etc. It is therefore problem dependent.

ENTRY OUTPF, ENTRY OUTP3

This prints out the fields of dependent variables.

ENTRY OUTP1

This prints out the variables at a preselected node and information related to residual sources evaluated in the subroutine SOLVE prior to updating of the variables. The index controlling the calling of this section is IPRSL.

ENTRY OUTPER

This prints out information related to the residual-source values specially evaluated here for the whole field, to give a true indication of the state of convergence. The indices controlling the calling of this section are IPFRS1 and IPFRS2.

Subroutine PRINT

This is a core subroutine, which prints variable-values in the 2-D field, along with the coordinate distances of the node locations. The number of columns in the field printed out as a single block is controlled by the variable NUMCOL, which is set in BLOCK DATA.

Subroutine SOLVE

This is a core subroutine embodying the TDMA. After the coefficients of the finite-difference equations have been set up in the subroutine COEFF, and suitably modified in the BOUND2, this subroutine solves the equations. To increase efficiency, two separate sections are provided, one for use with a non-unity relaxation-factor, the other for use with a unity relaxation-factor (i.e. no under-relaxation at all). Residual sources are also calculated here if required.

Subroutine SOURCE

This is a problem-dependent subroutine. All the source terms for the equations are specified here.

Subroutine TEST

This is a core subroutine. Its main function is to print information for program testing. The TEST itself is never called; but, some or all of the seven sections there, each defined by an entry name, may be activated.

Chapter 5

Results and Discussion

A major part of this study has been the development of the computer code, as discussed so far, for a solid fuel ramjet combustor. Now the purpose of this chapter is to discuss the use of the program to predict the flowfields of SFRJ combustors. All calculations have been done with solid fuel, polyethylene (C_2H_4), which is burnt with air in the SFRJ. To check the validity of the numerical predictions, both the diffusion flame model and the turbulent diffusion model have been tested against some experimental results, by carrying out several calculations. However, main attention has been given to comparison of the two combustion models.

5.1 Results from the Diffusion Flame Model

Table 5.1 lists the geometry, inlet and boundary conditions used in the computer code, which experimental results are available through Prins Maurits Laboratory TNO, the Netherlands [8, 9, 23, 11]. The combustion chamber being discussed is cylindrical in form, so the flow can be considered as axisymmetric. The length of the

chamber is 0.3 m, the diameter is 0.045 m and the stepheight is 0.015 m. Ethylene (C_2H_4) is used as fuel and at the inlet a mixture of 23.1% O_2 and 76.9% N_2 is blown into the combustion chamber. The grid system used is 30×17 non-equidistant grid. The solution is assumed to have converged when the sum of the normalized absolute residuals has fallen below 0.001. The flowfields calculated by the computer program are represented using contourplots.

Figure 5.1 shows the normalized velocity field in the x-direction. The area of the reverse flow can be clearly distinguished in this figure. It also shows the point at the downstream end of the recirculation region where the flow attaches and begins a boundary flow. Large velocity gradients can also be found near the inlet at the edge of the recirculating flow, where the velocities of the flow change rapidly from the inlet velocity 162 m/s to zero or even negative value (Table 5.2). Table 5.3 shows the radial velocities in the field. As the flow gets more developed towards the exit, the radial velocities become smaller and smaller.

The contours of the calculated temperature-field are plotted in Figure 5.2. The numerical data are also given in Table 5.3. It can be shown that the maximum temperatures lie between 2900 K and 3000 K. Normally at such high temperatures, dissociation of gaseous and molecules will occur. But in the present chemical sub-model, this effect cannot be taken into account. Consequently, it leads the model to overpredict the temperature-field. In spite of that, the code can still be used to gain a good qualitative insight of temperature distribution. From Figure 5.2 and Table 5.3, it can be clearly seen that the temperature gradients are large near the solid fuel wall. Also found are large temperature gradients just after the step, where the

temperatures are found to increase rapidly from the air inlet temperature 300 K to the temperatures of about 2800 K. This may be attributed to the sudden expansion, where the incoming flow meets the recirculating flow containing a relatively large amount of fuel that is lifted up by a vortex from the solid wall region. This results in large gradients of mixture fraction and hence in the large temperature gradients, since the temperature is strongly coupled to the mixture fraction. So the temperatures inside the recirculating region reach the highest values because of intense mixing generated by the vortex. As the flow moves downstream, the mixing process increases, so the peak temperature approaches gradually to the solid wall. Downstream of the recirculation zone, the maximum temperatures occur very close to the fuel wall, which shows that oxygen can penetrate into the region near the wall and react with the fuel vapourized from the fuel grain. Due to diffusion of reaction heat from the burning zone to the centre of the chamber, the cold flow entering at the inlet is heated and at the centreline temperatures are increasing downstream. Therefore isotherms are moving down towards the axis as they are approaching the end of the chamber.

Figure 5.3 shows the static pressure field within the combustion chamber. The incoming flow at the inlet has a sudden expansion, which leads to a rapid drop in static pressure. When the flow comes to the end of the expansion zone, its pressures reach their lowest levels in the flowfield. Thereafter, the pressures are recovering and are increasing in the flow direction to a maximum value. As the flow approaches the end of the chamber, it becomes more and more developed. Therefore, the velocity gradients in the flow direction become smaller and smaller

(zero if Poiseuille flow). Thus, the pressure difference in the flow direction becomes the only main force to drive the flow downstream. This explains why the pressures are decreased towards the end of the chamber. The maximum pressures occurring in the middle of the chamber might be caused by strong pressure gradients which are due to the redevelopment of the boundary layer after the recirculation zone. At the outlet pressure gradients are relatively small.

The density of the chemically reacting flow is a function of pressure, temperature, and mass fractions of species at the location. The density field in the SFRJ combustion chamber is also plotted in Figure 5.4. From the figure, it can be seen that the densities inside the recirculation region are relatively low. This is caused by very high temperatures and low pressures in this zone. However, the densities just outside this region are comparatively high near the inlet because the cold incoming fuel is not yet heated up, which results in large density gradients there. At the centreline the densities are decreasing as the flow moves downstream. Downstream of the recirculation zone near the wall, the densities are increasing in the flow direction.

For the mixture fraction field shown in Figure 5.5, large gradients occur at the edge of the recirculation zone near the inlet, where the oxygen-bearing incoming flow meets the fuel-bearing recirculating flow generated by the vortex, therefore resulting in a high degree of mixing there and hence relatively large gradients of mixture fraction. Inside the recirculation region, the mixture fractions reach their highest values because of a strong mixing between the fuel and oxygen, thus leading to extremely high temperatures there, which also can be seen in the temperature field (Figure 5.2). Hence, the recirculation region is not only essential to flame stabilization but

also beneficial to promoting complete combustion. As discussed earlier in Chapter 3, when using the diffusion flame model, combustion will take place at a thin flame sheet at the location where the mixture fraction equals the mixture fraction for stoichiometry (0.06438, which is calculated from Eq. (3.11)). The flame position can be clearly distinguished from the mixture fraction field in Figure 5.5, and is approaching the solid wall in the flow direction. Downstream of the recirculation zone, the flame sheet lies nearly on the pyrolyzing wall. At the lean side of this flame front where $f < f_{st}$, only oxygen, products and inerts (here only nitrogen is considered) are present whereas at the rich side, $f > f_{st}$, only fuel, products and inerts are found, which will be confirmed later by the mass fraction fields of the fuel, oxygen, nitrogen and products shown in Figures 5.8 to 5.11.

The distribution of the turbulence kinetic energy is given in Figure 5.6. The maximum turbulence kinetic energies are found at the interface of the incoming flow and recirculating flow, where the velocity gradients reach highest levels. Also at these locations, the turbulence kinetic energy gradients are relatively large. At the wall and at the centre of chamber the turbulence kinetic energies are low. This is because the solid wall tends to slow down the flow and thus depress turbulence activities near it. At the centreline, the flow becomes more stable, so the turbulence kinetic energies are reduced. As the flow moves downstream towards the end of the chamber, it becomes more and more developed, so the turbulence kinetic energies are getting smaller and smaller.

The distribution of the turbulence energy dissipation rate in the chamber as shown in Figure 5.7 is similar to that of turbulence kinetic energy. At the interface of

the incoming flow and recirculating flow, the turbulence dissipation rates reach their highest levels, and the gradients are also very large. Downstream of the recirculation zone, as the flow gets more developed towards the outlet, the turbulence dissipation rates decrease gradually. Near the solid wall and at the centre of the chamber the turbulence energy dissipation rates are relatively low, and the reasons are the same as those for the turbulence kinetic energy.

As discussed earlier in Chapter 3, both of the combustion models incorporated in the code can take into account five species such as the fuel C_2H_4 , oxygen O_2 , nitrogen N_2 and the products CO_2 , H_2O . The products CO_2 , H_2O here are treated as a whole to facilitate the analyses of the computed mass fraction fields. The mass fraction distributions of these species are contourplotted in Figures 5.8 to 5.11. The values of these mass fractions are supplied in Tables 5.5 to 5.8. From the figures and tables, it can be shown that near the inlet the composition of the gases corresponds nearly to that of air, and almost no combustion products are found. At the interface of the incoming flow and recirculating flow, large gradients are found for all the species, which may be caused by a strong mixing there. As the flow moves further downstream, the composition at the centreline is still close to the composition of the air at the inlet, but small amounts of the combustion products may also be found, moreover, the amounts are increasing in the axial direction. Oxygen is consumed gradually toward the end of the chamber and, therefore, its content is diminishing. The mass fraction of the fuel increases with diminishing distance from the wall, whereas the mass fractions of O_2 and N_2 decrease. Since the assumption made in the diffusion flame combustion model cannot allow the fuel

and oxygen to coexist at the same location, the fuel and oxygen occupy each area separately in the chamber. From Figure 5.8 and Table 5.6, the fuel is found merely around the upper corner inside the recirculation region, and is believed to be stirred up by a vortex generated by a sudden expansion. This area provides the chemical reaction with the fuel needed, and the constant heat released from the reaction is used to warm up the rest of the solid fuel grain. So this fuel-rich region is very useful to promoting stable combustion. Downstream of this area, no fuel is found, even at the grid points close to the solid fuel wall. This leads us to believe that the reaction occurs near the interface of the flow and fuel wall. The oxygen distribution as seen in Figure 5.9 and Table 5.5 shows that oxygen can diffuse into the region very close to the solid fuel wall, and confirms once again that the chemical reaction takes place in the area near the fuel grain. The peak temperature distribution in Figure 5.2 and Table 5.5 also confirms this conclusion.

5.2 Results from the Turbulent Diffusion Flame Model

A great disadvantage of the diffusion flame combustion model, as discussed early in Chapter 3, is that the influence of turbulence on combustion is neglected. Thus in the model, mixture fraction is assumed to have no fluctuation, as in laminar flows, and mass fractions are directly related to the value of the mixture fraction at a given point at any instant time. Turbulence does not affect the mass fraction directly, which is clearly not true in turbulent flows, realistically. But in the follow-

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A resolution test chart featuring various patterns of vertical and horizontal lines. The patterns are arranged in a grid-like fashion, with some patterns being larger and more prominent than others. Numerical values are placed next to the patterns, indicating the resolution level. The values include 1.0, 1.1, 1.25, 1.4, 1.6, 1.8, 2.0, 2.2, 2.5, 2.8, 3.2, 3.6, 4.0, 4.5, 5.0, 5.6, 6.3, 7.1, 8.0, 9.0, 10.0, 11.2, 12.5, 14.0, 16.0, 18.0, 20.0, 22.5, 25.0, 28.0, 32.0, 36.0, 40.0, 45.0, 50.0, 56.0, 63.0, 71.0, 80.0, 90.0, 100.0, 112.0, 125.0, 140.0, 160.0, 180.0, 200.0, 225.0, 250.0, 280.0, 320.0, 360.0, 400.0, 450.0, 500.0, 560.0, 630.0, 710.0, 800.0, 900.0, 1000.0, 1120.0, 1250.0, 1400.0, 1600.0, 1800.0, 2000.0, 2250.0, 2500.0, 2800.0, 3200.0, 3600.0, 4000.0, 4500.0, 5000.0, 5600.0, 6300.0, 7100.0, 8000.0, 9000.0, 10000.0.

ing turbulent diffusion flame model, the effect of turbulence on the mass fraction distributions of fuel, oxidizer and products is taken into account by relating the fluctuation in mixture fraction to fluctuations in mass fractions. Statistical means of these mass fractions can be obtained from weighting their instantaneous values with the Probability Density Function (see Eq. (3.39), Eq.(3.41)). Therefore, the species concentrations are no longer unique functions of mixture fraction, as in the diffusion flame model. As a consequence, the mean concentrations of the reactants are increased above the 'laminar value' predicted by the diffusion flame model at the same mean mixture fraction due to the effect of turbulence. The mean product concentration is correspondingly reduced. So less heat is released from the reaction, resulting in a lower temperature. This situation has often been described qualitatively by the term 'unmixedness' [51, 59, 60].

The same geometry and boundary conditions of the SFRJ combustor as listed in Table 5.1 are used for the calculation of the flowfields with the turbulent diffusion flame model. During the computation, the same convergence criteria are applied to ensure conservations of all the finite-difference equations involved. For the turbulent combustion model, one more variable, the variance of the mixture fraction, is needed to solve in order to determine the exact value of the probability of mass fraction at a certain location of the flowfield. In addition, the integral appearing in Eqs. (3.39) and (3.41) is solved with the Simpson approach and calculated in the subroutine INTEGRAL. The beta function is solved by calling a couple of special function routines taken from the SLATEC mathematical library, which is resident in the APOLLO system of Mechanical Engineering at Carleton University. The same

computational grid system is used. As compared with the diffusion flame model, the turbulent diffusion flame model is more complex. The number of routines involved in the execution of the program is considerably larger than for the former. In addition, the integral and beta function must be solved at every grid point, so the computing time required for each iterative step is expensively larger. Moreover, nearly double the number of sweeps is needed to achieve the desired solution over the same computational domain. Therefore, the code with the turbulent diffusion flame model is far more expensive to use, compared with the one with the diffusion flame model. However, its deficiency may be compensated for by a more reliable prediction of the flow in a SFRJ combustor.

Figures 5.12 to 5.23 and Tables 5.9 to 5.15 display the calculated flowfields in the combustion chamber. As we can see from Figure 5.12 and Tables 5.9 to 5.10, the velocity field does not differ significantly from the one obtained from the diffusion flame model. In other words, the combustion model used here does not affect the prediction of the velocity field very much.

However, the temperature field (Figure 5.13 and Table 5.11) does change significantly. The main difference between these temperature distributions is in the recirculation zone, where the temperatures are much lower for the turbulent diffusion flame model, although the temperatures in the other areas are also predicted lower than those obtained with the diffusion flame model. The maximum temperatures are found to be around 2300 K, and considerably lower than those predicted by the other combustion model. This is because the turbulent diffusion flame model can allow the fuel and oxygen to exist at the same location, being a time-average

of the instantaneous situation, it leads to the phenomenon of 'unmixedness'. The fuel and oxygen mass fractions can overlap each other in the flowfield. The mean concentrations of the reactants are increased, as compared with those obtained with the diffusion flame model. The mean product concentrations are correspondingly reduced, hence less heat is released from the combustion, thus, the lower temperatures are predicted in the chamber. This phenomenon of 'unmixedness' plays an important role in the recirculation region, because, there, a relatively large amount of the fuel is transported by the vortex from the wall into this area and turbulence intensity is highest. In other regions, the fuel is burnt quickly very near the wall. Thus, it can be deduced that for more intensely turbulent flow, the temperatures in the recirculation will be further reduced, due to the fact that the influence of turbulence on combustion ('unmixedness') is larger at higher turbulence levels. This behaviour is confirmed by the studies of Elands [10, 11]. In spite of relatively lower predicted temperatures, the validation with experimentally obtained results will still fail because dissociation of molecules and atoms, playing an important role at high temperatures, cannot be taken into account in this turbulent combustion model. However, the magnitudes of the calculated temperatures are believed to be closer to the values attained in reality.

The mass fractions of all the species in the flowfield are plotted in Figures 5.19 to 5.22 and Tables 5.12 to 5.15. For the fuel and oxygen, unlike the diffusion flame model, the mass fractions predicted by the turbulent diffusion flame model are found to have no discontinuity in their distributions. It means the fuel and oxygen can coexist over the entire chamber. The mass fraction of the fuel increases

with diminishing distance from the wall, whereas the mass fractions of O_2 and N_2 decrease.

In principle, the combustion can take place at any location where at a certain time the fuel and oxygen coexist, but exactly where the combustion takes place depends on the instantaneous situation. So for the time-averaged situation, the resulting flame zone will be thicker than that using the diffusion flame model. Moreover, the position of the flame front is closer to the solid wall compared with the position of flame sheet predicted by the diffusion flame model, and the maximum temperatures in Figure 5.13 and Table 5.11 also occur closer to the solid wall.

Figure 5.23 shows the distribution of the mass fraction variance. It is found that the variance gradients are very high at the interface of the incoming flow and recirculation region. The variances at and under the entrance of the chamber also reach the highest values. The reason is that the gradients of the mixture fraction are high in these regions, thus resulting in a large production of the variance in the transport equation of the variance (Eq. (3.28)). The special boundary condition at the wall discussed in Chapter 3 seems to work satisfactorily.

During the calculation using the turbulent diffusion flame model, special attention is given to the distribution of the beta Probability Density Function. It is found that the beta P.D.F is very small in the area near the centreline of the chamber, and the values of the mass fractions are hardly affected by weighting them with the P.D.F. But the beta Probability Density Function has a significant influence on the mass fraction distributions at the location where the mixture fractions are near the stoichiometric value f_{st} (0.06438).

From the above comparisons of the two combustion models, it may be concluded that the velocity fields do not differ very much, but the temperature and mass fraction distributions are significantly different. The turbulent diffusion flame model yields more realistic results than the diffusion flame model, although the effect of dissociation is still not taken into account. It is recommended to use the turbulent diffusion flame model, although its calculation requires more computing time. The diffusion flame model, however, is still a good, efficient and fast tool for preliminary calculations.

5.3 Other Calculations Carried Out

Since the author devoted most of his efforts to the development of the computer code for SFRJ combustors, as has been discussed so far, not much time was spent on calculations of flowfields at various inlet flow conditions, although it is very important to the complete validation of the present computer code. As the regression rate plays an important role in the performance of an SFRJ and it appears to be relatively constant during combustion, so, at present, the regression rate was chosen to be the prime parameter this validation is based on. In the following, a comparison between calculated and observed local mean regression rate data is given. Besides, the dependency of the mean regression rate on inlet air mass flow was calculated. Other studies such as the regression rate in relation to chamber pressure, inlet air temperature, and stepheight, etc., will be left for future work.

The computer codes assumes a steady state flow and combustion process. This

is in strong contrast with the actual situation, where, due to a regular vortex shedding at the inlet, locally highly fluctuating quantities like velocities, temperatures and species concentrations can be expected. Nevertheless, a relatively constant regression rate during the combustion of PE with air is observed in the experiments by Elands, et al [9]. In the experiments [9], the mean regression rates were obtained from weight loss measurements whereas the local mean regression rates were obtained by measuring the inner grain profile after combustion. Normally, highest regression rates occur at the end of the recirculation zone and are believed to correspond with the reattachment point. Figure 5.24 compares the calculated and experimentally observed local mean regression rates along the fuel grain. In general, the agreement between theoretical and experimental results is quite good. But, it is found that both models predict the maximum regression rate to occur upstream of where it is observed in the experimental data, and have similar profiles. This early peak in the regression rate results from the models predicting a shorter reattachment length than was found experimentally. This may be attributed to the inability of the $k - \epsilon$ turbulence model to predict, accurately, the separated flow behind a rearward facing step.

The mean regression rate is obtained by averaging the predicted local regression rate. In Figure 5.25, the mean regression rate is given as a function of the inlet air mass flow. The theoretical results are computed using the diffusion flame model. From the figure, it is observed that the predicted dependency of the regression rate on the air mass flow is stronger than for the experimental one. The difference between the calculated and measured regression rate data is small at low air mass

flows but increases with increasing flow rates. A closer examination of the regression rate behaviour reveals that this difference is especially apparent in the recirculation region. This is possibly due to the inability of the $k - \epsilon$ turbulence closure model in combination with the wall-functions, to accurately predict the flowfield and heat transfer behind the step.

Chapter 6

Conclusions and Recommendations

The primary objective of this thesis was to develop a computer code capable of predicting the flowfields of SFRJ combustors. For this purpose, the DRAGON code was developed, in which two combustion models were adopted. Both combustion models, the diffusion flame model and turbulent diffusion flame model, yields results which are expected from theory. But the turbulent diffusion flame model predicts results that are more realistic than the results predicted by the diffusion flame model, especially for the temperature field and mass fraction field. The main deficiency of the diffusion flame concept is that dissociation of molecules and atoms, playing an important role at high temperatures, cannot be taken into account, thus resulting in the over-prediction of the temperatures. Therefore any validation with experimentally obtained results for the temperature field will fail. Since only one single-step chemical reaction and the five species such as C_2H_4 , O_2 , N_2 , CO_2 , H_2O are considered in the code, the formation of pollutants cannot be predicted. The $k - \epsilon$ turbulence closure model has shown some deficiencies in the prediction of the flows and heat

flux in the recirculation zone. However, more calculations and an extensive study to compare the calculated results with the experimentally obtained results are needed to completely assess the validity of this computer code for predicting the flow in a solid fuel ramjet combustor.

In the future, some research work can be suggested to improve the predictability of the present code and obtain results which are more realistic. Those recommendations are presented as follows.

- The DRAGON computer code does not include radiative heat transfer to the fuel surface, and completely ignores an important role radiative heat transfer plays in combustion. This limits the utility of the code, since many all-hydrocarbon fuels produce significant amounts of radiative transfer through the generation of carbon particulate in the flame zone. The experiments [9] showed that for pressures above $6 \times 10^5 \text{ N/m}^2$, soot is formed and distributed over the chamber. It is necessary to incorporate a radiation model in the present program. In early literature surveys, a two-dimensional radiant heat flux model applicable to axisymmetrical geometries developed by Lowes [54] and subsequently extended three-dimensional flux model proposed by Marco, et al [55] are found very interesting, and might be considered as good choices in the future incorporation.
- Finite chemical kinetics model should be incorporated in the computer code to improve the prediction of the temperature field and the mixture composition, since it takes dissociation into account. For this purpose, more chemical species are necessary to be included, and more chemical reactions are needed to be

added for the formation of these species. The formation of these species, of course, is kinetically controlled. The prediction of NO_2 and CO formation should also be included in the program in order to monitor the emission of such pollutants from solid fuel ramjet.

- The $k - \epsilon$ turbulence closure model showed some deficiencies in predicting the separated flows arising from a sudden expansion. The proper modeling of the flow would probably require a higher order turbulence model. More research should be carried out to find a better alternative for the code. In addition, a so-called bounded-skew hybrid difference (BSHD) scheme [56, 30] might be considered in the present code to discretize the equations. This scheme takes into account the local direction of the flow and thereby greatly reduces the 'skewness error' which, in two-dimensional flows, is the largest contribution to false diffusion.
- The computer code should be made time dependent to take into account the regressing fuel wall and expanding combustion chamber. This could be done by a quasi-steady flow model, in which the combustion process can be divided into many time periods, and at each time step, the steady flow is assumed. There is also a need to extend the program into a three-dimensional code capable of modeling the two other important SFRJ geometries, side-dump and bypass.
- The extension of the computer code to allow for the combustion of various solid fuels for SFRJ, especially boron-containing fuels, is considered necessary. It

is well known that boron is a potential fuel candidate for airbreathing propulsion systems because of its high volumetric heat of combustion. However, realization of this energy is not straightforward, since it is difficult to ignite and maintain combustion of boron particles. It would be useful, therefore, to develop a theoretical model to analyze and characterize the behaviour of individual boron particles in the flowfield of an SFRJ combustor. The computer code should also be allowed to take into account the influence of the local gaseous flowfield on trajectory, thermal response, and chemical reactions of the boron particles. The King model [57, 58] would be considered as a good reference and starting base of the future research on this subject.

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Table 2.1 $k - \epsilon$ turbulence model empirical constants

C_1	C_2	C_D	σ_k	σ_ϵ	κ	E
1.43	1.92	0.09	1.0	1.3	0.4	9.0

Table 2.2 Governing equation parameters

ϕ	Γ_ϕ	S_ϕ
1	0	0
u	$\mu_t + \mu$	$-\frac{\partial P_{eff}}{\partial x} + \nabla \cdot [(\mu_t + \mu) \frac{\partial \vec{V}}{\partial x}]$
v	$\mu_t + \mu$	$-\frac{\partial P_{eff}}{\partial r} + \nabla \cdot [(\mu_t + \mu) \frac{\partial \vec{V}}{\partial r}] - 2 \frac{(\mu_t + \mu)v}{r^2}$
k	$(\mu_t + \mu)/\sigma_k$	$G + PV - \rho\epsilon$
ϵ	$(\mu_t + \mu)/\sigma_\epsilon$	$C_1 \frac{\epsilon}{k} (G + PV) - C_2 \rho \frac{\epsilon^2}{k}$
$\tilde{h}$	$(\mu_t + \mu)/\sigma_t$	0
f	$(\mu_t + \mu)/\sigma_f$	0
m_{N_2}	$(\mu_t + \mu)/\sigma_{N_2}$	0
g	$(\mu_t + \mu)/\sigma_g$	$C_{g1} \mu_t \frac{\partial I}{\partial x} \frac{\partial I}{\partial x} + C_{g1} \mu_t \frac{\partial I}{\partial r} \frac{\partial I}{\partial r} - C_{g2} \rho \frac{\epsilon}{k} g$

Note: $\sigma_f = \sigma_{N_2} = 0.7, \sigma_g = 0.9, \sigma_t = 1.0, \sigma_{g1} = 2.8, \sigma_{g2} = 2.0$

$$P_{eff} = P + \frac{2}{3}(\rho k + \mu_t \nabla \cdot \vec{V})$$

$$G = \mu_t \{ 2 [(\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial r})^2 + (\frac{v}{r})^2] + (\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x})^2 \} - \frac{2}{3}(\rho k + \mu_t \nabla \cdot \vec{V}) \nabla \cdot \vec{V}$$

$$PV = -(\overline{u'' \frac{\partial p}{\partial x}} + \overline{v'' \frac{\partial p}{\partial r}}) = -\frac{\mu}{\sigma_t} \frac{1}{\rho^2} (\frac{\partial \bar{p}}{\partial x} \frac{\partial \bar{p}}{\partial x} + \frac{\partial \bar{p}}{\partial r} \frac{\partial \bar{p}}{\partial r})$$

$$\nabla = \frac{\partial}{\partial x} \vec{i} + \frac{1}{r} \frac{\partial}{\partial r} r \vec{j}$$

$$\vec{V} = u \vec{i} + v \vec{j}$$

Note: The Schmidt number is chosen as unity in the energy equation.

Table 5.1 Geometry, boundary conditions and grid system for the calculation

chamber length, L	0.3 m
chamber diameter, D	0.045 m
step height, h	0.015 m
inlet velocity, u_{in}	162 m/s
inlet temperature, T_{in}	300 K
inlet pressure, P_{in}	450000 N/m ²
inlet mass fraction of O_2 , $m_{O_2,in}$	0.231
inlet mass fraction of N_2 , $m_{N_2,in}$	0.769
turbulence intensity factor, FACTKE	0.1
length scale factor FACTED,	0.03
wall temperature, T_{wall}	800 K
wall mass fraction of C_2H_4 , $m_{C_2H_4,wall}$	1.0
grid points	30 × 17
Near wall grid cell centre located at 0.9667 times the radius

Table 5.2(a) Axial velocity (m/s) (Diffusion flame model)

y (m)	x	0.000	0.011	0.021	0.032	0.043	0.054	0.064	0.075	0.086	0.096
0.0225	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.02175	0.0	0.0	-23.4	-42.9	-48.3	-44.1	-36.	-26.5	-16.9	-7.01	2.58
0.02025	0.0	0.0	-21.2	-36.4	-37.1	-31.2	-22.7	-13.5	-4.29	4.73	12.6
0.01875	0.0	0.0	-18.6	-28.7	-26.	-19.	-1.06	-1.94	6.55	14.5	21.1
0.01725	0.0	0.0	-13.3	-18.9	-12.8	-5.12	2.83	10.7	18.1	24.8	30.4
0.01575	0.0	0.0	-12.2	-6.24	3.23	11.1	18.2	24.8	30.9	36.3	40.7
0.01425	0.0	0.0	-8.83	10.9	22.6	29.9	35.7	40.6	45.1	48.9	52.1
0.01275	0.0	0.0	-1.6	33.6	45.9	51.8	55.4	58.2	60.6	62.7	64.4
0.01125	0.0	0.0	24.	63.5	73.6	76.6	77.3	77.4	77.5	77.5	77.6
0.00975	0.0	0.0	89.	103.	105.	103.	101.	97.6	95.1	93.	91.2
0.00825	0.0	0.0	139.	139.	135.	129.	123.	118.	113.	109.	105.
0.00675	162.0	160.	158.	154.	148.	142.	135.	129.	123.	118.	110.
0.00525	162.0	162.	161.	159.	157.	153.	147.	142.	136.	130.	120.
0.00375	162.0	162.	162.	161.	159.	157.	154.	150.	145.	139.	129.
0.00225	162.0	163.	162.	161.	160.	158.	156.	154.	150.	146.	140.
0.00075	162.0	163.	162.	161.	160.	159.	157.	155.	152.	148.	142.
0.0000	162.0	163.	162.	161.	160.	159.	157.	155.	152.	148.	142.

Table 5.2(b) Axial velocity (m/s) (Diffusion flame model)

	0.214	0.225	0.236	0.246	0.257	0.268	0.279	0.289	0.300
0.0225	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.02175	69.4	73.	76.4	79.6	82.2	84.1	86.	88.1	88.1
0.02025	74.4	78.1	81.5	84.8	87.7	90.3	92.7	95.6	95.6
0.01875	76.9	80.3	83.5	86.6	89.3	91.8	94.3	97.	97.
0.01725	79.	82.1	85.	87.8	90.4	92.8	95.	97.5	97.5
0.01575	81.1	83.8	86.5	89.	91.4	93.6	95.7	97.8	97.8
0.01425	83.3	85.6	87.9	90.2	92.3	94.3	96.2	98.2	98.2
0.01275	85.5	87.4	89.4	91.4	93.3	95.1	96.8	98.5	98.5
0.01125	87.7	89.2	90.9	92.6	94.2	95.9	97.4	98.8	98.8
0.00975	89.8	91.	92.3	93.7	95.2	96.6	98.	99.2	99.2
0.00825	91.9	92.7	93.7	94.8	96.	97.3	98.5	99.5	99.5
0.00675	93.7	94.2	94.9	95.8	96.8	97.9	99.	99.8	99.8
0.00525	95.3	95.4	95.9	96.6	97.5	98.5	99.4	100.	100.
0.00375	96.6	96.4	96.7	97.3	98.	98.9	99.8	100.	100.
0.00225	97.4	97.2	97.3	97.8	98.4	99.2	100.	100.	100.
0.00075	97.9	97.5	97.6	98.	98.6	99.3	100.	101.	101.
0.0000	97.9	97.5	97.6	98.	98.6	99.3	100.	101.	101.

Table 5.2(c) Axial velocity (m/s) (Diffusion flame model)

y (m) x	0.214	0.225	0.236	0.246	0.257	0.268	0.279	0.289	0.300
0.0225	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.02175	69.4	73.	76.4	79.6	82.2	84.1	86.	88.1	88.1
0.02025	74.4	78.1	81.5	84.8	87.7	90.3	92.7	95.6	95.6
0.01875	76.9	80.3	83.5	86.6	89.3	91.8	94.3	97.	97.
0.01725	79.	82.1	85.	87.8	90.4	92.8	95.	97.5	97.5
0.01575	81.1	83.8	86.5	89.	91.4	93.6	95.7	97.8	97.8
0.01425	83.3	85.6	87.9	90.2	92.3	94.3	96.2	98.2	98.2
0.01275	85.5	87.4	89.4	91.4	93.3	95.1	96.8	98.5	98.5
0.01125	87.7	89.2	90.9	92.6	94.2	95.9	97.4	98.8	98.8
0.00975	89.8	91.	92.3	93.7	95.2	96.6	98.	99.2	99.2
0.00825	91.9	92.7	93.7	94.8	96.	97.3	98.5	99.5	99.5
0.00675	93.7	94.2	94.9	95.8	96.8	97.9	99.	99.8	99.8
0.00525	95.3	95.4	95.9	96.6	97.5	98.5	99.4	100.	100.
0.00375	96.6	96.4	96.7	97.3	98.	98.9	99.8	100.	100.
0.00225	97.4	97.2	97.3	97.8	98.4	99.2	100.	100.	100.
0.00075	97.9	97.5	97.6	98.	98.6	99.3	100.	101.	101.
0.0000	97.9	97.5	97.6	98.	98.6	99.3	100.	101.	101.

Table 5.3(c) Radial velocity (m/s) (Diffusion flame model)

$y \times$	0.00	0.020	0.040	0.060	0.080	0.100	0.120	0.140	0.160	0.180
0.0225	-0.057	-0.06	-0.062	-0.065	-0.068	-0.070	-0.071	-0.072	-0.073	0.000
0.0210	0.052	-0.046	-0.105	-0.186	-0.106	-0.015	-0.022	0.003	0.000	0.000
0.0195	0.058	0.008	0.078	-0.003	0.009	0.028	-0.004	0.058	0.000	0.000
0.0180	0.061	0.469	0.005	0.192	0.062	0.142	0.098	0.187	0.000	0.000
0.0165	0.035	0.706	0.513	0.374	0.311	0.262	0.209	0.315	0.000	0.000
0.0150	1.16	0.905	0.688	0.528	0.437	0.367	0.307	0.421	0.000	0.000
0.0135	1.34	1.06	0.821	0.645	0.514	0.448	0.384	0.497	0.000	0.000
0.0120	1.45	1.15	0.909	0.723	0.598	0.502	0.435	0.541	0.000	0.000
0.0105	1.49	1.19	0.946	0.758	0.627	0.526	0.459	0.555	0.000	0.000
0.0090	1.46	1.17	0.934	0.750	0.620	0.519	0.455	0.538	0.000	0.000
0.0075	1.36	1.09	0.871	0.701	0.578	0.484	0.425	0.494	0.000	0.000
0.0060	1.19	0.955	0.762	0.613	0.505	0.423	0.371	0.426	0.000	0.000
0.0045	0.960	0.766	0.611	0.492	0.405	0.338	0.297	0.337	0.000	0.000
0.0030	0.673	0.536	0.427	0.344	0.283	0.236	0.207	0.234	0.000	0.000
0.0015	0.346	0.276	0.220	0.177	0.145	0.121	0.107	0.119	0.000	0.000
0.0000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 5.4(a) Temperature (K) (Diffusion flame model)

$y \text{ (m)} \times$	0.000	0.005	0.016	0.027	0.038	0.048	0.059	0.070	0.080	0.091
0.0225	800	800	800	800	800	800	800	800	800	800
0.02175	2990	2990	2990	2990	2980	2880	2750	2670	2630	2290
0.02025	2990	2990	2990	2810	2520	2320	2180	2080	2020	1830
0.01875	2990	2990	2990	2590	2290	2080	1940	1840	1760	1640
0.01725	2990	2990	2940	2440	2130	1910	1770	1660	1590	1490
0.01575	2990	2990	2840	2320	1990	1770	1620	1510	1440	1360
0.01425	2990	2990	2720	2190	1860	1630	1480	1380	1310	1240
0.01275	2990	2990	2530	2030	1700	1480	1340	1240	1180	1130
0.01125	2990	2990	2270	1790	1490	1300	1180	1100	1050	1010
0.00975	2630	2630	1790	1410	1200	1070	993	941	909	889
0.00825	1130	1130	964	886	839	807	787	774	768	767
0.00675	300	340	392	444	496	542	578	605	627	645
0.00525	300	300	317	333	356	386	423	462	499	533
0.00375	300	300	304	308	316	328	346	371	404	440
0.00225	300	300	301	302	305	310	317	330	350	380
0.00075	300	300	300	301	302	305	309	316	329	351
0.0000	300	300	300	301	302	305	309	316	329	351

Table 5.4(b) Temperature (K) (Diffusion flame model)

$y \text{ (m)} \times$	0.112	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.199
0.0225	870	870	870	870	870	870	870	870	870	870
0.02175	2130	2130	2190	2200	2220	2240	2280	2320	2370	2440
0.02025	1760	1770	1720	1720	1720	1730	1740	1760	1770	1820
0.01875	1570	1540	1520	1510	1510	1520	1530	1540	1560	1580
0.01725	1430	1400	1380	1370	1370	1370	1380	1390	1410	1430
0.01575	1310	1240	1260	1250	1250	1260	1270	1280	1300	1320
0.01425	1200	1170	1160	1150	1150	1160	1170	1180	1200	1220
0.01275	1090	1070	1060	1050	1060	1070	1080	1100	1120	1140
0.01125	984	970	964	967	975	989	1010	1030	1050	1070
0.00975	877	872	875	883	898	916	938	963	988	1010
0.00825	769	776	788	805	826	851	878	906	935	964
0.00675	664	683	706	732	761	792	825	858	890	922
0.00525	565	596	630	665	703	741	780	818	854	888
0.00375	479	521	564	609	656	701	745	787	826	863
0.00225	428	464	515	568	621	672	721	765	807	846
0.00075	386	433	488	546	603	658	708	755	797	837
0.0000	386	433	488	546	603	658	708	755	797	837

Table 5.4(c) Temperature (K) (Diffusion flame model)

$y \text{ (m)} \times$	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	800	800	800	800	800	800	800	800	800	800
0.02175	2510	2600	2700	2820	2920	2930	2940	2940	2940	2940
0.02025	1860	1900	1940	1990	2040	2090	2150	2200	2260	2260
0.01875	1610	1630	1670	1700	1730	1760	1790	1820	1860	1860
0.01725	1450	1480	1500	1530	1550	1580	1600	1630	1650	1650
0.01575	1340	1360	1380	1410	1430	1450	1470	1500	1520	1520
0.01425	1240	1270	1290	1310	1330	1360	1380	1400	1420	1420
0.01275	1160	1190	1210	1230	1260	1280	1300	1320	1340	1340
0.01125	1100	1120	1150	1170	1190	1220	1240	1260	1280	1280
0.00975	1040	1070	1090	1120	1140	1160	1190	1210	1230	1230
0.00825	993	1020	1050	1070	1100	1120	1140	1170	1190	1190
0.00675	953	983	1010	1040	1060	1090	1110	1130	1150	1150
0.00525	921	952	982	1010	1040	1060	1080	1110	1130	1130
0.00375	897	930	960	988	1020	1040	1060	1090	1110	1100
0.00225	881	915	946	975	1000	1030	1050	1070	1100	1100
0.00075	873	907	939	968	995	1020	1050	1070	1090	1090
0.0000	873	907	939	968	995	1020	1050	1070	1090	1090

Table 5.5(a) Oxygen mass fraction (Diffusion flame model)

[illegible]

Table 5.5(b) Oxygen mass fraction (Diffusion flame model)

$y \rightarrow x$	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.072	0.071	0.070	0.069	0.067	0.065	0.062	0.058	0.053	0.046
0.02025	0.113	0.115	0.116	0.116	0.116	0.115	0.113	0.112	0.109	0.106
0.01875	0.130	0.132	0.134	0.134	0.134	0.134	0.133	0.132	0.130	0.128
0.01725	0.143	0.145	0.146	0.147	0.147	0.147	0.146	0.145	0.143	0.141
0.01575	0.153	0.155	0.157	0.157	0.157	0.157	0.156	0.155	0.153	0.151
0.01425	0.162	0.164	0.166	0.166	0.166	0.166	0.164	0.163	0.161	0.159
0.01275	0.171	0.173	0.174	0.174	0.173	0.172	0.171	0.170	0.168	0.166
0.01125	0.180	0.181	0.181	0.181	0.180	0.179	0.177	0.176	0.174	0.172
0.00975	0.188	0.189	0.188	0.188	0.186	0.185	0.183	0.181	0.179	0.177
0.00825	0.197	0.196	0.195	0.194	0.192	0.190	0.188	0.186	0.183	0.181
0.00675	0.205	0.203	0.201	0.199	0.197	0.195	0.192	0.189	0.187	0.184
0.00525	0.212	0.210	0.207	0.204	0.202	0.199	0.196	0.193	0.190	0.187
0.00375	0.218	0.215	0.212	0.209	0.205	0.202	0.198	0.195	0.192	0.189
0.00225	0.223	0.219	0.216	0.212	0.208	0.204	0.200	0.197	0.193	0.190
0.00075	0.225	0.222	0.218	0.213	0.209	0.205	0.201	0.198	0.194	0.191
0.0000	0.225	0.222	0.218	0.213	0.209	0.205	0.201	0.198	0.194	0.191

Table 5.5(c) Oxygen mass fraction (Diffusion flame model)

0.2175	0.219	0.220	0.220	0.241	0.252	0.263	0.273	0.294	0.295	0.300
0.225	0.220	0.220	0.220	0.200	0.200	0.200	0.200	0.200	0.200	0.200
0.2275	0.219	0.221	0.221	0.210	0.200	0.200	0.200	0.200	0.200	0.200
0.2225	0.203	0.200	0.206	0.201	0.207	0.203	0.209	0.203	0.208	0.208
0.2175	0.226	0.223	0.221	0.218	0.215	0.213	0.210	0.207	0.205	0.205
0.2125	0.240	0.238	0.235	0.233	0.231	0.229	0.227	0.225	0.223	0.223
0.21575	0.250	0.248	0.246	0.244	0.242	0.240	0.238	0.236	0.234	0.234
0.21425	0.258	0.256	0.254	0.252	0.250	0.248	0.246	0.245	0.243	0.243
0.21275	0.264	0.262	0.260	0.258	0.256	0.255	0.253	0.251	0.249	0.249
0.21125	0.270	0.268	0.266	0.264	0.262	0.260	0.258	0.256	0.255	0.255
0.20975	0.275	0.272	0.270	0.268	0.266	0.264	0.262	0.261	0.259	0.259
0.20825	0.278	0.276	0.274	0.272	0.270	0.268	0.266	0.264	0.262	0.262
0.20675	0.282	0.279	0.277	0.275	0.273	0.271	0.269	0.267	0.265	0.265
0.20525	0.284	0.282	0.279	0.277	0.275	0.273	0.271	0.269	0.267	0.267
0.20375	0.286	0.284	0.281	0.279	0.277	0.275	0.273	0.271	0.269	0.269
0.20225	0.288	0.285	0.282	0.280	0.278	0.276	0.274	0.272	0.270	0.270
0.20075	0.288	0.285	0.283	0.280	0.278	0.276	0.274	0.272	0.270	0.270
0.2000	0.288	0.285	0.283	0.280	0.278	0.276	0.274	0.272	0.270	0.270

Table 5.6(a) Nitrogen mass fraction (Diffusion flame model)

[illegible]

Table 5.6(b) Nitrogen mass fraction (Diffusion flame model)

y (m) x	0.192	0.192	0.193	0.194	0.195	0.195	0.196	0.197	0.198	0.198
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.725	0.725	0.724	0.724	0.724	0.723	0.723	0.722	0.721	0.720
0.02025	0.744	0.744	0.744	0.744	0.744	0.744	0.744	0.743	0.743	0.742
0.01875	0.747	0.748	0.748	0.748	0.748	0.748	0.748	0.748	0.747	0.747
0.01725	0.750	0.751	0.751	0.751	0.751	0.751	0.751	0.750	0.750	0.750
0.01575	0.752	0.753	0.753	0.753	0.753	0.753	0.753	0.753	0.752	0.752
0.01425	0.754	0.755	0.755	0.755	0.755	0.755	0.755	0.754	0.754	0.754
0.01275	0.756	0.757	0.757	0.757	0.757	0.756	0.756	0.756	0.755	0.755
0.01125	0.758	0.758	0.758	0.758	0.758	0.758	0.758	0.757	0.757	0.756
0.00975	0.760	0.760	0.760	0.760	0.759	0.759	0.759	0.758	0.758	0.757
0.00825	0.762	0.762	0.761	0.761	0.761	0.760	0.760	0.759	0.759	0.758
0.00675	0.763	0.763	0.763	0.762	0.762	0.761	0.761	0.760	0.760	0.759
0.00525	0.765	0.764	0.764	0.763	0.763	0.762	0.761	0.761	0.760	0.760
0.00375	0.766	0.766	0.765	0.764	0.763	0.763	0.762	0.761	0.761	0.760
0.00225	0.767	0.767	0.766	0.765	0.764	0.763	0.762	0.762	0.761	0.760
0.00075	0.768	0.767	0.766	0.765	0.764	0.763	0.763	0.762	0.761	0.760
0.0000	0.768	0.767	0.766	0.765	0.764	0.763	0.763	0.762	0.761	0.760

Table 5.6(c) Nitrogen mass fraction (Diffusion flame model)

y (m) x	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.720	0.726	0.724	0.722	0.719	0.717	0.714	0.711	0.708	0.708
0.02025	0.742	0.741	0.740	0.739	0.738	0.737	0.736	0.735	0.734	0.734
0.01875	0.746	0.746	0.745	0.745	0.744	0.744	0.743	0.743	0.742	0.742
0.01725	0.749	0.749	0.749	0.748	0.748	0.747	0.747	0.746	0.746	0.746
0.01575	0.752	0.751	0.751	0.750	0.750	0.749	0.749	0.749	0.748	0.748
0.01425	0.753	0.753	0.752	0.752	0.752	0.751	0.751	0.750	0.750	0.750
0.01275	0.755	0.754	0.754	0.753	0.753	0.753	0.752	0.752	0.751	0.751
0.01125	0.756	0.755	0.755	0.755	0.754	0.754	0.753	0.753	0.753	0.753
0.00975	0.757	0.756	0.756	0.756	0.755	0.755	0.754	0.754	0.754	0.754
0.00825	0.758	0.757	0.757	0.756	0.756	0.755	0.755	0.755	0.754	0.754
0.00675	0.758	0.758	0.757	0.757	0.756	0.756	0.756	0.755	0.755	0.755
0.00525	0.759	0.758	0.758	0.757	0.757	0.757	0.756	0.756	0.755	0.755
0.00375	0.759	0.759	0.758	0.758	0.757	0.757	0.756	0.756	0.756	0.756
0.00225	0.760	0.759	0.759	0.758	0.758	0.757	0.757	0.756	0.756	0.756
0.00075	0.760	0.759	0.759	0.758	0.758	0.757	0.757	0.756	0.756	0.756
0.0000	0.760	0.759	0.759	0.758	0.758	0.757	0.757	0.756	0.756	0.756

Table 5.7(c) Fuel mass fraction (Diffusion flame model)

[illegible]

Table 5.8(a) Product mass fraction (Diffusion flame model)

$y \text{ (m)}$	x	0.000	0.005	0.016	0.027	0.038	0.048	0.059	0.070	0.080	0.091
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.000	0.267	0.273	0.277	0.280	0.270	0.254	0.245	0.242	0.204	
0.02025	0.000	0.271	0.278	0.259	0.224	0.201	0.186	0.176	0.169	0.151	
0.01875	0.000	0.273	0.280	0.232	0.197	0.174	0.459	0.148	0.141	0.129	
0.01725	0.000	0.274	0.274	0.215	0.179	0.156	0.140	0.130	0.122	0.113	
0.01575	0.000	0.275	0.262	0.200	0.164	0.140	0.125	0.114	0.107	0.100	
0.01425	0.000	0.275	0.247	0.185	0.149	0.126	0.110	0.100	0.093	0.087	
0.01275	0.000	0.276	0.225	0.168	0.132	0.110	0.096	0.086	0.080	0.076	
0.01125	0.000	0.276	0.195	0.142	0.111	0.092	0.080	0.072	0.068	0.064	
0.00975	0.000	0.237	0.142	0.103	0.082	0.070	0.062	0.058	0.055	0.051	
0.00825	0.000	0.075	0.060	0.052	0.048	0.045	0.043	0.042	0.041	0.041	
0.00675	0.000	0.004	0.080	0.013	0.017	0.021	0.024	0.027	0.029	0.030	
0.00525	0.000	0.000	0.001	0.003	0.005	0.007	0.011	0.014	0.017	0.020	
0.00375	0.000	0.000	0.000	0.000	0.001	0.002	0.004	0.006	0.009	0.012	
0.00225	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.004	0.007	
0.00075	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.004	
0.0000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.004	

Table 5.8(b) Product mass fraction (Diffusion flame model)

$y \text{ (m)} \times$	0.102	0.112	0.122	0.134	0.145	0.155	0.166	0.177	0.188	0.199
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.193	0.195	0.195	0.197	0.199	0.202	0.206	0.211	0.217	0.224
0.02025	0.143	0.141	0.140	0.140	0.140	0.141	0.143	0.145	0.148	0.151
0.01875	0.122	0.120	0.118	0.117	0.117	0.118	0.119	0.121	0.123	0.125
0.01725	0.107	0.104	0.103	0.102	0.102	0.102	0.103	0.105	0.107	0.109
0.01575	0.095	0.092	0.090	0.090	0.090	0.090	0.091	0.093	0.095	0.097
0.01425	0.083	0.081	0.080	0.079	0.079	0.080	0.081	0.083	0.085	0.087
0.01275	0.072	0.071	0.070	0.070	0.070	0.071	0.073	0.074	0.077	0.079
0.01125	0.062	0.061	0.060	0.060	0.062	0.063	0.065	0.067	0.069	0.072
0.00975	0.052	0.051	0.052	0.053	0.054	0.056	0.058	0.061	0.063	0.066
0.00825	0.042	0.042	0.044	0.045	0.047	0.050	0.052	0.055	0.058	0.061
0.00675	0.032	0.034	0.036	0.038	0.041	0.044	0.047	0.051	0.054	0.057
0.00525	0.023	0.026	0.029	0.032	0.036	0.039	0.043	0.047	0.050	0.054
0.00375	0.016	0.019	0.023	0.027	0.031	0.036	0.040	0.044	0.047	0.051
0.00225	0.010	0.014	0.019	0.023	0.028	0.033	0.037	0.042	0.045	0.049
0.00075	0.007	0.011	0.016	0.021	0.027	0.032	0.036	0.041	0.045	0.049
0.0000	0.007	0.011	0.016	0.021	0.027	0.032	0.036	0.041	0.045	0.049

Table 5.8(c) Product mass fraction (Diffusion flame model)

$y \text{ (m)} \times$	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.233	0.243	0.255	0.268	0.280	0.279	0.278	0.277	0.276	0.276
0.02025	0.155	0.160	0.165	0.170	0.175	0.180	0.186	0.192	0.199	0.199
0.01875	0.128	0.131	0.134	0.137	0.140	0.143	0.147	0.150	0.154	0.154
0.01725	0.111	0.114	0.116	0.119	0.121	0.124	0.127	0.129	0.132	0.132
0.01575	0.099	0.101	0.104	0.106	0.108	0.111	0.113	0.115	0.118	0.118
0.01425	0.089	0.091	0.094	0.096	0.099	0.101	0.103	0.105	0.107	0.107
0.01275	0.081	0.083	0.086	0.088	0.091	0.093	0.095	0.097	0.099	0.099
0.01125	0.074	0.077	0.080	0.082	0.084	0.086	0.089	0.090	0.093	0.093
0.00975	0.069	0.071	0.074	0.076	0.079	0.081	0.083	0.085	0.088	0.088
0.00825	0.064	0.067	0.069	0.072	0.074	0.077	0.079	0.081	0.083	0.083
0.00675	0.060	0.063	0.066	0.068	0.071	0.073	0.076	0.078	0.080	0.080
0.00525	0.057	0.060	0.063	0.066	0.068	0.071	0.073	0.075	0.077	0.077
0.00375	0.054	0.058	0.061	0.063	0.066	0.069	0.071	0.073	0.076	0.076
0.00225	0.053	0.056	0.059	0.062	0.065	0.067	0.070	0.072	0.074	0.074
0.00075	0.052	0.053	0.058	0.061	0.064	0.067	0.069	0.071	0.074	0.074
0.0000	0.052	0.053	0.058	0.061	0.064	0.067	0.069	0.071	0.074	0.074

Table 5.9(a) Axial velocity (m/s) (Turbulent diffusion flame model)

y (m) $\times$	0.107	0.118	0.129	0.139	0.150	0.161	0.171	0.182	0.193	0.204
0.0225	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.02175	19.00	26.71	33.83	40.38	46.38	51.83	56.74	61.09	64.93	68.34
0.02025	26.83	34.00	40.63	46.75	52.39	57.56	62.26	66.48	70.29	73.76
0.01875	33.36	39.86	45.89	51.48	56.64	61.38	65.72	69.64	73.21	76.48
0.01725	40.54	46.21	51.50	56.43	60.99	65.21	69.08	72.60	75.84	78.83
0.01575	48.58	53.27	57.69	61.84	65.70	69.29	72.62	75.68	78.51	81.16
0.01425	57.47	61.06	64.49	67.74	70.81	73.68	76.39	78.91	81.29	83.56
0.01275	67.16	69.51	71.84	74.14	76.25	78.14	80.06	82.00	84.17	86.02
0.01125	77.55	78.56	79.64	80.78	81.96	83.18	84.46	85.77	87.10	88.50
0.00975	88.49	88.03	87.78	87.73	87.85	88.13	88.60	89.23	90.01	90.95
0.00825	99.71	97.74	96.08	94.75	93.74	93.03	92.66	92.59	92.80	93.27
0.00675	110.9	107.4	104.3	101.6	99.42	97.71	96.49	95.73	95.38	95.39
0.00525	121.4	116.5	112.0	108.0	104.6	101.9	99.90	98.51	97.64	97.22
0.00375	130.5	124.5	118.8	113.5	109.1	105.4	102.7	100.8	99.46	98.70
0.00225	137.4	130.7	123.9	117.6	112.3	108.0	104.7	102.3	100.7	99.73
0.00075	141.0	134.0	126.7	119.8	114.0	109.3	105.7	103.2	101.4	100.3
0.0000	141.0	134.0	126.7	119.8	114.0	109.3	105.7	103.2	101.4	100.3

Table 5.9(b) Axial velocity (m/s) (Turbulent diffusion flame model)

y (m) $\times$	0.107	0.118	0.129	0.139	0.150	0.161	0.171	0.182	0.193	0.204
0.0225	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.02175	19.00	26.71	33.83	40.38	46.38	51.83	56.74	61.09	64.93	68.34
0.02025	26.83	34.00	40.63	46.75	52.39	57.56	62.26	66.48	70.29	73.76
0.01875	33.36	39.86	45.89	51.48	56.64	61.38	65.72	69.64	73.21	76.48
0.01725	40.54	46.21	51.50	56.43	60.99	65.21	69.08	72.60	75.84	78.83
0.01575	48.58	53.27	57.69	61.84	65.70	69.29	72.62	75.68	78.51	81.16
0.01425	57.47	61.06	64.49	67.74	70.81	73.68	76.39	78.91	81.29	83.56
0.01275	67.16	69.51	71.84	74.14	76.25	78.14	80.06	82.00	84.17	86.02
0.01125	77.55	78.56	79.64	80.78	81.96	83.18	84.46	85.77	87.10	88.50
0.00975	88.49	88.03	87.78	87.73	87.85	88.13	88.60	89.23	90.01	90.95
0.00825	99.71	97.74	96.08	94.75	93.74	93.03	92.66	92.59	92.80	93.27
0.00675	110.9	107.4	104.3	101.6	99.42	97.71	96.49	95.73	95.38	95.39
0.00525	121.4	116.5	112.0	108.0	104.6	101.9	99.90	98.51	97.64	97.22
0.00375	130.5	124.5	118.8	113.5	109.1	105.4	102.7	100.8	99.46	98.70
0.00225	137.4	130.7	123.9	117.6	112.3	108.0	104.7	102.3	100.7	99.73
0.00075	141.0	134.0	126.7	119.8	114.0	109.3	105.7	103.2	101.4	100.3
0.0000	141.0	134.0	126.7	119.8	114.0	109.3	105.7	103.2	101.4	100.3

Table 5.9(c) Axial velocity (m. s) (Turbulent diffusion flame model)

0.0100	0.214	0.225	0.236	0.246	0.257	0.268	0.279	0.289	0.300
0.0225	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
0.0350	0.425	0.430	0.435	0.440	0.445	0.450	0.455	0.460	0.465
0.0475	0.532	0.535	0.538	0.541	0.544	0.547	0.550	0.553	0.556
0.0600	0.640	0.642	0.644	0.646	0.648	0.650	0.652	0.654	0.656
0.0725	0.748	0.750	0.752	0.754	0.756	0.758	0.760	0.762	0.764
0.0850	0.856	0.858	0.860	0.862	0.864	0.866	0.868	0.870	0.872
0.0975	0.964	0.966	0.968	0.970	0.972	0.974	0.976	0.978	0.980
0.1100	1.072	1.074	1.076	1.078	1.080	1.082	1.084	1.086	1.088
0.1225	1.180	1.182	1.184	1.186	1.188	1.190	1.192	1.194	1.196
0.1350	1.288	1.290	1.292	1.294	1.296	1.298	1.300	1.302	1.304
0.1475	1.396	1.398	1.400	1.402	1.404	1.406	1.408	1.410	1.412
0.1600	1.504	1.506	1.508	1.510	1.512	1.514	1.516	1.518	1.520
0.1725	1.612	1.614	1.616	1.618	1.620	1.622	1.624	1.626	1.628
0.1850	1.720	1.722	1.724	1.726	1.728	1.730	1.732	1.734	1.736
0.1975	1.828	1.830	1.832	1.834	1.836	1.838	1.840	1.842	1.844
0.2100	1.936	1.938	1.940	1.942	1.944	1.946	1.948	1.950	1.952
0.2225	2.044	2.046	2.048	2.050	2.052	2.054	2.056	2.058	2.060
0.2350	2.152	2.154	2.156	2.158	2.160	2.162	2.164	2.166	2.168
0.2475	2.260	2.262	2.264	2.266	2.268	2.270	2.272	2.274	2.276
0.2600	2.368	2.370	2.372	2.374	2.376	2.378	2.380	2.382	2.384
0.2725	2.476	2.478	2.480	2.482	2.484	2.486	2.488	2.490	2.492
0.2850	2.584	2.586	2.588	2.590	2.592	2.594	2.596	2.598	2.600
0.2975	2.692	2.694	2.696	2.698	2.700	2.702	2.704	2.706	2.708
0.3100	2.800	2.802	2.804	2.806	2.808	2.810	2.812	2.814	2.816
0.3225	2.908	2.910	2.912	2.914	2.916	2.918	2.920	2.922	2.924
0.3350	3.016	3.018	3.020	3.022	3.024	3.026	3.028	3.030	3.032
0.3475	3.124	3.126	3.128	3.130	3.132	3.134	3.136	3.138	3.140
0.3600	3.232	3.234	3.236	3.238	3.240	3.242	3.244	3.246	3.248
0.3725	3.340	3.342	3.344	3.346	3.348	3.350	3.352	3.354	3.356
0.3850	3.448	3.450	3.452	3.454	3.456	3.458	3.460	3.462	3.464
0.3975	3.556	3.558	3.560	3.562	3.564	3.566	3.568	3.570	3.572
0.4100	3.664	3.666	3.668	3.670	3.672	3.674	3.676	3.678	3.680
0.4225	3.772	3.774	3.776	3.778	3.780	3.782	3.784	3.786	3.788
0.4350	3.880	3.882	3.884	3.886	3.888	3.890	3.892	3.894	3.896
0.4475	3.988	3.990	3.992	3.994	3.996	3.998	4.000	4.002	4.004
0.4600	4.096	4.098	4.100	4.102	4.104	4.106	4.108	4.110	4.112
0.4725	4.204	4.206	4.208	4.210	4.212	4.214	4.216	4.218	4.220
0.4850	4.312	4.314	4.316	4.318	4.320	4.322	4.324	4.326	4.328
0.4975	4.420	4.422	4.424	4.426	4.428	4.430	4.432	4.434	4.436
0.5100	4.528	4.530	4.532	4.534	4.536	4.538	4.540	4.542	4.544
0.5225	4.636	4.638	4.640	4.642	4.644	4.646	4.648	4.650	4.652
0.5350	4.744	4.746	4.748	4.750	4.752	4.754	4.756	4.758	4.760
0.5475	4.852	4.854	4.856	4.858	4.860	4.862	4.864	4.866	4.868
0.5600	4.960	4.962	4.964	4.966	4.968	4.970	4.972	4.974	4.976
0.5725	5.068	5.070	5.072	5.074	5.076	5.078	5.080	5.082	5.084
0.5850	5.176	5.178	5.180	5.182	5.184	5.186	5.188	5.190	5.192
0.5975	5.284	5.286	5.288	5.290	5.292	5.294	5.296	5.298	5.300
0.6100	5.392	5.394	5.396	5.398	5.400	5.402	5.404	5.406	5.408
0.6225	5.500	5.502	5.504	5.506	5.508	5.510	5.512	5.514	5.516
0.6350	5.608	5.610	5.612	5.614	5.616	5.618	5.620	5.622	5.624
0.6475	5.716	5.718	5.720	5.722	5.724	5.726	5.728	5.730	5.732
0.6600	5.824	5.826	5.828	5.830	5.832	5.834	5.836	5.838	5.840
0.6725	5.932	5.934	5.936	5.938	5.940	5.942	5.944	5.946	5.948
0.6850	6.040	6.042	6.044	6.046	6.048	6.050	6.052	6.054	6.056
0.6975	6.148	6.150	6.152	6.154	6.156	6.158	6.160	6.162	6.164
0.7100	6.256	6.258	6.260	6.262	6.264	6.266	6.268	6.270	6.272
0.7225	6.364	6.366	6.368	6.370	6.372	6.374	6.376	6.378	6.380
0.7350	6.472	6.474	6.476	6.478	6.480	6.482	6.484	6.486	6.488
0.7475	6.580	6.582	6.584	6.586	6.588	6.590	6.592	6.594	6.596
0.7600	6.688	6.690	6.692	6.694	6.696	6.698	6.700	6.702	6.704
0.7725	6.796	6.798	6.800	6.802	6.804	6.806	6.808	6.810	6.812
0.7850	6.904	6.906	6.908	6.910	6.912	6.914	6.916	6.918	6.920
0.7975	7.012	7.014	7.016	7.018	7.020	7.022	7.024	7.026	7.028
0.8100	7.120	7.122	7.124	7.126	7.128	7.130	7.132	7.134	7.136
0.8225	7.228	7.230	7.232	7.234	7.236	7.238	7.240	7.242	7.244
0.8350	7.336	7.338	7.340	7.342	7.344	7.346	7.348	7.350	7.352
0.8475	7.444	7.446	7.448	7.450	7.452	7.454	7.456	7.458	7.460
0.8600	7.552	7.554	7.556	7.558	7.560	7.562	7.564	7.566	7.568
0.8725	7.660	7.662	7.664	7.666	7.668	7.670	7.672	7.674	7.676
0.8850	7.768	7.770	7.772	7.774	7.776	7.778	7.780	7.782	7.784
0.8975	7.876	7.878	7.880	7.882	7.884	7.886	7.888	7.890	7.892
0.9100	7.984	7.986	7.988	7.990	7.992	7.994	7.996	7.998	8.000
0.9225	8.092	8.094	8.096	8.098	8.100	8.102	8.104	8.106	8.108
0.9350	8.200	8.202	8.204	8.206	8.208	8.210	8.212	8.214	8.216
0.9475	8.308	8.310	8.312	8.314	8.316	8.318	8.320	8.322	8.324
0.9600	8.416	8.418	8.420	8.422	8.424	8.426	8.428	8.430	8.432
0.9725	8.524	8.526	8.528	8.530	8.532	8.534	8.536	8.538	8.540
0.9850	8.632	8.634	8.636	8.638	8.640	8.642	8.644	8.646	8.648
0.9975	8.740	8.742	8.744	8.746	8.748	8.750	8.752	8.754	8.756
1.0100	8.848	8.850	8.852	8.854	8.856	8.858	8.860	8.862	8.864
1.0225	8.956	8.958	8.960	8.962	8.964	8.966	8.968	8.970	8.972
1.0350	9.064	9.066	9.068	9.070	9.072	9.074	9.076	9.078	9.080
1.0475	9.172	9.174	9.176	9.178	9.180	9.182	9.184	9.186	9.188
1.0600	9.280	9.282	9.284	9.286	9.288	9.290	9.292	9.294	9.296
1.0725	9.388	9.390	9.392	9.394	9.396	9.398	9.400	9.402	9.404
1.0850	9.496	9.498	9.500	9.502	9.504	9.506	9.508	9.510	9.512
1.0975	9.604	9.606	9.608	9.610	9.612	9.614	9.616	9.618	9.620
1.1100	9.712	9.714	9.716	9.718	9.720	9.722	9.724	9.726	9.728
1.1225	9.820	9.822	9.824	9.826	9.828	9.830	9.832	9.834	9.836
1.1350	9.928	9.930	9.932	9.934	9.936	9.938	9.940	9.942	9.944
1.1475	10.036	10.038	10.040	10.042	10.044	10.046	10.048	10.050	10.052
1.1600	10.144	10.146	10.148	10.150	10.152	10.154	10.156	10.158	10.160
1.1725	10.252	10.254	10.256	10.258	10.260	10.262	10.264	10.266	10.268
1.1850	10.360	10.362	10.364	10.366	10.368	10.370	10.372	10.374	10.376
1.1975	10.468	10.470	10.472	10.474	10.476	10.478	10.480	10.482	10.484
1.2100	10.576	10.578	10.580	10.582	10.584	10.586	10.588	10.590	10.592
1.2225	10.684	10.686	10.688	10.690	10.692	10.694	10.696	10.698	10.700
1.2350	10.792	10.794	10.796	10.798	10.800	10.802	10.804	10.806	10.808
1.2475	10.900	10.902	10.904	10.906	10.908	10.910	10.912	10.914	10.916
1.2600	11.008	11.010	11.012	11.014	11.016	11.018	11.020	11.022	11.024
1.2725	11.116	11.118	11.120	11.122	11.124	11.126	11.128	11.130	11.132
1.2850	11.224	11.226	11.228	11.230	11.232	11.234	11.236	11.238	11.240
1.2975	11.332	11.334	11.336	11.338	11.340	11.342	11.344	11.346	11.348
1.3100	11.440	11.442	11.444	11.446	11.448	11.450	11.452	11.454	11.456
1.3225	11.548	11.550	11.552	11.554	11.556	11.558	11.560	11.562	11.564
1.3350	11.656	11.658	11.660	11.662	11.664	11.666	11.668	11.670	11.672
1.3475	11.764	11.766	11.768	11.770	11.772	11.774	11.776	11.778	11.780
1.3600	11.872	11.874	11.876	11.878	11.880	11.882	11.884	11.886	11.888
1.3725	11.980	11.982	11.984	11.986	11.988	11.990	11.992	11.994	11.996
1.3850	12.088	12.090	12.092	12.094	12.096	12.098	12.100	12.102	12.104
1.3975	12.196	12.198	12.200	12.202	12.204	12.206	12.208	12.210	12.212
1.4100	12.304	12.306	12.308	12.310	12.312	12.314	12.316	12.318	12.320
1.4225	12.412	12.414	12.416	12.418	12.420	12.422	12.424	12.426	12.428
1.4350	12.520	12.522	12.524	12.526	12.528	12.530	12.532	12.534	12.536
1.4475	12.628	12.630	12.632	12.634	12.636	12.638	12.640	12.642	12.644

Table 5.10(a) Radial velocity (m/s) (Turbulent diffusion flame model)

[illegible]

Table 5.10(b) Radial velocity (m/s) (Turbulent diffusion flame model)

0.1225	0.266	0.365	0.464	0.563	0.663	0.763	0.863	0.964	1.065
0.1210	0.242	0.345	0.451	0.558	0.664	0.770	0.874	0.980	1.087
0.1195	0.249	0.356	0.465	0.572	0.679	0.786	0.891	0.996	1.103
0.1180	0.231	0.347	0.459	0.568	0.676	0.783	0.888	0.993	1.099
0.1165	0.249	0.355	0.463	0.571	0.678	0.785	0.890	0.995	1.100
0.1150	0.270	0.378	0.487	0.595	0.703	0.810	0.916	1.022	1.128
0.1135	0.286	0.395	0.505	0.614	0.722	0.829	0.935	1.041	1.147
0.1120	0.295	0.405	0.516	0.625	0.733	0.840	0.945	1.051	1.157
0.1105	0.312	0.423	0.535	0.644	0.752	0.858	0.963	1.068	1.174
0.1090	0.328	0.440	0.553	0.662	0.770	0.876	0.981	1.086	1.192
0.1075	0.339	0.452	0.566	0.675	0.783	0.888	0.993	1.098	1.204
0.1060	0.347	0.461	0.576	0.685	0.793	0.898	1.003	1.108	1.214
0.1045	0.361	0.476	0.592	0.701	0.809	0.914	1.019	1.124	1.230
0.1030	0.368	0.484	0.601	0.710	0.818	0.923	1.028	1.133	1.239
0.1015	0.377	0.495	0.613	0.722	0.830	0.935	1.040	1.145	1.251
0.1000	0.386	0.507	0.620	0.732	0.840	0.945	1.050	1.155	1.261

Table 5.10(c) Radial velocity (m/s) (Turbulent diffusion flame model)

[illegible]

Table 5.11(a) Temperature (K) (Turbulent diffusion flame model)

γ (°) $\times$	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	800	800	800	800	800	800	800	800	800	800
0.02175	2404	2404	2298	2137	2035	1971	1937	1939	1969	1973
0.02025	2225	2225	2066	1861	1733	1651	1603	1581	1579	1496
0.01875	2054	2054	1867	1742	1604	1515	1461	1431	1419	1362
0.01725	2217	2217	1997	1854	1638	1414	1256	1122	1037	1267
0.01575	2189	2189	1831	1575	1423	1225	1065	1230	1212	1134
0.01425	2169	2169	1751	1494	1338	1239	1179	1144	1126	1039
0.01275	2155	2155	1645	1398	1244	1148	1085	1052	1035	1022
0.01125	2084	2084	1508	1268	1129	1038	989	963	947	941
0.00975	1653	1653	1262	1070	970	909	877	862	859	862
0.00825	906	906	820	783	764	754	752	755	764	777
0.00675	300	357	423	485	539	582	614	640	668	694
0.00525	300	306	324	351	387	431	479	523	566	606
0.00375	300	300	303	312	326	349	382	423	472	522
0.00225	300	300	300	302	307	317	333	362	402	454
0.00075	300	300	300	300	302	307	317	335	367	416
0.0000	300	300	300	300	302	307	317	335	367	416

Table 5.11(b) Temperature (K) (Turbulent diffusion flame model)

γ (°) $\times$	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	800	800	800	800	800	800	800	800	880	800
0.02175	1789	1804	1822	1843	1867	1895	1927	1962	2000	2039
0.02025	1480	1483	1492	1505	1522	1542	1564	1589	1616	1644
0.01875	1351	1351	1358	1369	1384	1401	1422	1444	1467	1491
0.01725	1255	1255	1261	1272	1287	1305	1325	1347	1369	1393
0.01575	1173	1173	1181	1193	1209	1227	1248	1271	1294	1317
0.01425	1091	1093	1109	1123	1141	1161	1184	1207	1231	1255
0.01275	1018	1023	1035	1051	1072	1095	1127	1153	1178	1203
0.01125	942	956	972	992	1015	1041	1069	1105	1132	1159
0.00975	870	885	905	930	964	993	1023	1054	1083	1120
0.00825	795	820	847	877	910	950	984	1016	1048	1079
0.00675	721	753	787	829	867	905	949	985	1019	1051
0.00525	646	691	735	780	829	873	914	959	995	1029
0.00375	577	631	689	743	795	847	892	933	977	1012
0.00225	516	584	650	715	772	829	876	919	965	1001
0.00075	482	557	629	700	761	820	868	913	959	995
0.0000	482	557	629	700	761	820	868	913	959	995

Table 5.11(c) Temperature (K) (Turbulent diffusion flame model)

y (m) $\times$	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	800	800	800	800	800	800	800	800	880	900
0.02175	2080	2120	2160	2197	2232	2262	2289	2310	2325	2325
0.02025	1672	1702	1731	1760	1788	1815	1841	1864	1885	1885
0.01875	1515	1539	1564	1587	1611	1633	1654	1673	1692	1692
0.01725	1415	1439	1461	1483	1505	1526	1545	1563	1581	1581
0.01575	1340	1363	1386	1408	1429	1449	1469	1486	1504	1504
0.01425	1279	1303	1325	1348	1369	1389	1409	1427	1445	1445
0.01275	1228	1252	1275	1298	1320	1341	1360	1379	1398	1398
0.01125	1184	1209	1234	1257	1279	1300	1320	1339	1359	1359
0.00975	1147	1173	1198	1222	1245	1267	1287	1307	1326	1326
0.00825	1116	1143	1169	1193	1217	1239	1260	1280	1300	1300
0.00675	1081	1118	1145	1170	1194	1217	1238	1258	1278	1278
0.00525	1060	1099	1126	1152	1176	1199	1221	1241	1261	1261
0.00375	1045	1075	1112	1138	1163	1186	1208	1229	1249	1249
0.00225	1034	1065	1103	1129	1154	1177	1200	1221	1241	1241
0.00075	1029	1060	1098	1125	1150	1173	1195	1216	1237	1237
0.0000	1029	1060	1098	1125	1150	1173	1195	1216	1237	1237

Table 5.12(a) Oxygen mass fraction (Turbulent diffusion flame model)

$y \text{ (m)} \times$	0.000	0.005	0.016	0.027	0.038	0.048	0.059	0.070	0.080	0.091
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.000	0.016	0.035	0.054	0.066	0.073	0.077	0.076	0.073	0.094
0.02025	0.000	0.031	0.062	0.086	0.100	0.108	0.113	0.115	0.115	0.124
0.01875	0.000	0.038	0.074	0.100	0.114	0.122	0.128	0.130	0.131	0.137
0.01725	0.000	0.043	0.083	0.109	0.124	0.133	0.138	0.141	0.142	0.146
0.01575	0.000	0.047	0.091	0.118	0.133	0.142	0.147	0.150	0.151	0.154
0.01425	0.000	0.049	0.100	0.127	0.141	0.150	0.155	0.158	0.160	0.162
0.01275	0.000	0.052	0.112	0.137	0.151	0.159	0.164	0.167	0.168	0.169
0.01125	0.000	0.063	0.127	0.149	0.161	0.169	0.173	0.175	0.176	0.176
0.00975	0.000	0.113	0.150	0.167	0.175	0.180	0.183	0.184	0.184	0.193
0.00825	0.000	0.182	0.188	0.191	0.193	0.193	0.193	0.193	0.192	0.190
0.00675	0.231	0.226	0.220	0.215	0.211	0.207	0.205	0.202	0.200	0.197
0.00525	0.231	0.230	0.229	0.227	0.224	0.220	0.216	0.212	0.208	0.205
0.00375	0.231	0.231	0.231	0.230	0.229	0.227	0.224	0.220	0.216	0.212
0.00225	0.231	0.231	0.231	0.231	0.230	0.230	0.228	0.226	0.222	0.218
0.00075	0.231	0.231	0.231	0.231	0.230	0.230	0.229	0.228	0.225	0.221
0.0000	0.231	0.231	0.231	0.231	0.230	0.230	0.229	0.228	0.225	0.221

Table 5.12(b) Oxygen mass fraction (Turbulent diffusion flame model)

$y \text{ (m)} \times$	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.092	0.090	0.088	0.085	0.083	0.079	0.076	0.072	0.067	0.063
0.02025	0.124	0.124	0.123	0.121	0.119	0.117	0.115	0.112	0.109	0.106
0.01875	0.137	0.137	0.136	0.135	0.133	0.131	0.129	0.127	0.124	0.122
0.01725	0.147	0.147	0.146	0.144	0.143	0.141	0.139	0.136	0.134	0.131
0.01575	0.155	0.154	0.153	0.152	0.150	0.148	0.146	0.144	0.141	0.139
0.01425	0.162	0.162	0.160	0.159	0.157	0.155	0.152	0.150	0.147	0.145
0.01275	0.169	0.168	0.167	0.165	0.163	0.161	0.158	0.155	0.152	0.150
0.01125	0.176	0.174	0.173	0.171	0.168	0.166	0.163	0.159	0.157	0.154
0.00975	0.182	0.180	0.179	0.176	0.173	0.170	0.167	0.164	0.161	0.158
0.00825	0.189	0.186	0.184	0.181	0.178	0.174	0.171	0.167	0.164	0.161
0.00675	0.195	0.192	0.189	0.185	0.181	0.178	0.174	0.170	0.167	0.164
0.00525	0.201	0.197	0.193	0.189	0.185	0.181	0.177	0.173	0.169	0.166
0.00375	0.207	0.202	0.197	0.192	0.188	0.183	0.179	0.175	0.171	0.167
0.00225	0.212	0.206	0.201	0.195	0.190	0.184	0.180	0.176	0.172	0.168
0.00075	0.215	0.209	0.202	0.196	0.191	0.185	0.181	0.177	0.172	0.169
0.0000	0.215	0.209	0.202	0.196	0.191	0.185	0.181	0.177	0.172	0.169

Table 5.12(c) Oxygen mass fraction (Turbulent diffusion flame model)

y	x	0.000	0.005	0.010	0.015	0.020	0.025	0.030	0.035	0.040	0.045
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.058	0.053	0.048	0.043	0.039	0.034	0.030	0.027	0.024	0.024	0.024
0.02025	0.103	0.100	0.096	0.093	0.090	0.087	0.084	0.081	0.078	0.078	0.078
0.01875	0.119	0.116	0.114	0.111	0.109	0.106	0.104	0.101	0.099	0.099	0.099
0.01725	0.129	0.127	0.124	0.122	0.119	0.117	0.115	0.113	0.111	0.111	0.111
0.01575	0.136	0.134	0.132	0.129	0.127	0.125	0.123	0.121	0.119	0.119	0.119
0.01425	0.142	0.140	0.138	0.136	0.133	0.131	0.129	0.127	0.125	0.125	0.125
0.01275	0.147	0.145	0.142	0.140	0.138	0.136	0.133	0.131	0.129	0.129	0.129
0.01125	0.151	0.149	0.146	0.144	0.142	0.139	0.137	0.135	0.133	0.133	0.133
0.00975	0.155	0.152	0.150	0.147	0.145	0.143	0.141	0.139	0.137	0.137	0.137
0.00825	0.158	0.155	0.152	0.150	0.148	0.145	0.143	0.141	0.139	0.139	0.139
0.00675	0.161	0.157	0.155	0.152	0.150	0.147	0.145	0.143	0.142	0.142	0.142
0.00525	0.163	0.159	0.156	0.154	0.151	0.149	0.147	0.145	0.143	0.143	0.143
0.00375	0.164	0.161	0.158	0.155	0.153	0.150	0.148	0.146	0.144	0.144	0.144
0.00225	0.165	0.162	0.159	0.156	0.154	0.151	0.149	0.147	0.145	0.145	0.145
0.00075	0.166	0.163	0.159	0.156	0.154	0.152	0.149	0.147	0.145	0.145	0.145
0.00000	0.166	0.163	0.159	0.156	0.154	0.152	0.149	0.147	0.145	0.145	0.145

Table 5.13(a) Nitrogen mass fraction (Turbulent diffusion flame model)

y	x	0.000	0.005	0.010	0.015	0.020	0.025	0.030	0.035	0.040	0.045
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.000	0.665	0.684	0.698	0.705	0.709	0.711	0.711	0.709	0.720	0.720
0.02025	0.000	0.678	0.700	0.712	0.719	0.723	0.725	0.726	0.726	0.731	0.731
0.01875	0.000	0.684	0.706	0.717	0.724	0.728	0.731	0.732	0.732	0.735	0.735
0.01725	0.000	0.687	0.710	0.721	0.728	0.732	0.735	0.736	0.737	0.739	0.739
0.01575	0.000	0.690	0.713	0.725	0.732	0.736	0.738	0.740	0.740	0.742	0.742
0.01425	0.000	0.692	0.717	0.729	0.735	0.739	0.741	0.743	0.743	0.744	0.744
0.01275	0.000	0.693	0.722	0.733	0.739	0.743	0.745	0.746	0.746	0.747	0.747
0.01125	0.000	0.698	0.728	0.738	0.743	0.746	0.748	0.749	0.749	0.750	0.750
0.00975	0.000	0.722	0.738	0.745	0.749	0.751	0.752	0.752	0.752	0.752	0.752
0.00825	0.000	0.750	0.753	0.754	0.755	0.756	0.756	0.756	0.755	0.755	0.755
0.00675	0.769	0.767	0.765	0.764	0.762	0.761	0.760	0.759	0.759	0.758	0.758
0.00525	0.769	0.769	0.768	0.767	0.767	0.765	0.764	0.763	0.762	0.760	0.760
0.00375	0.769	0.769	0.769	0.769	0.768	0.768	0.767	0.766	0.764	0.763	0.763
0.00225	0.769	0.769	0.769	0.769	0.769	0.768	0.768	0.767	0.766	0.765	0.765
0.00075	0.769	0.769	0.769	0.769	0.769	0.769	0.768	0.768	0.767	0.766	0.766
0.00000	0.769	0.769	0.769	0.769	0.769	0.769	0.768	0.768	0.767	0.766	0.766

Table 5.13(b) Nitrogen mass fraction (Turbulent diffusion flame model)

γ (m) $\times$	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.719	0.719	0.719	0.718	0.717	0.716	0.714	0.712	0.710	0.708
0.02025	0.731	0.731	0.731	0.730	0.730	0.729	0.728	0.727	0.726	0.724
0.01875	0.736	0.736	0.736	0.735	0.735	0.734	0.734	0.732	0.732	0.731
0.01725	0.739	0.739	0.739	0.739	0.738	0.738	0.737	0.736	0.735	0.735
0.01575	0.742	0.742	0.742	0.742	0.741	0.741	0.740	0.739	0.738	0.737
0.01425	0.745	0.745	0.745	0.744	0.744	0.743	0.742	0.741	0.741	0.740
0.01275	0.747	0.747	0.747	0.747	0.746	0.745	0.744	0.743	0.743	0.742
0.01125	0.749	0.750	0.749	0.749	0.748	0.747	0.746	0.745	0.744	0.743
0.00975	0.752	0.752	0.751	0.750	0.751	0.749	0.748	0.747	0.746	0.745
0.00825	0.755	0.754	0.753	0.752	0.753	0.750	0.749	0.748	0.747	0.746
0.00675	0.757	0.756	0.755	0.754	0.754	0.752	0.750	0.749	0.748	0.747
0.00525	0.759	0.758	0.757	0.755	0.755	0.753	0.751	0.750	0.749	0.748
0.00375	0.761	0.760	0.758	0.757	0.756	0.754	0.752	0.751	0.750	0.748
0.00225	0.763	0.761	0.759	0.758	0.756	0.754	0.753	0.751	0.750	0.749
0.00075	0.764	0.762	0.760	0.758	0.756	0.754	0.753	0.751	0.750	0.749
0.0000	0.764	0.762	0.760	0.758	0.756	0.754	0.753	0.751	0.750	0.749

Table 5.13(c) Nitrogen mass fraction (Turbulent diffusion flame model)

γ (m) $\times$	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.705	0.702	0.699	0.695	0.691	0.687	0.683	0.679	0.674	0.674
0.02025	0.723	0.721	0.720	0.718	0.716	0.714	0.712	0.710	0.708	0.708
0.01875	0.730	0.728	0.727	0.726	0.725	0.723	0.722	0.721	0.719	0.719
0.01725	0.734	0.733	0.732	0.730	0.729	0.728	0.727	0.726	0.725	0.725
0.01575	0.736	0.736	0.735	0.734	0.733	0.732	0.730	0.730	0.729	0.729
0.01425	0.739	0.738	0.737	0.736	0.735	0.734	0.733	0.732	0.732	0.732
0.01275	0.741	0.740	0.739	0.738	0.737	0.736	0.735	0.735	0.734	0.734
0.01125	0.742	0.741	0.741	0.740	0.739	0.738	0.737	0.736	0.735	0.735
0.00975	0.744	0.743	0.742	0.741	0.740	0.739	0.738	0.738	0.737	0.737
0.00825	0.745	0.744	0.743	0.742	0.741	0.740	0.740	0.738	0.738	0.738
0.00675	0.746	0.745	0.744	0.743	0.742	0.741	0.740	0.740	0.739	0.739
0.00525	0.747	0.746	0.745	0.744	0.743	0.742	0.741	0.740	0.739	0.739
0.00375	0.747	0.746	0.745	0.745	0.743	0.742	0.742	0.741	0.740	0.740
0.00225	0.748	0.747	0.746	0.745	0.744	0.743	0.742	0.741	0.740	0.740
0.00075	0.748	0.747	0.746	0.745	0.744	0.743	0.742	0.741	0.740	0.740
0.0000	0.748	0.747	0.746	0.745	0.744	0.743	0.742	0.741	0.740	0.740

Table 5.14(a) Fuel mass fraction (Turbulent diffusion flame model)

y (m) x	0.0	0.005	0.016	0.027	0.038	0.048	0.059	0.070	0.080	0.091
0.0225	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02175	0.999	0.981	0.959	0.946	0.940	0.936	0.934	0.934	0.936	0.927
0.02025	0.999	0.966	0.946	0.935	0.931	0.928	0.926	0.925	0.926	0.922
0.01875	0.999	0.961	0.941	0.932	0.927	0.924	0.923	0.922	0.921	0.919
0.01725	0.999	0.957	0.938	0.929	0.925	0.922	0.920	0.919	0.919	0.917
0.01575	0.999	0.955	0.936	0.927	0.922	0.920	0.918	0.917	0.916	0.915
0.01425	0.999	0.953	0.933	0.925	0.920	0.917	0.916	0.915	0.914	0.914
0.01275	0.999	0.952	0.930	0.922	0.918	0.915	0.914	0.913	0.912	0.912
0.01125	0.999	0.948	0.925	0.919	0.915	0.913	0.912	0.911	0.911	0.910
0.00975	0.999	0.931	0.919	0.914	0.912	0.910	0.910	0.909	0.909	0.909
0.00825	0.999	0.911	0.909	0.908	0.908	0.907	0.907	0.907	0.907	0.907
0.00675	0.999	0.909	0.902	0.903	0.903	0.904	0.905	0.905	0.905	0.906
0.00525	0.999	0.902	0.905	0.908	0.901	0.902	0.902	0.903	0.904	0.904
0.00375	0.999	0.900	0.902	0.904	0.905	0.907	0.901	0.902	0.901	0.903
0.00225	0.999	0.900	0.900	0.902	0.903	0.904	0.906	0.908	0.901	0.902
0.00075	0.999	0.900	0.900	0.901	0.902	0.903	0.904	0.905	0.908	0.901
0.0000	0.999	0.900	0.900	0.901	0.902	0.903	0.904	0.905	0.908	0.901

Table 5.14(b) Fuel mass fraction (Turbulent diffusion flame model)

y (m) x	0.102	0.112	0.123	0.134	0.145	0.155	0.166	0.177	0.188	0.198
0.0225	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02175	0.027	0.027	0.027	0.027	0.028	0.029	0.030	0.032	0.033	0.035
0.02025	0.021	0.021	0.021	0.021	0.021	0.022	0.022	0.023	0.024	0.024
0.01875	0.018	0.018	0.018	0.018	0.018	0.019	0.019	0.019	0.020	0.021
0.01725	0.016	0.016	0.016	0.016	0.016	0.016	0.017	0.017	0.018	0.018
0.01575	0.015	0.014	0.014	0.014	0.014	0.015	0.015	0.016	0.016	0.017
0.01425	0.013	0.013	0.013	0.013	0.013	0.013	0.014	0.014	0.015	0.015
0.01275	0.012	0.012	0.011	0.012	0.012	0.012	0.012	0.013	0.013	0.014
0.01125	0.010	0.010	0.010	0.010	0.011	0.011	0.011	0.011	0.012	0.013
0.00975	0.009	0.009	0.009	0.009	0.010	0.010	0.011	0.011	0.012	0.012
0.00825	0.007	0.008	0.008	0.008	0.009	0.009	0.010	0.010	0.011	0.011
0.00675	0.006	0.006	0.007	0.007	0.008	0.008	0.009	0.010	0.010	0.011
0.00525	0.005	0.005	0.006	0.006	0.007	0.008	0.008	0.010	0.010	0.010
0.00375	0.003	0.004	0.005	0.006	0.006	0.007	0.008	0.009	0.009	0.010
0.00225	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.008	0.009	0.010
0.00075	0.002	0.003	0.004	0.005	0.006	0.007	0.007	0.008	0.009	0.009
0.0000	0.002	0.003	0.004	0.005	0.006	0.007	0.007	0.008	0.009	0.009

Table 5.14(c) Fuel mass fraction (Turbulent diffusion flame model)

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Table 5.15(a) Product mass fraction (Turbulent diffusion flame model)

y (mm) x	0.000	0.005	0.016	0.027	0.038	0.048	0.059	0.070	0.080	0.091
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.000	0.238	0.222	0.202	0.189	0.181	0.178	0.178	0.182	0.159
0.02025	0.000	0.224	0.192	0.166	0.150	0.141	0.136	0.134	0.134	0.124
0.01875	0.000	0.210	0.179	0.151	0.135	0.125	0.119	0.116	0.115	0.110
0.01725	0.000	0.212	0.169	0.139	0.123	0.113	0.107	0.104	0.102	0.100
0.01575	0.000	0.208	0.160	0.130	0.113	0.103	0.097	0.094	0.092	0.089
0.01425	0.000	0.206	0.150	0.120	0.103	0.093	0.087	0.084	0.083	0.080
0.01275	0.000	0.203	0.136	0.109	0.093	0.083	0.077	0.074	0.073	0.072
0.01125	0.000	0.190	0.120	0.094	0.080	0.072	0.067	0.065	0.064	0.064
0.00975	0.000	0.134	0.093	0.074	0.064	0.059	0.056	0.055	0.055	0.056
0.00825	0.000	0.057	0.049	0.046	0.045	0.044	0.044	0.045	0.046	0.047
0.00675	0.000	0.006	0.012	0.018	0.024	0.028	0.031	0.033	0.036	0.039
0.00525	0.000	0.000	0.003	0.005	0.009	0.013	0.018	0.022	0.027	0.031
0.00375	0.000	0.000	0.000	0.001	0.003	0.005	0.008	0.013	0.017	0.022
0.00225	0.000	0.000	0.000	0.000	0.000	0.002	0.003	0.006	0.010	0.016
0.00075	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.004	0.007	0.012
0.0000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.004	0.007	0.012

Table 5.15(b) Product mass fraction (Turbulent diffusion flame model)

y (m) x	0.202	0.212	0.223	0.234	0.245	0.255	0.266	0.277	0.288	0.298
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.162	0.164	0.166	0.169	0.172	0.175	0.180	0.185	0.189	0.195
0.02025	0.124	0.124	0.126	0.128	0.130	0.132	0.135	0.138	0.142	0.145
0.01875	0.109	0.109	0.110	0.112	0.114	0.116	0.118	0.121	0.124	0.127
0.01725	0.098	0.098	0.099	0.101	0.103	0.105	0.107	0.110	0.113	0.116
0.01575	0.089	0.089	0.090	0.092	0.094	0.096	0.099	0.102	0.104	0.107
0.01425	0.080	0.080	0.081	0.084	0.087	0.089	0.092	0.095	0.098	0.100
0.01275	0.072	0.073	0.074	0.077	0.079	0.082	0.086	0.089	0.092	0.095
0.01125	0.064	0.066	0.068	0.070	0.073	0.076	0.079	0.084	0.087	0.090
0.00975	0.057	0.059	0.061	0.064	0.068	0.071	0.75	0.078	0.082	0.086
0.00825	0.049	0.052	0.055	0.059	0.062	0.067	0.071	0.074	0.078	0.081
0.00675	0.042	0.045	0.049	0.074	0.058	0.062	0.067	0.071	0.075	0.078
0.00525	0.034	0.039	0.044	0.049	0.054	0.059	0.063	0.068	0.072	0.076
0.00375	0.028	0.034	0.040	0.045	0.051	0.056	0.061	0.066	0.071	0.074
0.00225	0.022	0.029	0.036	0.043	0.049	0.055	0.060	0.064	0.069	0.073
0.00075	0.019	0.026	0.034	0.041	0.047	0.054	0.059	0.064	0.069	0.073
0.0000	0.019	0.026	0.034	0.041	0.047	0.054	0.059	0.064	0.069	0.073

Table 5.15(c) Product mass fraction (Turbulent diffusion flame model)

y (m) x	0.209	0.220	0.230	0.241	0.252	0.263	0.273	0.284	0.295	0.300
0.0225	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02175	0.200	0.205	0.210	0.215	0.219	0.223	0.227	0.230	0.232	0.232
0.02025	0.149	0.152	0.156	0.159	0.163	0.166	0.169	0.172	0.175	0.175
0.01875	0.130	0.133	0.136	0.139	0.142	0.144	0.147	0.149	0.152	0.152
0.01725	0.119	0.121	0.124	0.127	0.129	0.132	0.134	0.137	0.139	0.139
0.01575	0.110	0.113	0.116	0.118	0.121	0.123	0.126	0.128	0.130	0.130
0.01425	0.103	0.106	0.109	0.111	0.114	0.116	0.119	0.121	0.123	0.123
0.01275	0.098	0.100	0.103	0.106	0.109	0.111	0.114	0.116	0.118	0.118
0.01125	0.093	0.096	0.099	0.101	0.104	0.107	0.109	0.111	0.114	0.114
0.00975	0.089	0.092	0.095	0.098	0.100	0.103	0.105	0.108	0.110	0.110
0.00825	0.086	0.089	0.092	0.095	0.097	0.100	0.102	0.105	0.107	0.107
0.00675	0.082	0.086	0.089	0.092	0.095	0.098	0.100	0.102	0.105	0.105
0.00525	0.080	0.084	0.087	0.090	0.093	0.096	0.098	0.101	0.103	0.103
0.00375	0.078	0.081	0.086	0.089	0.092	0.094	0.097	0.099	0.102	0.102
0.00225	0.077	0.080	0.085	0.088	0.091	0.093	0.096	0.098	0.101	0.101
0.00075	0.076	0.080	0.084	0.087	0.090	0.093	0.095	0.098	0.100	0.100
0.0000	0.076	0.080	0.084	0.087	0.090	0.093	0.095	0.098	0.100	0.100

Figure 1.1 Schematic representation of a solid-fuel ramjet , Ref. 5

Figure 1.2 Schematic diagram of an SFRJ combustor showing the fluid dynamic and combustion characteristics , Ref. 40

Figure 1.3 Schematic representation of SFRJ combustion showing the flowfield in the flame stabilization region , Ref. 3

Storage of . axial velocities, u
radial velocities, v
all variables
other than u, v

Figure 2.1 The staggered grid system

Figure 2.2 An elementary control volume

Figure 2.3 Part of the grid system

Figure 3.1 Fuel and oxidizer feeds into the combustion chamber

Figure 3.2 Mass fraction distribution (Diffusion flame model)

r — regression rate

v_w — injection velocity at the wall

ρ_w — density of solid fuel

ρ_f — density of the flow adjacent to the wall

Figure 3.3 Mass balance at the solid fuel wall

Figure 3.4 Mass fraction distribution (Turbulent diffusion flame model)

Figure 3.5 Beta probability density function, Ref. 10

Figure 3.6 Determination of $\frac{\partial f}{\partial r}$ gradient

Figure 4.1 The flow chart

Figure 4.2 The computational grid system

Figure 4.3 Three types of cells

Figure 5.1 Normalized u-velocity field, $\bar{u} = u/u_m$ (Diffusion flame model)

Figure 5.2 Temperature field (K) (Diffusion flame model)

Figure 5.3 Pressure field (N/m^2) (Diffusion flame model)

Figure 5.4 Density field (kg/m^3) (Diffusion flame model)

Figure 5.5 Mixture fraction field (Diffusion flame model)

Figure 5.6 Turbulence kinetic energy field (m^2/s^2). (Diffusion flame model)

Figure 5.7 Turbulence energy dissipation rate field ($10^6 \text{ m}^2/\text{s}^3$)
(Diffusion flame model)

Figure 5.8 Fuel mass fraction field (Diffusion flame model)

Figure 5.9 Oxygen mass fraction field (Diffusion flame model)

Figure 5.10 Product mass fraction field (Diffusion flame model)

Figure 5.11 Nitrogen mass fraction field (Diffusion flame model)

Figure 5 12 Normalized velocity field, $\bar{u} \equiv u/u_m$ (Turbulent diffusion flame model)

Figure 5.13 Temperature field (K) (Turbulent diffusion flame model)

Figure 5.14 Pressure field (N/m^2) (Turbulent diffusion flame model)

Figure 5.15 Density field (kg/m^3) (Turbulent diffusion flame model)

Figure 5.16 Mixture fraction field (Turbulent diffusion flame model)

Figure 5.17 Turbulence kinetic energy field (m^2/s^2)
(Turbulent diffusion flame model)

Figure 5.18 Turbulence energy dissipation rate field ($10^6 \text{ m}^2/\text{s}^3$).
(Turbulent diffusion flame model)

Figure 5.19 Fuel mass fraction field (Turbulent diffusion flame model)

Figure 5.20 Oxygen mass fraction field (Turbulent diffusion flame model)

Figure 5.21 Product mass fraction field (Turbulent diffusion flame model)

Figure 5.22 Nitrogen mass fraction field (Turbulent diffusion flame model)

Figure 5.23 Mass fraction variance field (Turbulent diffusion flame model)

Figure 5.24 A comparison between calculated and observed local mean regression rate data.

Figure 5.25 Calculated and experimental regression rate data in relation to air mass flow (Diffusion flame model)

END

28·0|5·92

FIN