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MODELING OF HIGH SPEED CHEMICALLY REACTING FLOW-FIELDS

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ABSTRACT

The SPARK3D and SPARK3D-PNS computer programs have been developed to model 3-D supersonic, chemically reacting flow-fields. The SPARK3D code is a full Navier-Stokes solver, and is suitable for use in scramjet combustors and other regions where recirculation may be present. The SPARK3D-PNS is a parabolized Navier-Stokes solver and provides an efficient means of calculating steady-state combustor far-fields and nozzles. Each code has a generalized chemistry package, making modeling of any chemically reacting flow possible.

Research activities by the Langley group range from addressing fundamental theoretical issues to simulating problems of practical importance. Algorithmic development includes work on higher order and upwind spatial difference schemes. Direct numerical simulations employ these algorithms to address the fundamental issues of flow stability and transition, and the chemical reaction of supersonic mixing layers and jets. It is believed that this work will lend greater insight into phenomenological model development for simulating supersonic chemically reacting flows in practical combustors. Currently, the SPARK3D and SPARK3D-PNS codes are used to study problems of engineering interest, including various injector designs and 3-D combustor-nozzle configurations. Examples, which demonstrate the capabilities of each code are presented.

*Analytical Services and Materials, Inc.

OVERVIEW

- GROUP OBJECTIVES
- DESCRIPTION OF 2 AND 3-D CODES
- 3-D FULL NAVIER-STOKES
- 3-D PARABOLIZED NAVIER-STOKES
- 2 AND 3-D MIXING ENHANCEMENT
- CONCLUSIONS AND DIRECTIONS

OBJECTIVES

- THEORETICAL ISSUES
  - NUMERICS FOR SUPERSONIC CHEMICALLY REACTING FLOWS
    - Numerical Efficiency
    - Numerical Accuracy
    - Robustness
  - PHYSICAL ISSUES
    - Mixing Enhancement and Combustion
    - Transition to Turbulence
    - Phenomenological Turbulence Models
- APPLICATIONS
  - 3-D COMBUSTORS AND NOZZLES
    - SPARK3D
    - SPARK3D-PNS

SPARK 3-D

- 3-D NAVIER-STOKES AND CHEMISTRY
- FULLY ELLIPTIC STRUCTURE
- VISCOUS OR INVISCID CAPABILITIES
- TIME-ACCURATE OR LOCAL RELAXATION
- GENERALIZED CHEMISTRY ROUTINES
- LOW STORAGE FORMAT

GENERALIZED CHEMISTRY ROUTINE

- REAL GAS THERMODYNAMICS MODELS
  - POLYNOMIAL FITS FOR C_p, C_v, S, G
  - KINETIC THEORY BASED DIFFUSION MODELS
    - Sutherlands Law for μ_i and k_i
    - Wilkes law for μ and k
    - Binary or multicomponent diffusion models

- CHEMISTRY MODELS
  - FROZEN
  - EQUILIBRIUM
  - FINITE RATE CHEMISTRY (NS=9, NR=18)

NUMERICAL METHODS

- TRANSFORMED COORDINATES (ξ,η,ζ)
  - GEOMETRIC CONSERVATION LAW TERMS INCLUDED

- TEMPORAL INTEGRATION (2ND ORDER)
  - EXPLICIT FORMULATION FOR HYDRO-DYNAMIC TERMS
    - Allows local time stepping
  - EXPLICIT/IMPLICIT FORMULATION FOR CHEMICAL SOURCE TERMS

- FINITE DIFFERENCE SPATIAL DISCRETIZATION
  - STANDARD MACCORMACK (2ND ORDER)
  - GOTTLIEB MACCORMACK (4TH ORDER)
  - COMPACT MACCORMACK (4TH ORDER AT S.S.)
  - UPWIND (3RD ORDER)

CORNER FLOW

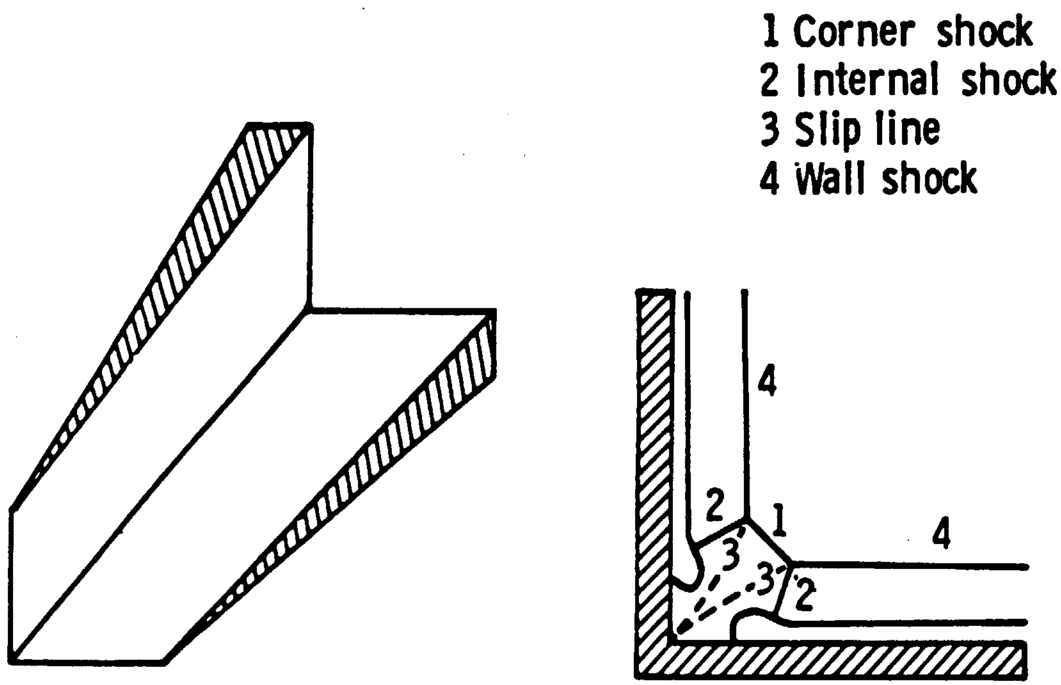
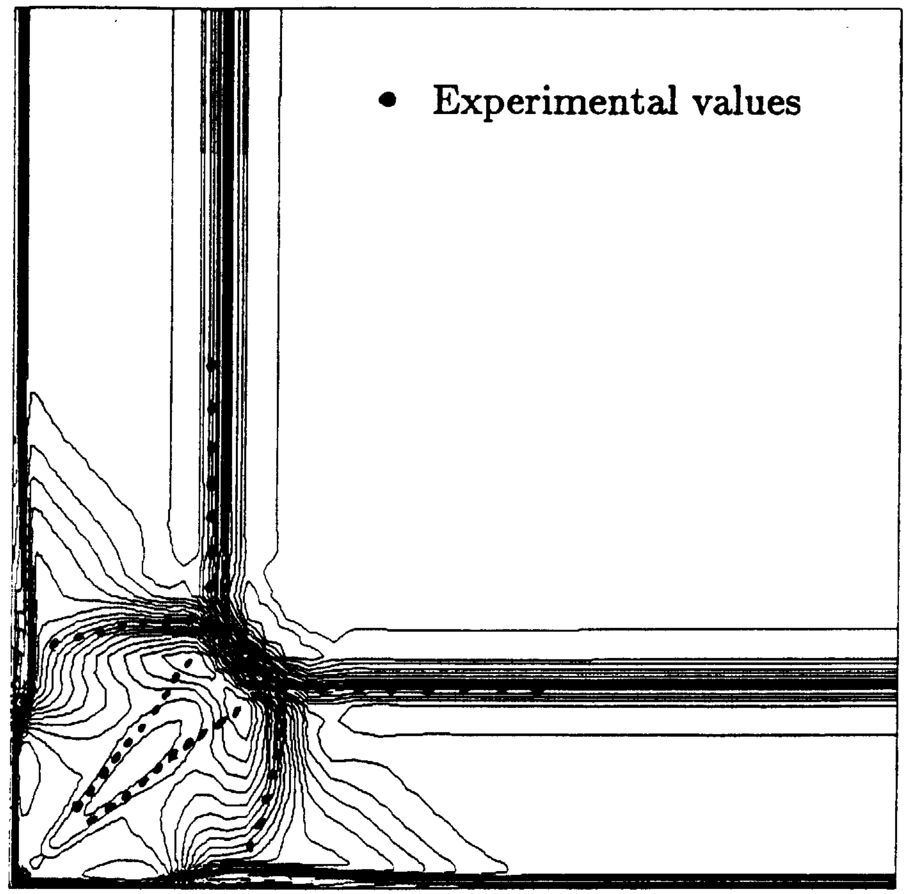


Figure 3.- Symmetric-wedge corner and schematic of corner flow.

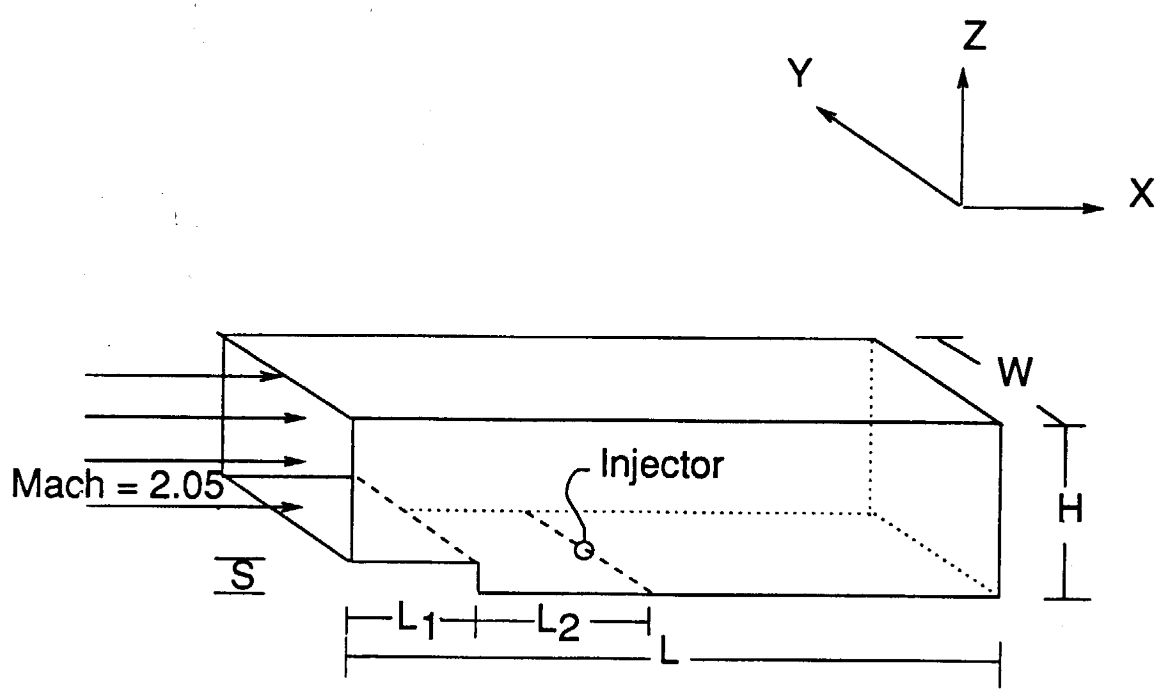
CORNER FLOW

Symmetric-Wedge Corner



Density Contours (Laminar Flow)

REARWARD STEP



$L = 7.0$ cm, $H = 1.8$ cm, $W = 2.9$ cm
$L_1 = 0.7$ cm, $L_2 = 1.2$ cm, $S = 0.3$ cm

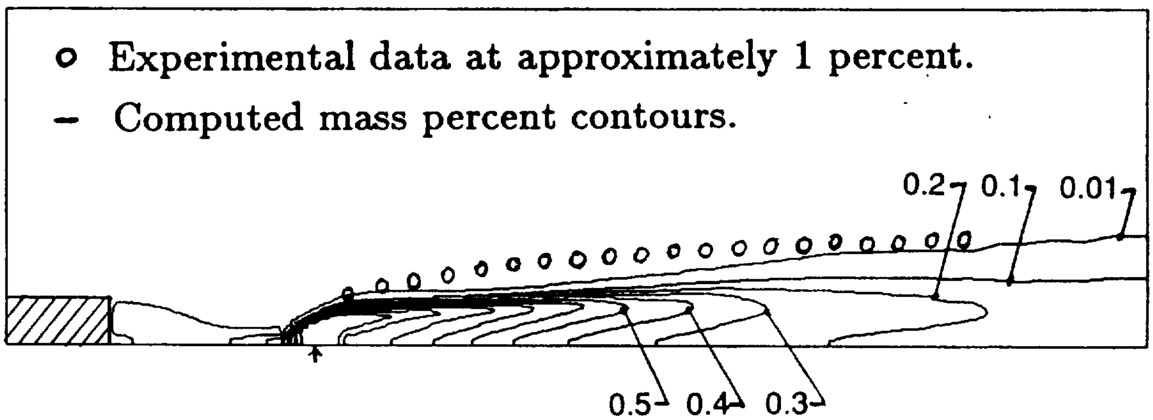
SPARK3D
REARWARD STEP COMPARISON

Mach = 2.05

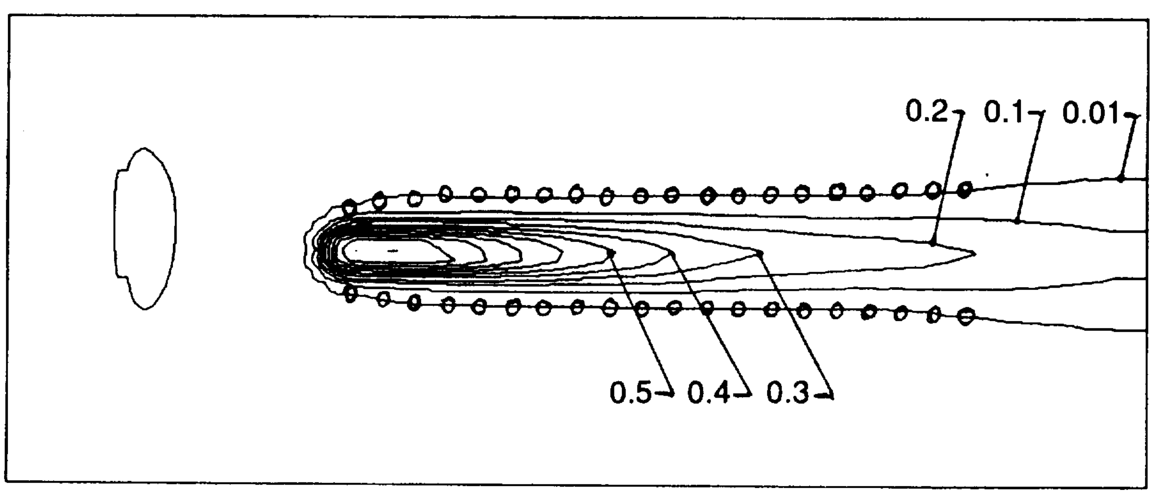
101 x 41 x 25 GRID

Qr = 0.39

JET PENETRATION IN X-Z PLANE AT Y = Y$_{\mathbb{C}}$



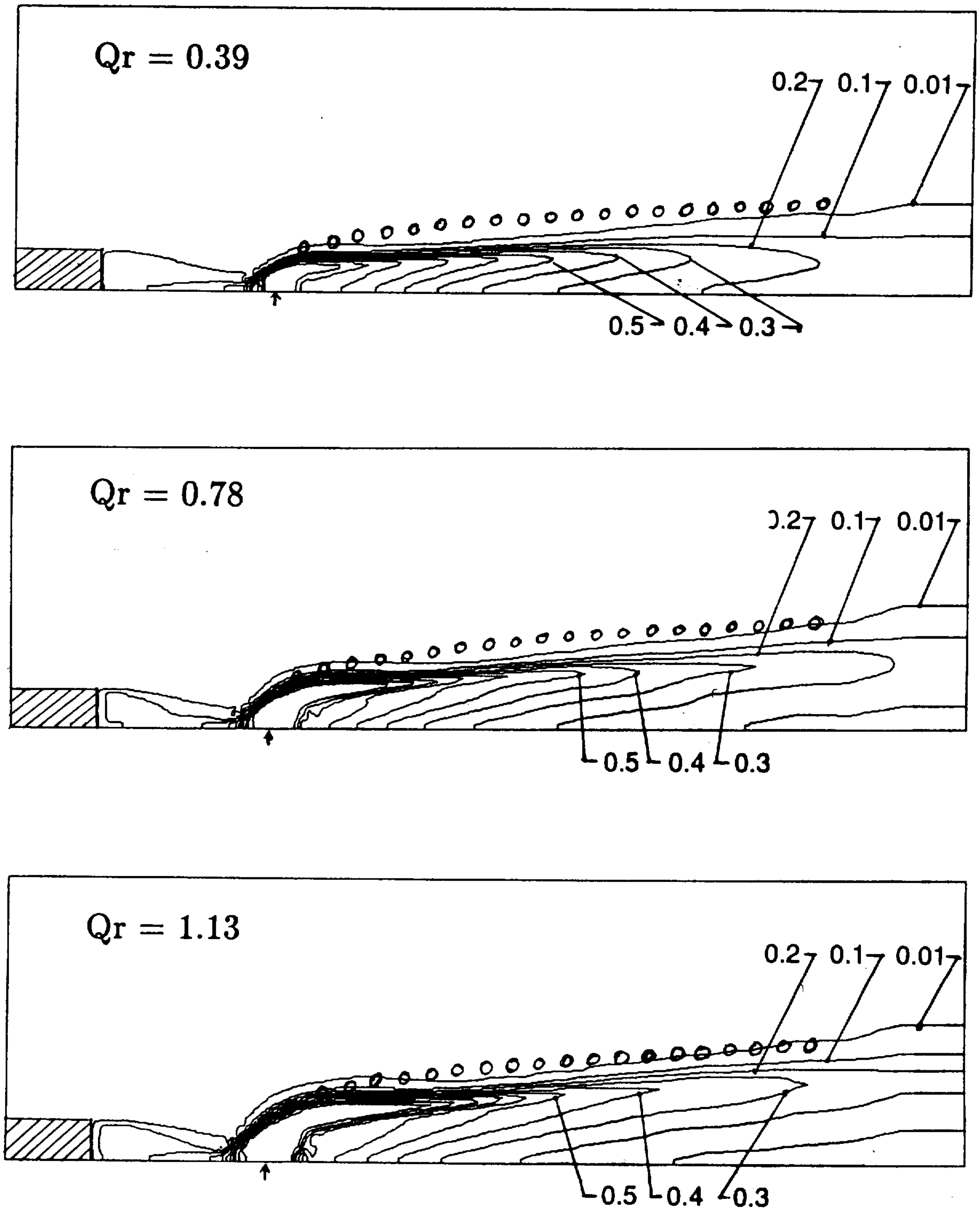
JET SPREAD IN X-Y PLANE AT Z = D



EXPERIMENTAL COMPARISON

Jet Penetration

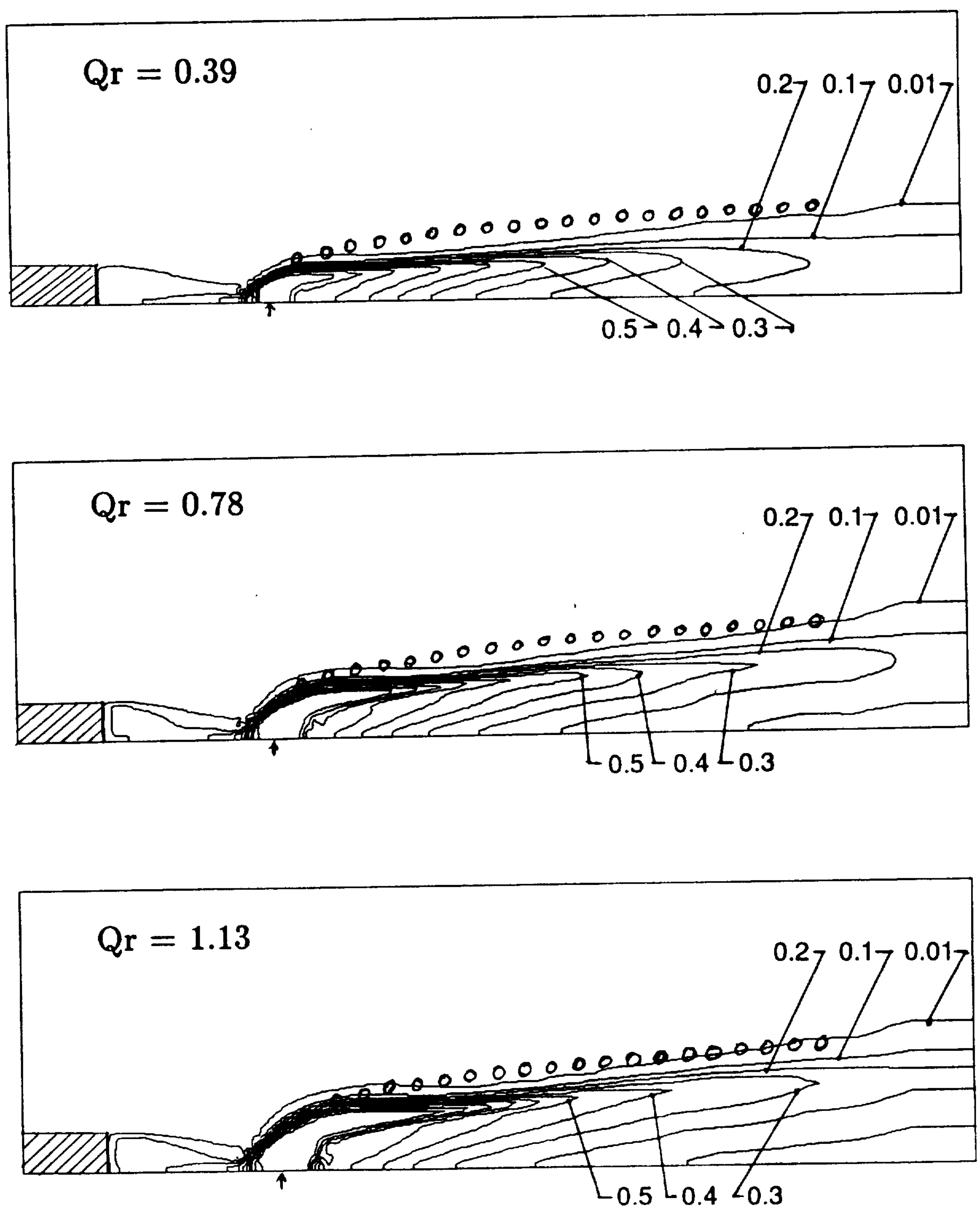
61 x 41 x 25 GRID



EXPERIMENTAL COMPARISON

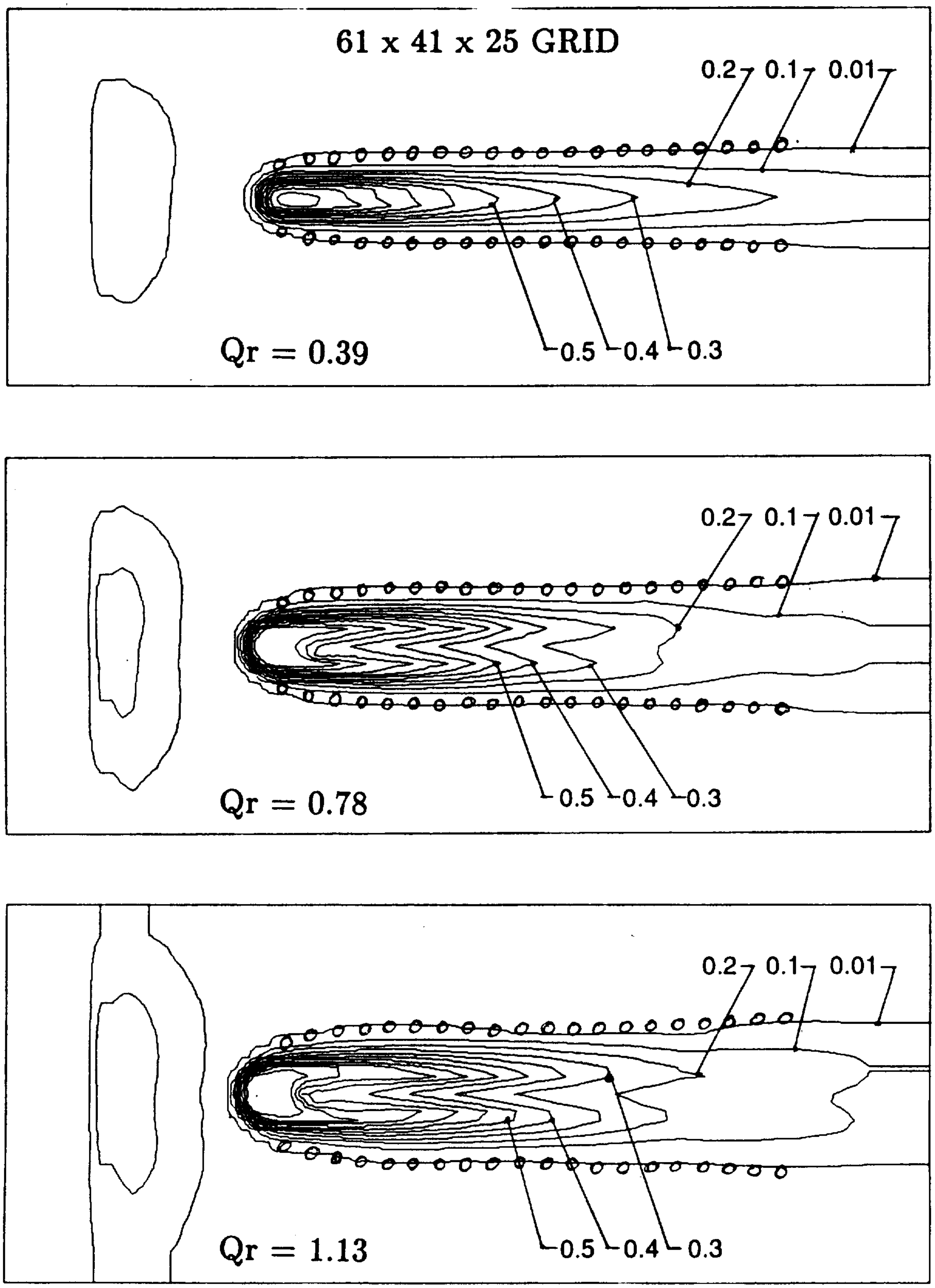
Jet Penetration

61 x 41 x 25 GRID



REARWARD STEP COMPARISON

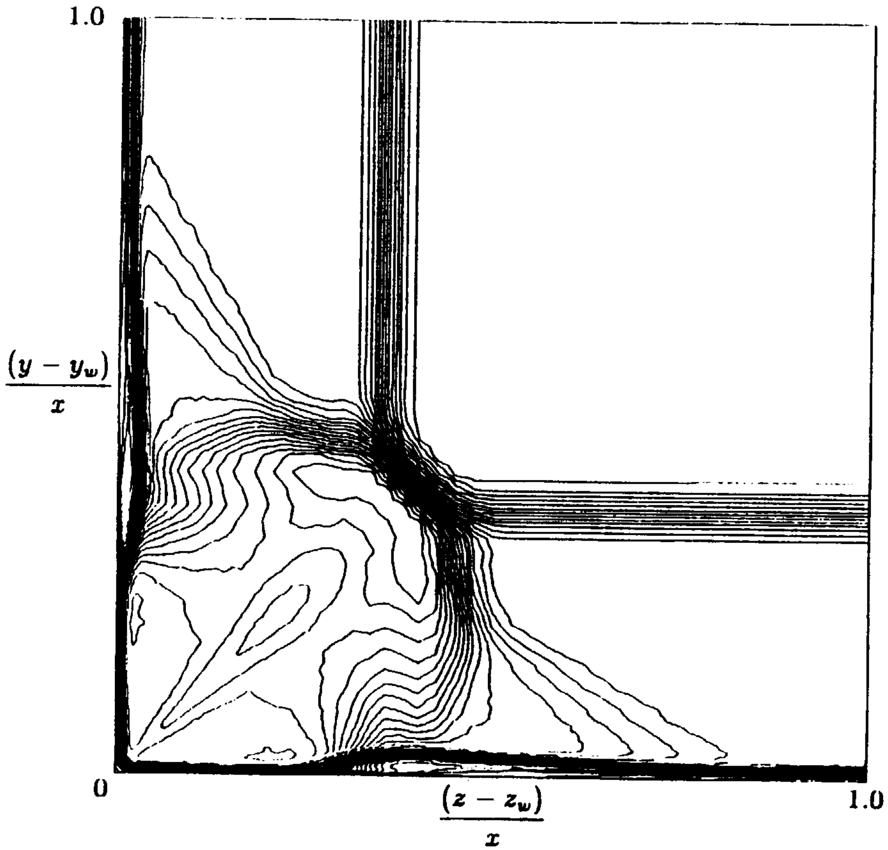
Jet Spread



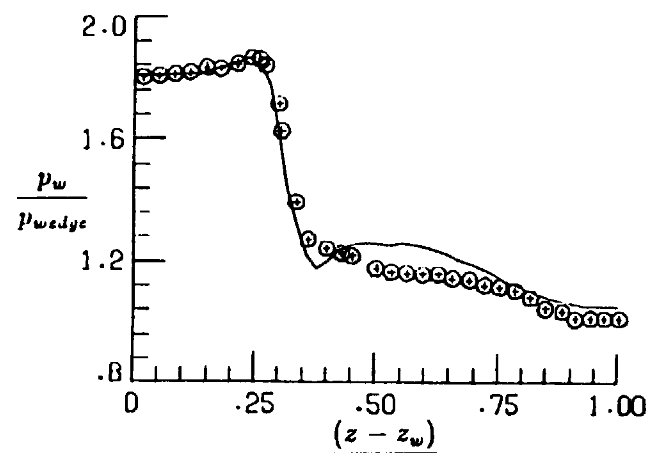
SPARK3D-PNS

- EXTENSION OF SPARK3D
- EFFICIENT SOLUTIONS OF STEADY 3-D PNS EQUATIONS
- FOR USE IN THE COMBUSTOR FAR-FIELD AND NOZZLE
- INTEGRATION SCHEME BASED ON 2ND ORDER MACCORMACK ALGORITHM

CORNER FLOW



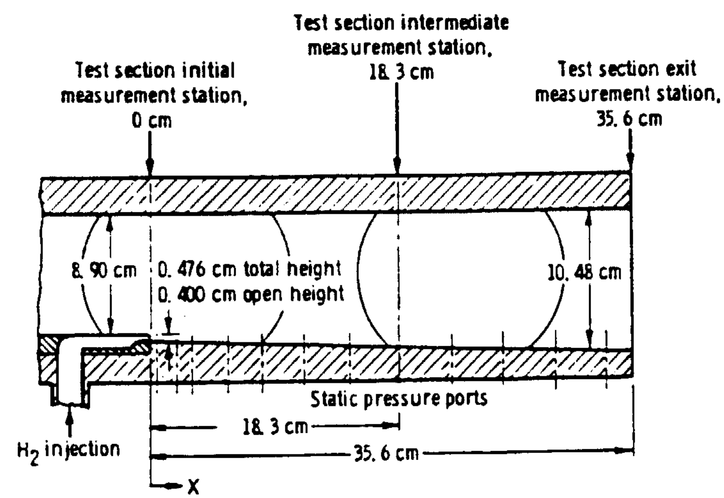
1. Computed density contours.



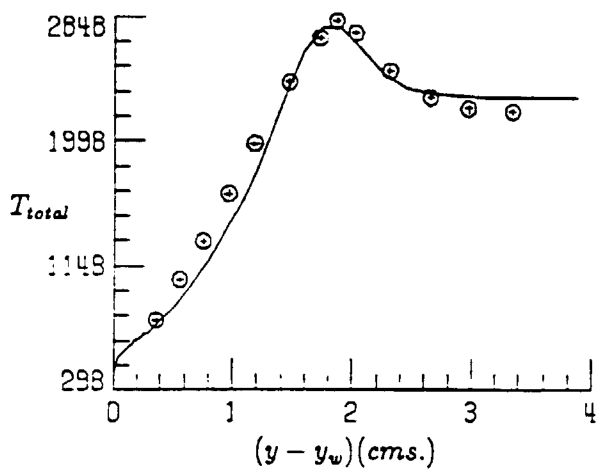
2. Wall pressure comparison.

BURROWS KURKOV

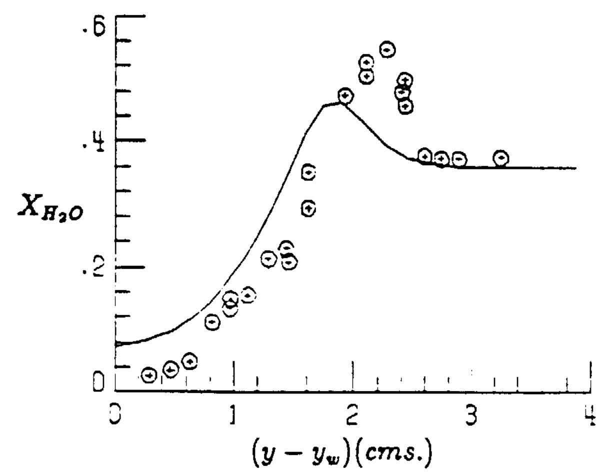
It involves Mach 1 H_2 injection in a Mach 2.44 vitiated-air stream. The flow conditions correspond to the experiments of Burrows and Kurkov. For the H_2 jet: $u = 1216$ m/s, $T = 254$ K and $f_{H_2} = 1.0$. For the vitiated-air stream: $u = 1764$ m/s, $T = 1270$ K, $f_{O_2} = 0.258$, $f_{N_2} = 0.486$ and $f_{H_2O} = 0.256$.



BURROWS KURKOV



1. Total temperature comparison.



2. H_2O mole fraction comparison.

MIXING ENHANCEMENT STUDIES

- FUEL-AIR MIXING DECREASES WITH INCREASING MACH NUMBER

- MIXING ENHANCEMENT MECHANISMS ARE REQUIRED AT HIGH COMBUSTOR MACH NUMBER

    - PLANAR SHOCKS
    - CURVED SHOCKS
    - SWIRL
    - ACOUSTIC FORCING

  } EXCITATION OF UNSTABLE MODES

- ENHANCEMENT BY SHOCKS IS EXAMINED IN THIS STUDY

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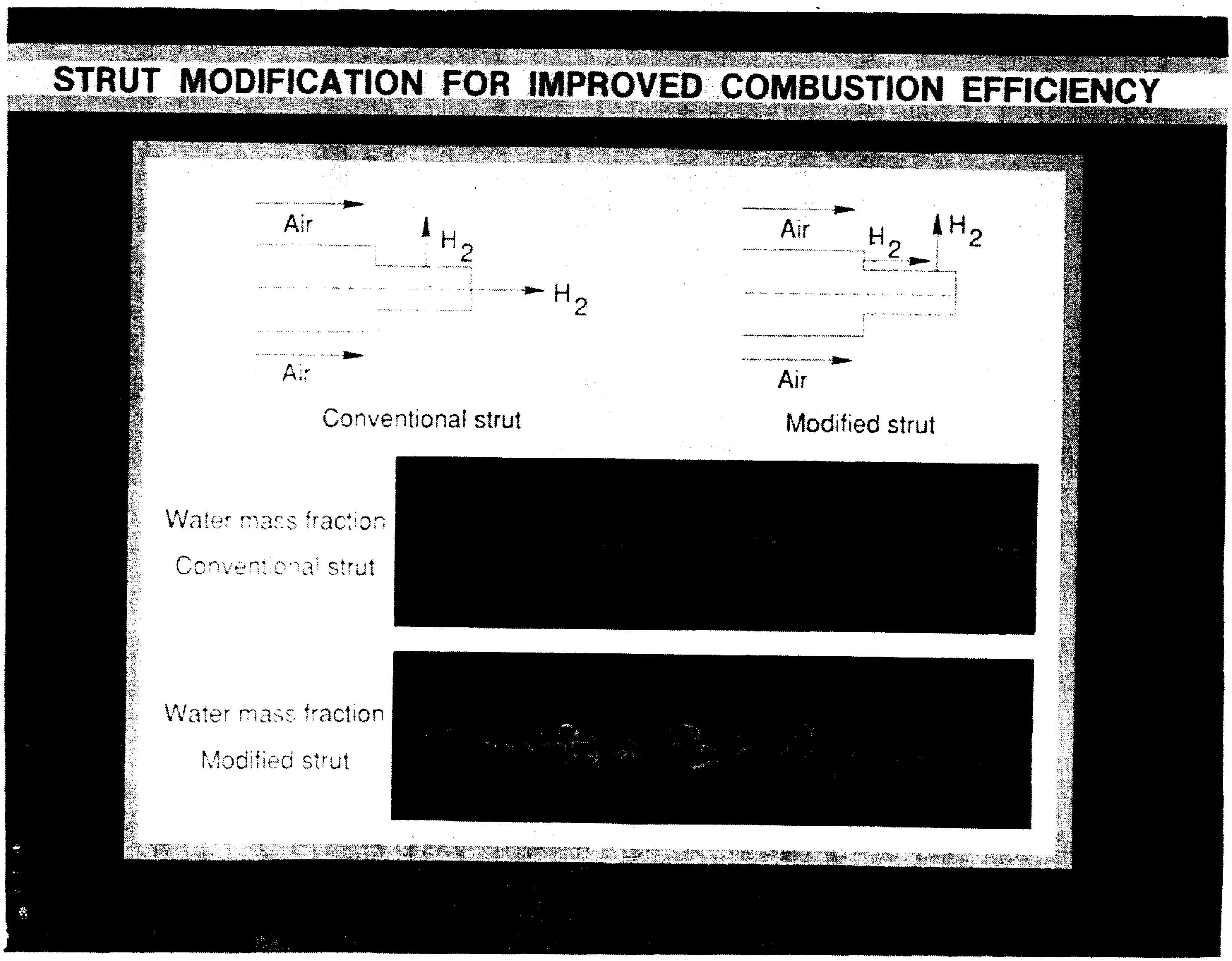
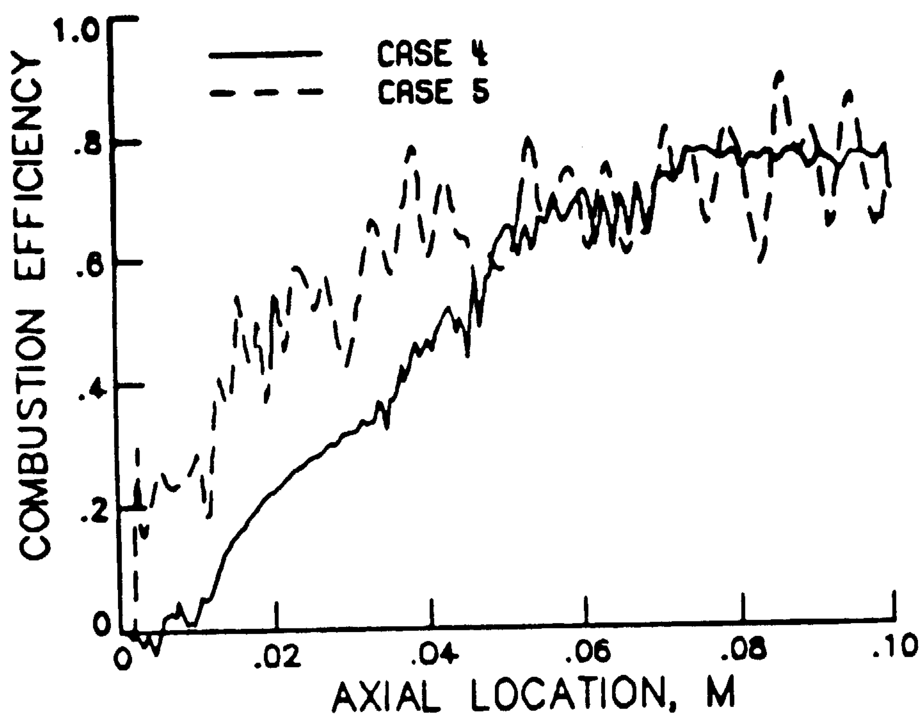
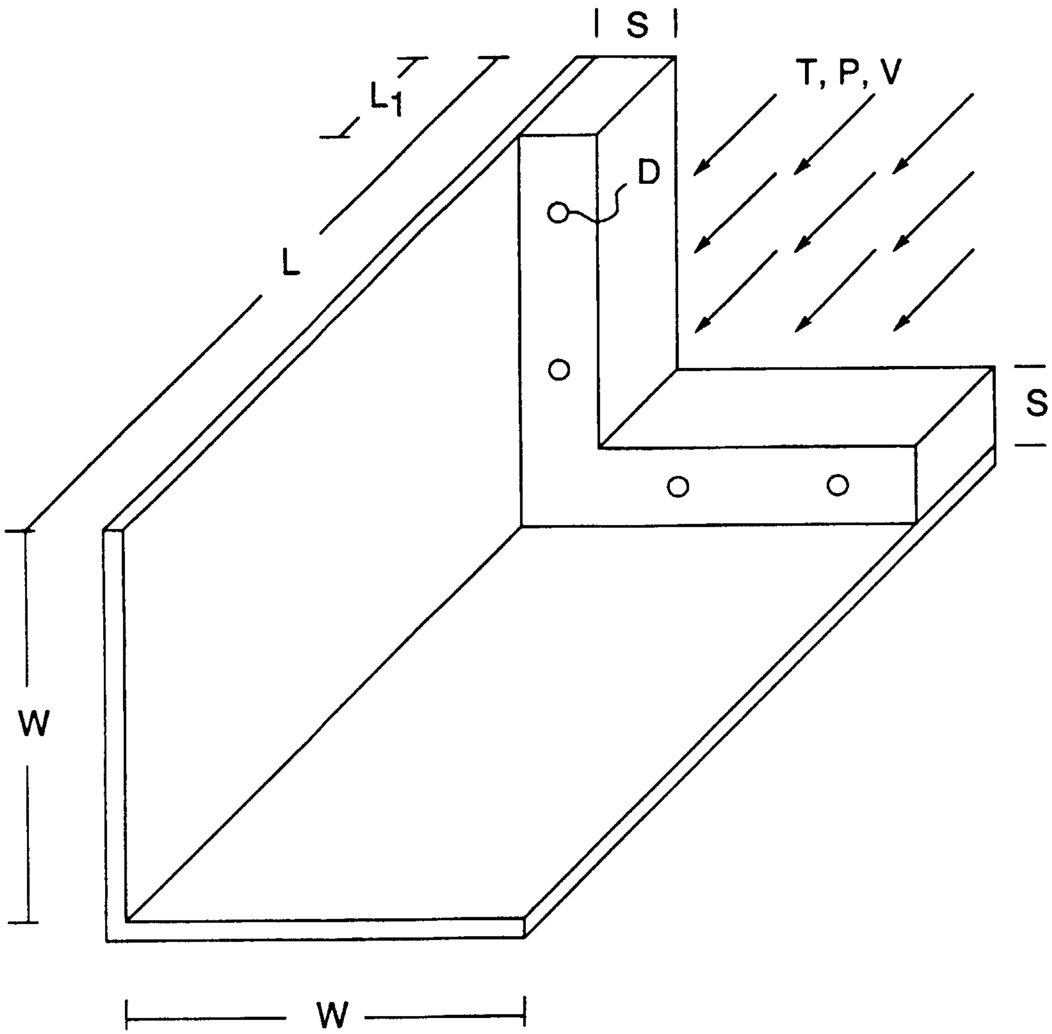


STRUT WITH TRANSVERSE - PARALLEL JETS



MODEL COMBUSTOR



L = 20.0 cm, W = 10.0 cm

S = 2.0 cm, L_1 = 1.5 cm, D = 3.5 mm

T = 1000 K, P = 0.5 atm, V = 1500 m/s

CONCLUSIONS

- COMPUTER PROGRAMS DEVELOPED TO MODEL 3-D SUPERSONIC CHEMICALLY REACTING FLOWFIELDS.

- FAVORABLE VALIDATION AGAINST AVAILABLE EXPERIMENTAL RESULTS

- BEING USED EXTENSIVELY IN THEORETICAL STUDIES AND IN ENGINEERING ENVIRONMENTS

DIRECTIONS

- ALGORITHMS
  - HIGHER ORDER AND COMPACT
  - UPWINDING
  - PARALLEL COMPUTING

- TRANSITION - TURBULENCE MODELING
  - COMPARISON WITH LINEAR STABILITY CODES
  - DIRECT SIMULATIONS OF SUPERSONIC JETS AND MIXING LAYERS
  - "DATABASE" FOR PHENOMINOLOGICAL MODELS

- PRODUCTION CODE SUPPORT