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**Modeling of Outgassing and Matrix Decomposition
in Carbon-Phenolic Composites
NASA Marshall Grant NAG8-295**

Semi-Annual Report
for the period January 1994-June 1994

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Submitted to Dr. Roy Sullivan
ED24
George C. Marshall Space Flight Center
MSFC, AL 35812

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by

Hugh L. McManus
Class of 1943 Assistant Professor
Principal Investigator

(NASA-CR-196319) MODELING OF
OUTGASSING AND MATRIX DECOMPOSITION
IN CARBON-PHENOLIC COMPOSITES
Semiannual Report, Jan. - Jun. 1994
(MIT) 52 p

TECHNOLOGY LABORATORY FOR ADVANCED COMPOSITES
Department of Aeronautics and Astronautics, Room 33-311
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, Massachusetts 02139

Introduction

This report summarizes the work done in the period January 1994 through June 1994 on the "Modeling of Outgassing and Matrix Decomposition in Carbon-Phenolic Composites" program.

Progress

Two threads of research have been followed. First, the thermodynamics approach was used to model the chemical and mechanical responses of composites exposed to high temperatures. This approach was first proposed by Sullivan [1]. The thermodynamics approach lends itself easily to the usage of variational principles. This thermodynamic-variational approach has been applied to the transpiration cooling problem. In transpiration cooling, a porous solid is cooled by gas flowing from the cool end to the hot end. The governing equation for the temperature distribution was obtained for the steady-state case.

The second thread is the development of a better algorithm to solve the governing equations resulted from modeling. The resulting nonlinear, partial differential equations are very complex. The complexities are increased even more when detailed material models are included such as multi-stage chemical reactions and non-ideal gases. Previously, implicit finite difference method was used to solve the governing equations. Although the implicit method is relatively stable, it was found that detailed material models cannot be easily incorporated into the implicit finite difference method. Explicit finite difference method is explored as an alternate numerical method to solve the governing equations. In the explicit method, detailed material models can be included into the algorithm much easier than the implicit method. The explicit method is also highly suitable for solution on massively parallel supercomputers such as SCOUT, MIT's new ARPA-sponsored Thinking Machines CM-5.

To demonstrate the feasibility of the explicit scheme in solving nonlinear partial differential equations, a sample problem was solved using SCOUT. The sample problem was a transpiration cooling problem, which resembles the composite ablative problem in that the solution requires solving simultaneously the continuity, energy, and momentum equations. Some interesting transient behaviors were captured such as stress waves and small spatial oscillations of transient pressure distribution. The results of this study were presented at NASA-Langley in April 1994. A set of viewgraphs from this presentation are attached.

Current Status

The thermodynamic-variational approach is currently being pursued. Using the approach, governing equations for material responses of composites exposed to high temperatures will be derived. Biot has done some extensive work in developing the thermodynamic-variational approach in references [2,3]. Our work will follow Biot's development closely.

The ablative composite code CHAR is being re-coded using the explicit finite difference method on the CM5 Massively Parallel Machine that MIT has acquired recently. After CHAR-CM5 is completed, the new thermodynamically-based material and reaction models will be included into the code to perform parametric studies.

References

- [1] Sullivan, R.M., "On the Constitutive Relations for the High-Temperature, Nonlinear Expansion of Polymeric Composites," AMD-Vol. 159, Mechanics of Composites, Materials Nonlinear Effects, Editor: M.W. Hyer, 1993, pp. 331-342.
- [2] Biot, M.A., "New Fundamental Concepts and Results in Thermodynamics with Chemical Application," Chemical Physics 22, 1977, pp. 183-198.
- [3] Biot, M.A., "Variational-Lagrangian Irreversible Thermodynamics of Initially-Stressed Solids with Thermomolecular Diffusion and Chemical Reactions," Journal of Mechanics and Physics of Solids, 1977, Vol. 25, pp. 289-307.

RESEARCH RELEVANT TO TRANSPIRATION COOLING OF AEROSPACE VEHICLES AT MIT

Prof. Hugh L. McManus
Class of 1943 Career Development Professor



Technology Laboratory for Advanced Composites
Department of Aeronautics and Astronautics
Massachusetts Institute of Technology

OUTLINE

Modeling of composite ablators

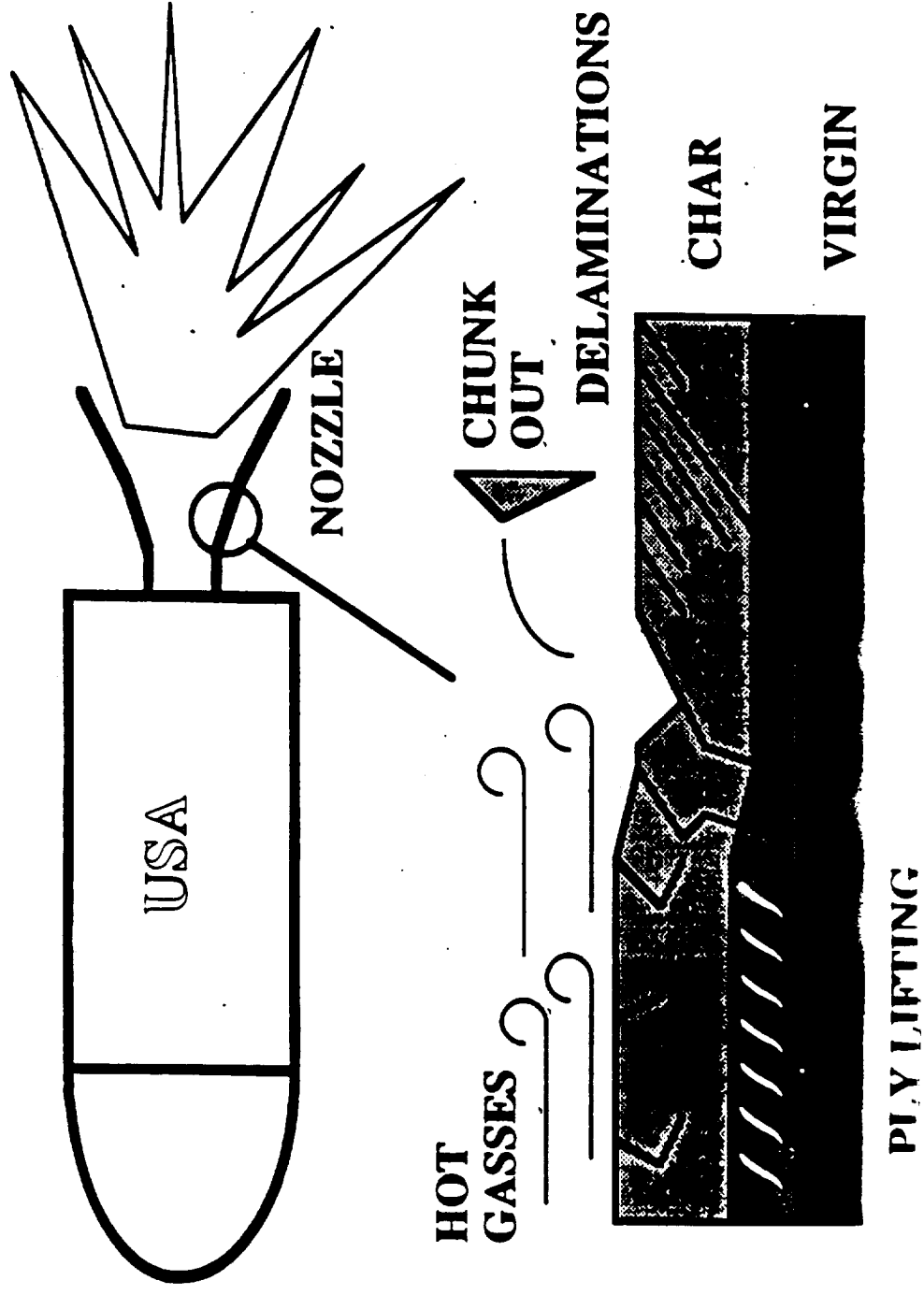
Advanced numerical methods

Transpiration cooling used as example problem

Functionally graded materials

Interdisciplinary hypersonics research program

COMPOSITE ABLATORS



Very large heat loads require ablative materials

Modeling Material Response

Problem:

Complex environments

Complex material responses:

Thermal

Chemical

Mechanical

Ugly (outgassing and gas flow, vol. desorption)

**Often outside the range of usual assumptions
(like linearity)**

Coupling between all of above...

How do we do this?

Modeling Approach

Given:

Environment

Material properties (may need a lot...)

Experimental observations of gross behavior

Propose:

Physical models of what material does

Formulate mathematically (and in FORTRAN)

Predict Behavior

Verify Experimentally

Trick is to model material as completely as required to capture critical behaviors

Why do this?

Quantitatively Accurate Model Allows:

Understanding why behavior exists
Determination of what factors affect it
Which direction to change these factors
Bounding (order of magnitude) calculations
Must be used in conjunction with testing

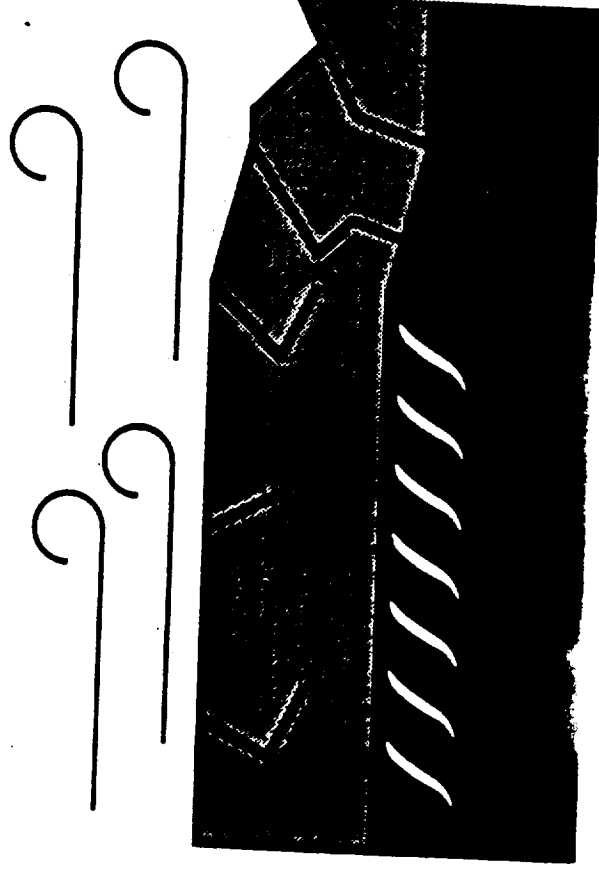
Qualitatively Accurate Model Allows:

Accurate assessment of response to environment
Design of parts suitable to environment

*Reports, user-tolerant computer codes facilitate utility
of models developed here*

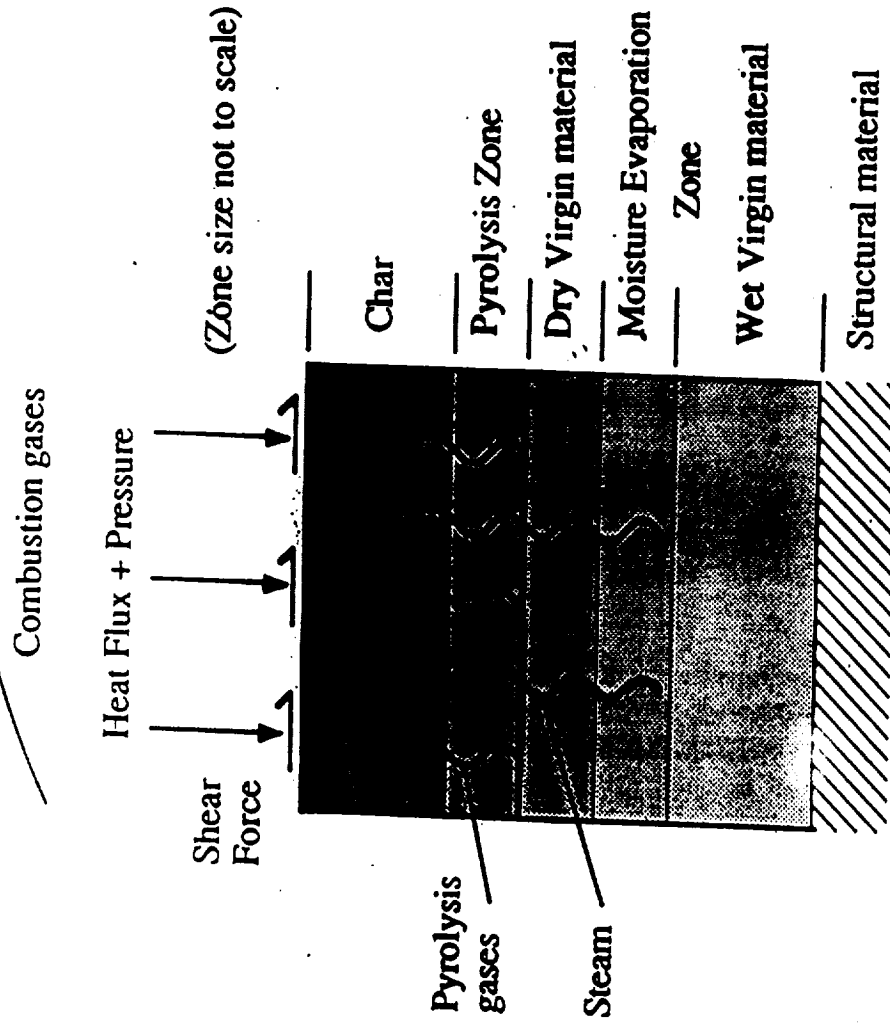
Chemical-Flow-Poro-Thermo-Structural Modeling:

Motivation: Ply Lifting of Rocket Nozzles



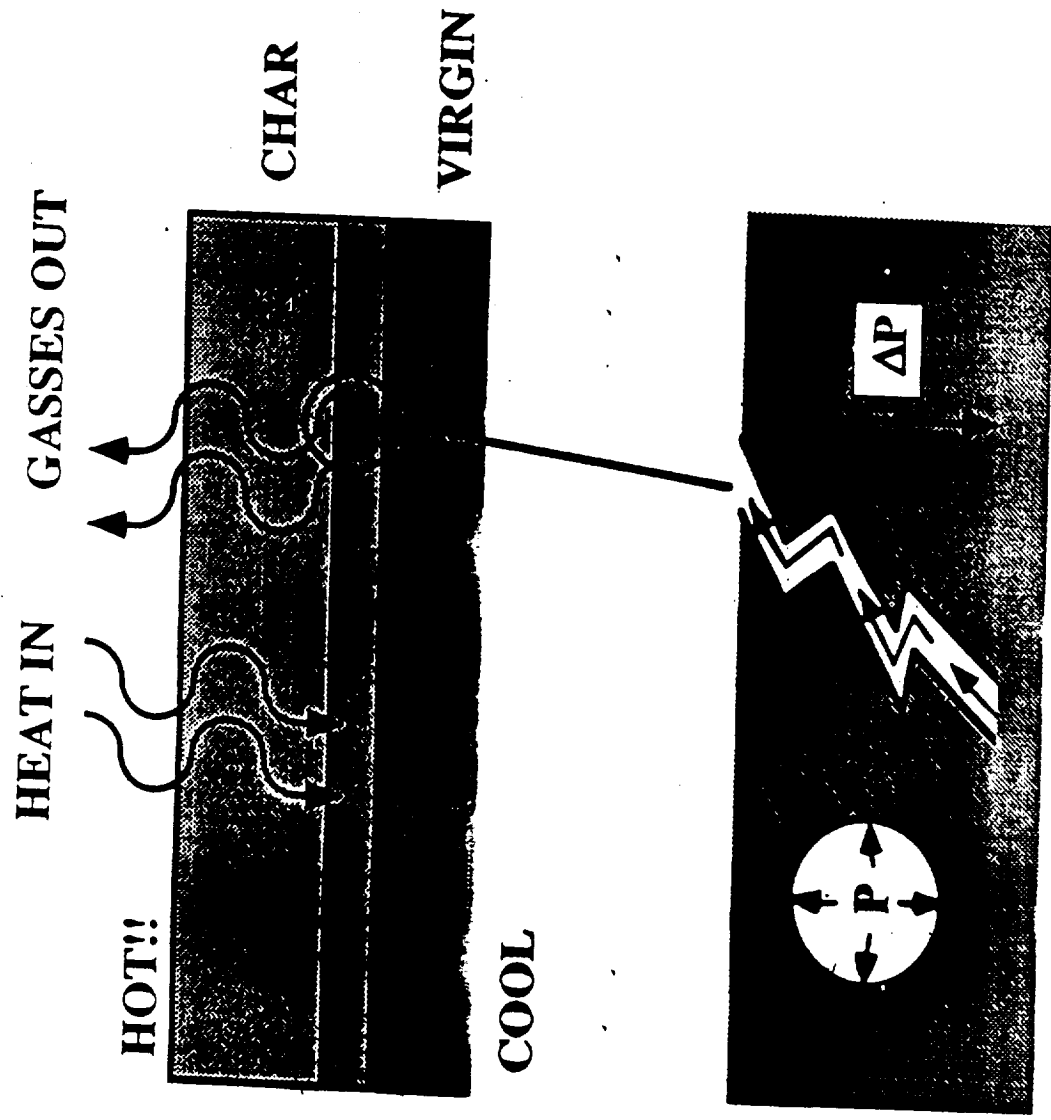
Shuttle Solid Rocket Motors (SRM) did
Next Generation (ASRM) does too!

Reaction Zones

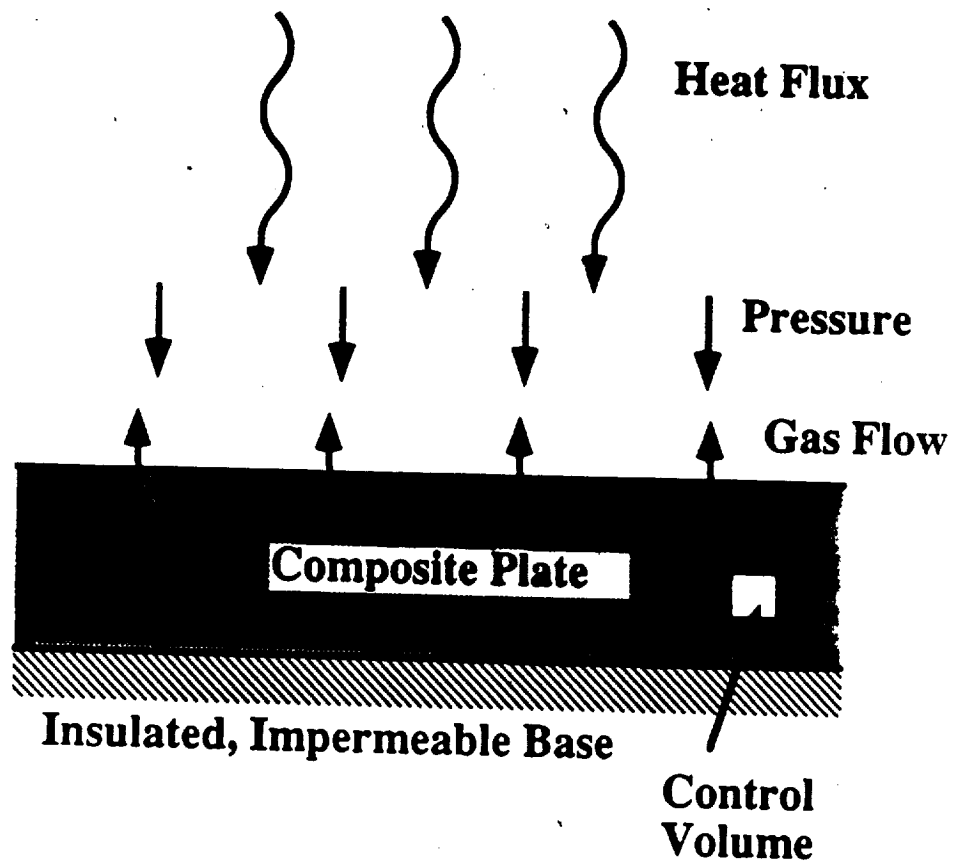


- Pyrolysis Zone and Moisture Evaporation Zone are very small
- Large pressure developed just below the Pyrolysis Zone
- Ply-lift is observed to occur just below the Pyrolysis Zone

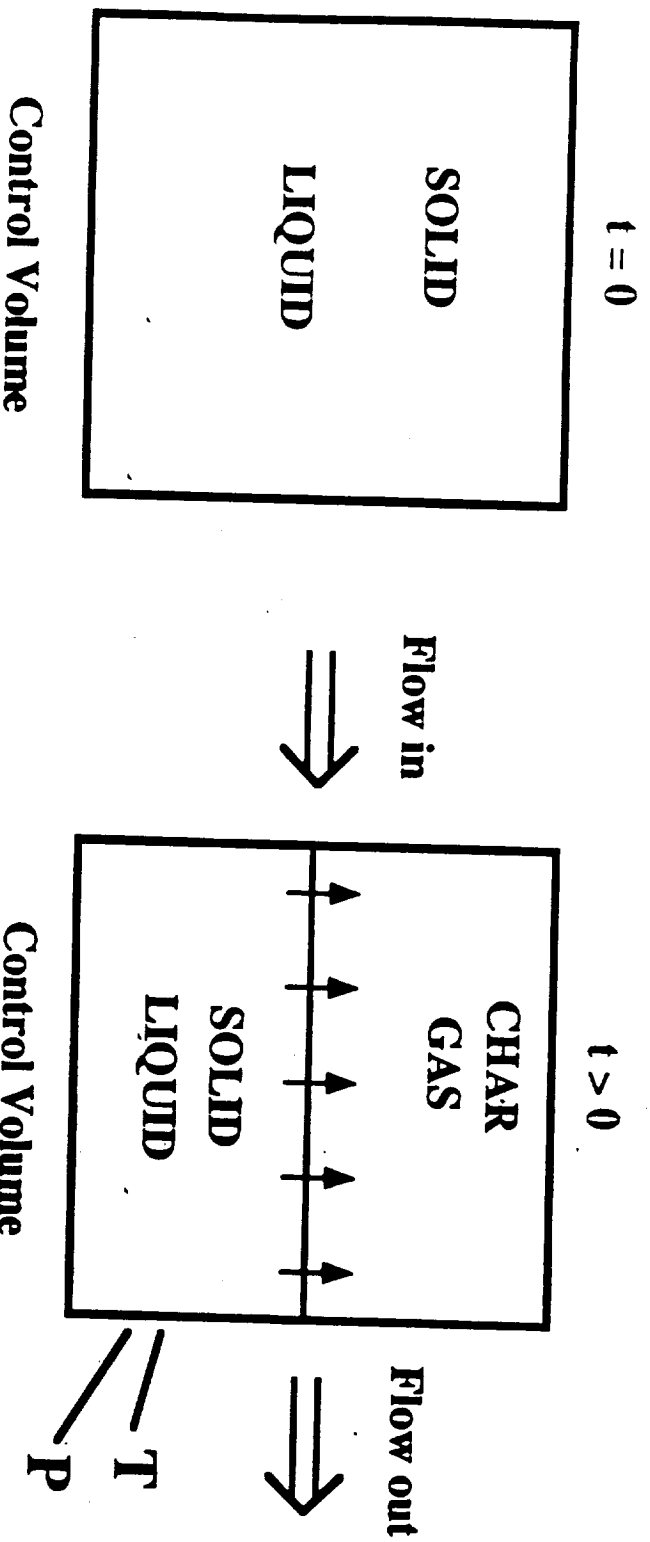
Internal Pressure



THERMOCHEMICAL MODEL



THERMOCHEMICAL MODEL



- Conservation of Mass
- Conservation of Energy
- Equations of State
- Darcy's Flow Law
- Reaction Kinetics

MECHANICAL MODEL

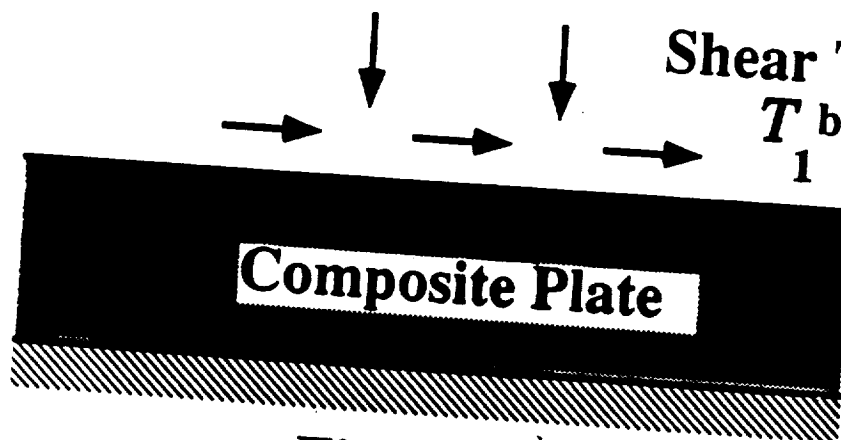
Pressure P_b

Normal Traction T_3^b

Shear Traction
 $T_1^b; T_2^b$

Composite Plate

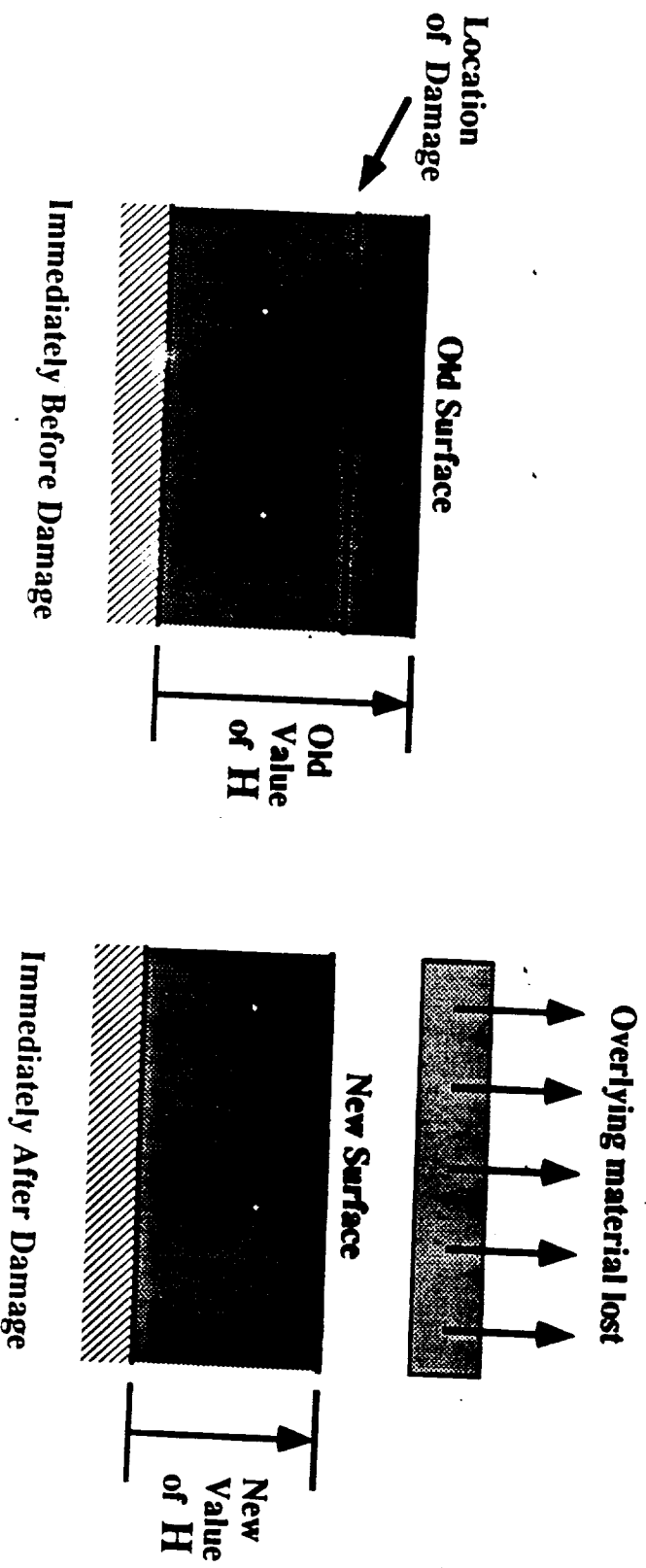
Fixed Base



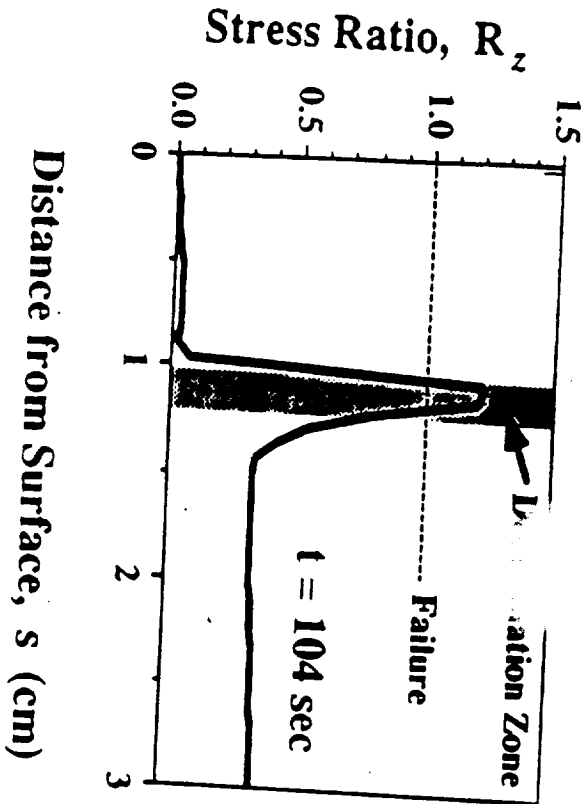
MECHANICAL MODEL

COMPOSITE FAILURE CRITERIA

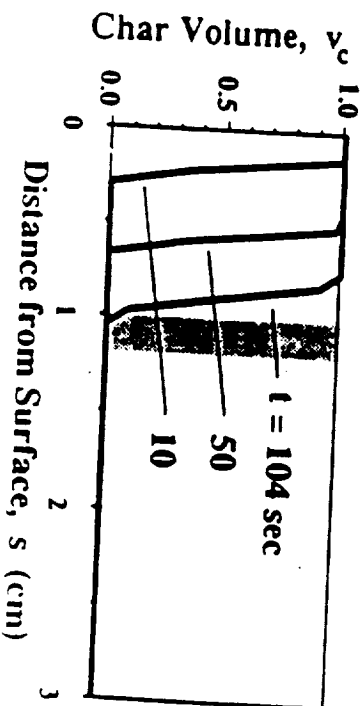
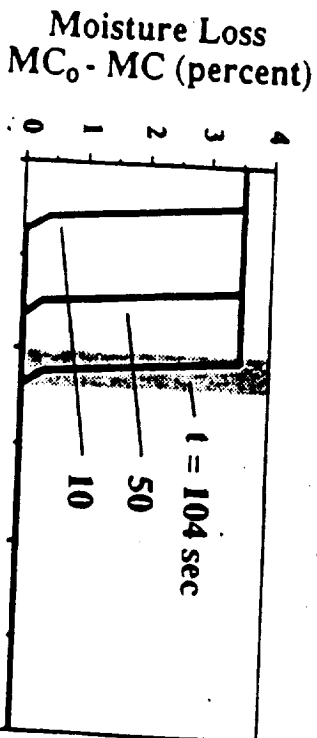
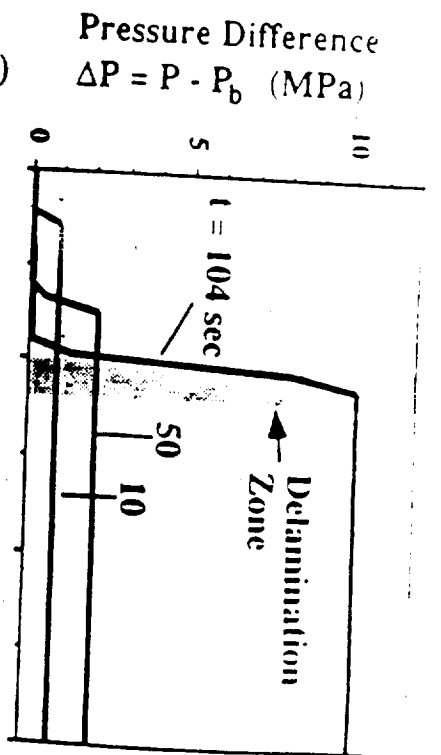
O MAXIMUM STRESS



Ply Lift Replication



Ply lift is a distinct event



It occurs in the zone between moisture loss and charring

Current Research

Qualitative predictive capability achieved

Unfortunately, quantitative analysis sensitive to messy details of analysis:

Reaction models

Water storage and release mechanisms

Permeability-stress interactions

Numerical Scheme

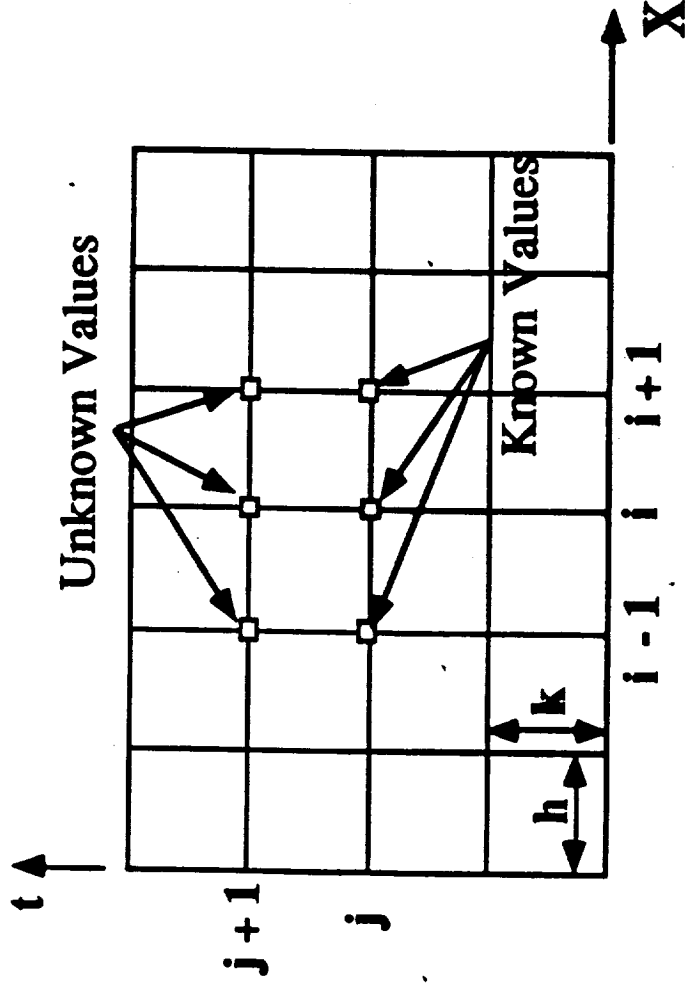
Exploring advanced models, as well as "revolutionary" approaches:

Thermodynamic description of material

Massively Parallel numerical models

ADVANCED NUMERICAL METHODS

-Implicit Method

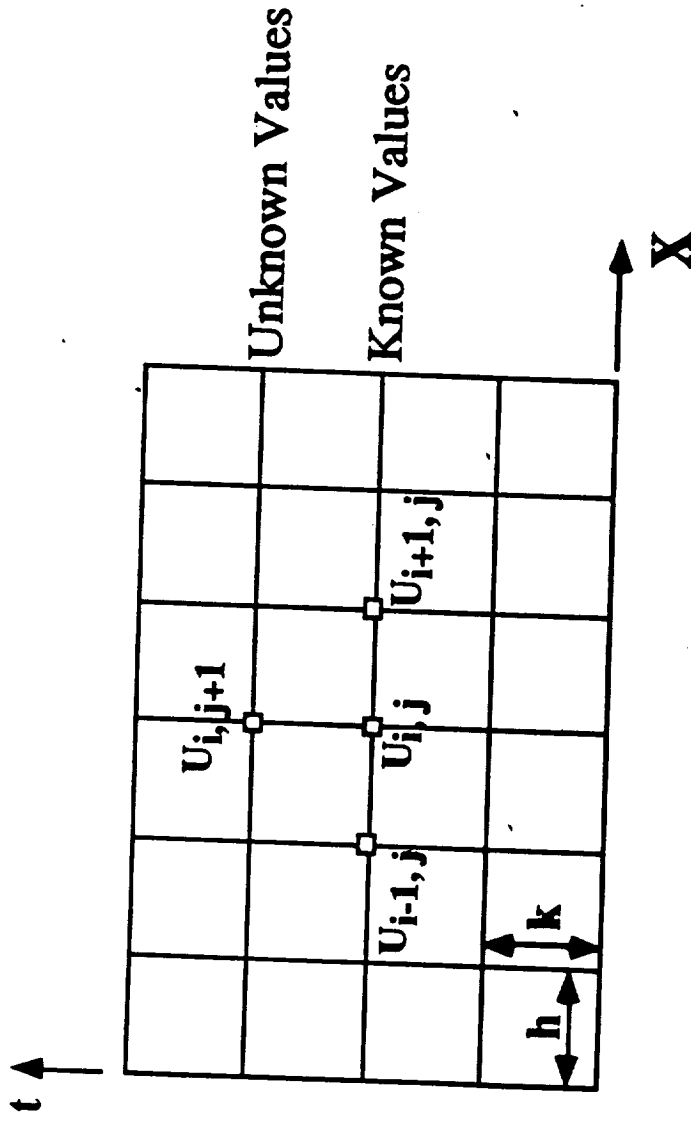


N equations with N unknowns

- More difficult to program
- Nonlinear equations need large iterations for convergence

Solution Method

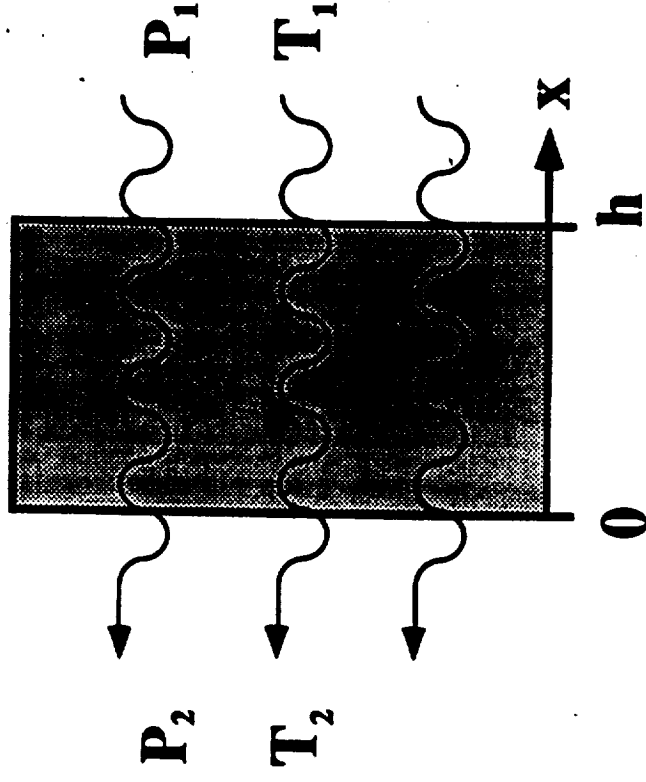
- ## - Explicit Method



Unknown at $t+\Delta t$ expressed in terms of knowns at t

- Simple algorithm
- Need small time steps

EXAMPLE PROBLEM: TRANSPIRATION COOLING



- Exact solutions of steady state temperature and pressure distributions available
- Explicit solution ran until steady state reached

Check Case #1

- Steady state temperature distribution

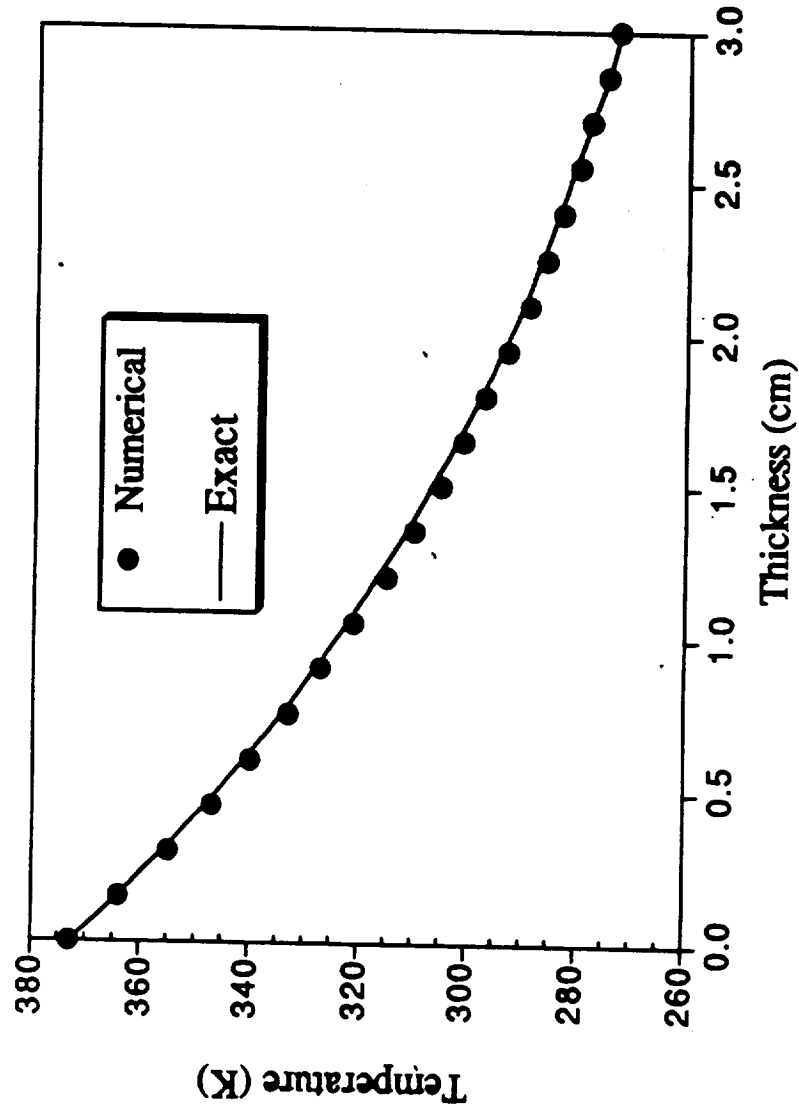
$$P_1 = 2 \text{ MPa}, P_2 = 1 \text{ MPa}$$

$$T_1 = 273 \text{ K}, T_2 = 373 \text{ K}$$

$$h = 3 \text{ cm}, \quad \dot{m}_g = 3.4 \text{ kg/m}^3 \text{ sec}$$

Check Case #1

Steady State Temperature Distribution



Check Case #2

- Steady state pressure distribution

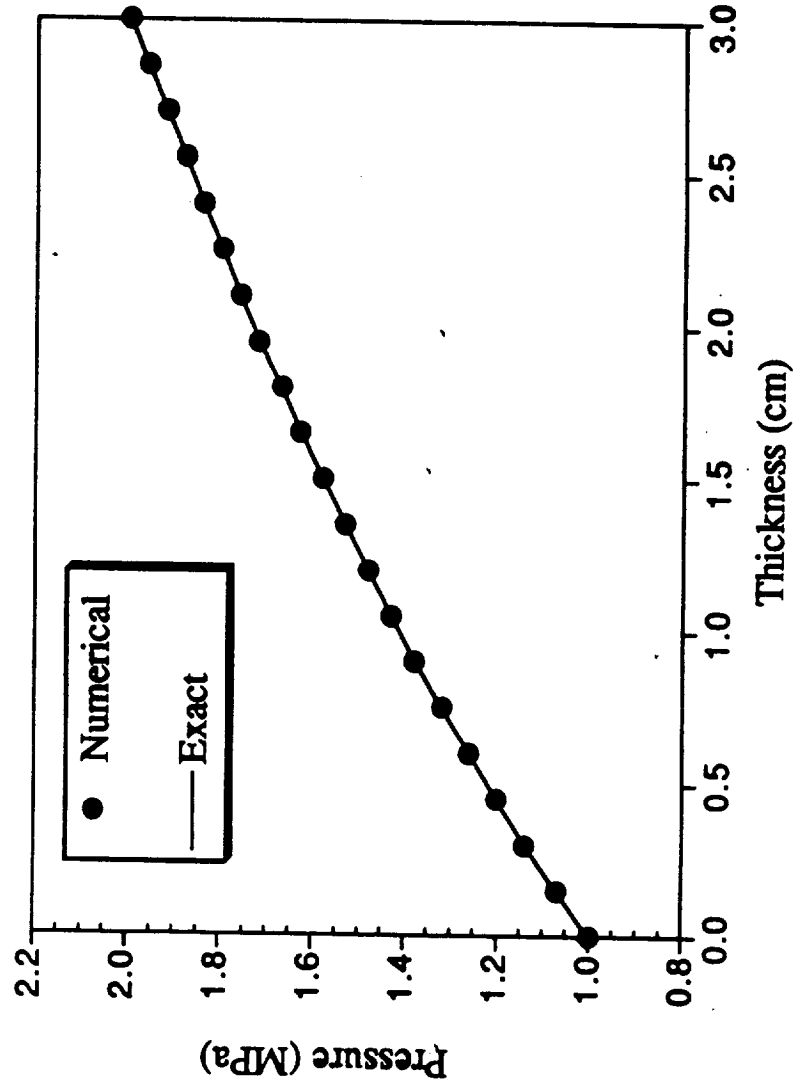
$$P_1 = 2 \text{ MPa}, P_2 = 1 \text{ MPa}$$

$$T_1 = 273 \text{ K}, T_2 = 273 \text{ K}$$

$$h = 3 \text{ cm}, \quad \dot{m}_g = 4.0 \text{ kg/m}^3 \text{ sec}$$

Check Case #2

Steady State Pressure Distribution



Parametric Studies

- Varying P_1
- Varying permeability
- Varying porosity

Variation in P_1

Parameters used

$$- P_1 = 2\text{MPa} \quad \dot{m}_g = 3.40 \text{ kg/m}^3 \text{ sec}$$

$$- P_1 = 5\text{MPa} \quad \dot{m}_g = 30.2 \text{ kg/m}^3 \text{ sec}$$

$$- P_1 = 20\text{MPa} \quad \dot{m}_g = 843 \text{ kg/m}^3 \text{ sec}$$

$$P_2 = 1 \text{ MPa}$$

$$T_1 = 273 \text{ }^\circ\text{K}$$

$$T_2 = 373 \text{ }^\circ\text{K}$$

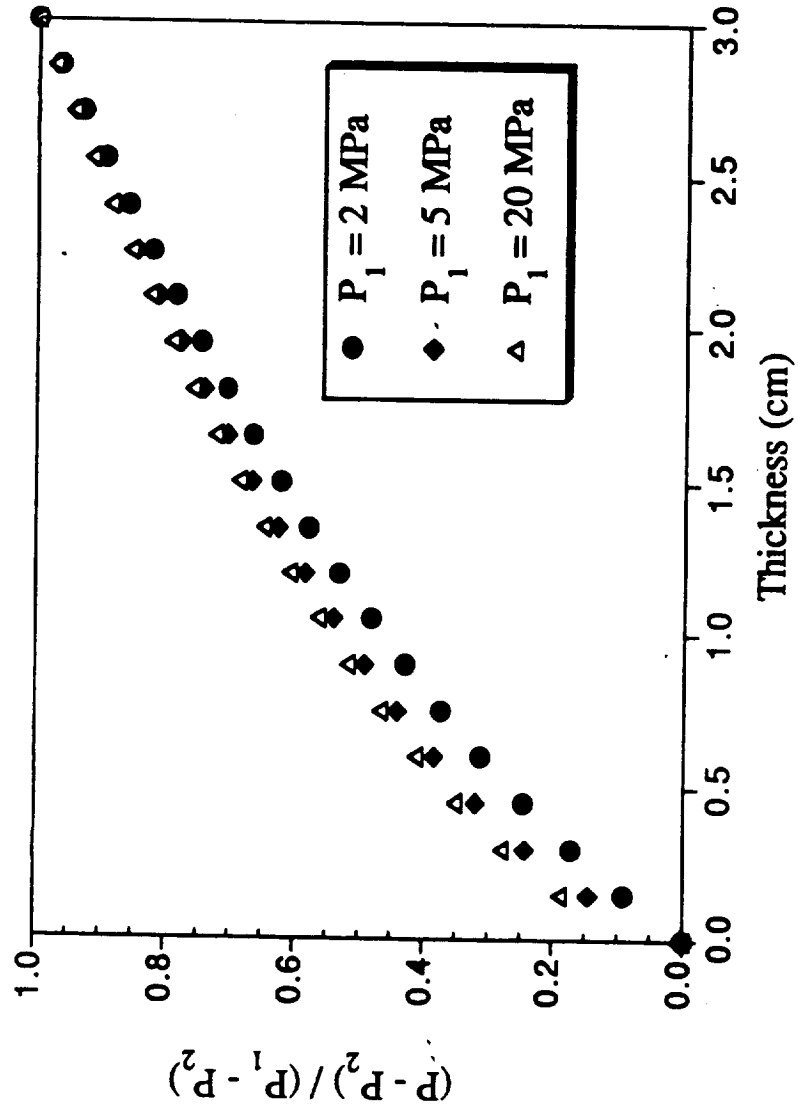
$$\text{porosity} = 0.05$$

$$\text{permeability} = 100 \times 10^{-15} \text{ m}^2$$

$$\text{viscosity} = 1 \times 10^{-5} \text{ kg/m sec}$$

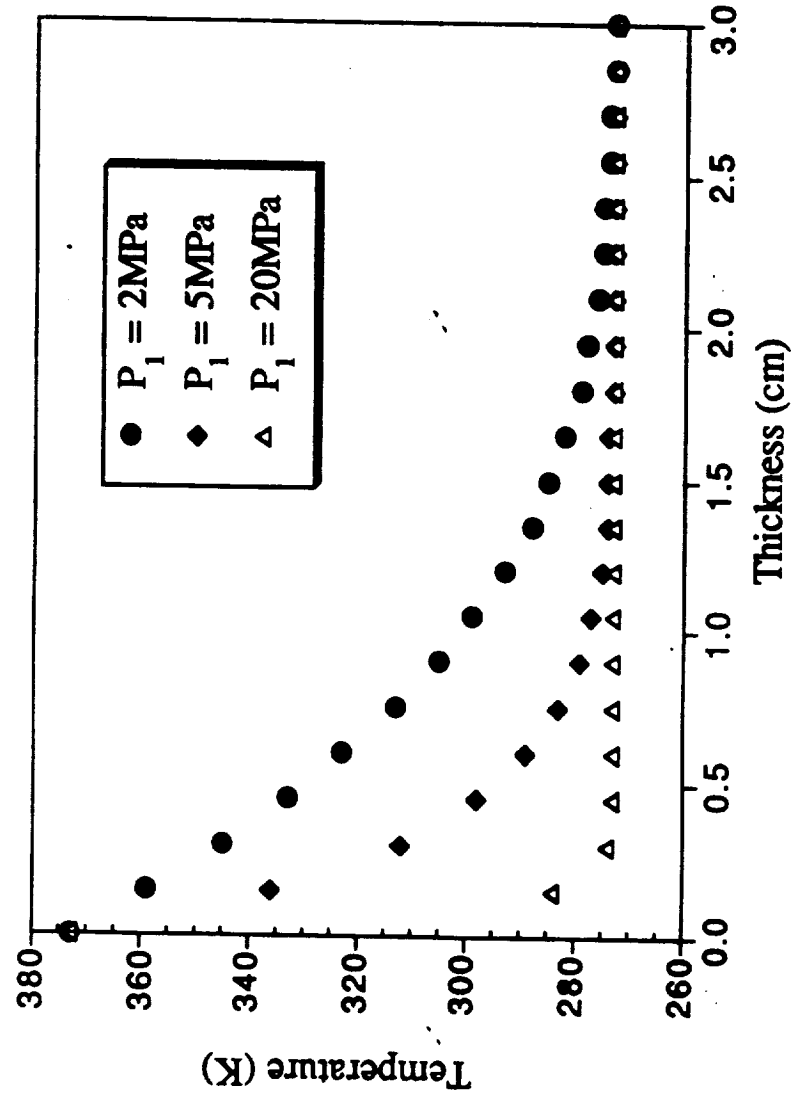
Variation in P_1

Steady State Pressure Distributions



Variation in P_1

Steady State Temperature Distributions



Variation in Permeability

Parameters used

- Permeability = $100 \times 10^{-16} \text{ m}^2$ $\dot{m}_g = 0.33 \text{ kg/m}^3 \text{ sec}$
- Permeability = $100 \times 10^{-15} \text{ m}^2$ $\dot{m}_g = 3.40 \text{ kg/m}^3 \text{ sec}$
- Permeability = $100 \times 10^{-14} \text{ m}^2$ $\dot{m}_g = 37.0 \text{ kg/m}^3 \text{ sec}$

$P_1 = 2 \text{ MPa}$

$P_2 = 1 \text{ MPa}$

$T_1 = 273 \text{ K}$

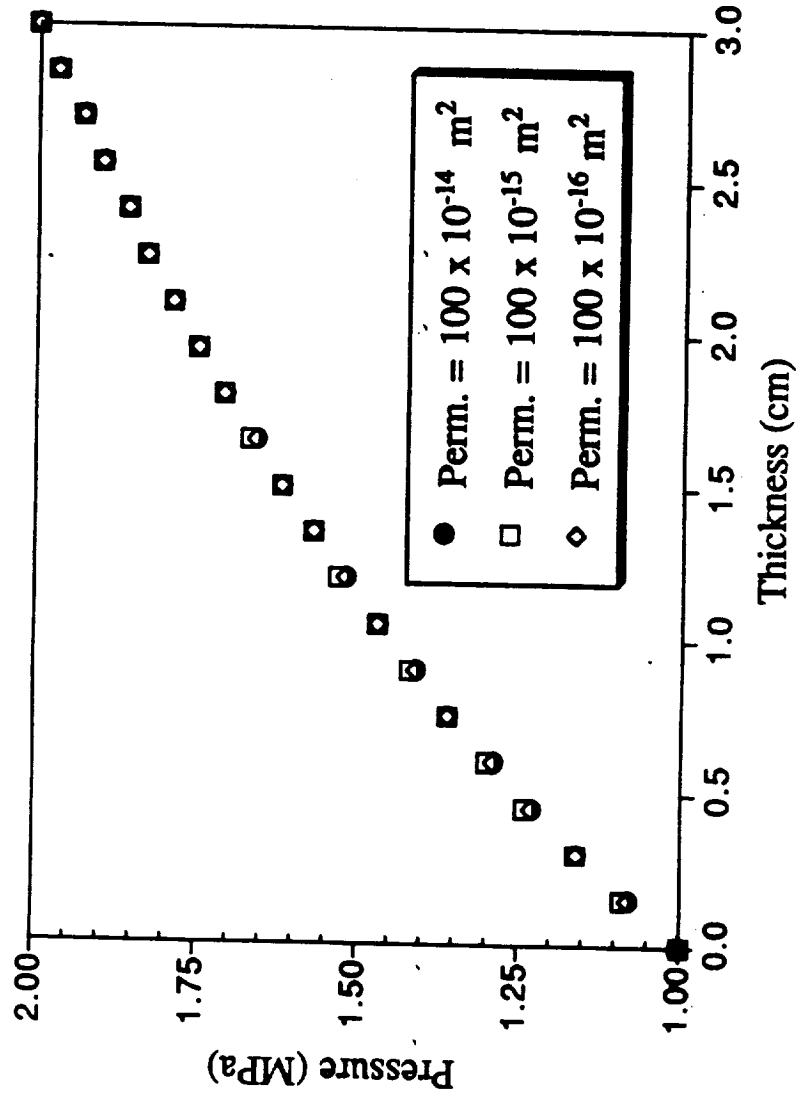
$T_2 = 373 \text{ K}$

porosity = 0.05

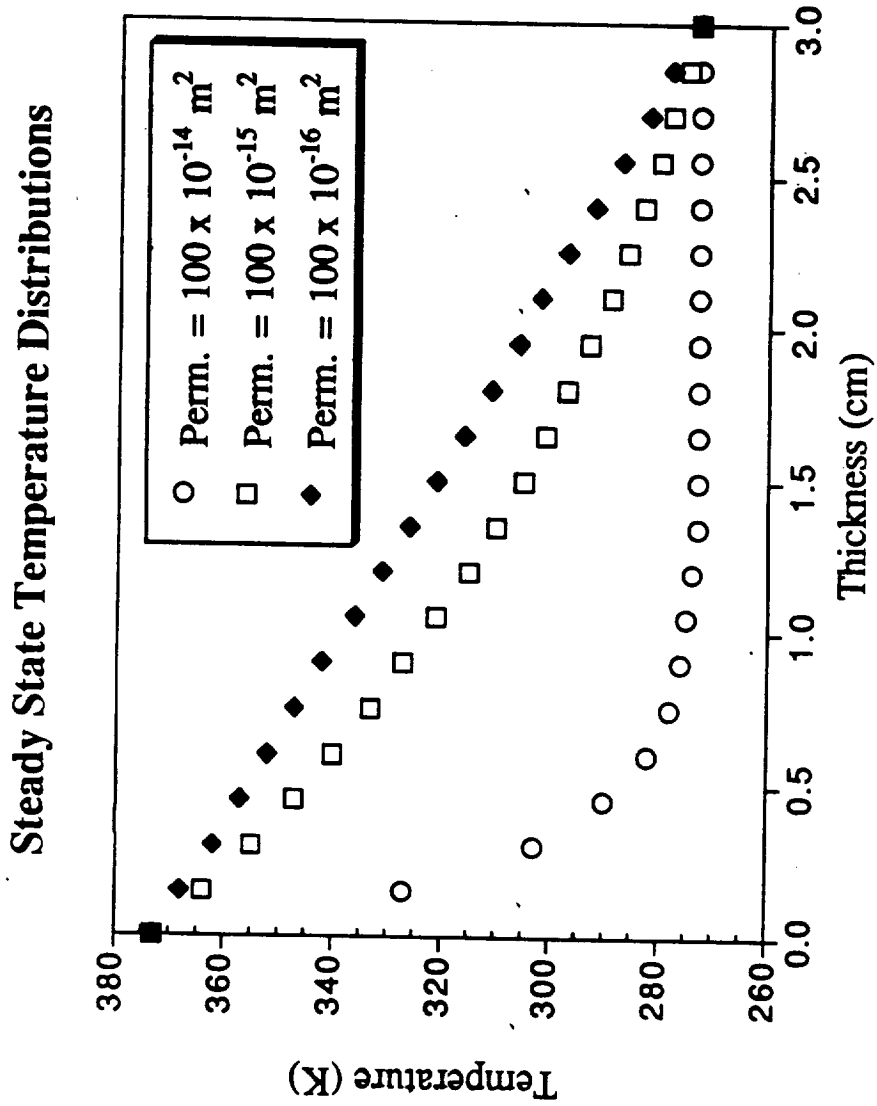
viscosity = $1 \times 10^{-4} \text{ kg/n sec}$

Variation in Permeability

Steady State Pressure Distributions



Variation in Permeability



Variation in Porosity

Parameters used

$$k = 150 \text{ W/m}^2\text{K}$$

$$C_{ps} = 167 \text{ J/kg K}$$

- porosity = 0.01 $k_{\text{effective}} = 149 \text{ W/m}^2\text{K}$ $C_{ps}^{\text{effective}} = 166 \text{ J/kg K}$
- porosity = 0.025 $k_{\text{effective}} = 146 \text{ W/m}^2\text{K}$ $C_{ps}^{\text{effective}} = 163 \text{ J/kg K}$
- porosity = 0.05 $k_{\text{effective}} = 143 \text{ W/m}^2\text{K}$ $C_{ps}^{\text{effective}} = 159 \text{ J/kg K}$

$$P_1 = 2 \text{ MPa}$$

$$P_2 = 1 \text{ MPa}$$

$$T_1 = 373 \text{ K}$$

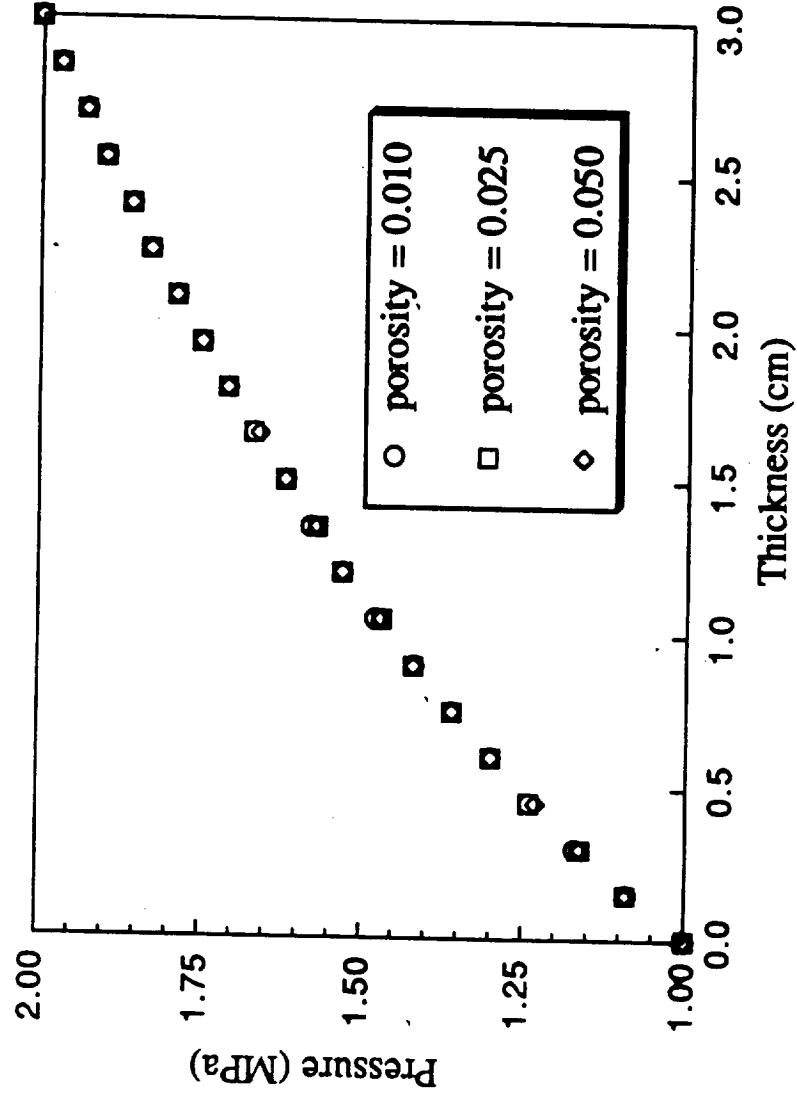
$$T_2 = 273 \text{ K}$$

$$\text{viscosity} = 1 \times 10^{-5} \text{ kg/m sec}$$

$$\text{permeability} = 100 \times 10^{-15} \text{ m}^2$$

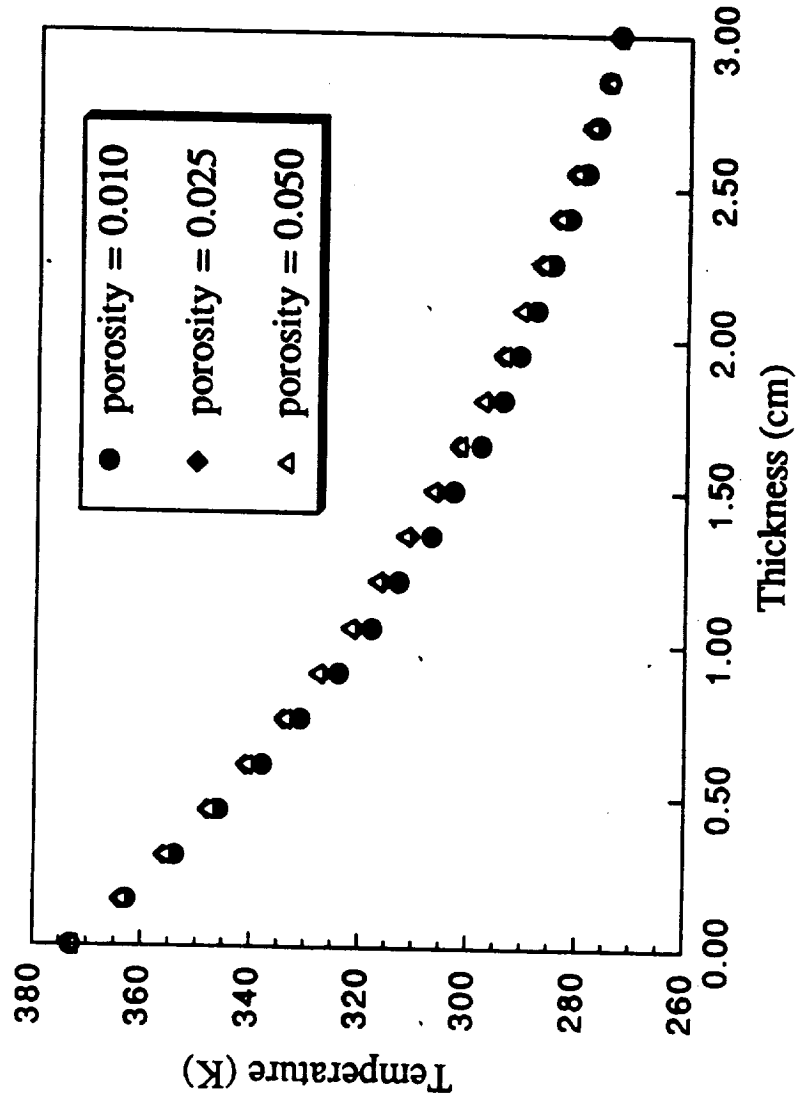
Variation in porosity

Steady State Pressure Distributions



Variation in Porosity

Steady State Temperature Distributions



Examples

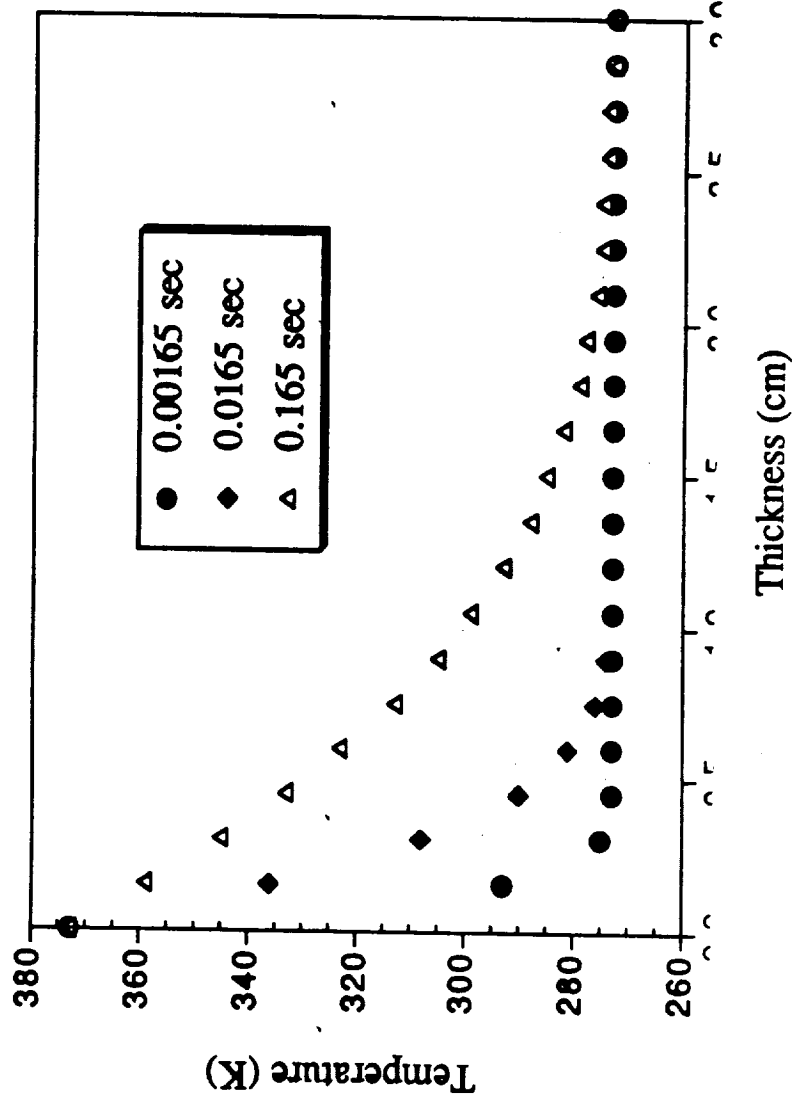
- Transient temperature distribution
- Transient pressure distribution

Parameters used

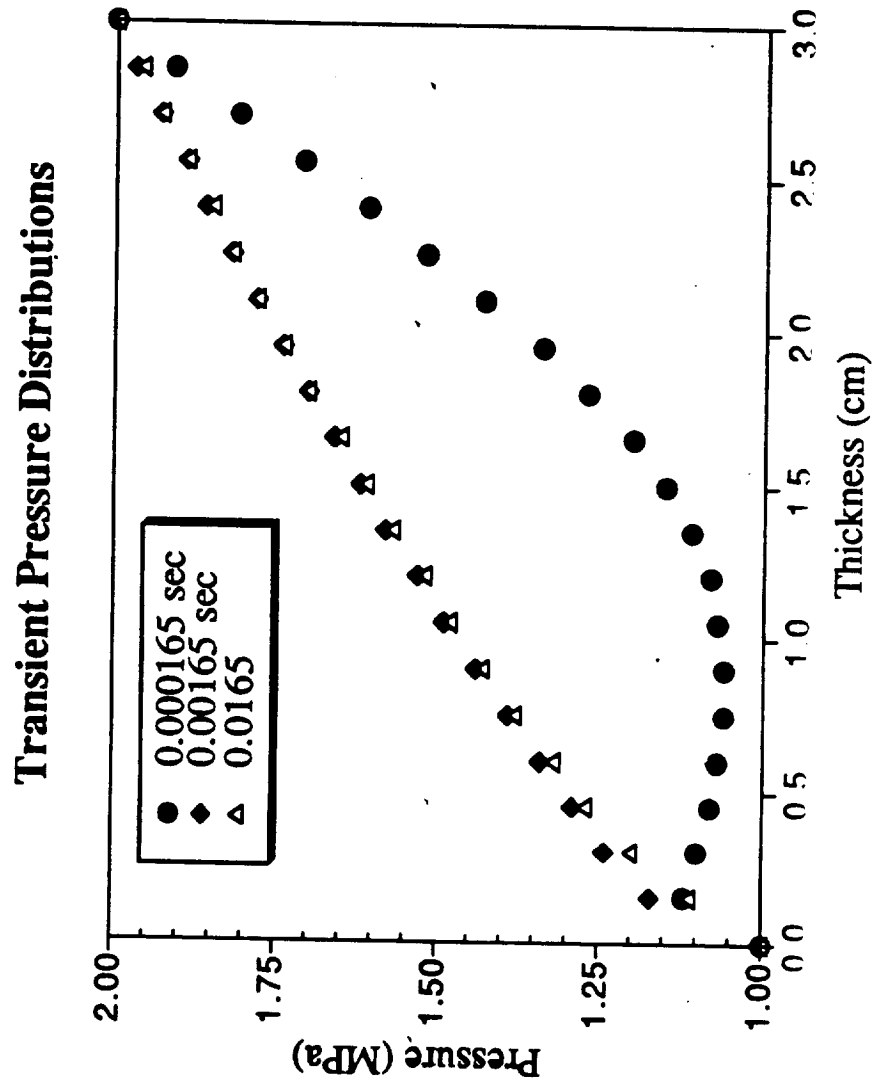
$P_1 = 2 \text{ MPa}$
 $P_2 = 1 \text{ MPa}$
 $T_1 = 273 \text{ K}$
 $T_2 = 373 \text{ K}$
permeability = $100 \times 10^{-15} \text{ m}^2$
viscosity = $1 \times 10^{-5} \text{ kg/m sec}$
porosity = 0.05

Transient Temperature Distributions

Transient Temperature Distributions



Transient Pressure Distributions



FUNCTIONALLY GRADED MATERIALS

**Materials with gradients
constituent fractions
microstructure
porosity/permeability**

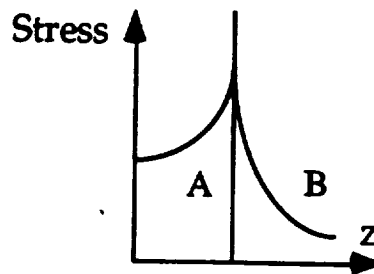
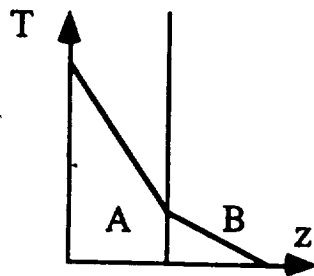
**Greatly expands material choices
material properties functions of location**

**Ideal for environments with sharp gradients
e.g. thermal**

ALTERNATE MATERIAL DESIGNS

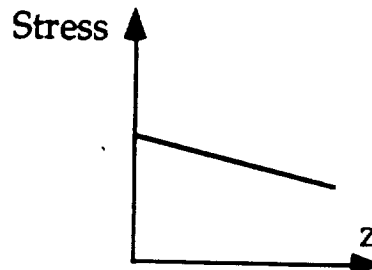
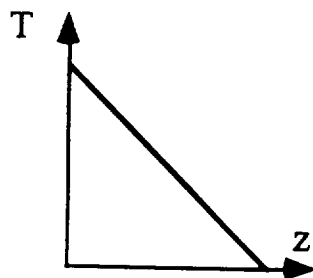
MULTIPLE MATERIALS

Design Parameters	Constraints	Problem
Material Choice (Two or more)	Available Materials Compatibility Joining Techniques	Stress Concentrations Weight Expense

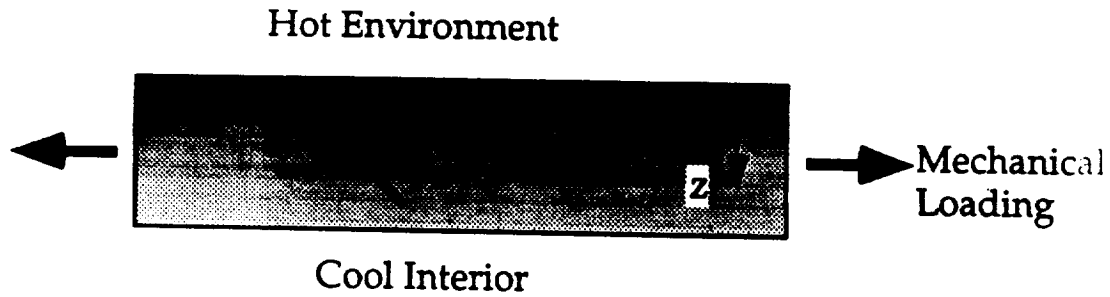


COMPOSITES

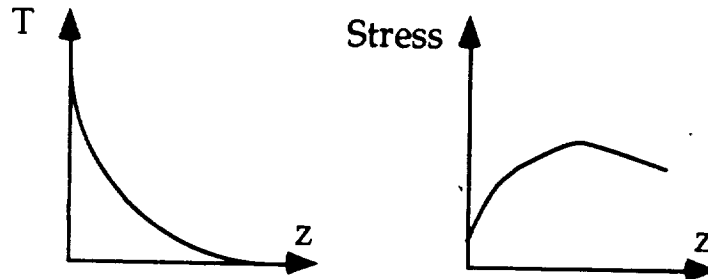
Design Parameters	Constraints	Problems
Constituents Volume Fractions Geometry	Available Materials Compatibility Processing Techniques	Spatial Uniformity 3rd Dimension



FGM MATERIAL DESIGNS



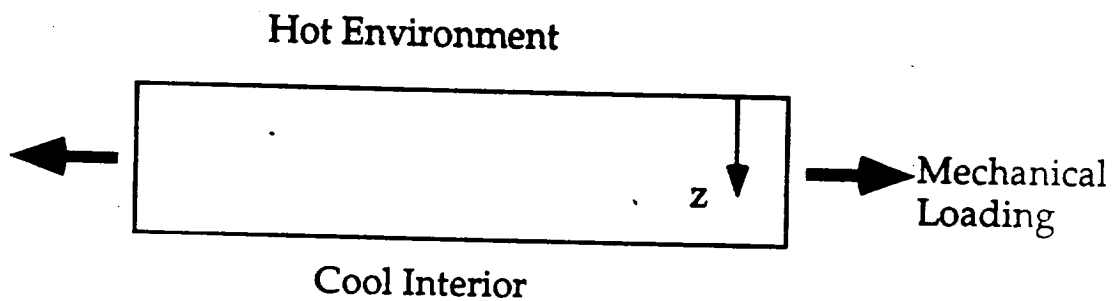
Design Parameters	Constraints	Problems
Constituents Volume Fractions Geometry ALL FUNCTIONS OF POSITION	Available Materials Compatibility PROCESSING	TBD



DESIGNING WITH FGM

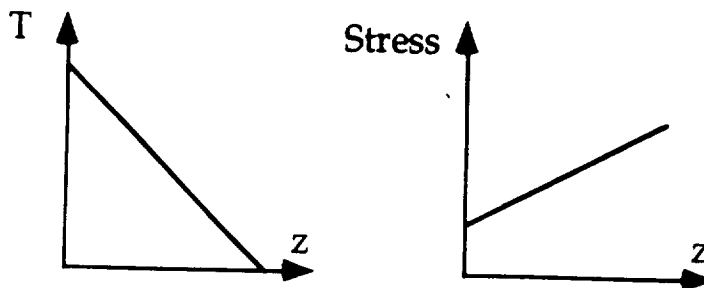
- FGM frees up the spatial distribution of material properties as design parameters
- This is a key advantage in problems with multiple functional requirements

EXAMPLE



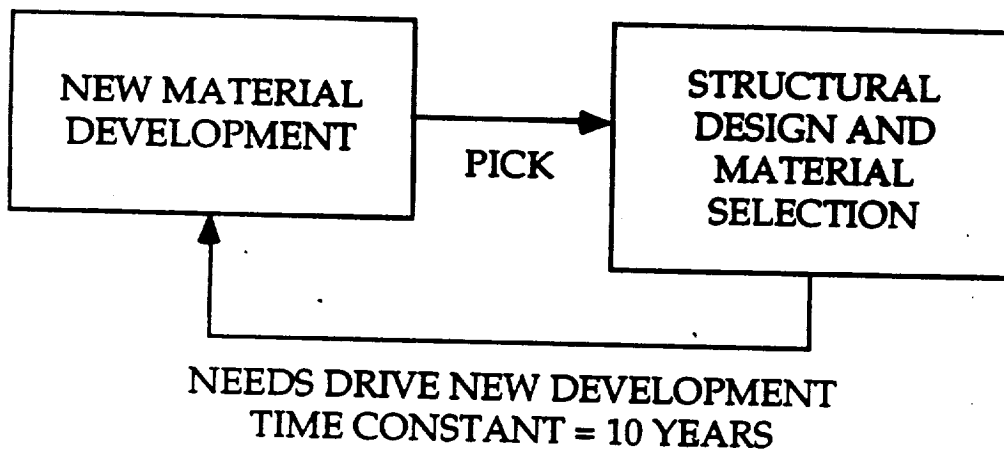
TRADITIONAL MATERIAL CHOICE

Design Parameters	Constraints	Problems
Material Choice	Available Materials	All props set by single choice May be no solution



INTEGRATED FGM DESIGN

TRADITIONAL MATERIAL SELECTION PROCESS

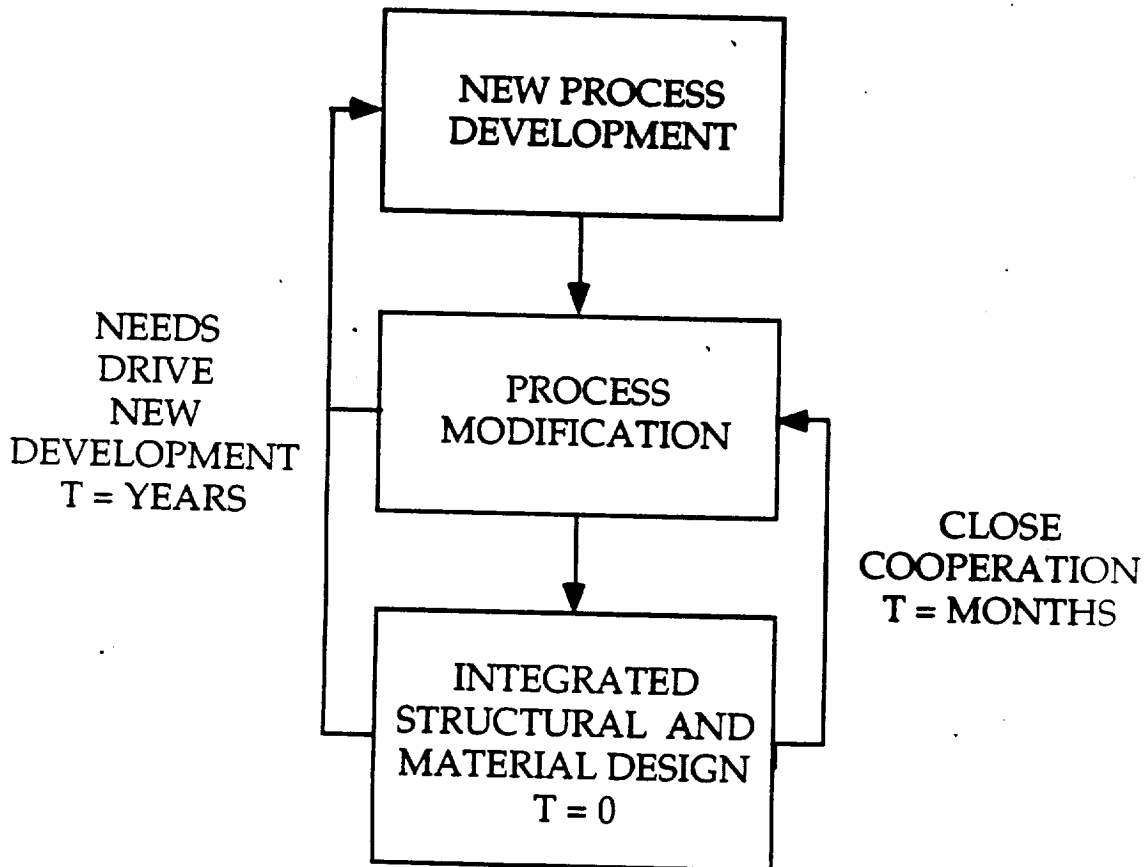


Decoupled material and structural design

Very long time before new materials are ready for application

INTEGRATED FGM DESIGN

Fully integrated design, and close cooperation between designers, analysts, and processors, critical for rapid exploitation of FGM



Parallels major initiative in the MIT Aeronautics and Astronautics Department in *Engineered Materials*

- Integration of material design into aerospace structural engineering
- Research and educational initiatives

TOOLS FOR INTEGRATED DESIGN

PROCESS MODELING

Given process parameters, what is the microstructure as a function of position?

MICROMECHANICS

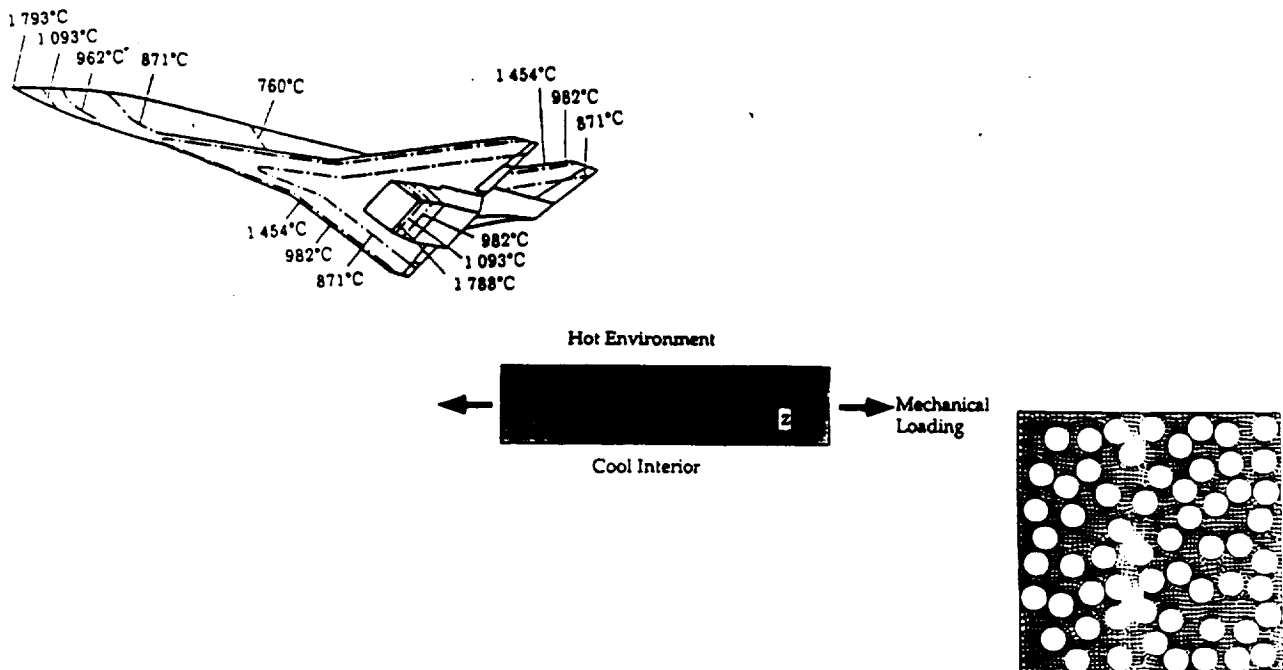
Given constituent properties, volume fractions, architectures and microstructures, what are the *local* bulk properties?

GRADIENT STRUCTURE ANALYSIS

Given local bulk properties as functions of position, what are the distributions of temperature, stresses, etc., also as functions of position?

GLOBAL STRUCTURAL ANALYSIS

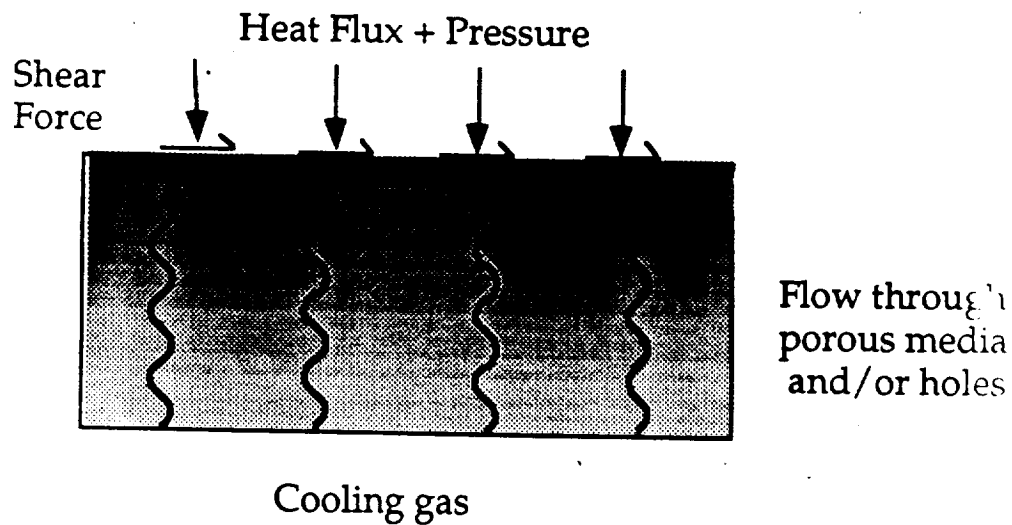
What is the response of the entire structure?



All these analyses must be coupled

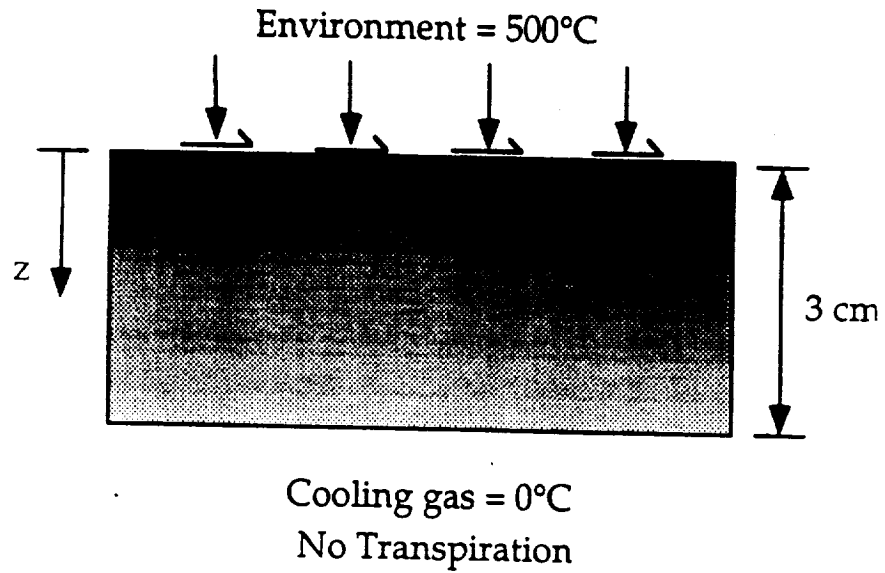
EXAMPLE DESIGN ANALYSIS

- Computer code adapted from charring ablator code CHAR
- Coupled thermal, porous flow, chemical reaction, and thermo-poro-elastic structural solutions
- Transient solutions for arbitrary thermal BCs, and several structural cases (coatings, plates)
- Simple FGM input
- Crude micromechanics
- Limited material failure and damage modeling capabilities

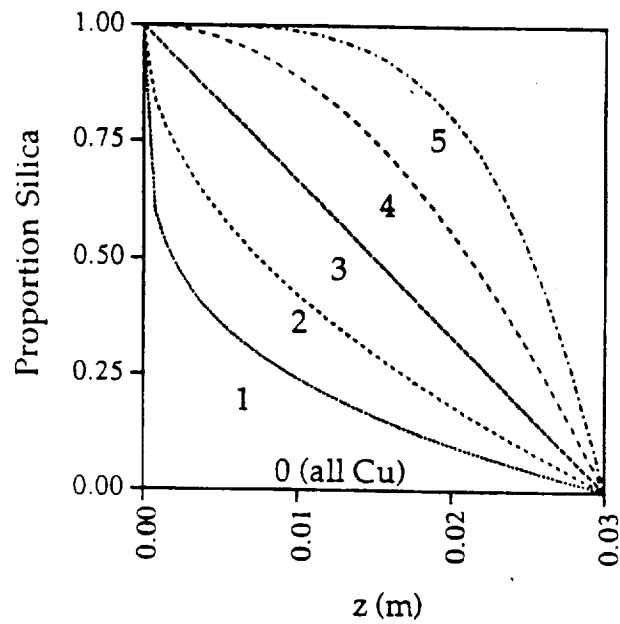


User-Specified Graded Material

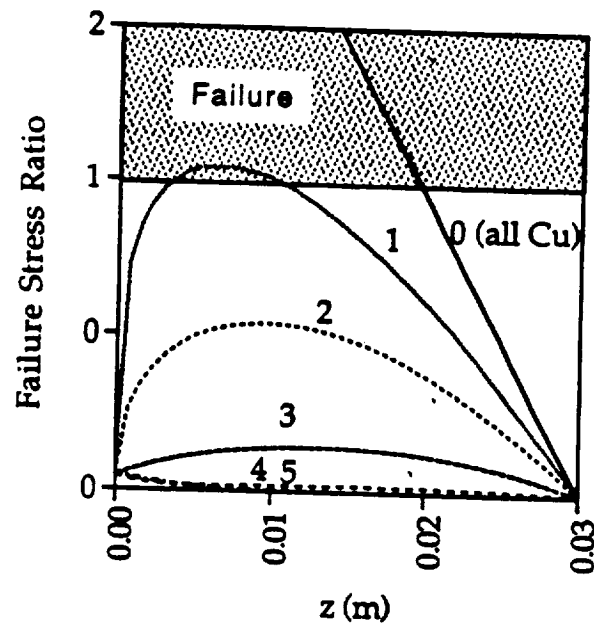
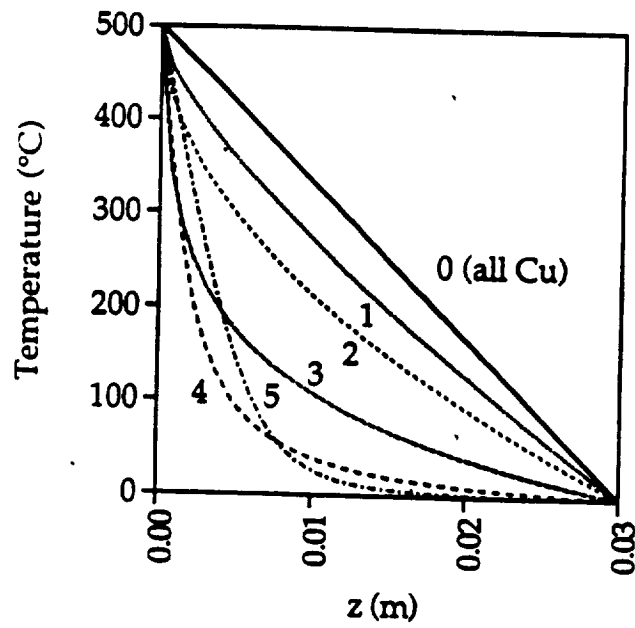
EXAMPLE CASE



Silica/Copper with Various Gradients



EXAMPLE CASE RESULTS



SUMMARY AND CHARGE

To apply FGM concepts to practical design problems as quickly as possible

- Bottleneck disciplines must be identified and worked on
- Existing processing, analysis and design capabilities must be integrated for FGM application

It is our hope that this workshop will

- Identify what can and cannot be done with existing technique
- Aid in the integration of existing knowledge
- Identify critical areas for research and development

INTERDISCIPLINARY HYPERSONICS PROGRAM

Coupled response of hypersonic vehicles
aerodynamic
thermal
structural
propulsion
control

Unique MIT department of Aero+Astro capability
fully integrated team
students will work on specific problems
several professors will supervise each student

HEAT TRANSFER PROBLEM

Hypersonic heat transfer very difficult to predict
depends on fine structure of flow
shock attachment
etc

Transpiration complicates things even further!

Include transpiration in this study?

SEND MONEY

