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MODELING OF TURBULENT SUPERSONIC H_2-AIR COMBUSTION WITH AN IMPROVED JOINT BETA PDF

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Abstract

Attempts at modeling recent experiments of Cheng et al.[1] indicated that discrepancies between theory and experiment can be a result of the form of assumed PDF and/or the turbulence model employed.[2] In this investigation, improvements in both the form of the assumed PDF and the turbulence model are presented. The results are again used to compare with measurements. Initial comparisons are encouraging.

Introduction

The successful design of scramjet engines requires the understanding of turbulent mixing and its effect on combustion at supersonic speeds. The availability of detailed measurements of composition and temperature and their variances in H_2-Air supersonic reacting shear layers provides the modeler with useful data to develop the codes that will eventually be used in the design. The first attempt at predicting the data of Ref. 1 indicated needed improvements in the form of the assumed PDF and the turbulence model.

The joint-Beta PDF used in Ref. 2 was developed by Girimaji[3] to study mixing. According to the model, all variances and covariances involving mass fractions depend on their mean values and an additional quantity which is the sum of their variances. Thus, using this PDF requires one additional model equation. The newly developed PDF that is presented below results in independent variances and covariances thus necessitating additional model equations. Because of the above, the present effort limits the joint-Beta PDF to the elemental mass fractions

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and employs a partial equilibrium assumption to relate the minor species to the elemental mass fractions. To accomplish this, an approach similar to that employed by Janicka and Kollmann[4] was used in conjunction with Table 1 (Ref. 5) to determine combined variables whose production rates are independent of the two-body reactions (the first fourteen reactions in Table 1). The minor species, O, H, OH, H_2O_2 and HO_2 are then expressed in terms of the elemental mass fractions and one of the combined variables using an equilibrium assumption.

The New Joint-Beta PDF

The elemental mass fractions obey the relation

$$s = x_1 + x_2 + x_3 = 1 \tag{1}$$

where x_j is the mass fraction of element 'j'. For H_2-air combustion, the PDF is assumed to have the form (reflecting the three elements H_2, O_2, and N_2)

$$F = \frac{1}{c}\left[x_3^{\beta-1}\,(1-x_3)^{\alpha-(\gamma_1+\gamma_2)}\,x_1^{\gamma_1-1}\,x_2^{\gamma_2-1}\,\delta(1-s)\right] \tag{2}$$

where δ is the Dirac delta function and c is a constant determined from a normalization condition. The parameters α, β, γ_1, and γ_2. can be expressed in terms of means, variances, and covariances by taking appropriate moments of the joint PDF, i.e.,

$$\overline{x_1} = \int x_1\, f\, dx_1\, dx_2\, dx_3 = \frac{\alpha}{\alpha+\beta}\,\frac{\gamma_1}{\gamma_1+\gamma_2}$$

$$\overline{x_1'^2} = \int (x_1-\overline{x_1})^2\, f\, dx_1\, dx_2\, dx_3 = \overline{x_1^2} - (\overline{x_1})^2$$

$$\overline{x_1' x_2'} = \int (x_1-\overline{x_1})\,(x_2-\overline{x_2})\, f\, dx_1\, dx_2\, dx_3 = \overline{x_1 x_2} - \overline{x_1}\;\overline{x_2} \tag{3}$$

with

$$\overline{x_1^2} = \frac{\alpha(\alpha+1)}{(\alpha+\beta)(\alpha+\beta+1)} \cdot \frac{\gamma_1(\gamma_1+1)}{(\gamma_1+\gamma_2)(\gamma_1+\gamma_2+1)}$$

$$\overline{x_1 x_2} = \frac{\alpha(\alpha + 1)}{(\alpha + \beta)(\alpha + \beta + 1)} \cdot \frac{\gamma_1 \gamma_2}{(\gamma_1 + \gamma_2)(\gamma_1 + \gamma_2 + 1)} \tag{4}$$

The parameters α, β, γ_1 and γ_2 follow from the expressions for $\overline{x_1} + \overline{x_2}$, $\overline{x_1'^2}$, $\overline{x_2'^2}$, $\overline{x_1' x_2'}$.

The Combined Variables

A general procedure has been developed which makes it possible to take a set of reactions, such as those indicated in Table 1, and determine the combined variables whose production rates are independent of the rates of the two-body reactions. For the set shown in Table 1, the combined variables are

$$\frac{Y^*_{O_2}}{W_{O_2}} = \frac{Y_{O_2}}{W_{O_2}} + \frac{Y_O}{W_O} + \frac{1}{2}\frac{Y_H}{W_H} + \frac{1}{2}\frac{Y_{OH}}{W_{OH}} + \frac{1}{2}\frac{Y_{HO_2}}{W_{HO_2}} \tag{5}$$

$$\frac{Y^*_{H_2}}{W_{H_2}} = \frac{Y_{H_2}}{W_{H_2}} + \frac{Y_O}{W_O} + \frac{3}{2}\frac{Y_H}{W_H} + \frac{1}{2}\frac{Y_{OH}}{W_{OH}} - \frac{1}{2}\frac{Y_{HO_2}}{W_{HO_2}} - \frac{Y_{H_2O_2}}{W_{H_2O_2}} \tag{6}$$

$$\frac{Y^*_{H_2O}}{W_{H_2O}} = \frac{Y_{H_2O}}{W_{H_2O}} - \frac{Y_o}{W_o} - \frac{Y_H}{W_H} + \frac{Y_{HO_2}}{W_{HO_2}} + 2\frac{Y_{H_2O_2}}{W_{H_2O_2}} \tag{7}$$

where W is the molecular weight.

The production rates of the combined variables are given by

$$\dot{w}^*_{O_2} = -W_{O_2}\left[\dot{w}_{15} + \dot{w}_{16} + \dot{w}_{17} - \dot{w}_{18}\right] \tag{8}$$

$$\dot{w}^*_{H_2} = -2W_{H_2}\left[\dot{w}_{15} + \dot{w}_{16} + \dot{w}_{17} - \dot{w}_{18}\right] \tag{9}$$

$$\dot{w}^*_{H_2O} = -2W_{H_2O}\left[\dot{w}_{15} + \dot{w}_{16} + \dot{w}_{17} - \dot{w}_{18}\right] \tag{10}$$

The Proposed Model

The elemental mass fractions, Z_O and Z_H and $Y^*_{H_2O}$, are the three independent quantities for which conservation of mass equations are solved. The remaining mass fractions, Y_O, Y_H, Y_{OH}, Y_{HO_2}, and $Y_{H_2O_2}$, are determined using an equilibrium assumption in terms of Z_O, Z_H, and $Y^*_{H_2O}$. The joint PDF describing temperature and concentration fluctuations is chosen as

$$G(T, Y^*_{H_2O}, Z_O, Z_H, Z_N) = f_1(T)\, f_2(Y^*_{H_2O})\, F(Z_O, Z_H, Z_N) \qquad (11)$$

In the present approach, $f_1(T)$ is a Gaussian PDF, f_2 is a single Beta PDF while F is the joint-Beta PDF indicated in equation (2).

Results and Discussion

A schematic of the experimental setup is shown in Figure 1, and Table 2 gives a summary of the burner exit conditions. Measurements were taken at axial locations of 0.85, 10.8, 32.3, 43.1, 64.7, and 86.1 inner diameters downstream of the burner.

A complex model of the type described above has to be developed step by step. Initial calculations compared the results of a full finite rate kinetic model calculation with those employing a partial equilibrium assumption. These calculations were carried out using a 91 × 91 grid on a domain of 4 × 4 inches. As a result, only comparisons for the first five axial stations are given. Figures 2-4 compare measured and calculated mole fractions of H_2O and OH and the temperature distribution. As is seen from the figures, the partial equilibrium assumption is an acceptable assumption especially at the downstream stations.

The paper will implement the full model and will present detailed comparisons with experiments of Ref. 1.

Acknowledgement

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Tables

Table 1. Chemistry Model

Reaction Number	Reaction	A	b	T_a
1	$H_2 + O_2 \rightarrow OH + OH$	.170E + 14	0.00	24157.0
2	$H + O_2 \rightarrow OH + O$	.120E + 18	-0.91	8310.5
3	$OH + H_2 \rightarrow H_2O + H$	.220E + 14	0.00	2591.8
4	$O + H_2 \rightarrow OH + H$	.506E + 05	2.67	3165.6
5	$OH + OH \rightarrow H_2O + O$	.630E + 13	0.00	548.6
6	$HO_2 + H \rightarrow H_2 + O_2$	.130E + 14	0.00	0.0
7	$HO_2 + H \rightarrow OH + OH$	.150E + 15	0.00	503.3
8	$HO_2 + O \rightarrow O_2 + OH$	.200E + 14	0.00	0.0
9	$HO_2 + OH \rightarrow H_2O + O_2$	.200E + 14	0.00	0.0
10	$HO_2 + H_2 \rightarrow H_2O_2 + H$	.301E + 12	0.00	9411.2
11	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	.200E + 13	0.00	0.0
12	$H + H_2O_2 \rightarrow H_2O + OH$	.100E + 14	0.00	1801.7
13	$O + H_2O_2 \rightarrow HO_2 + OH$	.280E + 14	0.00	3220.9
14	$OH + H_2O_2 \rightarrow H_2O + HO_2$	.700E + 13	0.00	722.2
15	$H + OH + M \rightarrow H_2O + M$	.221E + 23	-2.00	0.0
16	$H + H + M \rightarrow H_2 + M$	.730E + 18	-1.00	0.0
17	$H + O_2 + M \rightarrow HO_2 + M$	.230E + 19	-1.00	0.0
18	$H_2O_2 + M \rightarrow OH + OH + M$	.121E + 18	0.00	22898.8

Units of A are a multiple of $cm^3 \cdot mole^{-1} \cdot s^{-1}$

Table 2. Exit Conditions

Exit Conditions	Hydrogen Jet	Outer Jet	Ambient Air
Mach Number	1.0	2.0	0.0
Temperature, K	545.0	1250.0	300.0
Velocity, m/s	1780.0	1417.0	0.0
Pressure, MPa	0.112	0.107	0.101
Mass Fraction			
Y_{H_2}	1.0	0.0	0.0
Y_{O_2}	0.0	0.245	0.233
Y_{N_2}	0.0	0.580	0.757
Y_{H_2O}	0.0	0.175	0.010

Figures

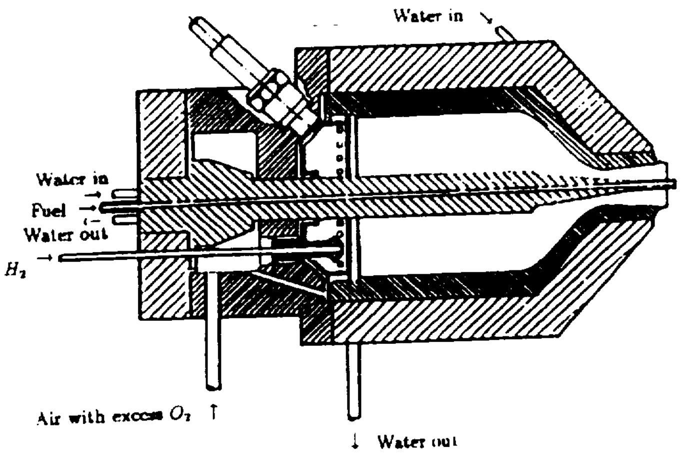

Figure 1: Schematic of test apparatus

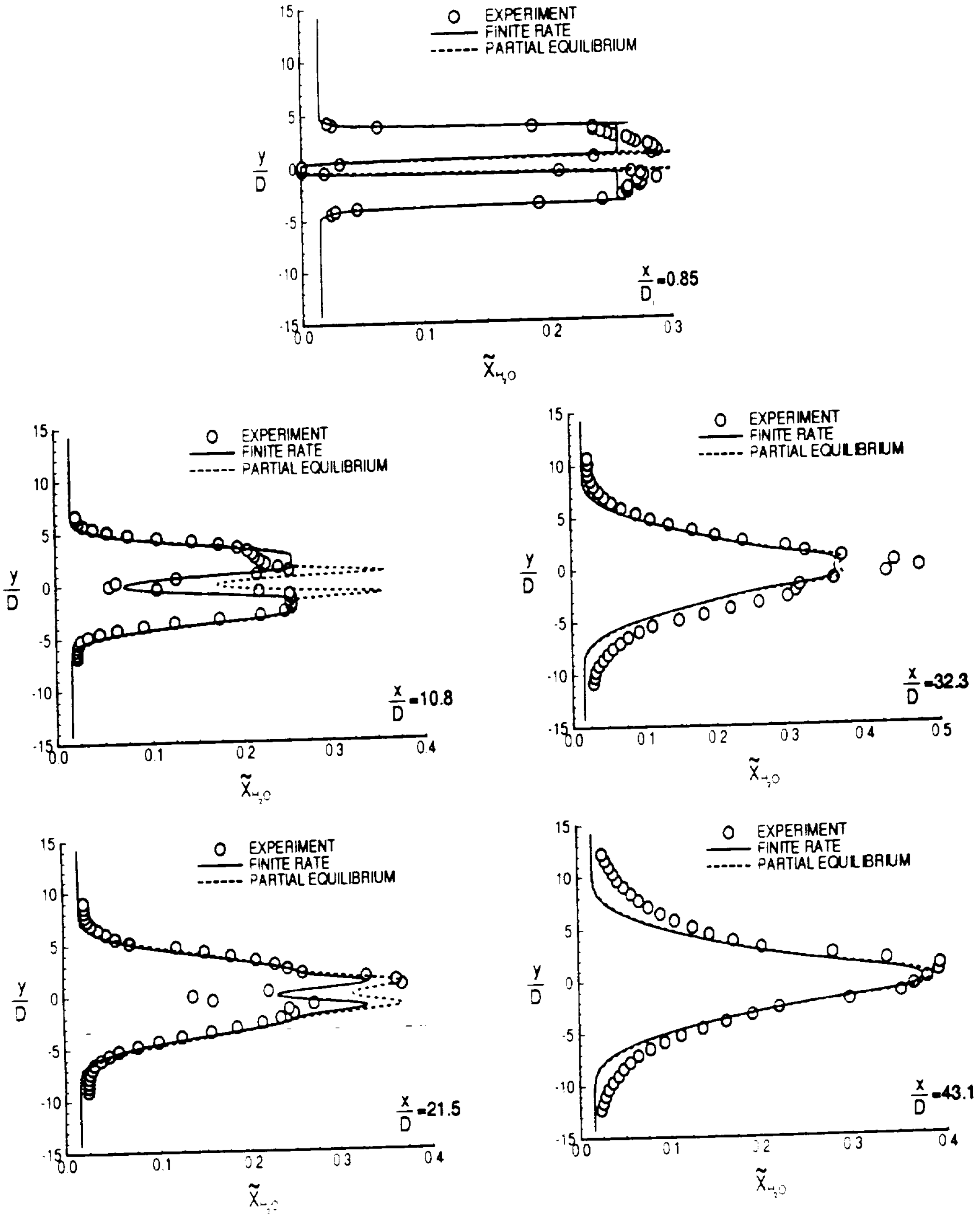

Figure 2: Mean H_2O Mole Fraction Comparisons Between Full Finite Rate Chemistry and Assuming Partial Equilibrium

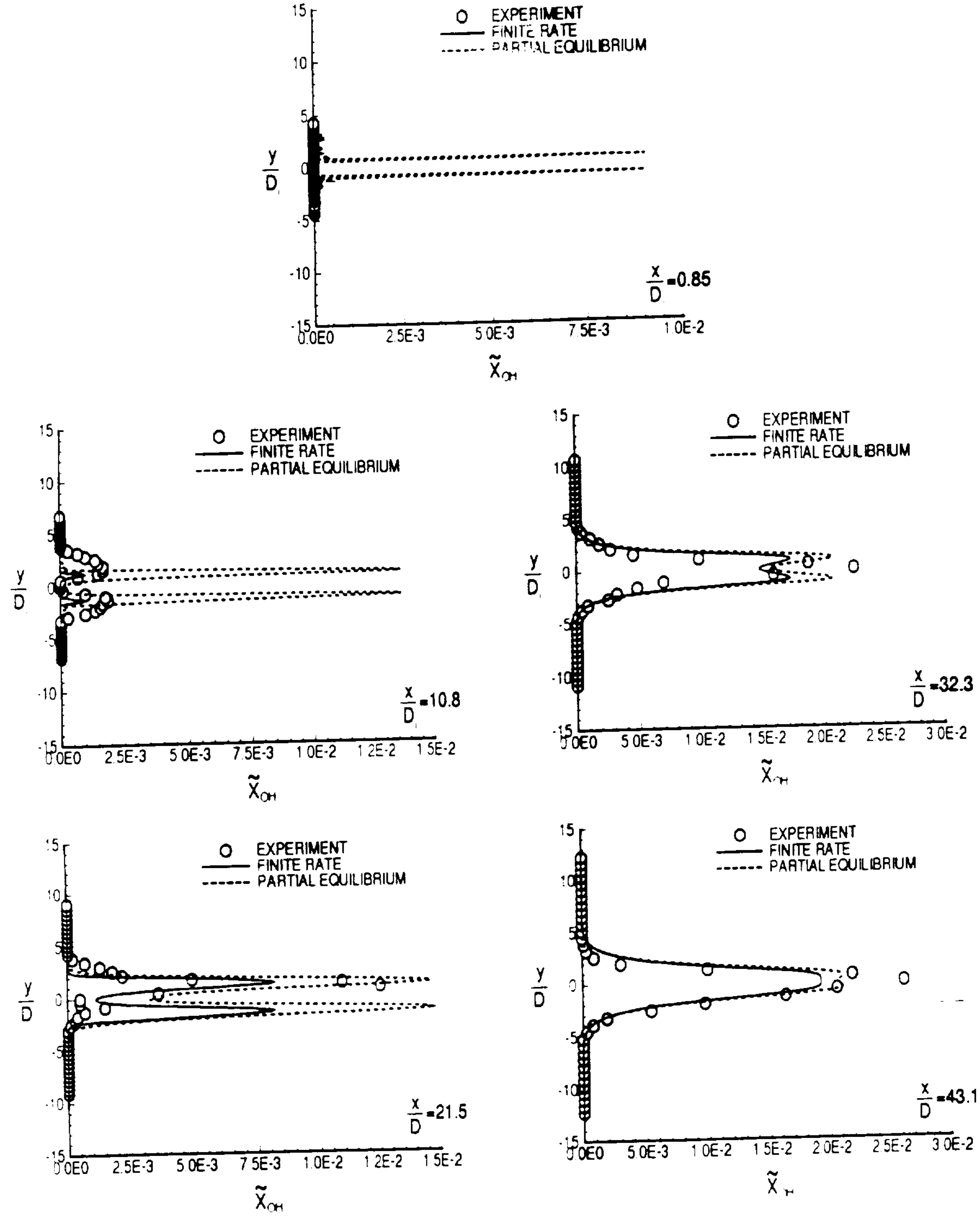

Figure 3: Mean OH Mole Fraction Comparisons Between Full Finite Rate Chemistry and Assuming Partial Equilibrium

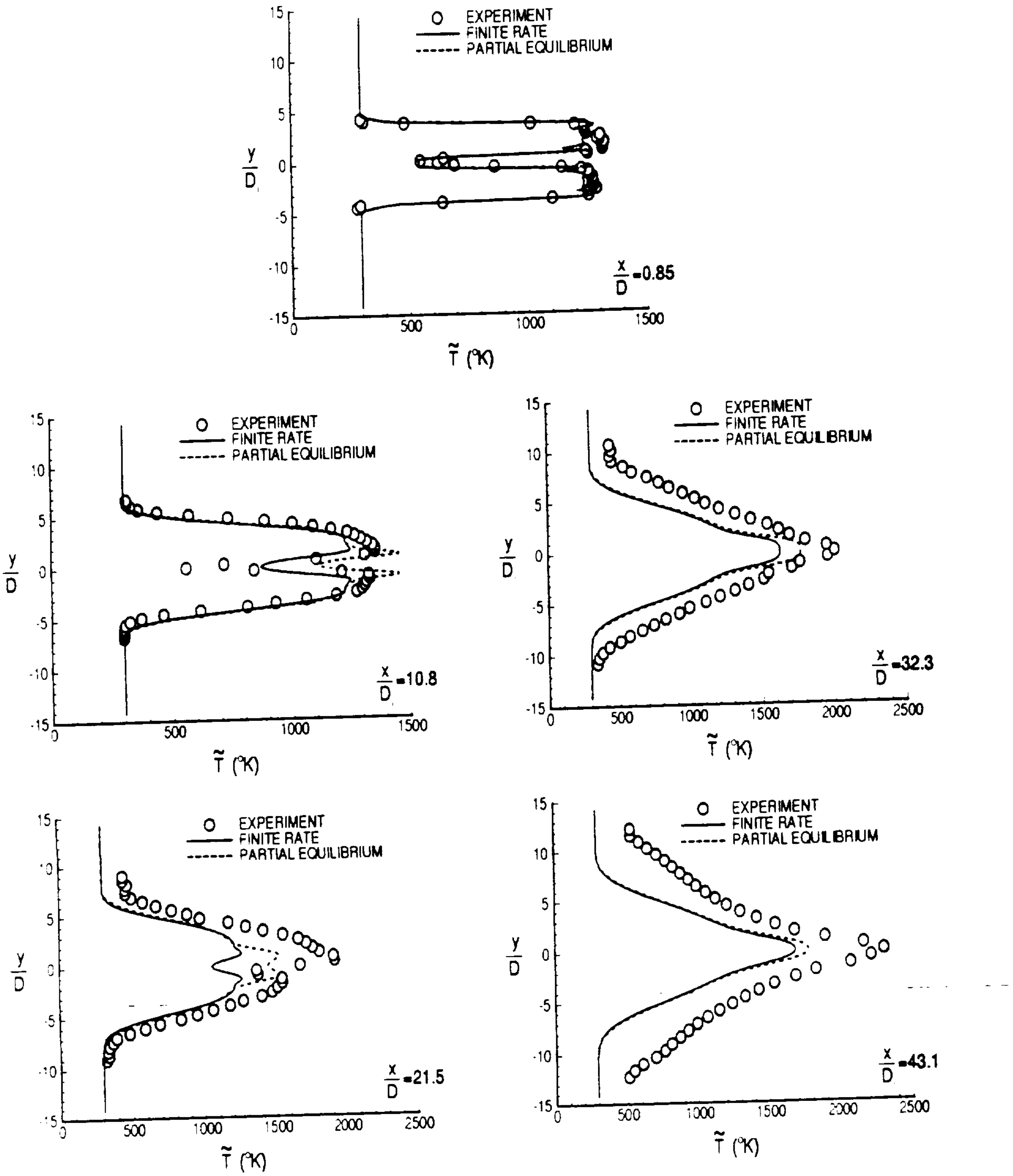

Figure 4: Mean Temperature Comparisons Between Full Finite Rate Chemistry and Assuming Partial Equilibrium