A Numerical Procedure for Analysis of Finite Rate Reacting Flows

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ABSTRACT

Combustion processes in rocket propulsion systems are characterized by the existence of multiple, vastly differing time and length scales, as well as flow-speeds at wide variation of Mach numbers. The chemical kinetics processes in the highly active reaction zone are characterized by much more smaller scales compared to fluid convective and diffusive time scales. An operator splitting procedure for transient finite rate chemistry problems has been developed using a pressure based method, which can be applied to all speed flows without difficulties. The splitting of chemical kinetics terms formed the fluid-mechanical terms of the species equation ameliorated the difficulties associated with the disparate time scales and stiffness in the set of equations which describes highly exothermic combustion. A combined efficient ordinary differential equations (O.D.E.) solver was used to integrate the effective chemical source terms over the residence time at each grid cell. One and two dimensional reacting flow situations were carried out to demonstrate and verify the current procedure. Different chemical kinetics with different degrees of nonlinearity have also been incorporated to test the robustness and generality of the proposed method.

A NUMERICAL PROCEDURE FOR ANALYSIS OF FINITE RATE REACTING FLOWS

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OBJECTIVE

- DEVELOP AN EFFICIENT ALGORITHM FOR FINITE RATE CHEMICAL REACTING FLOWS AT ALL-SPEED
- VALIDATE THE METHODOLOGY AT STEADY AND TRANSIENT FLOWS

BACKGROUND

- ENGINE COMBUSTOR IGNITION PROCESSES
- SHOCK-INDUCED COMBUSTION AND DETONATION
- IGNITION DELAY AND COMBUSTION EFFICIENCY
- SSME AND HYPERSONIC VEHICLE PROPULSION, etc.

NUMERICAL ISSUES

- FAST CHEMISTRY OF H2-O2 SYSTEM
- VERY SMALL CHEMICAL TIME SCALE COMPARE TO FLUID DYNAMICS TIME SCALE
- A SET OF STIFF NON-LINEAR PARTIAL DIFFERENTIAL EQUATIONS
- EXPENSIVE CPU TIME EVEN FOR TWO-DIMENSIONAL STUDY

NUMERICAL APPROACH

FINITE RATE CHEMISTRY MODEL

- **GENERAL SYSTEM OF CHEMICAL REACTION IN TERMS OF MASS FRACTION:**

$$\sum_i \upsilon_{ij} M_i = \sum_i \upsilon'_{ij} M'_i$$

$$\dot{\omega}_i = M_{Wi} \sum_j (\upsilon'_{ij} - \upsilon_{ij}) \left[K_{fj} \prod_i \left(\frac{\rho \alpha_i}{M_{Wi}}\right)^{\upsilon_{ij}} - K_{bj} \prod_i \left(\frac{\rho \alpha_i}{M_{Wi}}\right)^{\upsilon'_{ij}} \right]$$

- **SPECIES CONTINUITY EQUATION:**

$$\frac{\partial (\rho \alpha_i)}{\partial t} + \frac{\partial (\rho u_j \alpha_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\mu_{eff}}{\sigma_\alpha} \frac{\partial \alpha_i}{\partial x_j} \right) + \dot{\omega}_i$$

NUMERICAL APPROACH (cont.)

ODE SOLVER

- **DEFINE FLUID PARTICLE RESIDENCE TIME**

$$\Delta t_f = \left(\frac{u}{\Delta x} + \frac{v}{\Delta y} + \frac{w}{\Delta z} \right)^{-1}$$

- **INTEGRATE CHEMICAL KINETICS OVER** $\Delta t_c = \min(\Delta t_f, \Delta t)$ **WITH "DEBDF" ODE SOLVER**
- **CALCULATE CHEMICAL SOURCE TERM** $\dot{\omega}_i = \rho \frac{\alpha_i^* - \alpha_i^n}{\Delta t_c}$
- **OPERATOR-SPLITTING/POINT-IMPLICIT SCHEME**
- **AVOID TO SOLVE A SET OF NONLINEAR STIFF PDE EQUATIONS**

NUMERICAL APPROACH (cont.)

PENALTY FUNCTION (PF)

- **TIME STEP LIMITER FOR SPECIES EQUATIONS:**

$$\Delta t_s = \left[\rho(\Delta\alpha_i)_{assigned} / \dot{\omega}_i \right]_{\min}$$

- **ELEMENT BALANCE CONSTRAINTS:**

$$\sum_i \alpha_i = 1.0 \qquad and \qquad 0.0 \le \alpha_i \le 1.0$$

- **DEVISE A PENALTY FUNCTION** $P = \min(P_i)$

$$P_i = \frac{1.0 - \alpha_i^k}{\alpha_i^* - \alpha_i^k} \quad for \quad \alpha_i^* - \alpha_i^k > 0.0 \quad or \quad P_i = \frac{-\alpha_i^k}{\alpha_i^* - \alpha_i^k} \quad for \quad \alpha_i^* - \alpha_i^k < 0.0$$

- **ADJUST MASS FRACTION:** $\alpha_i^{k+1} = \alpha_i^k + (\alpha_i^* - \alpha_i^k) \cdot P$

- **ONLY FOR STEADY STATE CALCULATIONS**

NUMERICAL APPROACH (cont.)

NUMERICAL METHOD

- PRESSURE BASED FINITE DIFFERENCE NAVIER-STOKES FLOW SOLVER (FDNS)
- TIME-ACCURATE SOLUTION PROCEDURE
- HIGH ORDER CHAKRAVARTHY-OSHER (C-O) TVD SCHEME
- STANDARD & EXTENDED k-ε TURBULENCE MODELS WITH COMPRESSIBILITY CORRECTIONS
- CONJUGATE GRADIENT SQUARE (CGS) AND ADI SOLVER

VALIDATION

1. IGNITION DELAY

2. ONE-DIMENSIONAL DETONATION

3. SSME NOZZLE FLOW (PREMIXED)

4. BURROWS AND KURKOV DIFFUSION FLAME

VALIDATION (cont.)

1. IGNITION DELAY

- TO CHECK OUT THE CHEMICAL KINETICS MODELS, ODE SOLVER AND IMPLEMENTATION OF OPERATOR-SPLITTING SCHEME
- TEST CONDITIONS:
  STOICHIOMETRIC MIXTURE OF H2+AIR
  N2 IS CHEMICALLY INERT
  P_∞ = 101,325 Pa; U_∞ = 2,689 m/s; T_∞ = 1,000 K
- CHEMICAL KINETICS MODELS:
  2-STEP REACTION MODEL OF ROGERS AND CHINITZ
  9-STEP REACTION MODEL OF ANON

VALIDATION (cont.)

1. IGNITION DELAY (cont.)

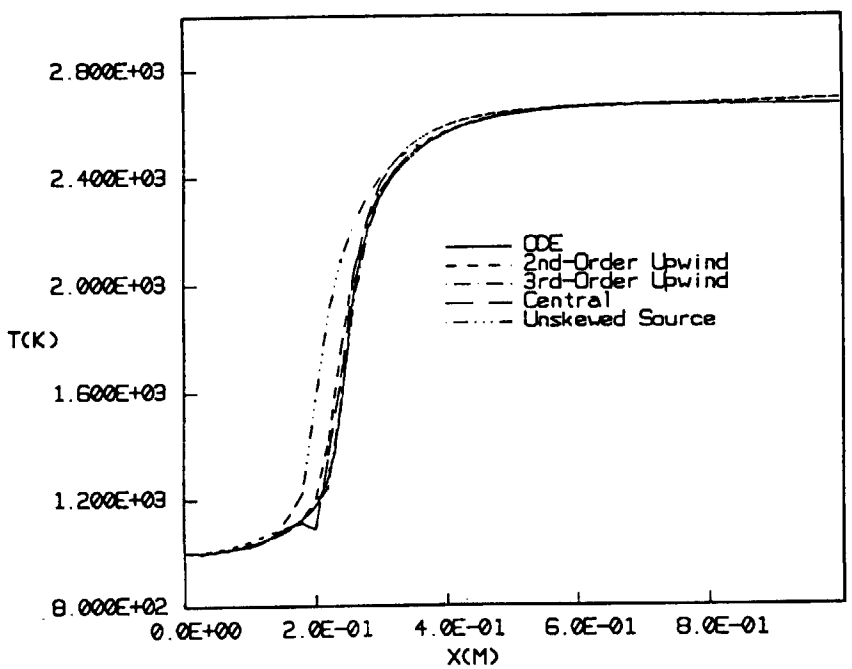
- **ODE SOLVER IN TIME DOMAIN:**

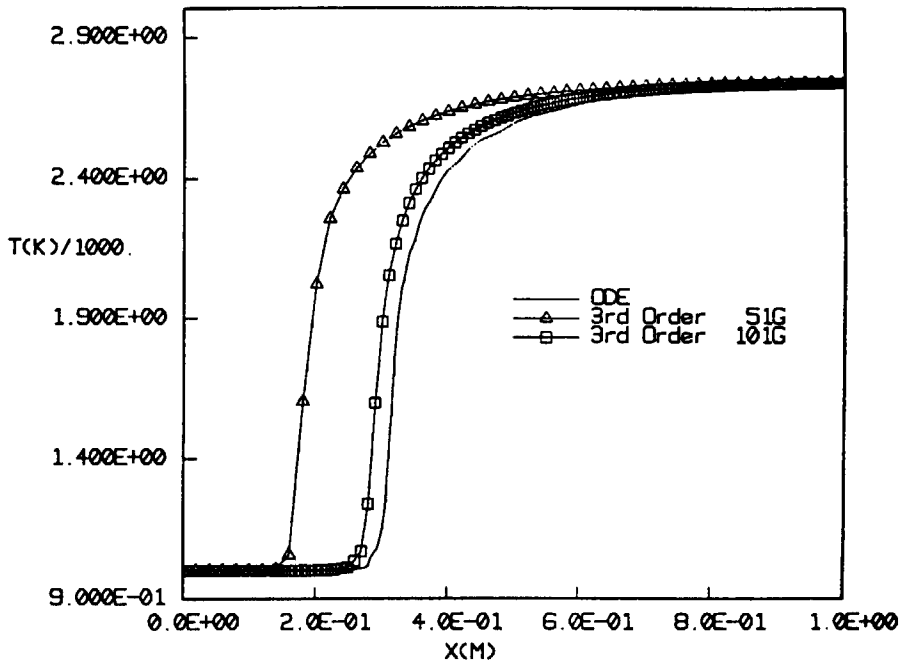
$$\rho \frac{d\alpha_i}{dt} = \omega_i$$

- **OPERATOR-SPLITTING IN SPATIAL DOMAIN:**

$$\rho u \frac{d\alpha_i}{dx} = \omega_i$$

- **CONSTANT P, ρ AND U**
- **THE IGNITION DELAY SHOULD BE SAME BY USING BOTH METHODS WITH** $x = u \cdot t$
- **CAREFUL CALIBRATION**
- **CONSISTENT RESULTS**





(a) 2-step reaction, 51 grids **(b) 9-step reaction**

Fig. 1 Temperature profiles in one-dimensional ignition delay calculation.

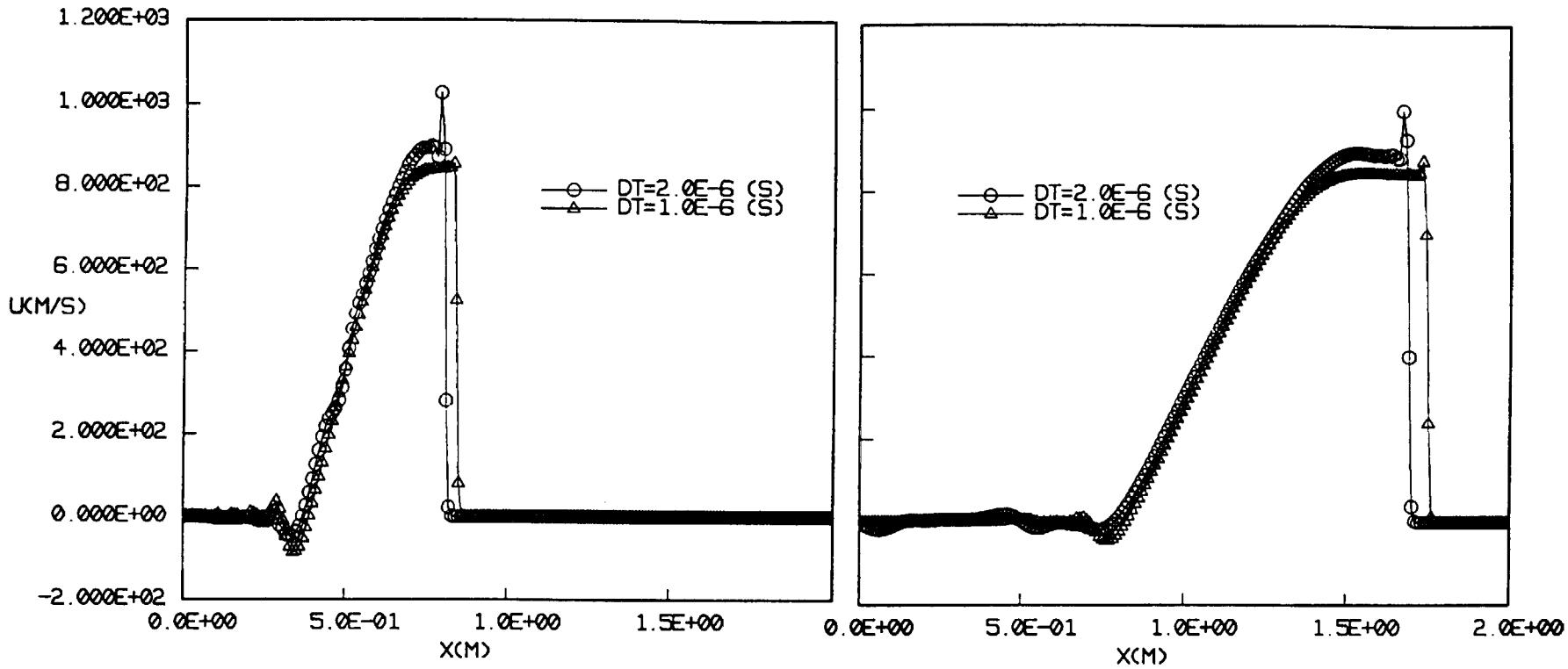
VALIDATION (cont.)

2. ONE-DIMENSIONAL DETONATION

- **STOICHIOMETRIC MIXTURE OF H2 AND O2**
  P_1 = 101,325 Pa; U_1 = 0.0 m/s; T_1 = 298 K;
  L=2.0 m; 201 UNIFORM GRIDS
- **9-STEP REACTION MODEL OF ANON**
- **HOT-SPOT AT X=0.0 m AND TIME=0.0 ms**

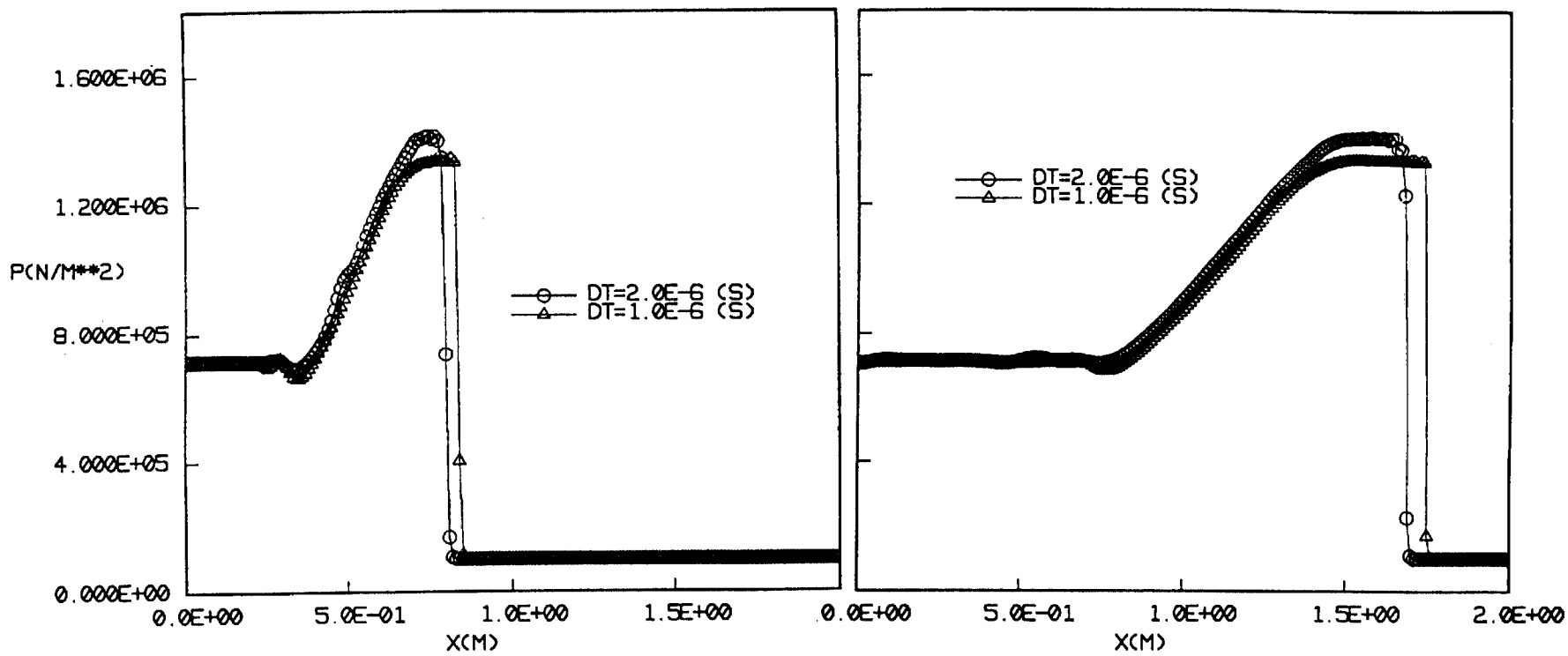
	DT=2μs	DT=1μs	DATA
Vw* (m/s)	2,950	3,000	2,819
P (MPa)	1.405	1.335	1.80
T (K)	3,617	3,592	3,583

* DETONATION WAVE SPEED



(a) Time=300μs **(b) Time=600μs**

Fig. 2 Velocity profiles at different times for one-dimensional detonation.



(a) Time=300μs **(b) Time=600μs**

Fig. 3 Pressure profiles at different times for one-dimensional detonation.

VALIDATION (cont.)

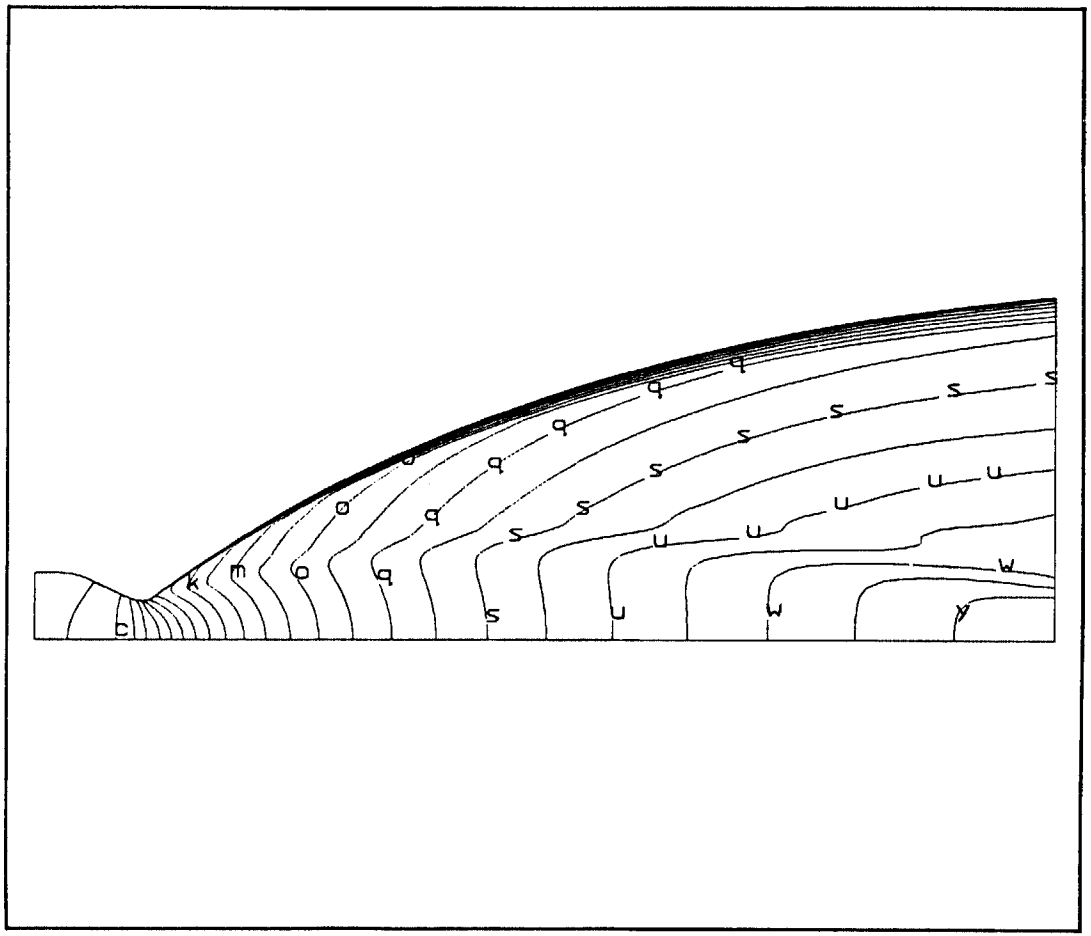
3. SSME NOZZLE FLOW (PREMIXED)

- SSME NOZZLE AT 100-PERCENT POWER LEVEL
- 9-STEP REACTION MODEL OF ANON
- 101X71 NON-UNIFORM GRIDS
- k-ε TURBULENCE MODEL

1229

	ITER	Ma**	Isp (s)	POINT STEP (μs)***
PF	1000	6.10	452.2	1,000
ODE	100*	6.09	452.2	28,000

*RESTART FROM PF; **AT CENTER LINE OF EXIT; *** IBM RISC/6000.



Prediction of the Mach number contour for SSME nozzle with ODE solver

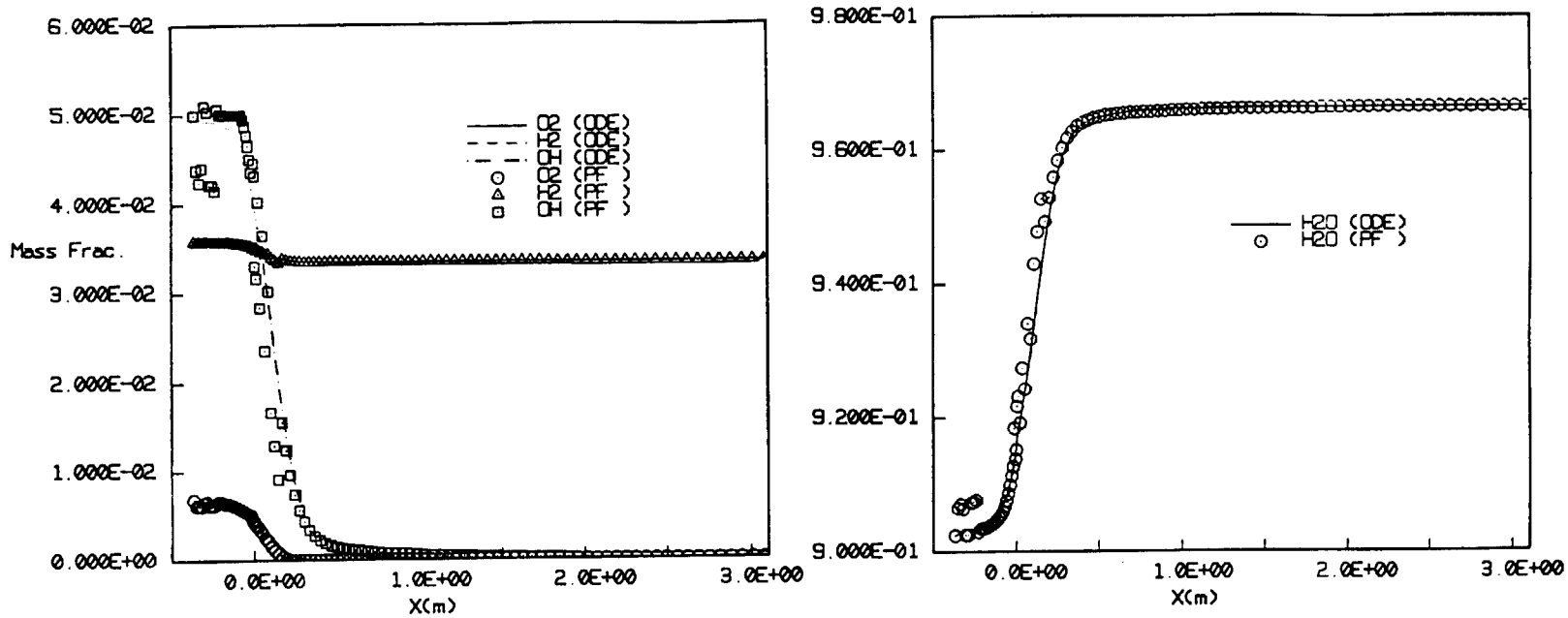
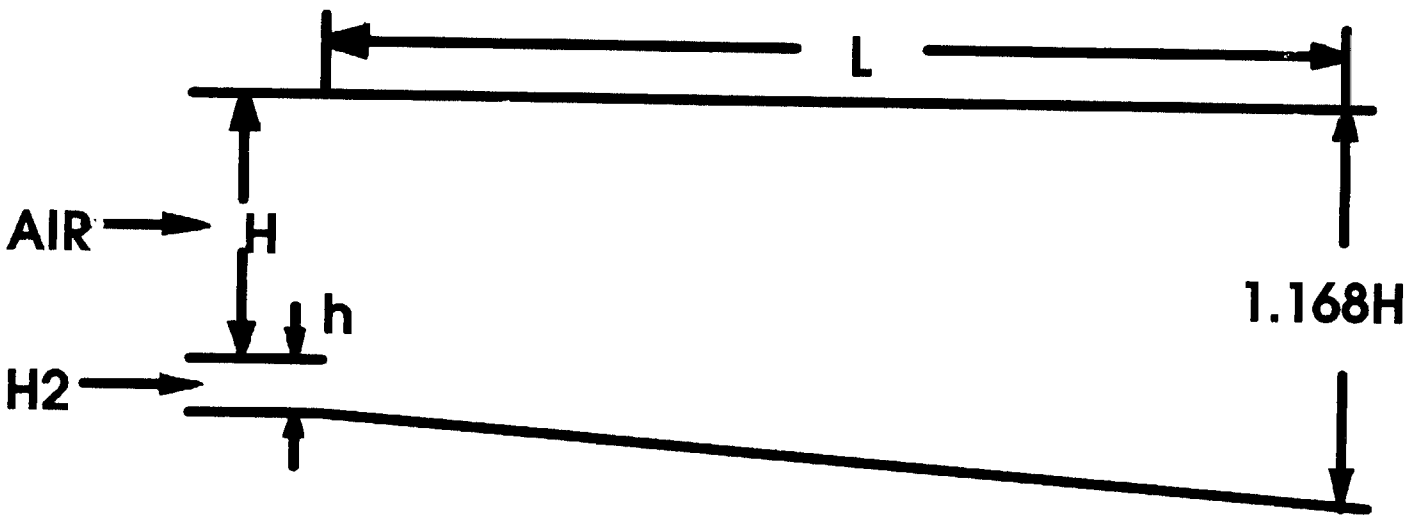


Fig. 4 Mass fraction profiles for SSME nozzle flow along the center line.

VALIDATION (cont.)

4. BURROWS AND KURKOV DIFFUSION FLAME



h=0.004m H=0.08976m L=0.356m

VALIDATION (cont.)

4. BURROWS AND KURKOV DIFFUSION FLAME (cont.)

	HYDROGEN JET	AIR STREAM VITIATED	AIR STREAM NON VITIATED
MACH NUMBER	1.00	2.44	2.44
TEMPERATURE, T, K	254	1270	1150
VELOCITY, U, m/s	1216	1764	1679
PRESSURE, P, MPa	0.1	0.1	0.1
MASS FRACTION:			
H2	1.00	0	0.000
O2	0	0.258	0.000
N2	0	0.486	0.744
H2O	0	0.256	0.256

- COMPUTATIONAL EFFICIENCY (RESIDUALS DROP 3 ORDER):
  - ODE: 300 TIME-STEP ITERATIONS, 3 HOUR CPU TIME*
  - PF: 900 TIME-STEP ITERATIONS, 0.8 HOUR CPU TIME*

*CPU TIME BASED ON IBM RISC/600

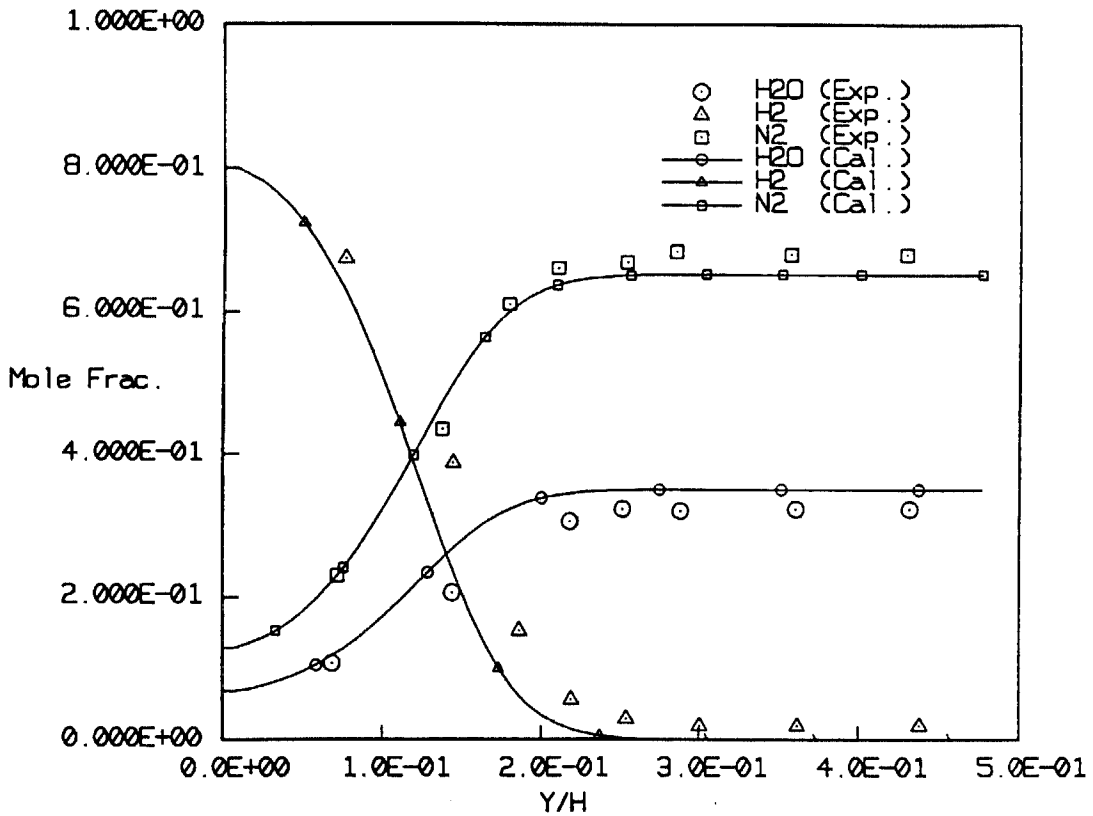


Fig. 5 Mole fraction profiles at x=35.6cm for Burrows and Kurkov's non-reacting case.

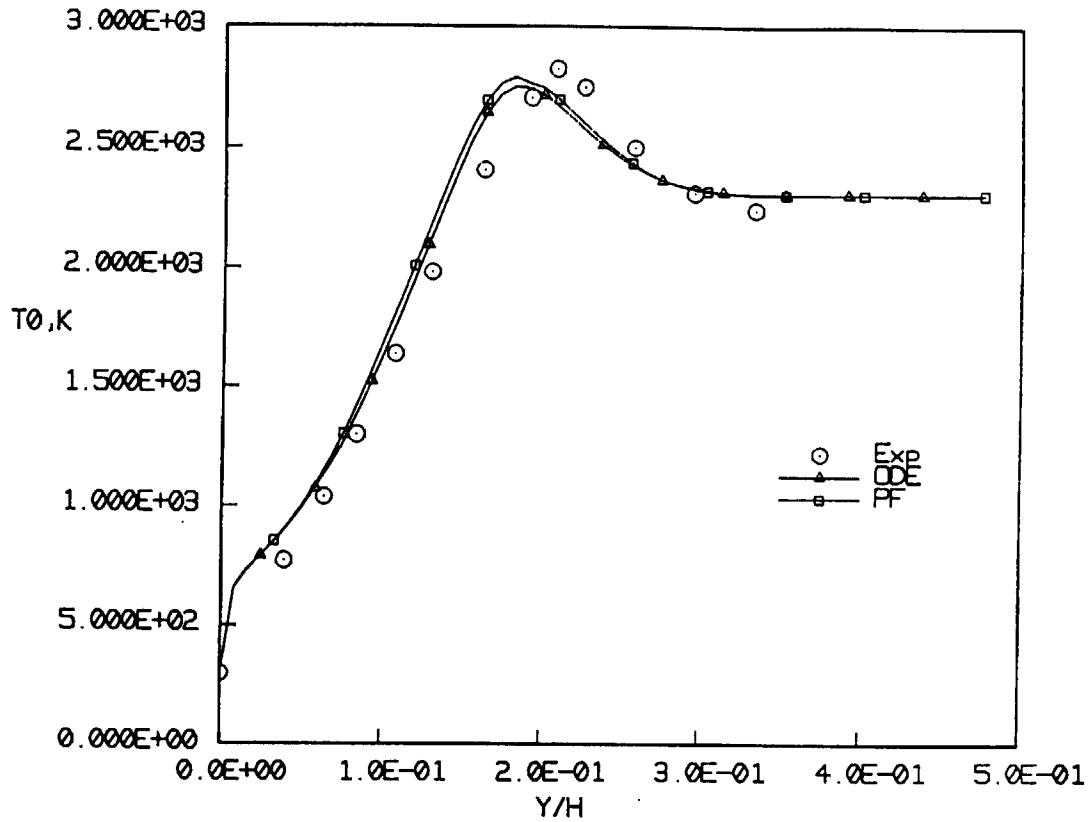


Fig. 6 Total temperature profiles at x=35.6cm for Burrows and Kurkov's reacting case.

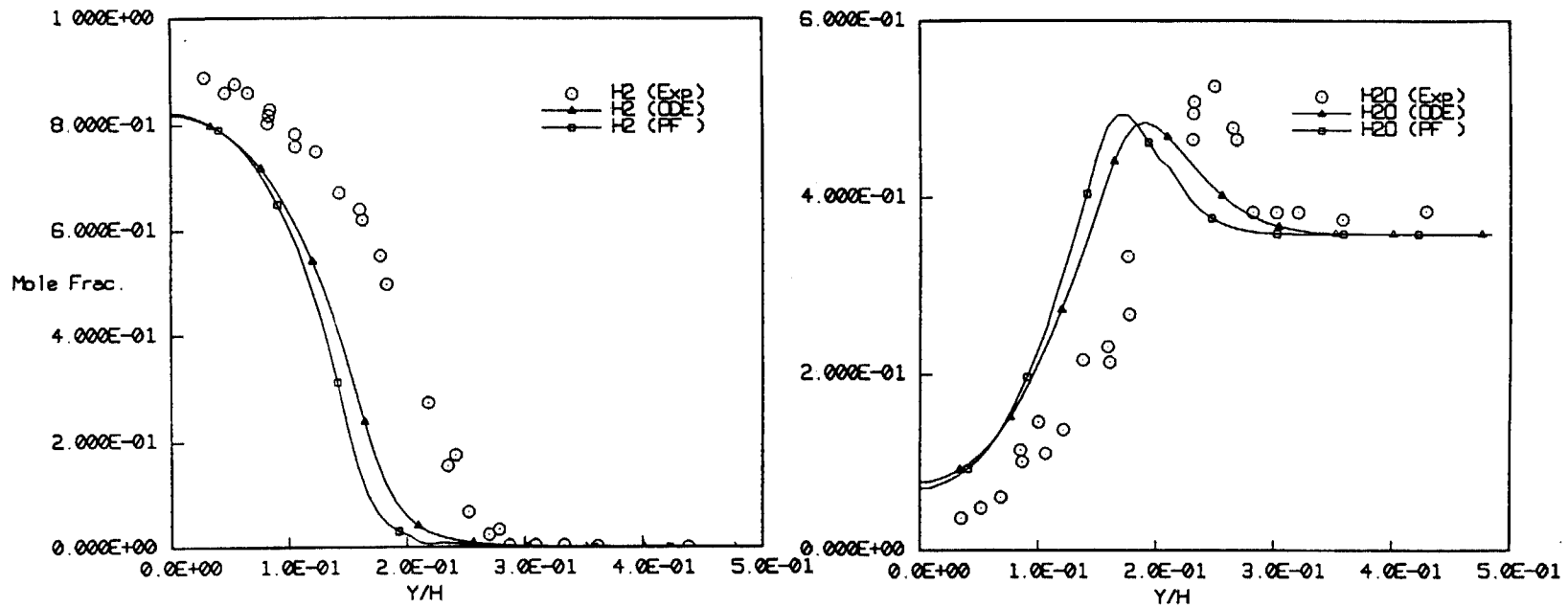


Fig. 7a Mole fraction profiles at x=35.6cm for Burrows and Kurkov's reacting case.

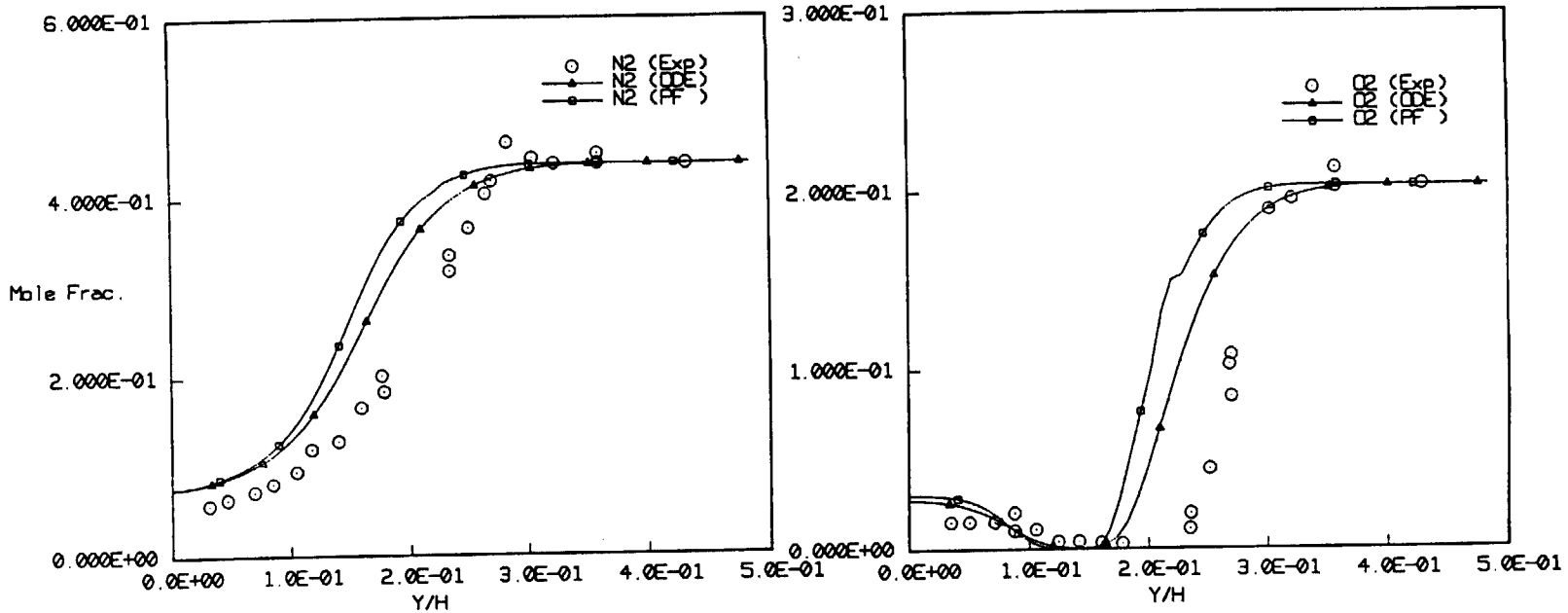


Fig. 7b Mole fraction profiles at x=35.6cm for Burrows and Kurkov's reacting case.

CONCLUSION

- SUCCESSFUL IMPLEMENTATION OF "DEBDF" ODE SOLVER AND CHEMICAL KINETICS
- PENALTY FUNCTION -- EFFICIENT; BUT MASS FRACTION OSCILLATION IN SOME CASES
- ODE SOLVER -- CAN BE APPLIED TO TRANSIENT CALCULATIONS
- EFFICIENCY CAN BE ACHIEVED BY THE COMBINATION OF PENALTY FUNCTION AND ODE SOLVER IN STEADY STATE CASE
- CONTINUE TO INVESTIGATE TIME ACCURATE FLAME PROPAGATION CALCULATION
- INCORPORATE SPRAY COMBUSTION MODELS