

Progress Towards an Efficient and General CFD Tool for Propulsion Design/Analysis

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The simulation of propulsive flows inherently involves chemical activity. Recent years have seen substantial strides made in the development of numerical schemes for reacting flowfields, in particular those involving finite-rate chemistry. However, finite-rate calculations are computationally intensive and require knowledge of the actual kinetics, which are not always known with sufficient accuracy. Alternatively, flow simulations based on the assumption of local chemical equilibrium are capable of obtaining physically reasonable results at far less computational cost.

The present study summarizes the development of efficient numerical techniques for the simulation of flows in local chemical equilibrium, whereby a "Black Box" chemical equilibrium solver is coupled to the usual gasdynamic equations. The generalization of the methods enables the modelling of any arbitrary mixture of thermally perfect gases, including air, combustion mixtures and plasmas. As demonstration of the potential of the methodologies, several solutions, involving reacting and perfect gas flows, will be presented. Included is a preliminary simulation of the SSME startup transient. Future enhancements to the proposed techniques will be discussed, including more efficient finite-rate and hybrid (partial equilibrium) schemes. The algorithms that have been developed and are being optimized provide for an efficient and general tool for the design and analysis of propulsion systems.

MISSISSIPPI STATE UNIVERSITY / National Science Foundation

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*Workshop for Computational Fluid Dynamic Applications
in Rocket Propulsion and Launch Vehicle Technology*
April 25-27, 1995
Huntsville, AL

ENGINEERING TO
RESEARCH CENTER 20
COMPUTATIONAL
FIELD SIMULATION
COMPLEX GEOMETRY / COMPLEX PHYSICS



Purpose

- Provide an overview of the development of a solver for reacting gas flows, which utilizes **EFFICIENT** numerical techniques and is capable of handling **ARBITRARY** mixtures.



MOTIVATIONS

- Finite-rate chemistry is **COMPLICATED** and **EXPENSIVE**

Chemical kinetics, actual reaction path are required.

N species continuity equations.

Finite-rate equations are extremely stiff for near equilibrium flows.

- Why not curvefits?

Limited to a particular mixture and range.



APPROACH

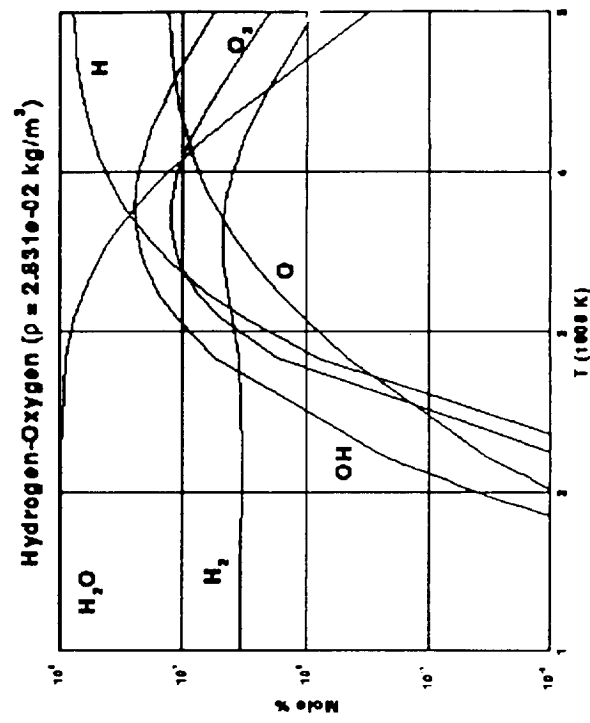
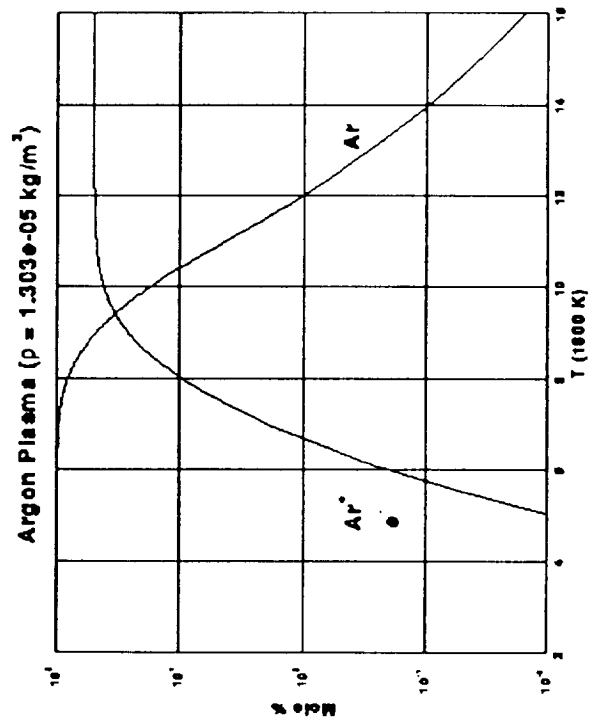
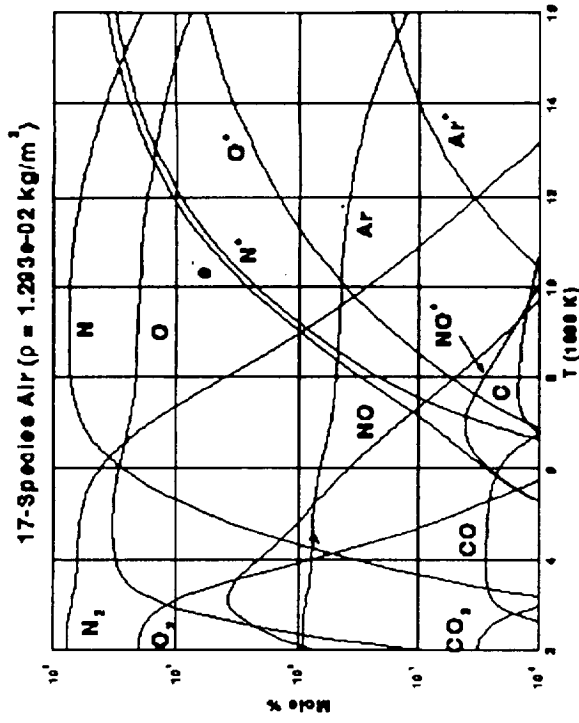
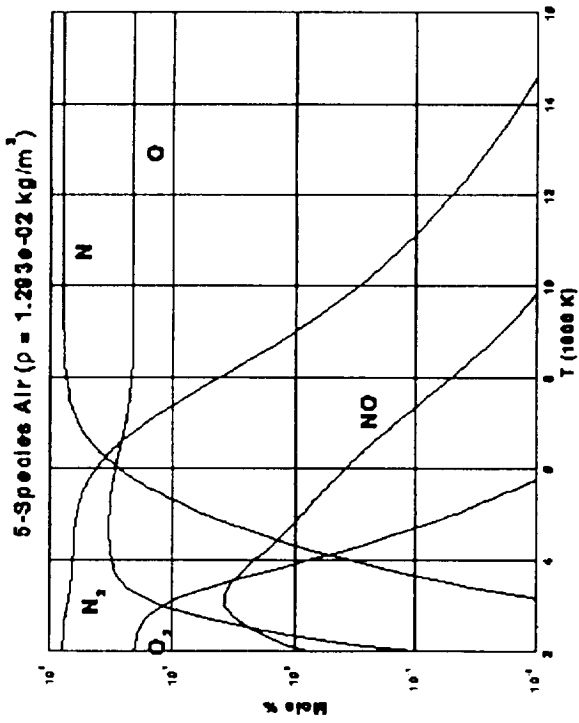
- Chemical equilibrium “Black Box” solver coupled to the “usual” gasdynamic equations
5 equations, not the N+4 equations required for finite-rate chemistry.
- An “off-the-shelf” multi-block flow solver is modified to handle “real gas” effects
Unstructured Block Implicit solver



BLACK BOX

- Provides chemical composition and thermodynamic properties
- Capable of handling **ARBITRARY** mixtures
 - 10 chemistry models available including air, combustion and plasma mixtures, as well as perfect gas.
- Variety of computational options
 - 2 Solution Methods: Mass Constraint & Degree of Advancement
 - 2 Rate Coefficient Models: Curvefit & Consistent
 - 2 Thermodynamic Models: Vibrational & Curvefit
- **EFFICIENT** and **ROBUST**

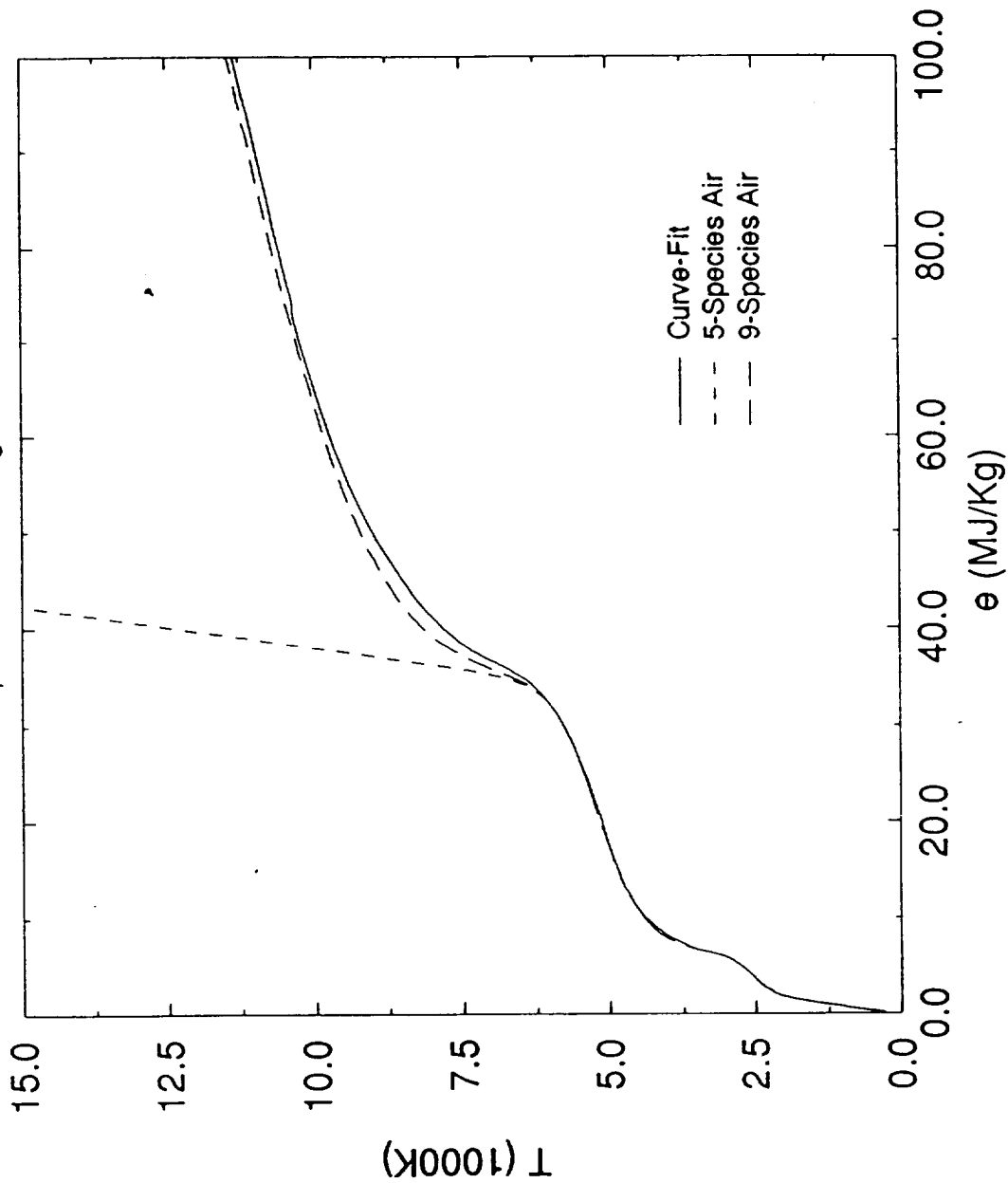






Temperature vs Internal Energy

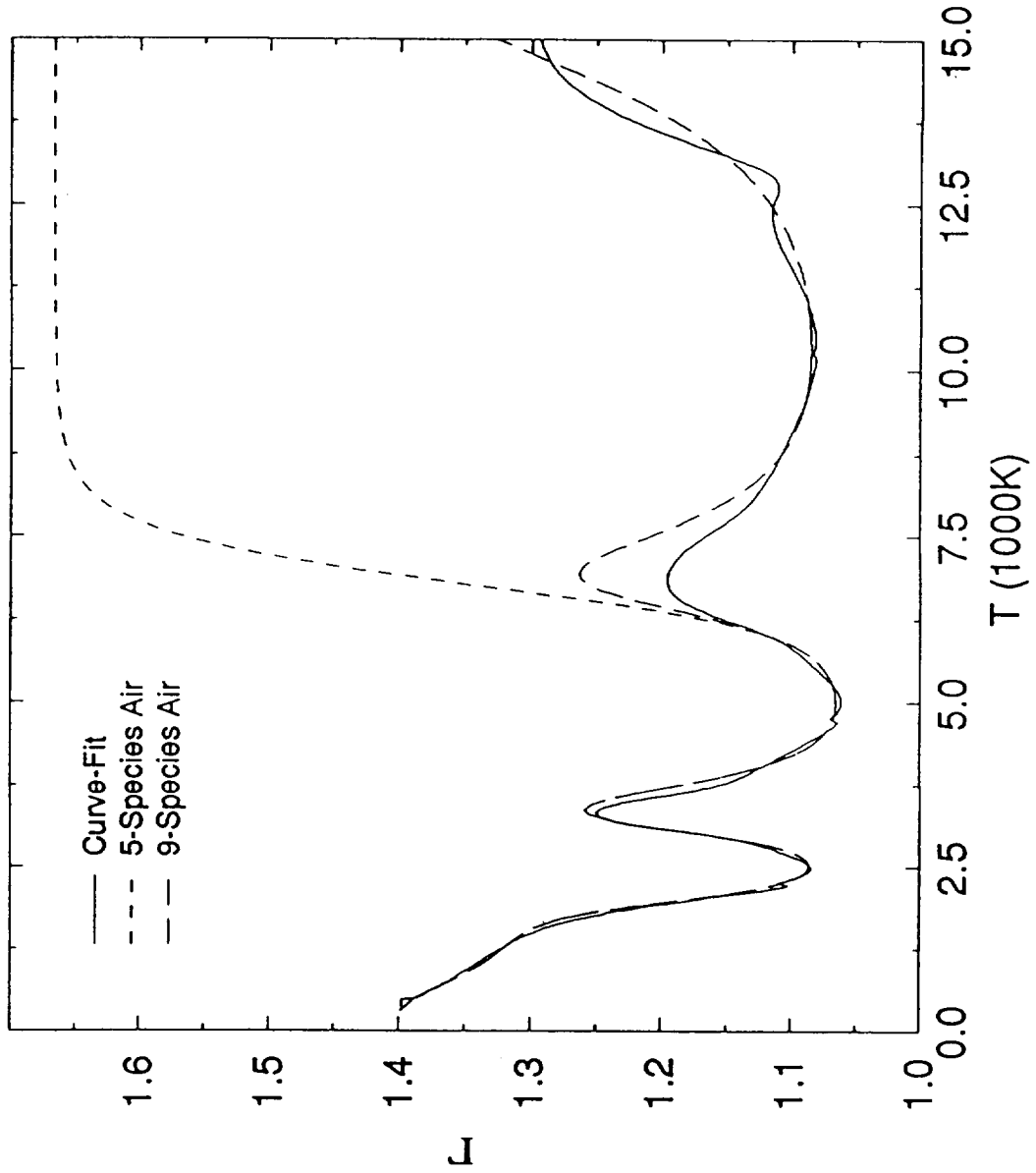
$\rho = 1.293 \cdot 10^{-4} \text{ kg/m}^3$





Isentropic Index vs Temperature

$\rho = 1.293 \cdot 10^{-4} \text{ kg/m}^3$



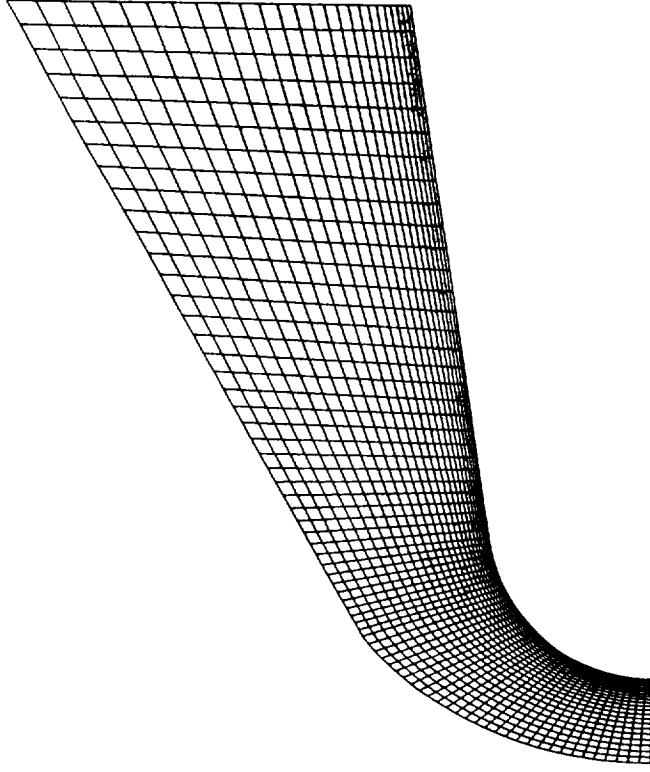
FLOW SOLVER

- Implicit, finite-volume, high-order TVD scheme.
- Modified 2-Pass solution algorithm
- Steger-Warming FVS used on LHS
- Approximate Riemann Solver used on RHS
- Unstructured multi-block capability using ...
 - “ribbon vector” storage,
 - block-structured grids, and
 - extraction-injection for block-to-block communication.



BLUNT CONE

- 9 degree half angle, 2.5 in. nose radius



- Flow conditions:

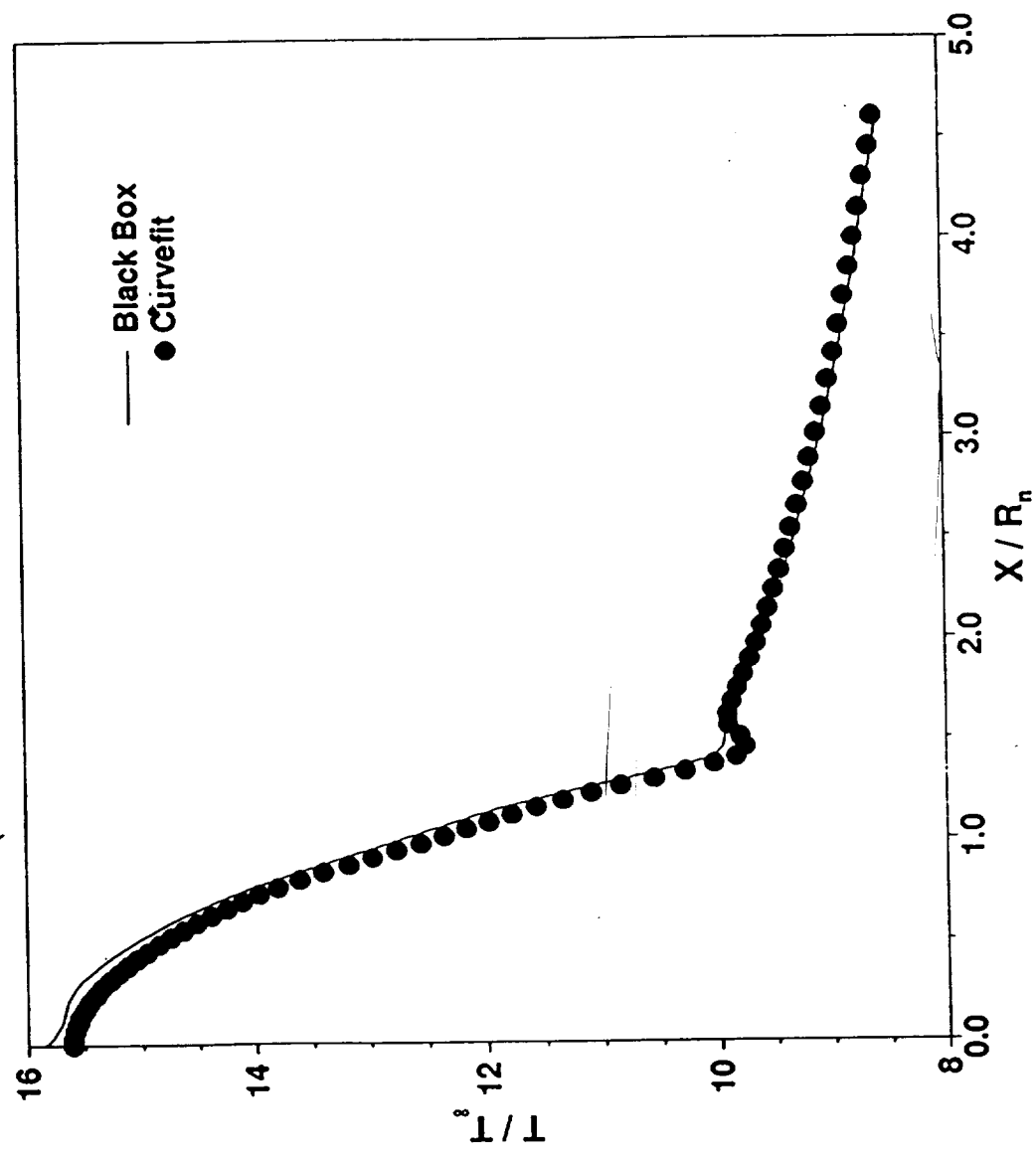
$$T_{\infty} = 223 \text{ K} \quad M_{\infty} = 10$$

$$p_{\infty} = 26.5 \text{ kPa} \quad \alpha_{\infty} = 0 \text{ degrees}$$





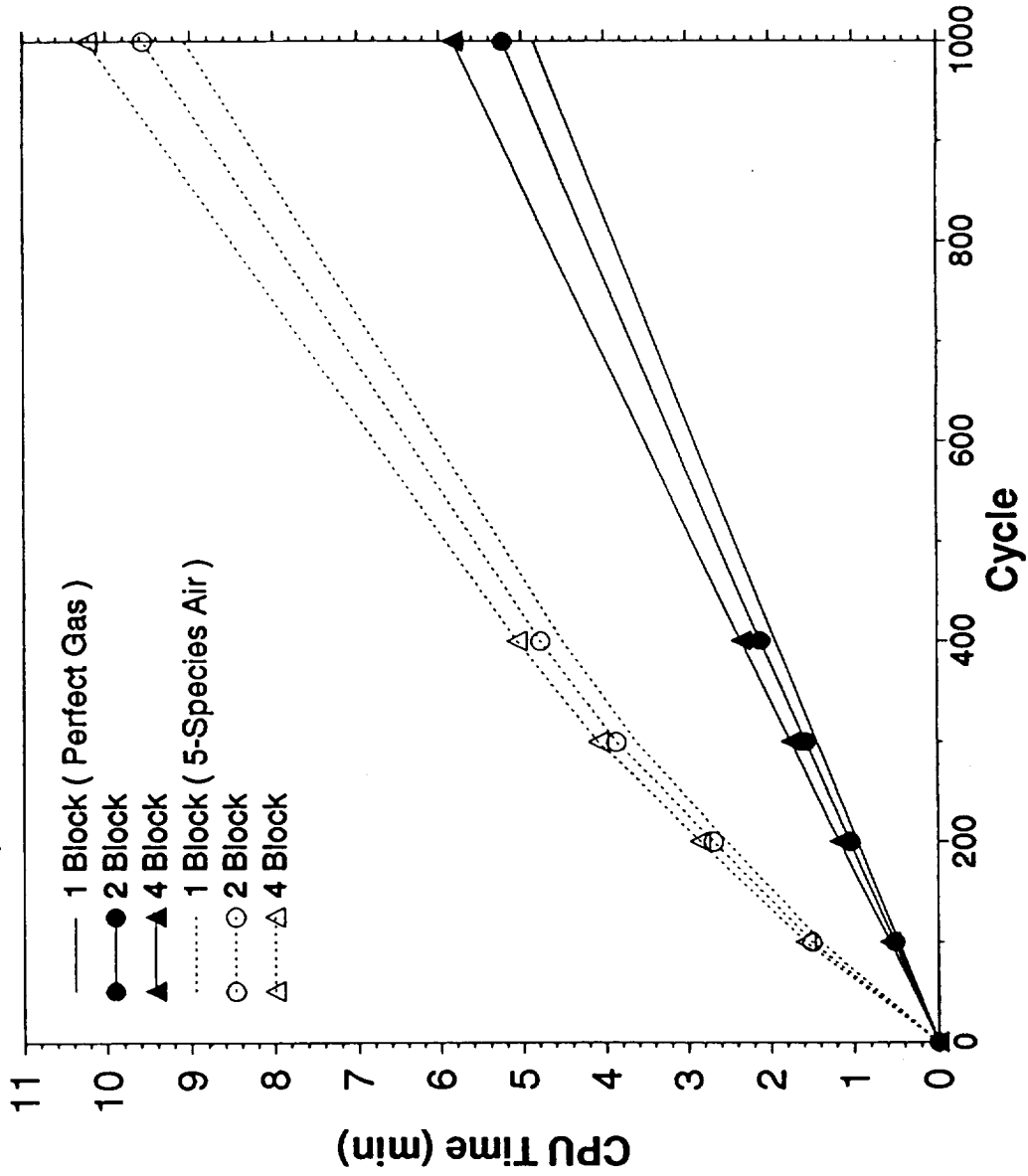
Black Box - Curvefit Comparison (Blunt Cone, Surface , Temperature)





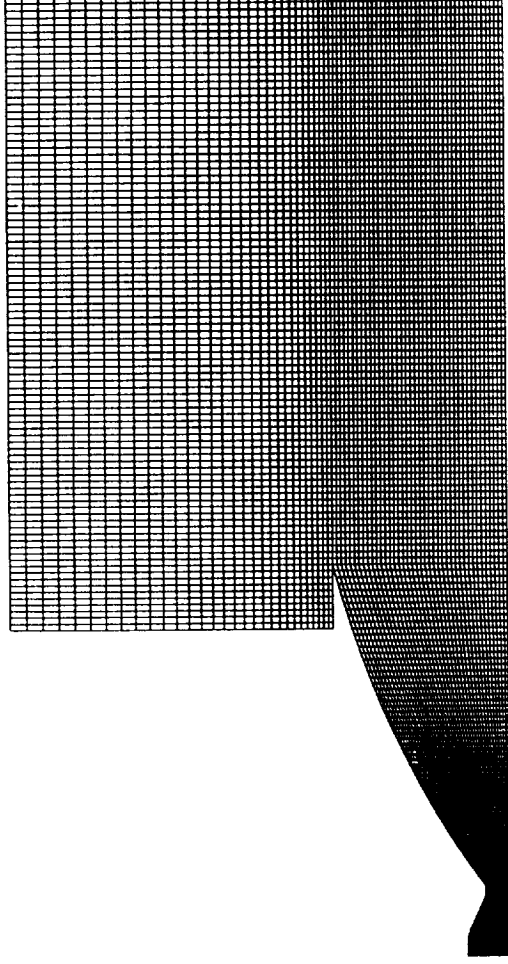
Timing Comparisons for Multi-Block Solver

(Blunt Cone, $M_\infty = 10$, Cray-YMP)



SSME NOZZLE

- 100% power @ sea level, mixture ratio 6:1



- Chamber conditions:

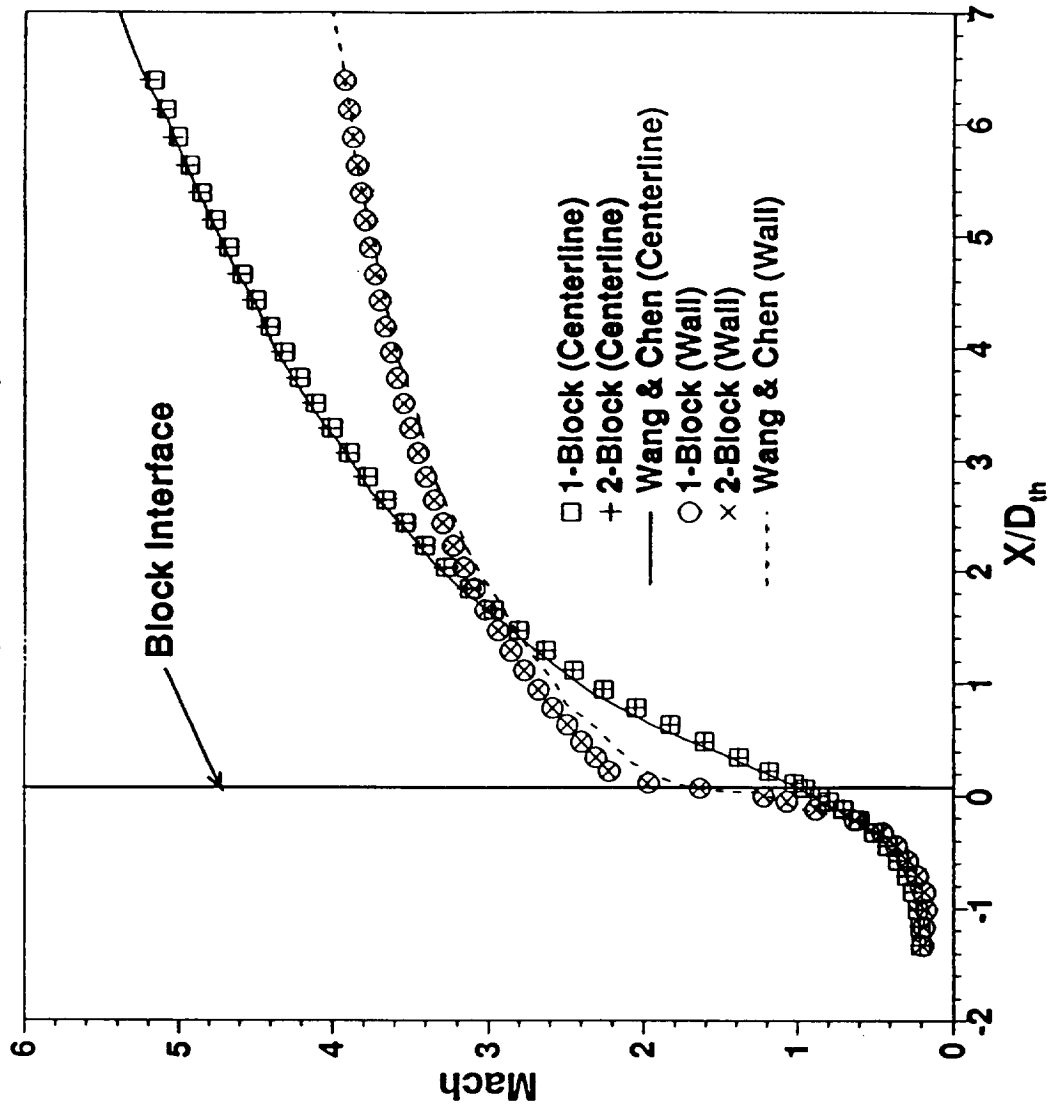
$$T_c = 3639 \text{ K} \quad M_c = 0.2$$

$$p_c = 20.24 \text{ MPa}$$



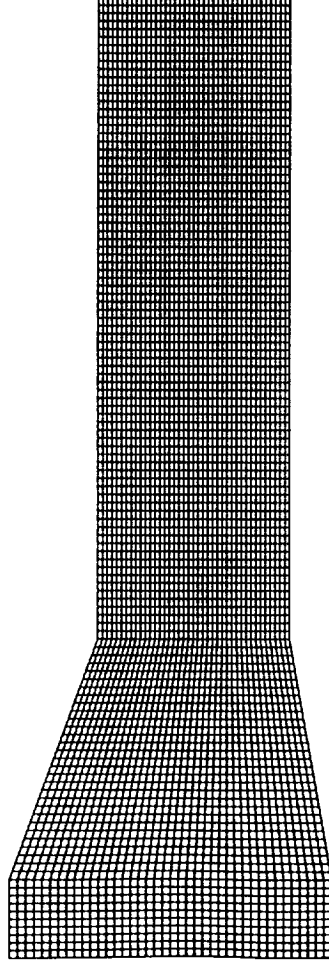


Mach Number Profiles (SSME Nozzle)



HYPERSONIC INLET

- 10 deg. lower and 20 deg. upper ramp



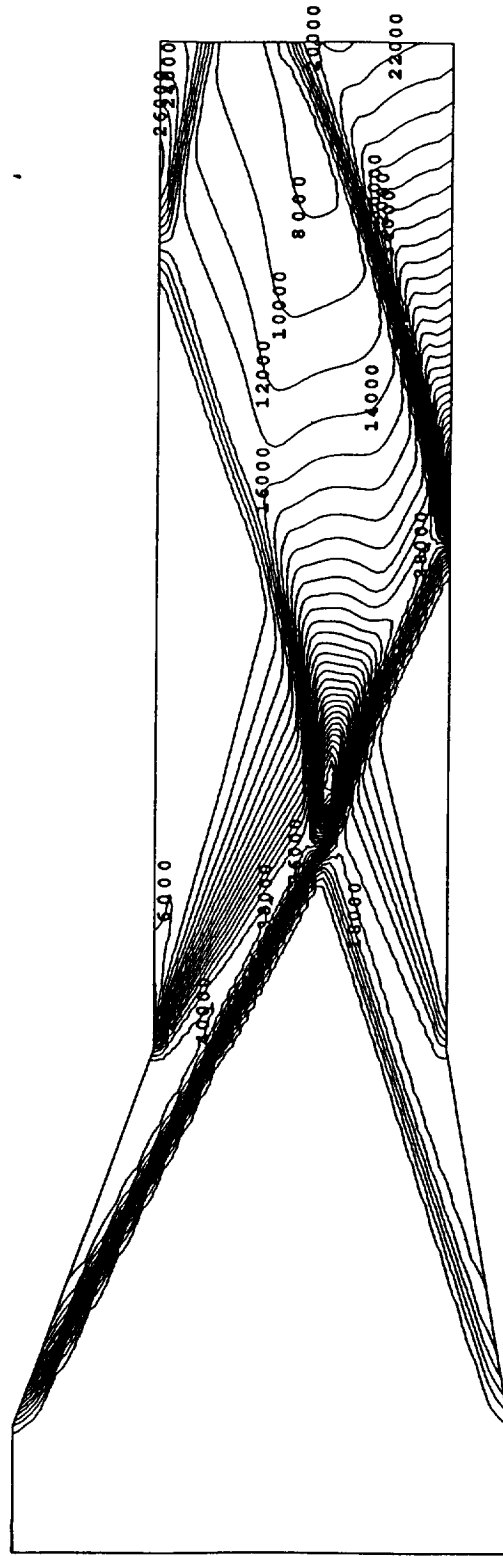
- Flow conditions:

$$M_{\infty} = 5 \quad p_{\infty} = 6.52 \text{ kPa}$$

$$\rho_{\infty} = 1.293 \times 10^{-2} \text{ kg/m}^3$$



Pressure Contours



WORK IN PROGRESS

- Viscous terms added
 - Parabolized Navier-Stokes (Turbulent)
 - Full Navier-Stokes (Laminar)
- Finite-rate chemistry
 - Improved numerical techniques
- Hybrid chemistry (partial equilibrium)
 - Elemental species continuity equations (allows for diffusion)
 - Kinetic species continuity equations coupled with “Black Box”
- Pre-conditioning for low-speed flows
- Parallelization



CONCLUSIONS

- An EFFICIENT and GENERAL solver for reacting gas flows has been developed, which...
can handle arbitrary mixtures,
uses efficient numerical techniques,
and
is applicable to propulsion design/analysis.



