# A k-ω-MULTIVARIATE BETA PDF FOR SUPERSONIC COMBUSTION

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## Introduction

In an attempt to study the interaction between combustion and turbulence in supersonic flows, an assumed PDF has been employed[1,2]. This makes it possible to calculate the time average of the chemical source terms that appear in the species conservation equations as

$$\bar{\dot{w}}_s = \int P(T, Y_1, ..., Y_u)\, \dot{w}_s\, dT\, dY_1 \ldots dY_n \qquad (1)$$

where $\dot{w}_s$ is the production rate of species s, P is the probability density function, T is the temperature and $Y_k$ is the mass faction of species k. The probability density function is assumed to have the form

$$P(T, Y_1, \ldots Y_n) = F_1(T)\, F_2(Y_1, ..., Y_k)$$

where $F_1$ is a Gaussian distribution and $F_2$ is the multivariate PDF developed by Girimaji[3], i.e.,

$$F_2(Y_1 \ldots Y_n) = \frac{1}{c}\, \delta(1 - s) \prod_{k=1}^{n} Y_k^{\beta_k - 1}$$

where

$$s = \Sigma Y_k\,, \quad c = \prod_{k=1}^{n} \Gamma(\beta_n)/\Gamma(\Sigma\beta_k)$$



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$\delta$ is the Dirac delta function, and n is the number of species present. The quantities $\beta_k$ appearing in the PDF can be determined in terms of the mean mass fractions and the sum of their variances, i.e.,

$$\beta_k = \bar{Y}_n\left(\frac{1 - S}{Q} - 1\right) \tag{5}$$

where

$$S = \Sigma(\bar{Y}_k)^2, \quad Q = \Sigma\,\overline{Y_k''^2} \tag{6}$$

In order to determine the averages indicated in equation (1), two transport equations, one for the temperature (enthalpy) variance and one for Q, are required. Model equations are formulated for such quantities and they can be written as

$$\frac{\partial}{\partial t}(\bar{\rho}\,\widetilde{h''^2}) + \frac{\partial}{\partial x_j}(\bar{\rho}\,\tilde{u}_j\,\widetilde{h''^2}) = \frac{\partial}{\partial x_j}\left[\left(\frac{\mu}{\bar{\rho}Pr} + \frac{\mu_t}{\bar{\rho}\,Pr_t}\right)\frac{\partial}{\partial x_j}\left(\bar{\rho}\,\widetilde{h''^2}\right)\right] + 2C_1\,\frac{\mu_t}{Pr}\left(\frac{\partial \tilde{h}}{\partial x_j}\right)^2 - \frac{\bar{\rho}\,\widetilde{h''^2}}{\tau} \tag{7}$$

$$\frac{\partial}{\partial t}(\bar{\rho}\,\bar{Q}) + \frac{\partial}{\partial x_j}(\bar{\rho}\,\tilde{u}_j\,\bar{Q}) = \frac{\partial}{\partial x_j}\left[\bar{\rho}\,(D + D_t)\frac{\partial \bar{Q}}{\partial x_j}\right] + 2\,\bar{\rho}\,D_t\left(\frac{\partial \tilde{Y}_k}{\partial x_j}\right)^2 + 2\Sigma\,\overline{\dot{w}_k Y_k''} - C_Q\,\frac{\bar{\rho}\,\bar{Q}}{\tau} \tag{8}$$

In the above equation D is the diffusion coefficient, $\mu$ is the viscosity, $C_1$ and $C_Q$ are model constants and $\tau$ is the turbulent time scale.

As is seen from equations (7) and (8), the turbulent time scale controls the evolution of both $(\widetilde{T''})^2$ and $\bar{Q}$. An algebraic model similar to that used by Eklund et al.[4] was used in Reference 2 in an attempt to predict the recent measurements of Cheng et al.[5] Predictions were satisfactory before ignition but were less satisfactory after ignition. One of the reasons for this behavior is the inadequacy of the algebraic turbulence model employed. Because of this, the objective of this work is to develop a k-$\omega$ model to remedy the situation.

## Results and Discussion

A full kinetic model based on the work of Jachimowski[6] is employed. It consists of eighteen reactions (Table 1) and allows for the presence of $H_2$, $O_2$, H, O, OH, $H_2O$, $HO_2$, $H_2O_2$ and treats $N_2$ as an inert. 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, 21.5, 32.3, 43.1, 64.7, and 86.1 inner diameters downstream of the burner.

It became evident that traditional model constants in the k-ω model were not appropriate for modeling the experiment under consideration. Because of this, we decided to develop, as a first step, a one-equation turbulence model based on the energy equation and then use it to develop the k-ω model. This first step is now complete.

Figures 2-4 show comparisons of mean temperature, mean $H_2O$, and rms $H_2O$ distributions. As is seen from the figures, there is a need to implement the full k-ω model.

The paper will implement the complete turbulence model and will present detailed comparisons with the measurements of Ref. 5.

## Acknowledgement

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## References

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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. |
| Temperature, K | 545 | 1250 | 300 |
| Velocity, m/s | 1780 | 1417 | 0. |
| Pressure, MPa | .112 | .107 | .101 |
| Mass Fraction | | | |
| $Y_{H_2}$ | 1. | 0. | 0. |
| $Y_{O_2}$ | 0. | .245 | .233 |
| $Y_{N_2}$ | 0. | .58 | .757 |
| $Y_{H_2O}$ | 0. | .175 | 0.01 |

# Figures

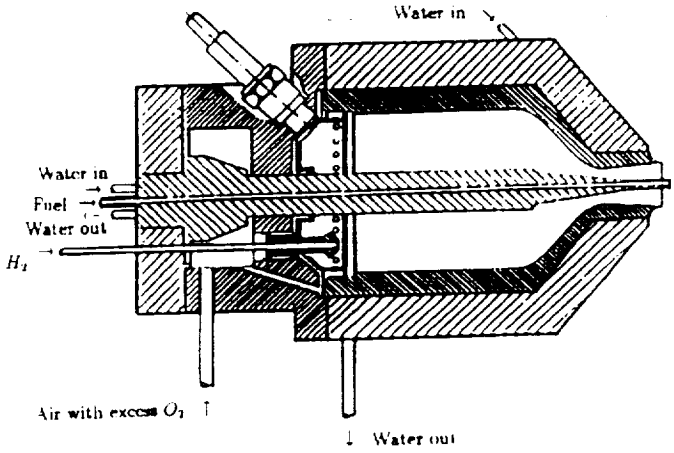


Figure 1: Schematic of test apparatus

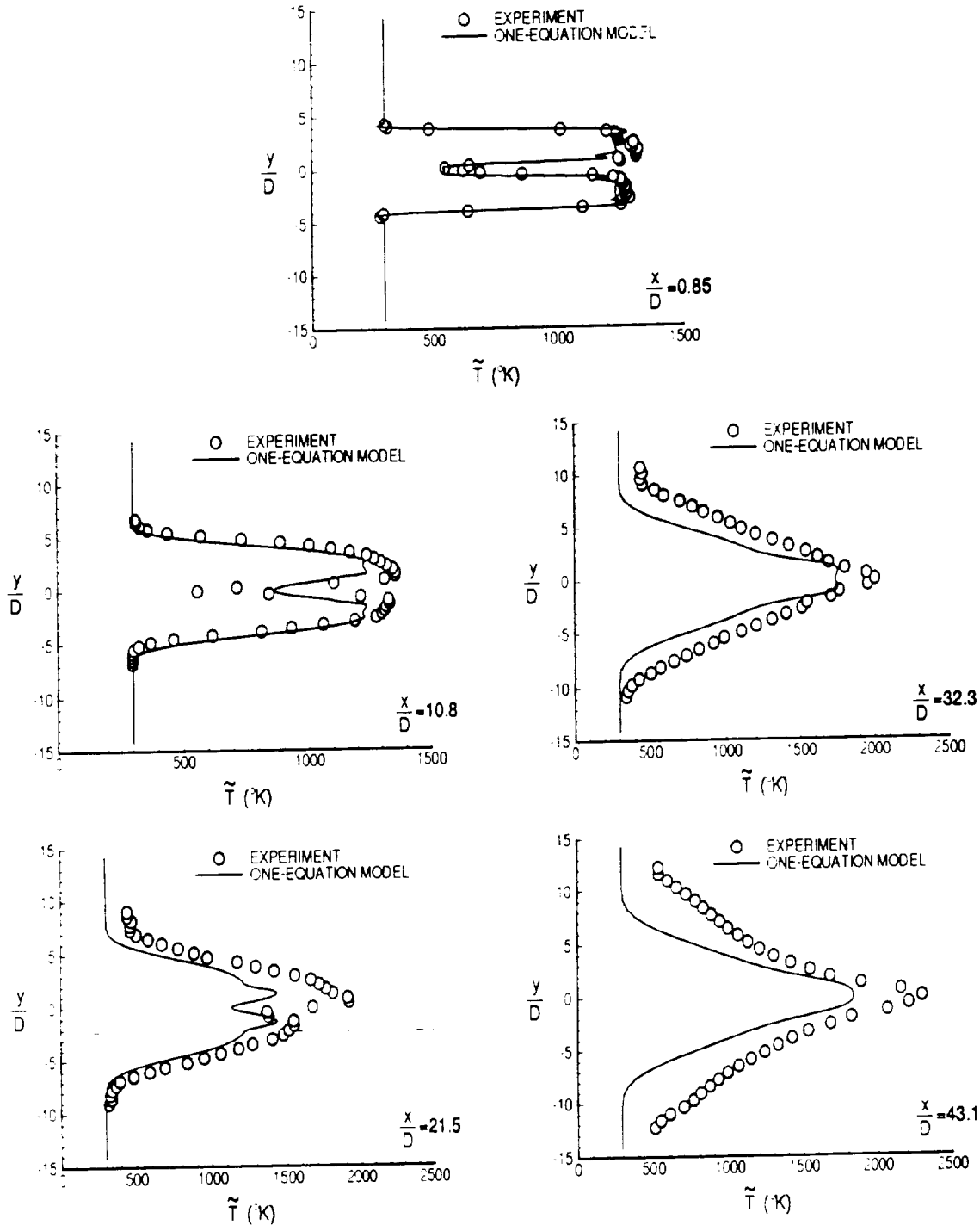


Figure 2: Mean Temperature Comparison With Experiment

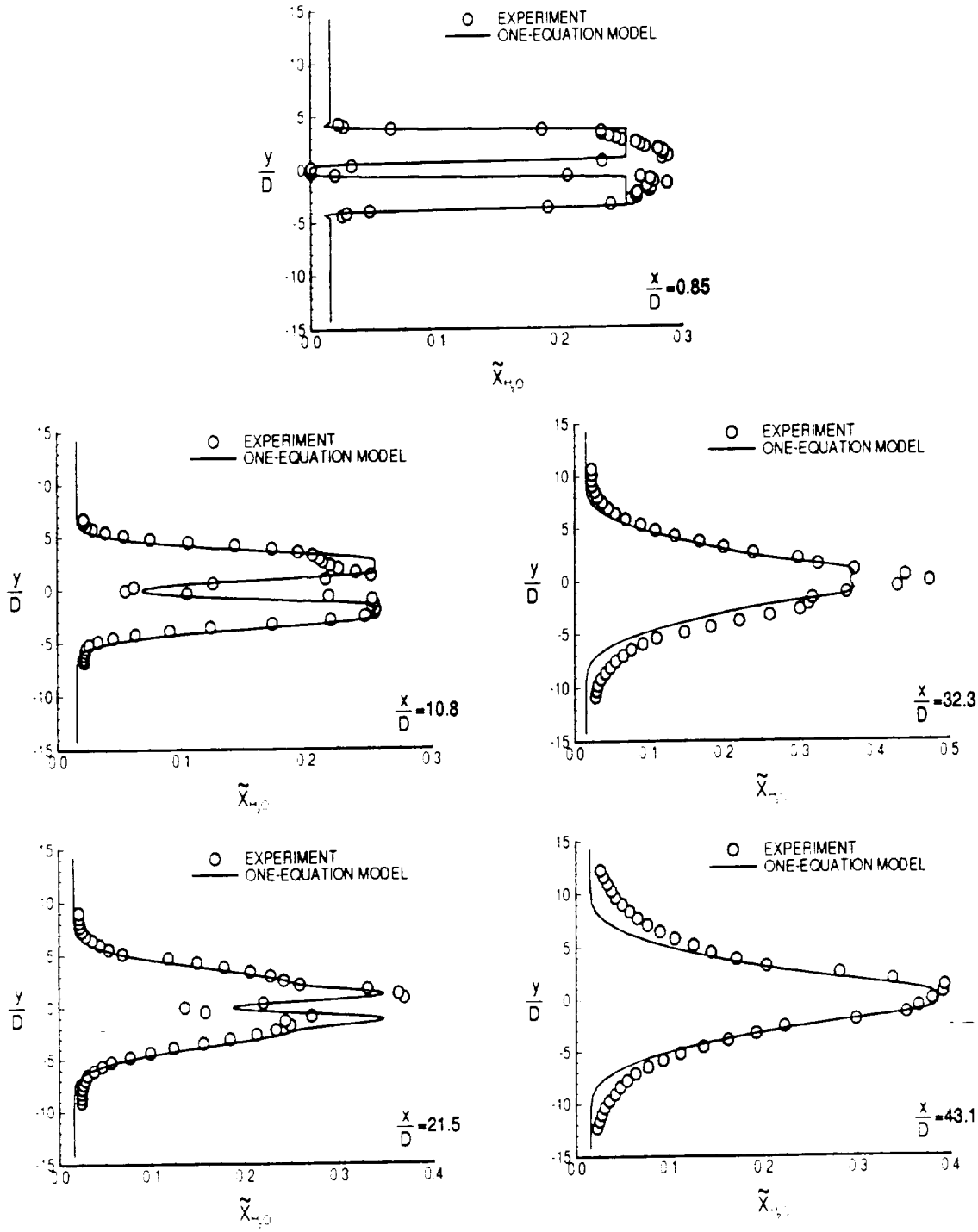


Figure 3: Mean $H_2O$ Mole Fraction Comparison With Experiment

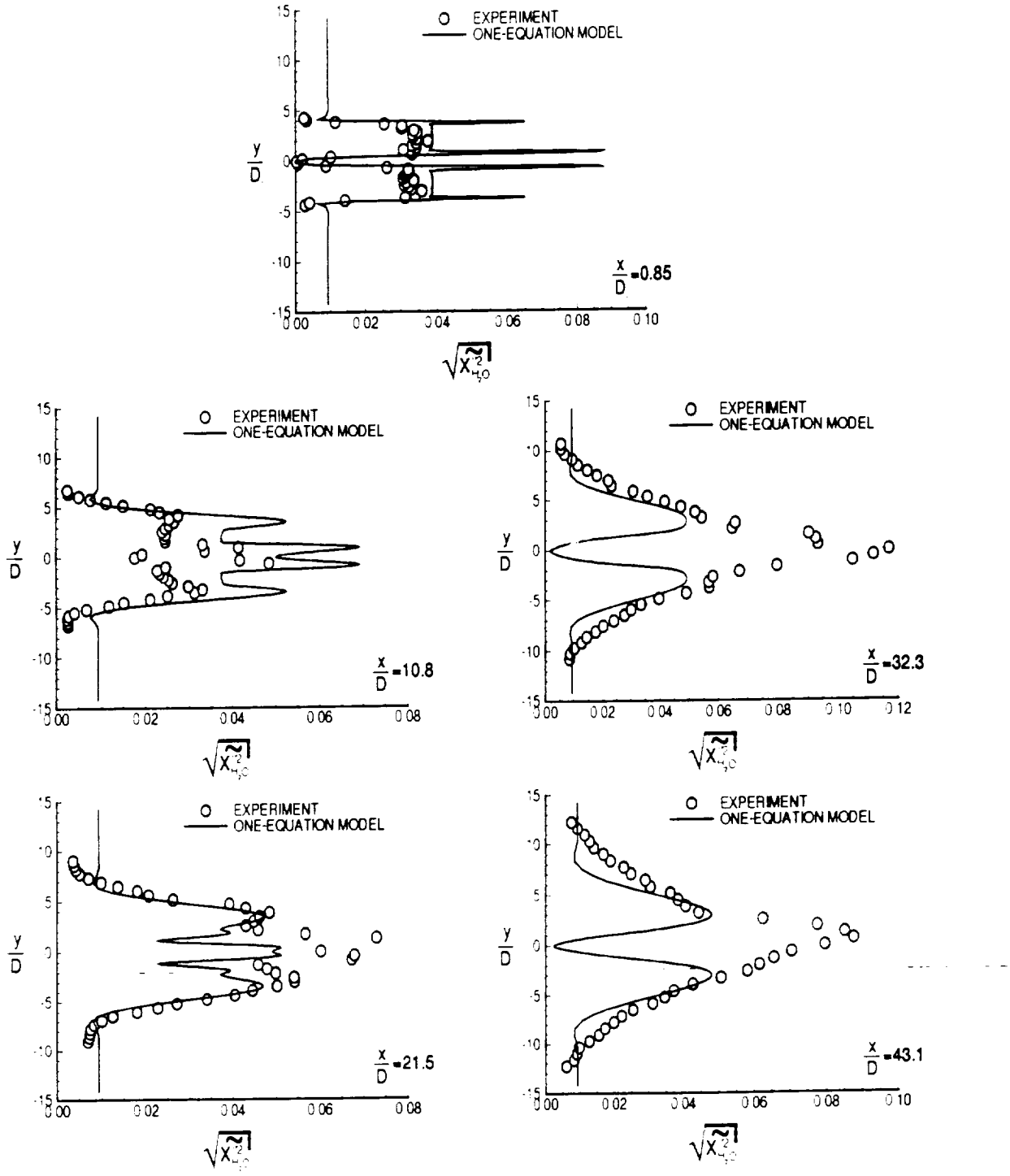


Figure 4: RMS $H_2O$ Mole Fraction Comparison With Experiment