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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

Submitted to Dr. Roy Sullivan
ED24
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by

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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 been 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

TELAC

Technology Laboratory for Advanced Composites
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OUTLINE

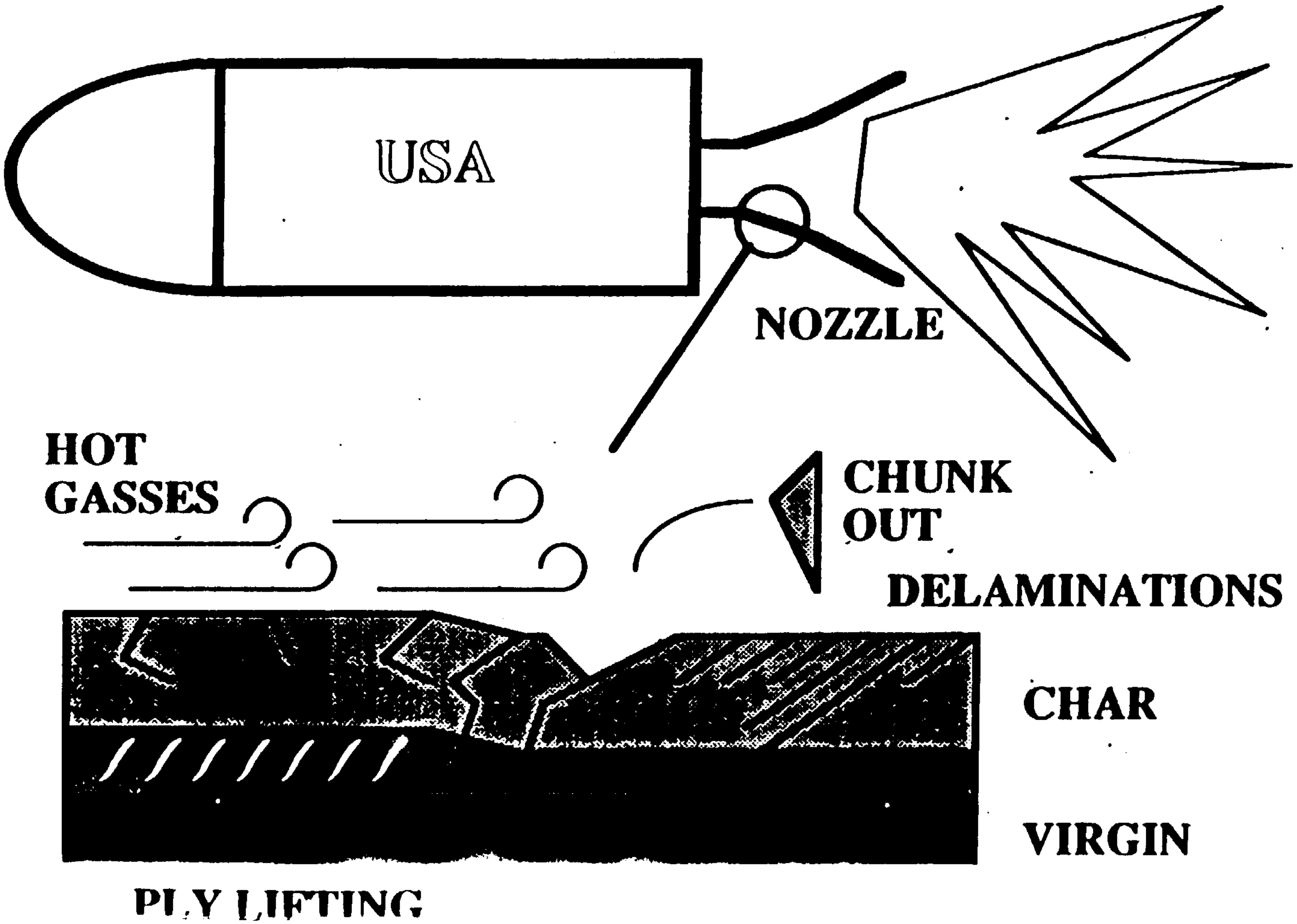
Modeling of composite ablators

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

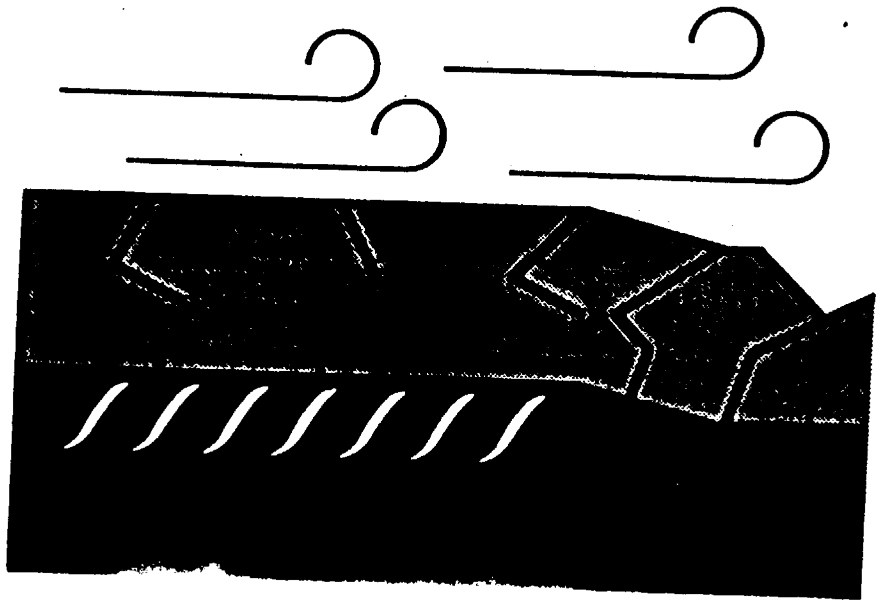
Must be used in conjunction with testing

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

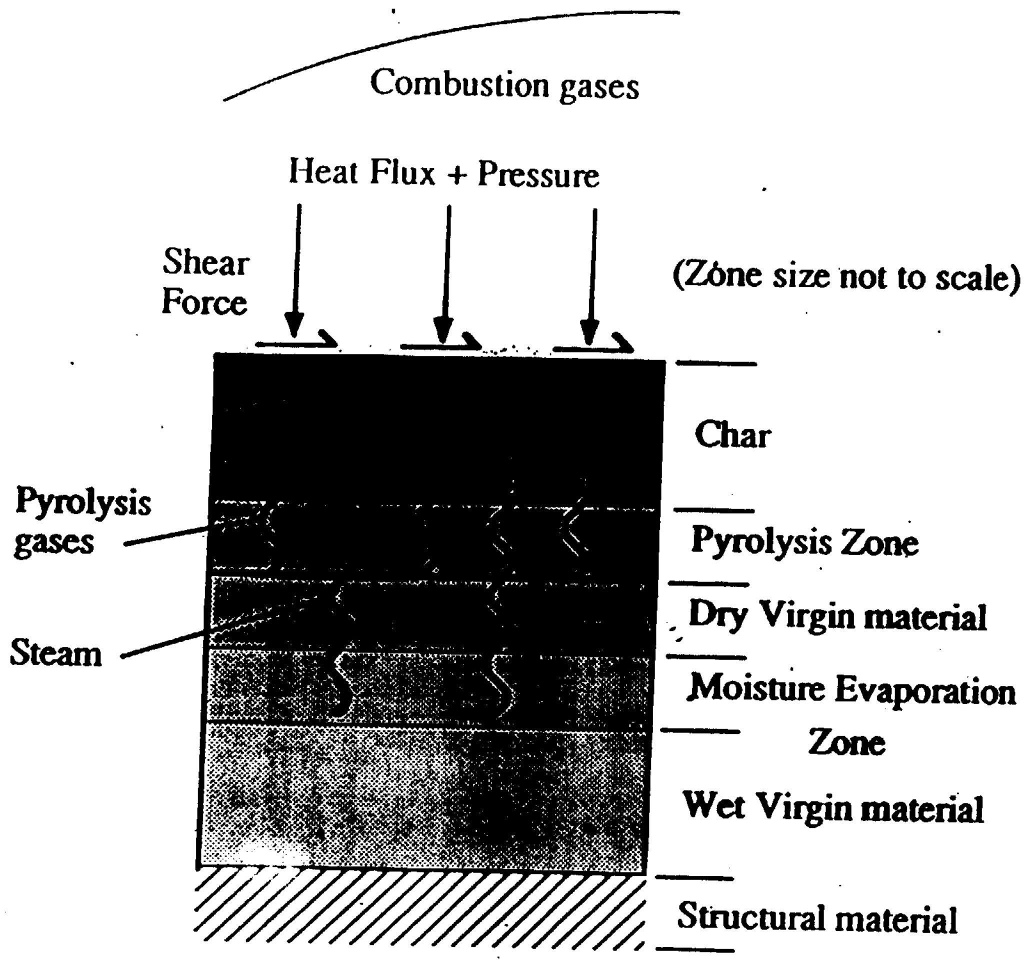
Chemical-Flow-Poro-Thermo-Structural Modeling:

Motivation: Ply Lifting of Rocket Nozzles



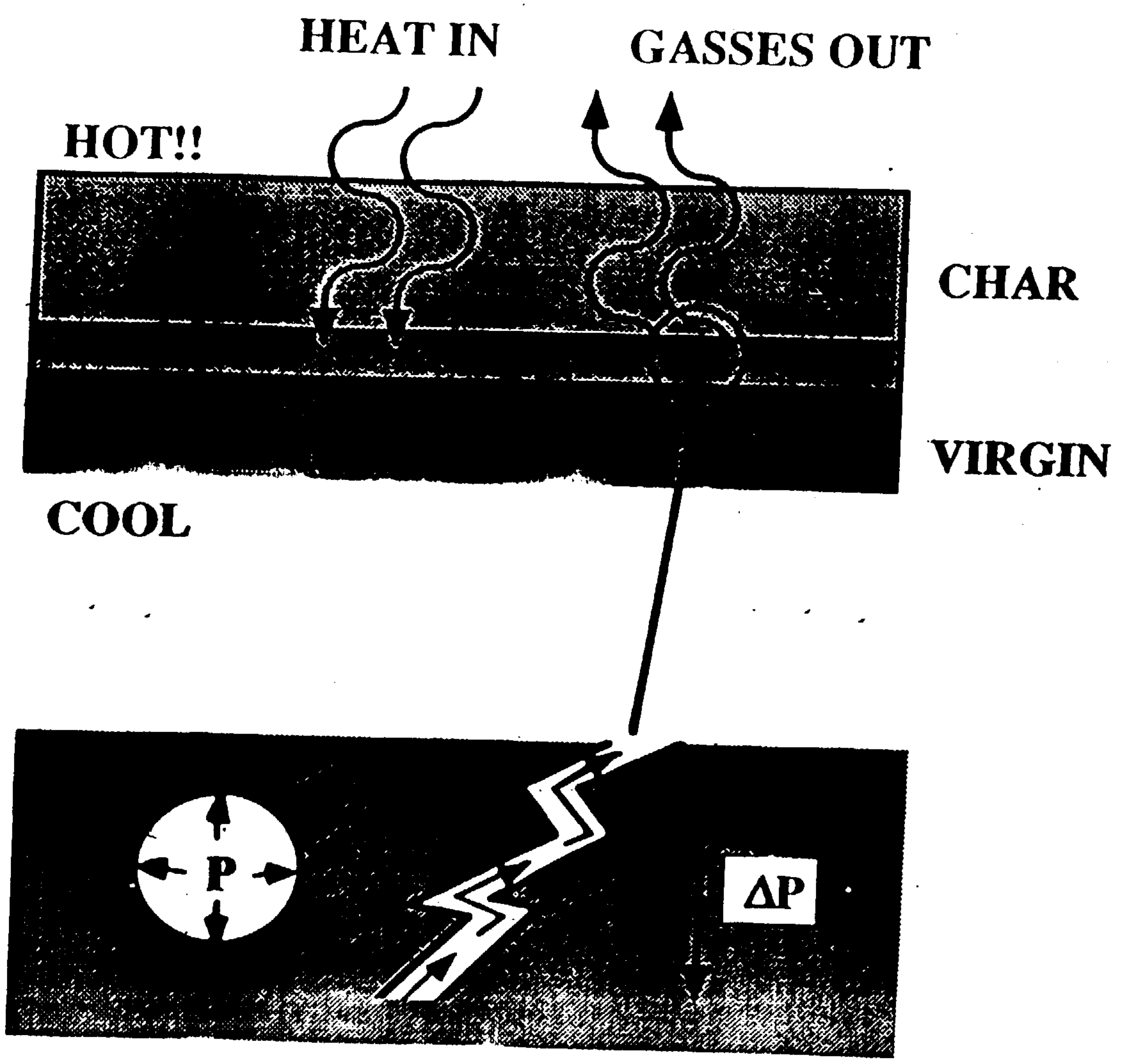
Shuttle Solid Rocket Motors (SRM) did
Next Generation (ASRM) does too!

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



HEAT IN

GASSES OUT

HOT!!

CHAR

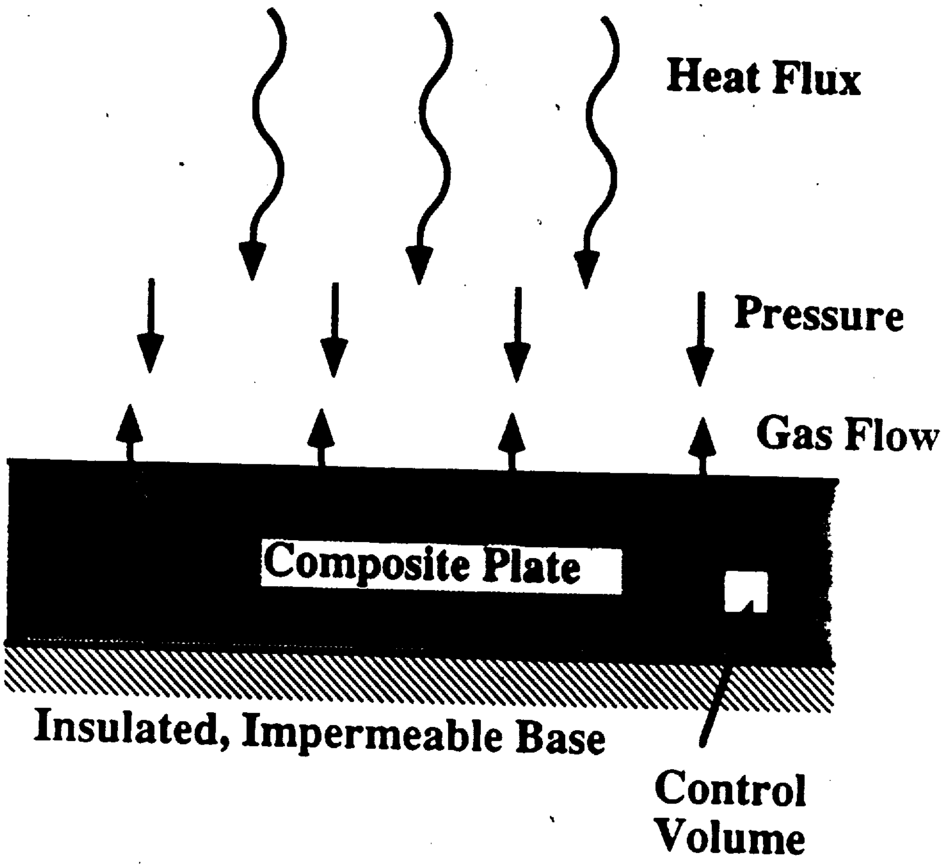
VIRGIN

COOL

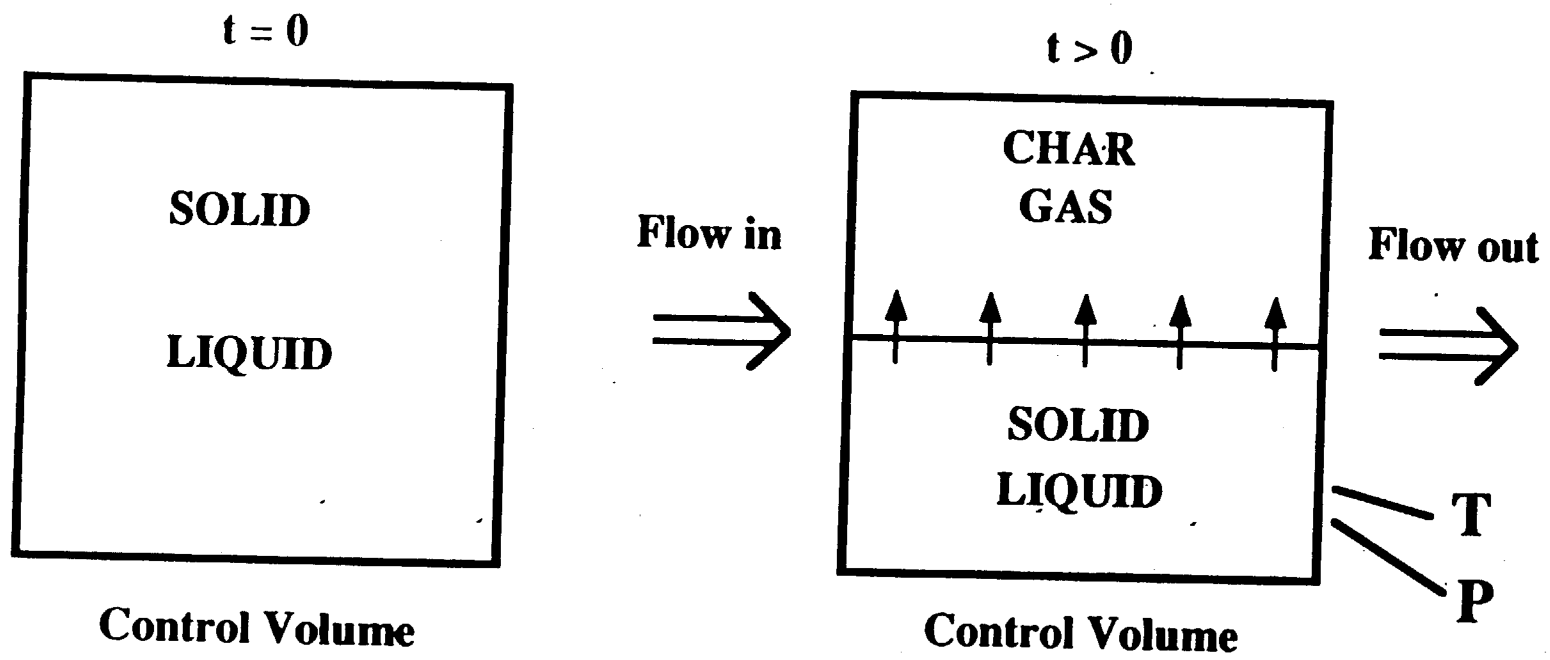
P

ΔP

THERMOCHEMICAL MODEL

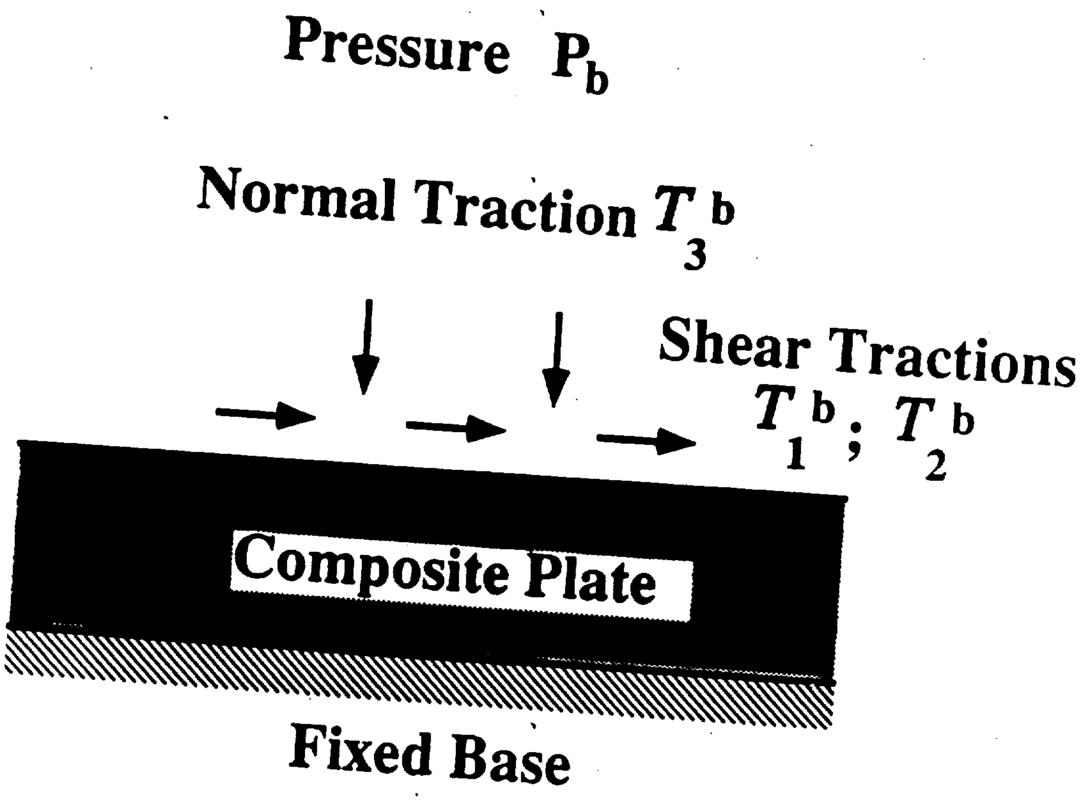


THERMOCHEMICAL MODEL



- 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 Tractions T_1^b; T_2^b

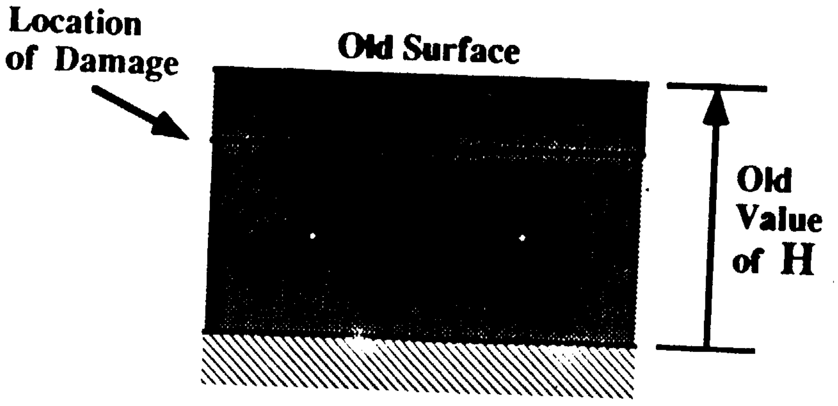
Composite Plate

Fixed Base

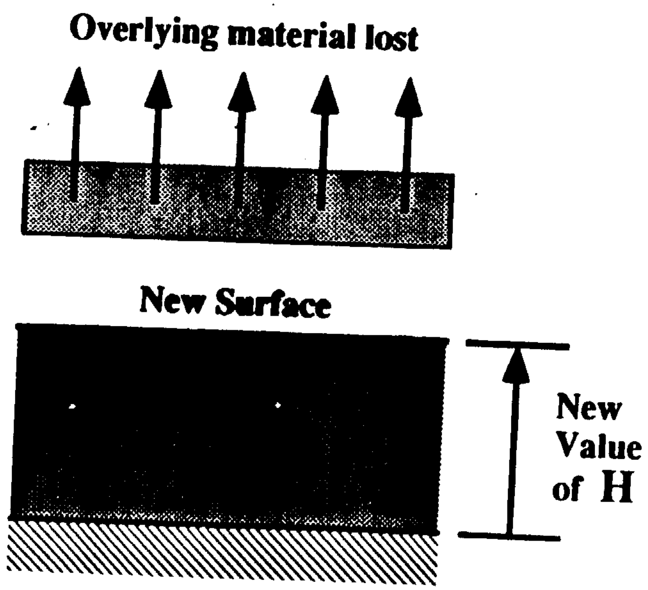
MECHANICAL MODEL

COMPOSITE FAILURE CRITERIA

- O MAXIMUM STRESS

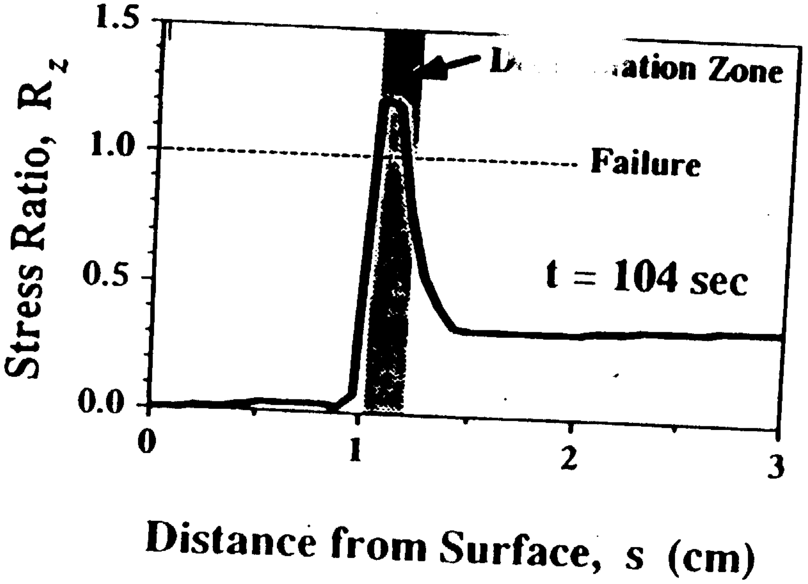


Immediately Before Damage

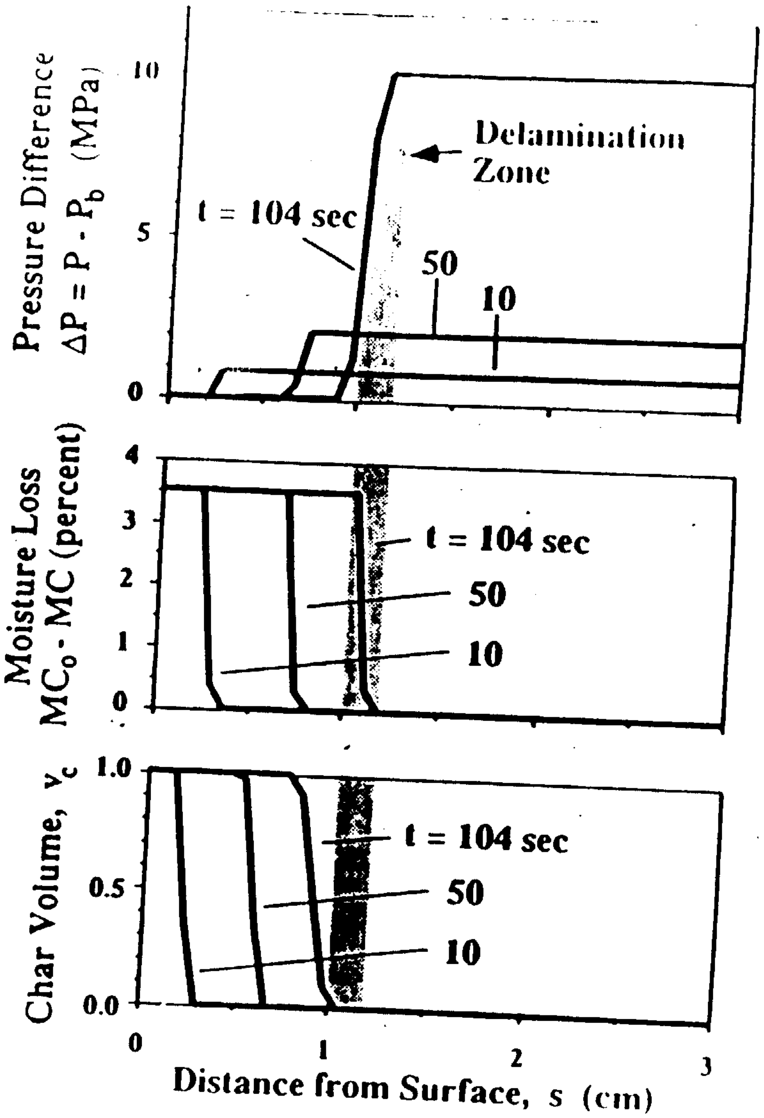


Immediately After Damage

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:

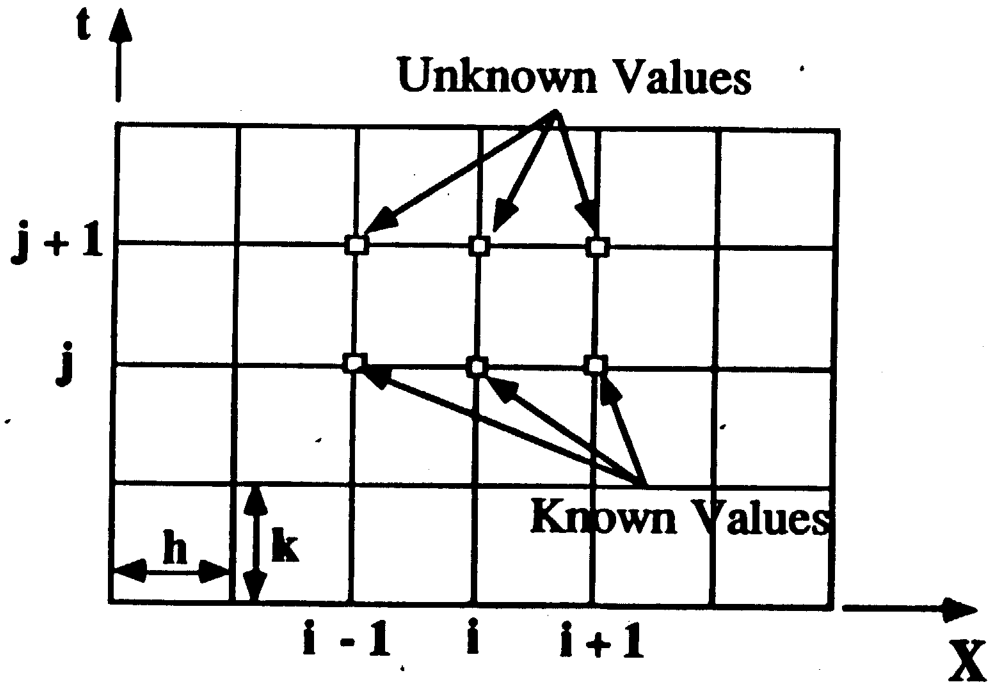
- Reaction models
- Water storage and release mechanisms
- Permeability-stress interactions
- Numerical Scheme

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

- Thermodynamic description of material
- Massively Parallel numerical models

ADVANCED NUMERICAL METHODS

-Implicit Method

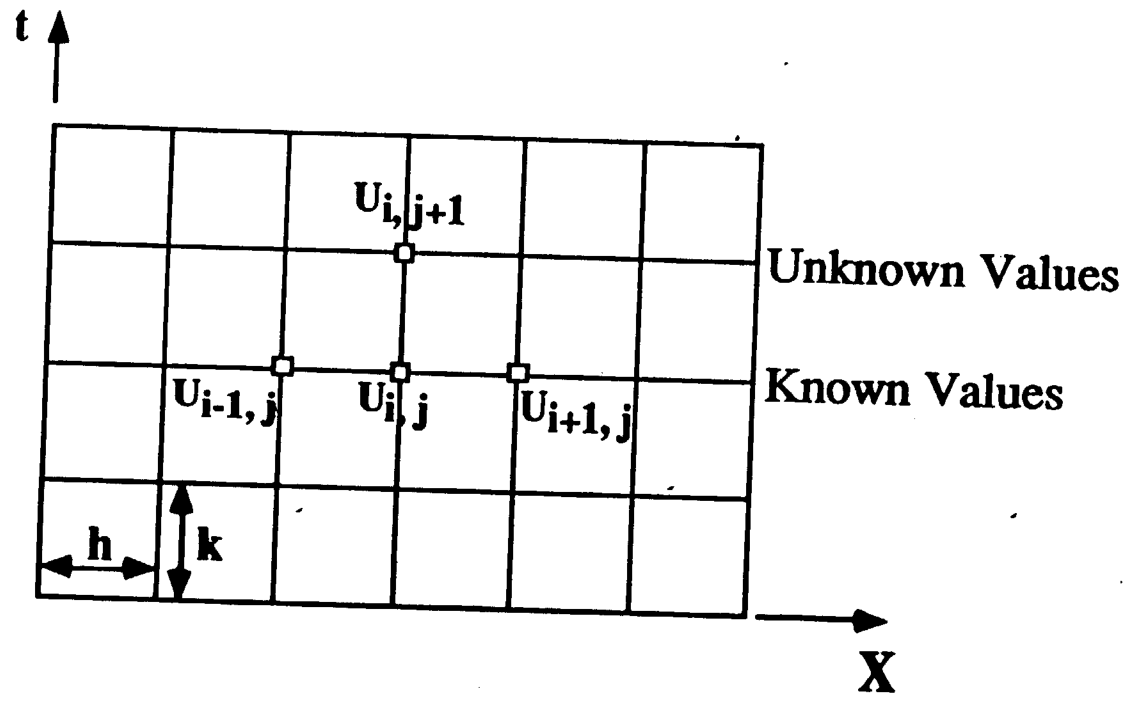


N equations with N unknowns

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

Solution Method

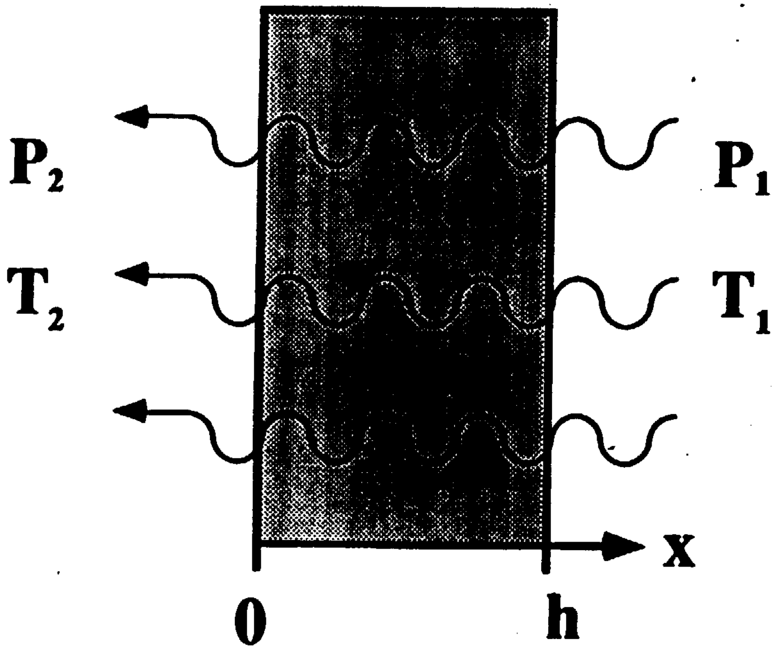
- Explicit Method



Unknown at t+Δt 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

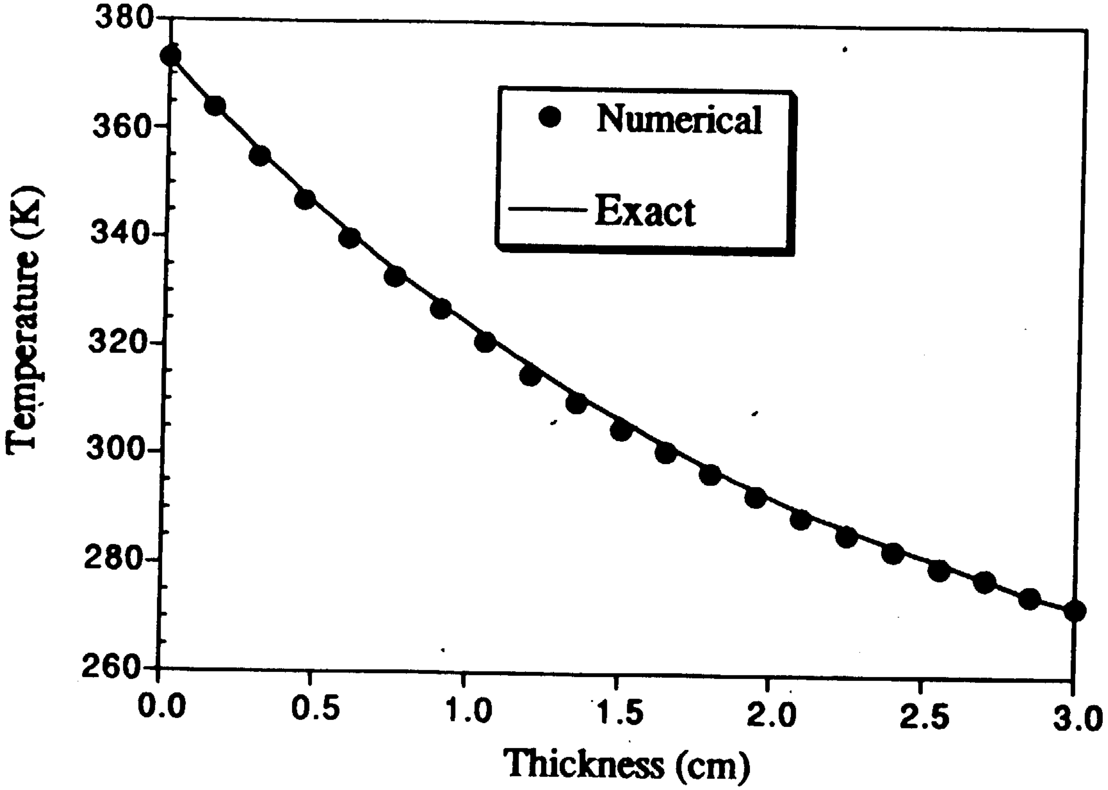
- Steady state temperature distribution

$P_1 = 2$ MPa, $P_2 = 1$ MPa

$T_1 = 273$ K, $T_2 = 373$ K

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

Check Case #1



Steady State Temperature Distribution

Check Case #2

- Steady state pressure distribution

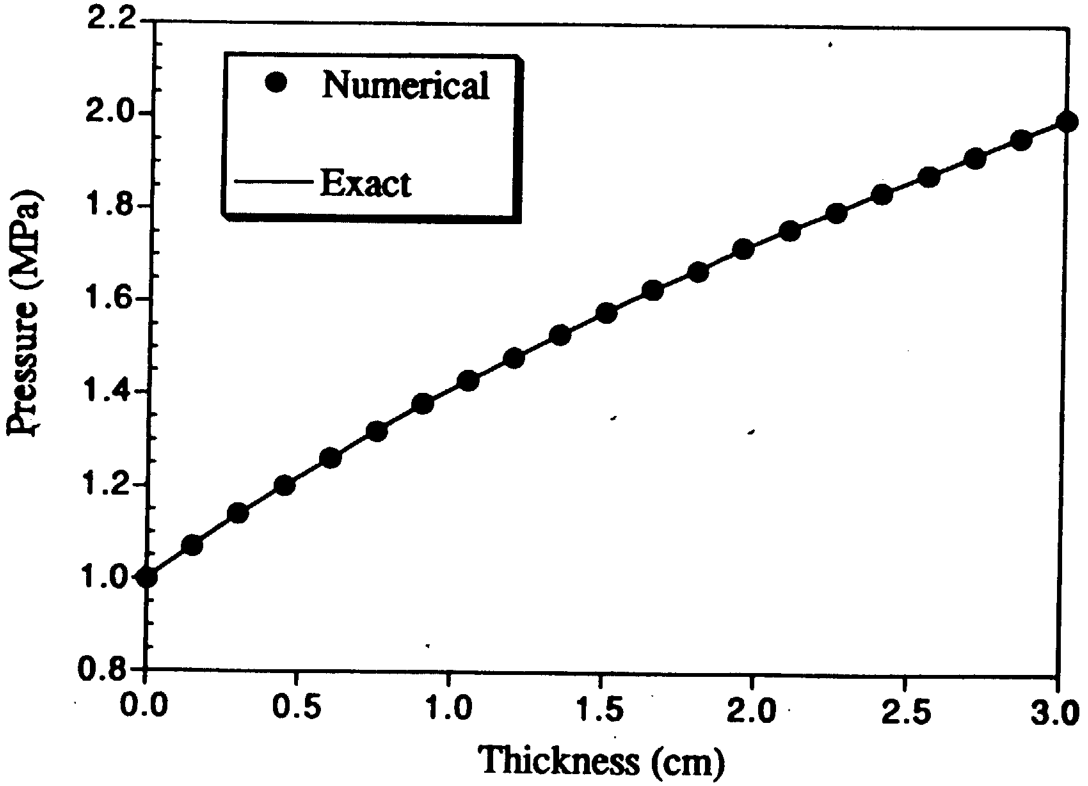
$P_1 = 2$ MPa, $P_2 = 1$ MPa

$T_1 = 273$ K, $T_2 = 273$ K

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

Check Case #2

Steady State Pressure Distribution



Parametric Studies

- Varying P_1
- Varying permeability
- Varying porosity

Variation in P_1

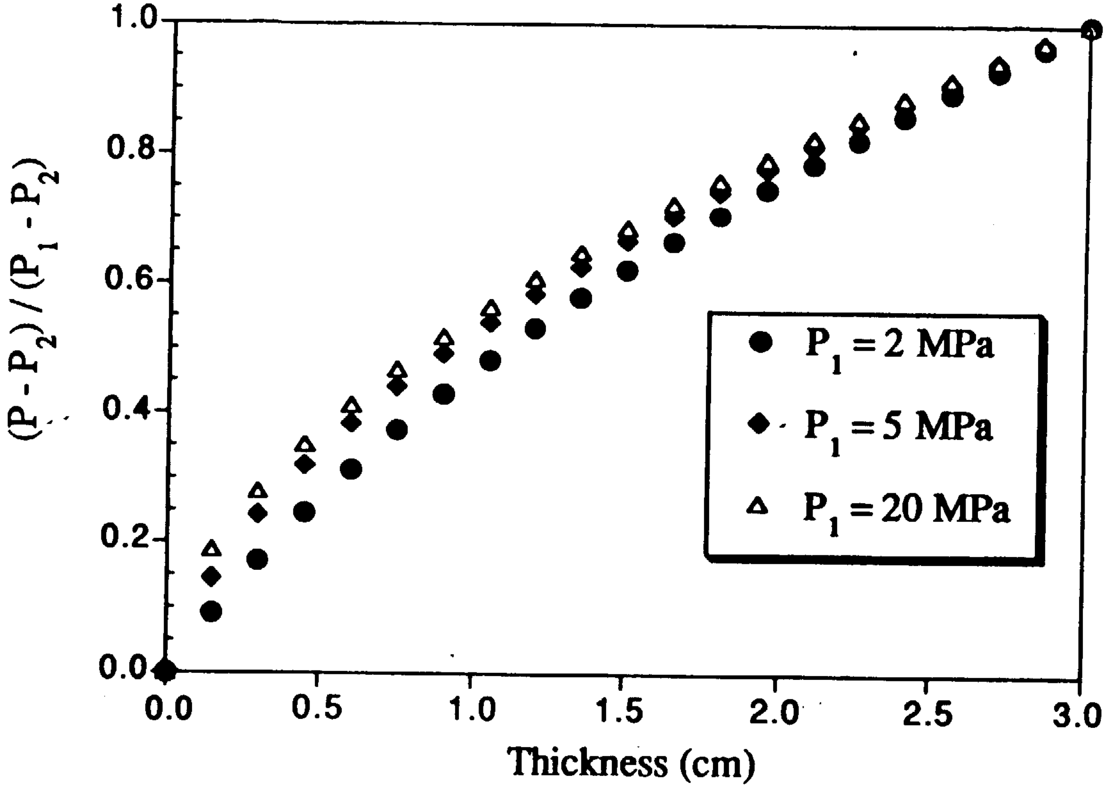
Parameters used

- $P_1 = 2\text{MPa}$ $\dot{m}_g = 3.40\ \text{kg/m}^3\ \text{sec}$
- $P_1 = 5\text{MPa}$ $\dot{m}_g = 30.2\ \text{kg/m}^3\ \text{sec}$
- $P_1 = 20\text{MPa}$ $\dot{m}_g = 843\ \text{kg/m}^3\ \text{sec}$

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

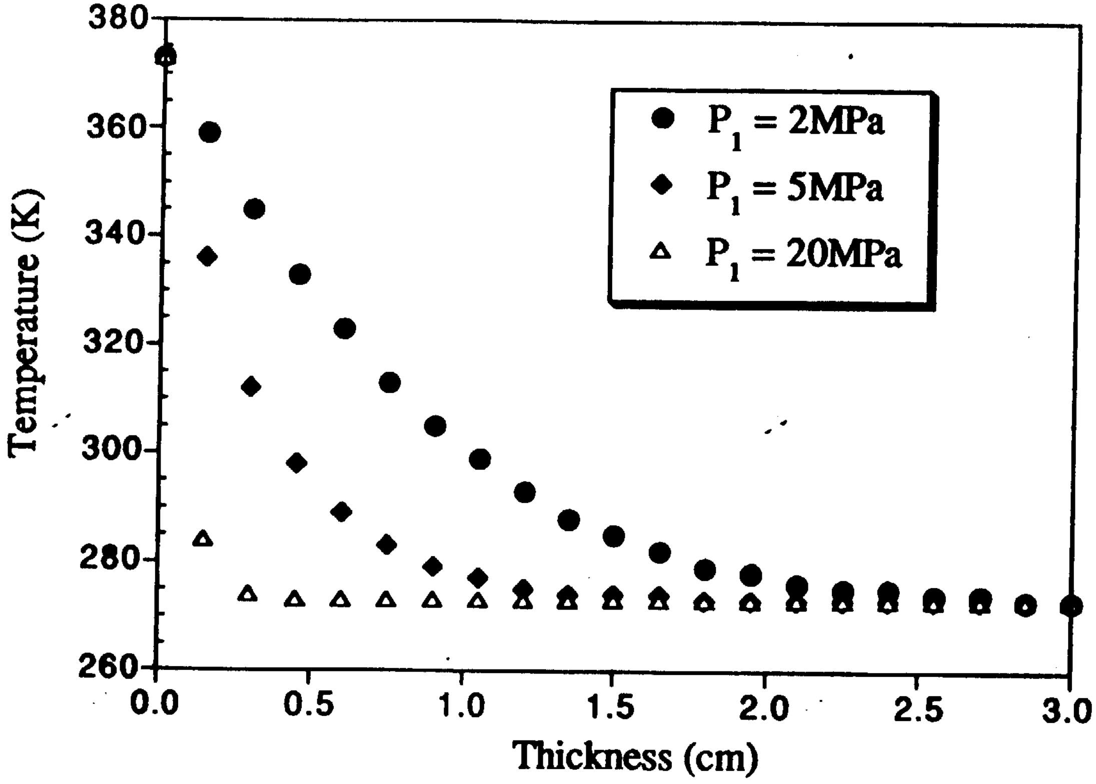
Variation in P_1

Steady State Pressure Distributions



Variation in P_1

Steady State Temperature Distributions



Variation in Permeability

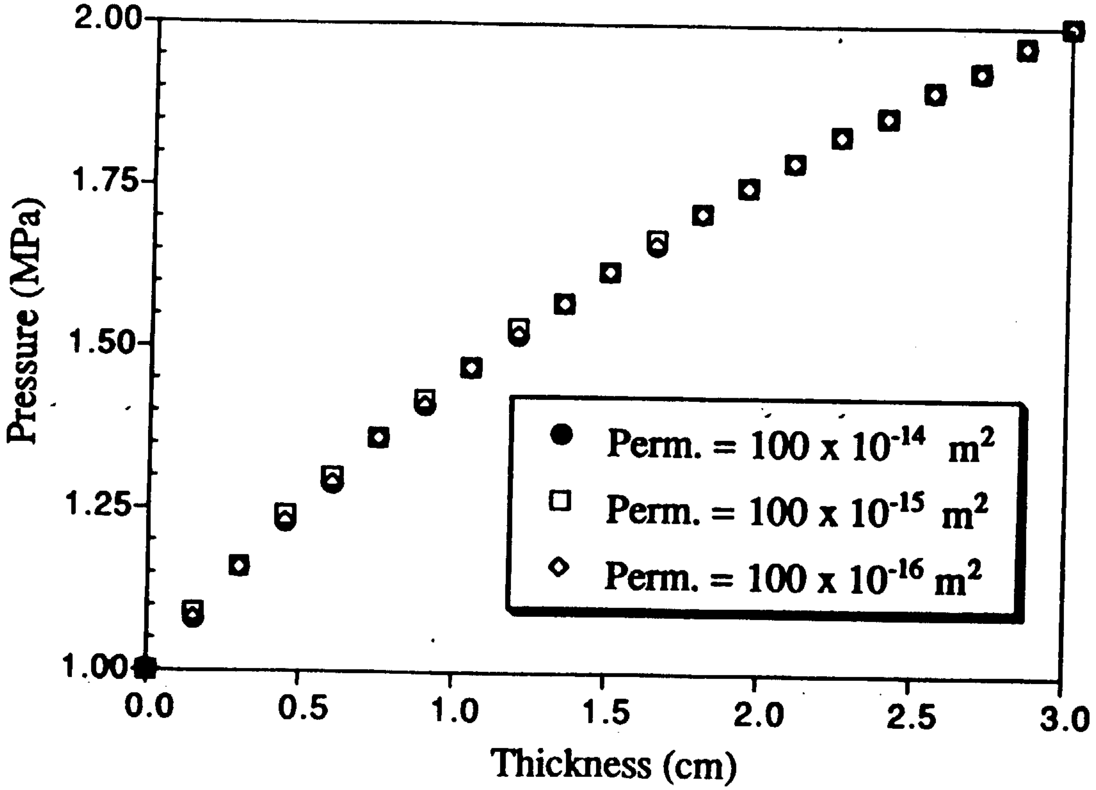
Parameters used

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

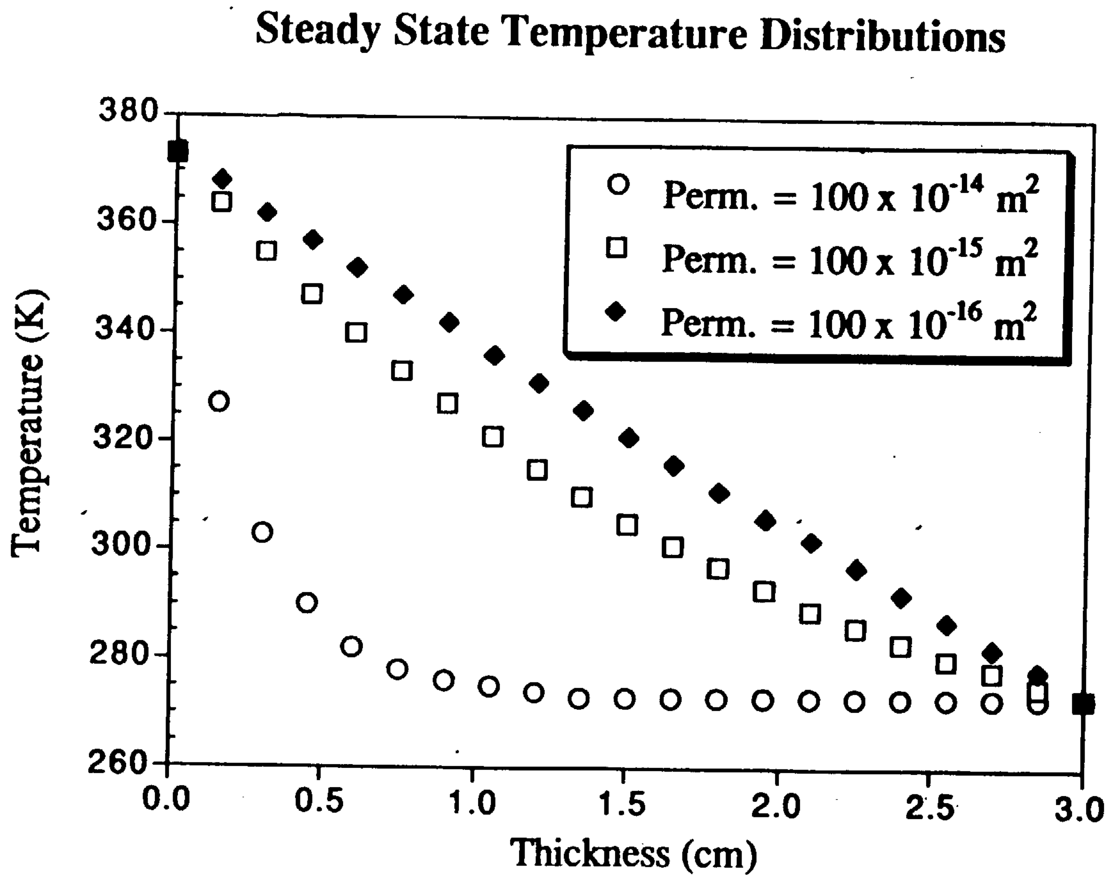
$P_1 =$ 2 MPa
$P_2 =$ 1 MPa
$T_1 =$ 273 K
$T_2 =$ 373 K
porosity = 0.05
viscosity = 1 x 10^{-}[illegible] kg/m sec

Variation in Permeability

Steady State Pressure Distributions



Variation in Permeability



Steady State Temperature Distributions

Variation in Porosity

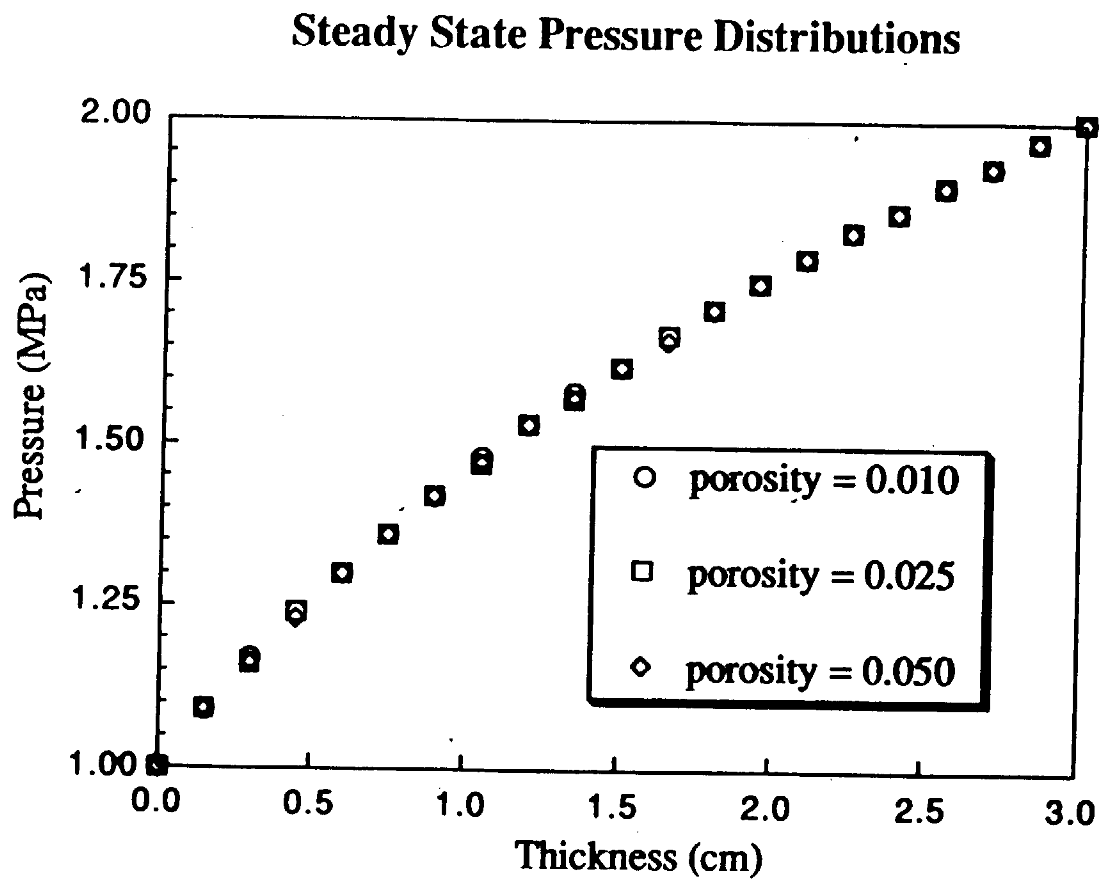
Parameters used

$k = 150\ W/m^2K$
$C_{ps} = 167$ J/kg K

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

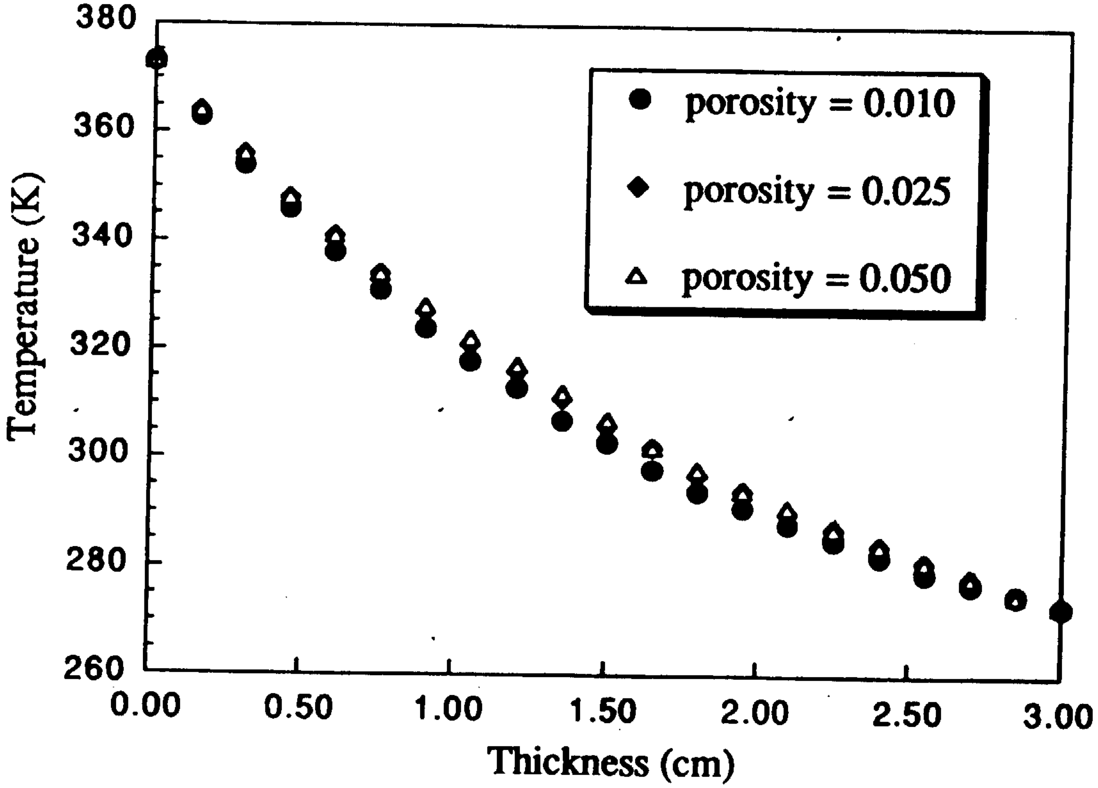
$P_1 =$ 2 MPa
$P_2 =$ 1 MPa
$T_1 =$ 373 K
$T_2 =$ 273 K
viscosity = 1×10^{-5} kg/m sec
permeability = $100 \times 10^{-15}\ m^2$

Variation in porosity



Variation in Porosity

Steady State Temperature Distributions



Examples

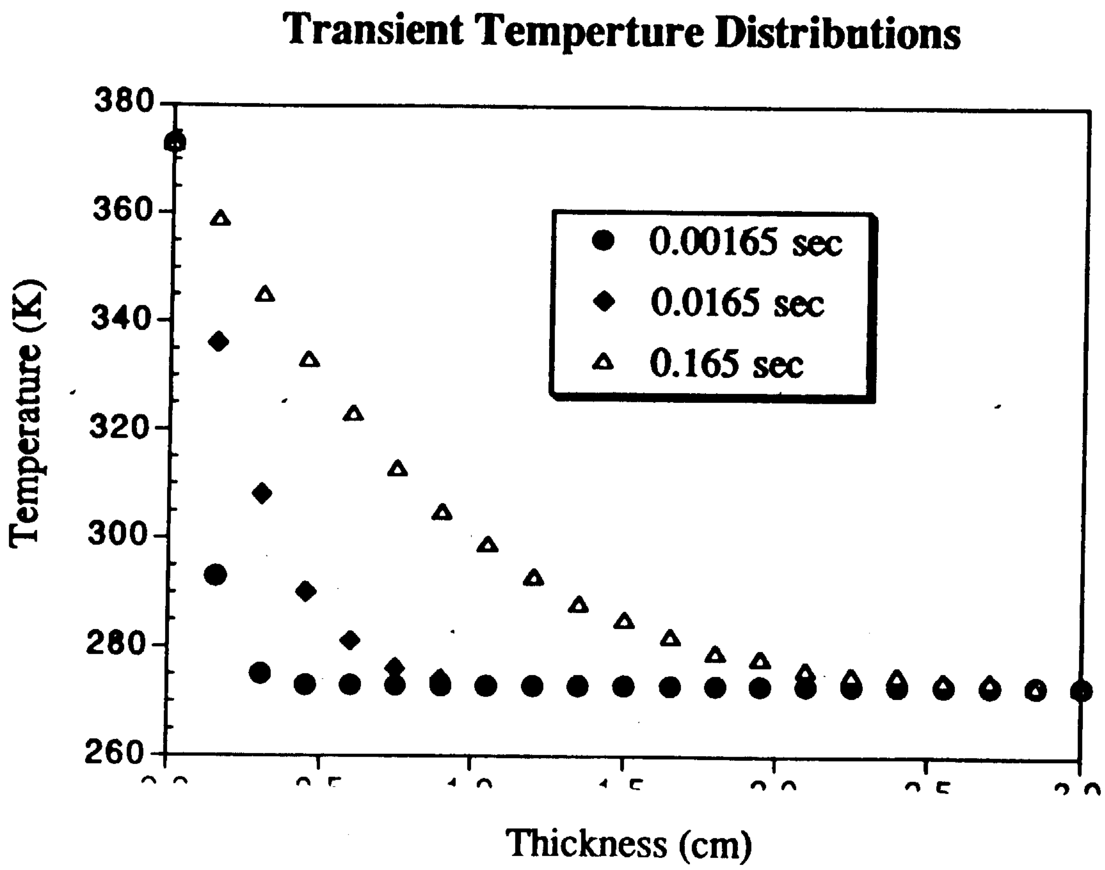
- Transient temperature distribution

- Transient pressure distribution

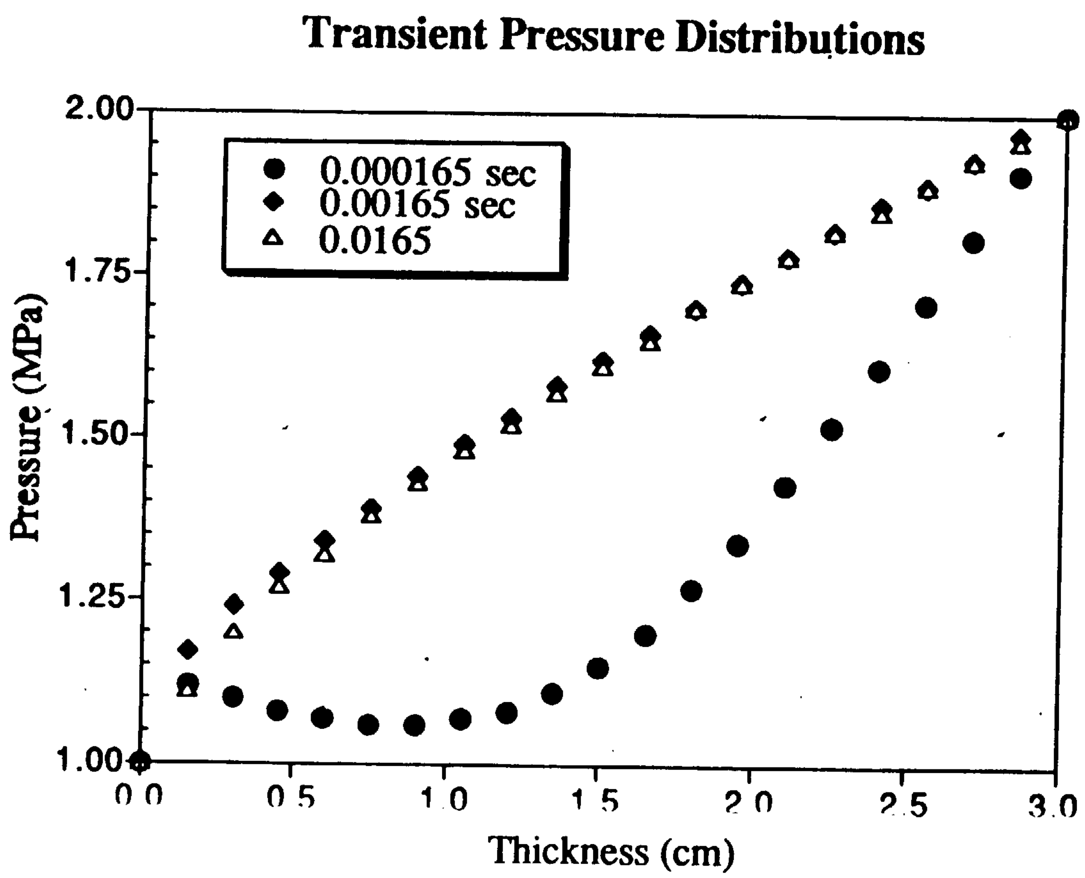
Parameters used

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

Transient Temperature Distributions



Transient Pressure Distributions



FUNCTIONALLY GRADED MATERIALS

Materials with gradients
  constituent fractions
  microstructure
  porosity/permeability

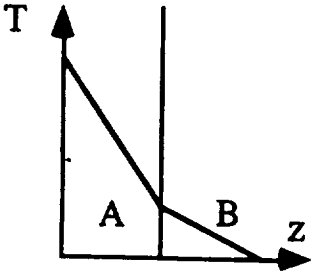
Greatly expands material choices
  material properties functions of location

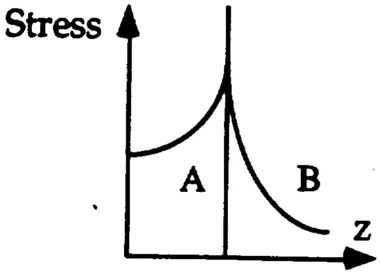
Ideal for environments with sharp gradients
  e.g. thermal

ALTERNATE MATERIAL DESIGNS

MULTIPLE MATERIALS

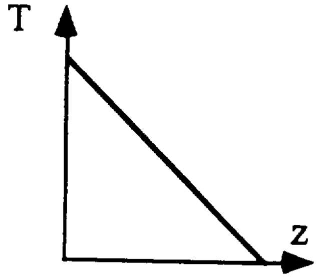
Design Parameters	Constraints	Problem
Material Choice	Available Materials	Stress Concentrations
(Two or more)	Compatibility	Weight
	Joining Techniques	Expense

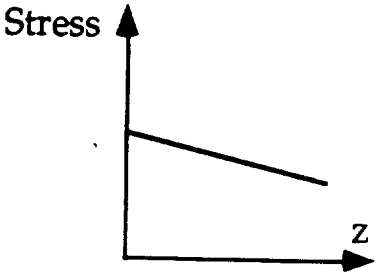




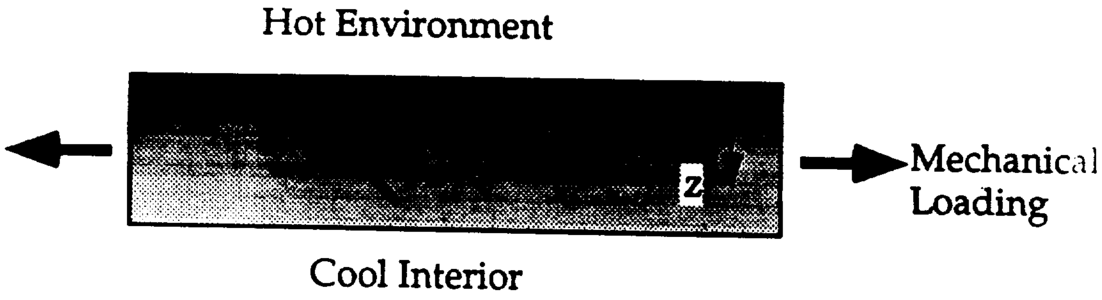
COMPOSITES

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





FGM MATERIAL DESIGNS

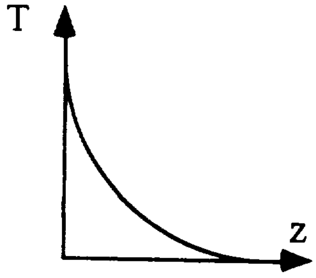


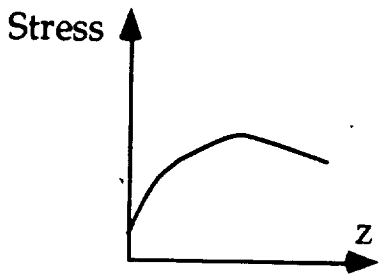
Hot Environment

Mechanical Loading

Cool Interior

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

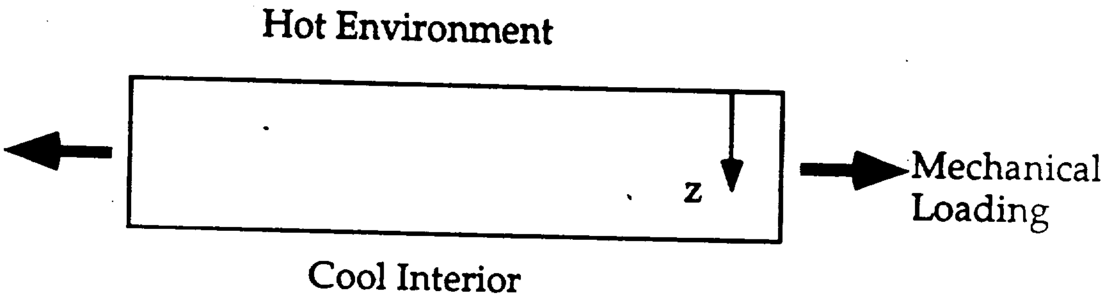




DESIGNING WITH FGM

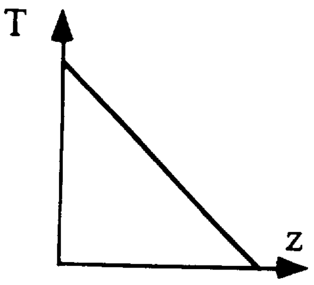
- FGM frees up the spatial distribution of material properties as design parameters
- This is a key advantage in problems with multiple functional requirements

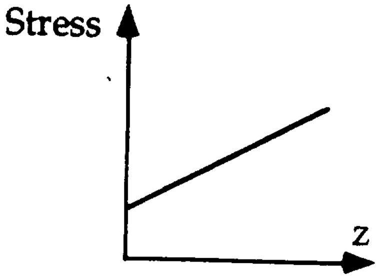
EXAMPLE



TRADITIONAL MATERIAL CHOICE

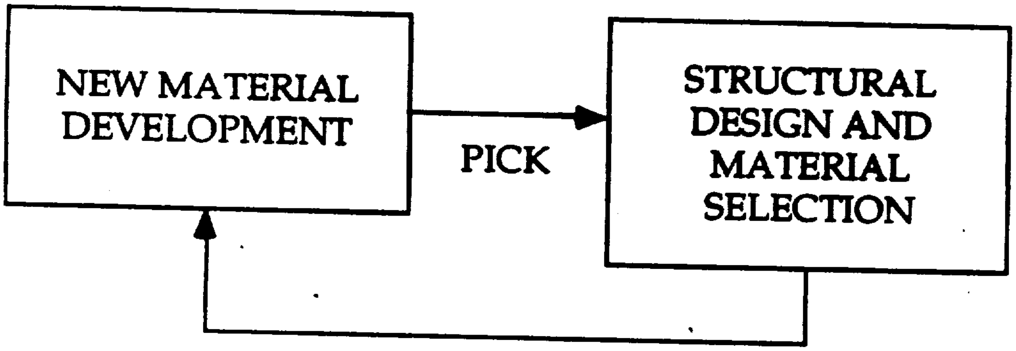
Design Parameters	Constraints	Problems
Material Choice	Available Materials	All props set by single choice May be no solution





INTEGRATED FGM DESIGN

TRADITIONAL MATERIAL SELECTION PROCESS



NEW MATERIAL DEVELOPMENT

PICK

STRUCTURAL DESIGN AND MATERIAL SELECTION

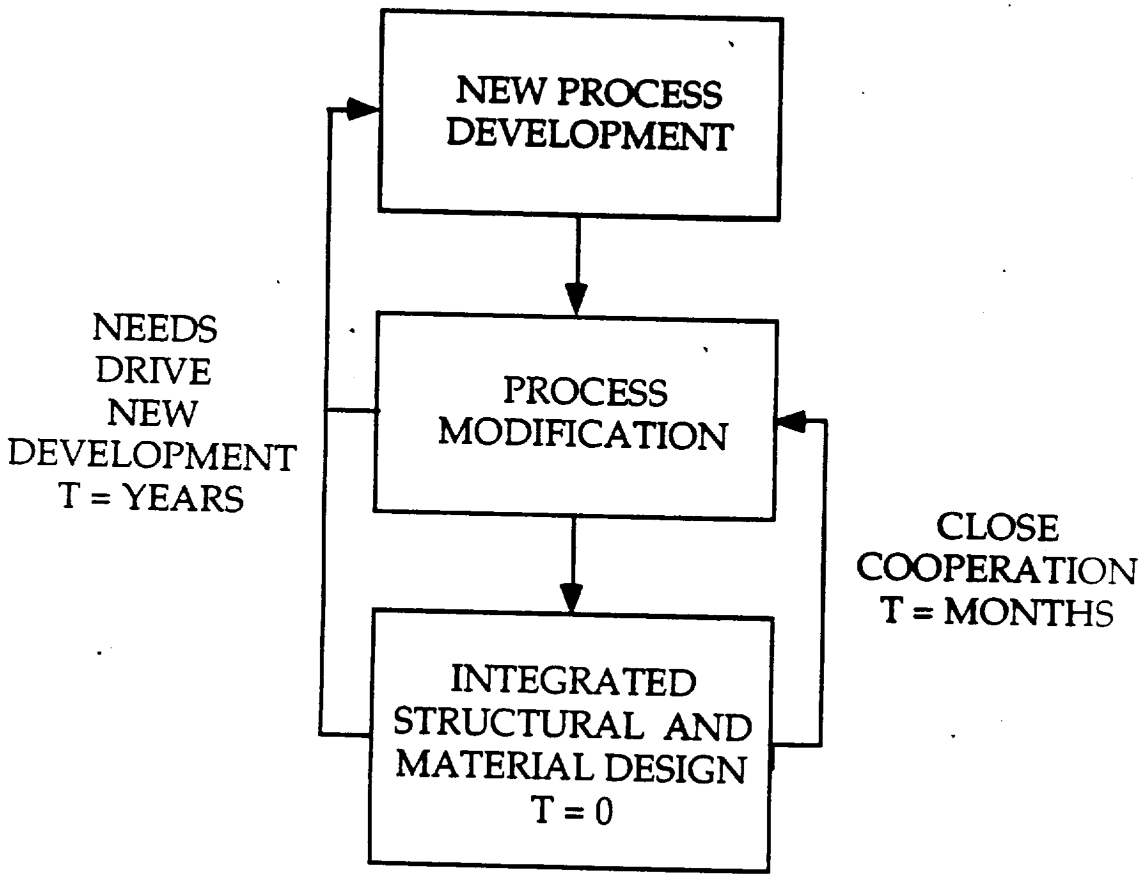
NEEDS DRIVE NEW DEVELOPMENT
TIME CONSTANT = 10 YEARS

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



NEW PROCESS DEVELOPMENT

PROCESS MODIFICATION

INTEGRATED STRUCTURAL AND MATERIAL DESIGN
T = 0

NEEDS DRIVE NEW DEVELOPMENT
T = YEARS

CLOSE COOPERATION
T = MONTHS

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

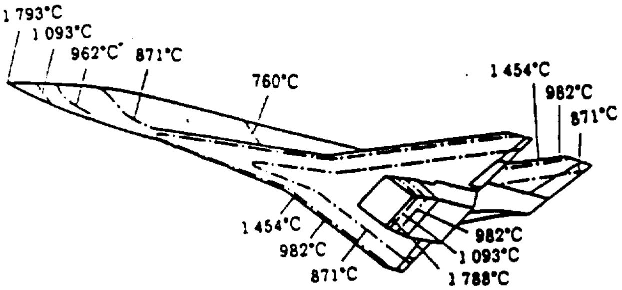
Given constituent properties, volume fractions, architectures and microstructures, what are the *local* bulk properties?

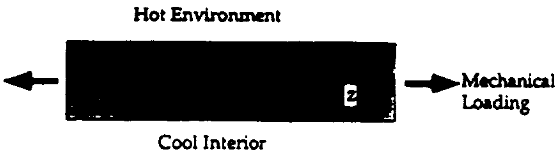
GRADIENT STRUCTURE ANALYSIS

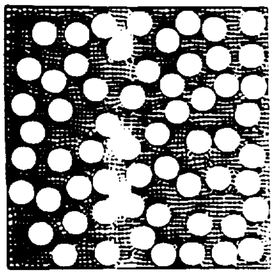
Given local bulk properties as functions of position, what are the distributions of temperature, stresses, etc., also as functions of position?

GLOBAL STRUCTURAL ANALYSIS

What is the response of the entire structure?



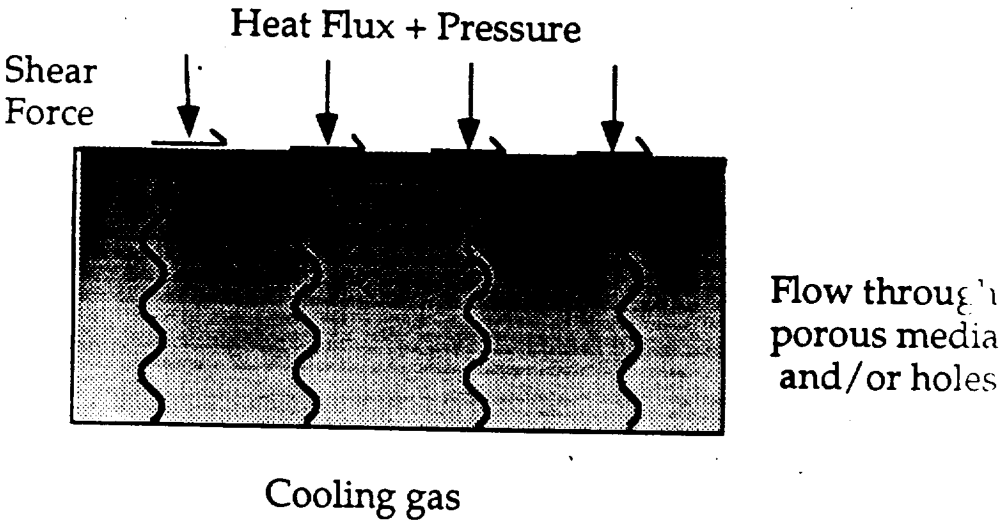




All these analyses must be coupled

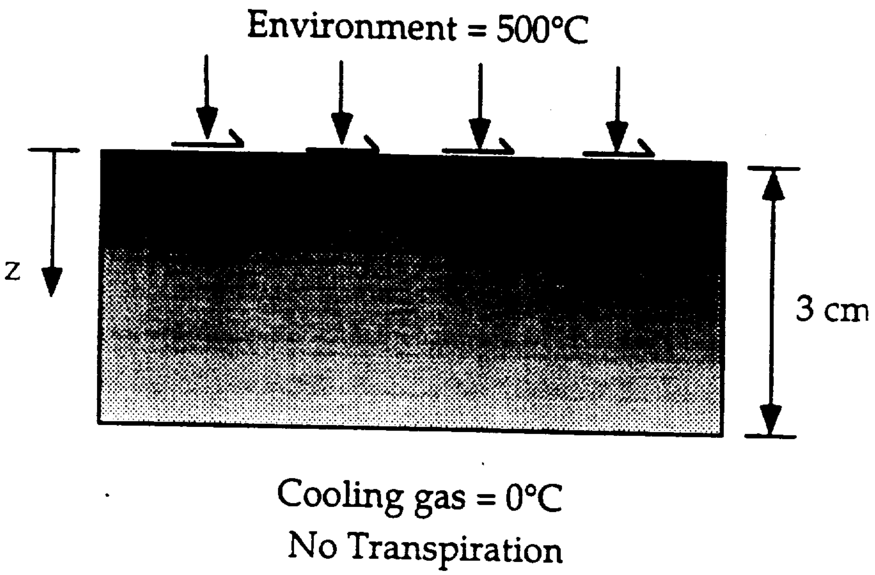
EXAMPLE DESIGN ANALYSIS

- 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

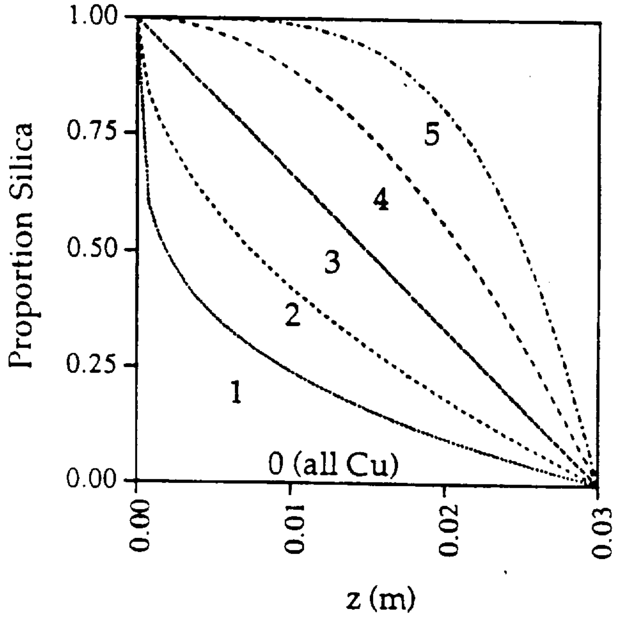


User-Specified Graded Material

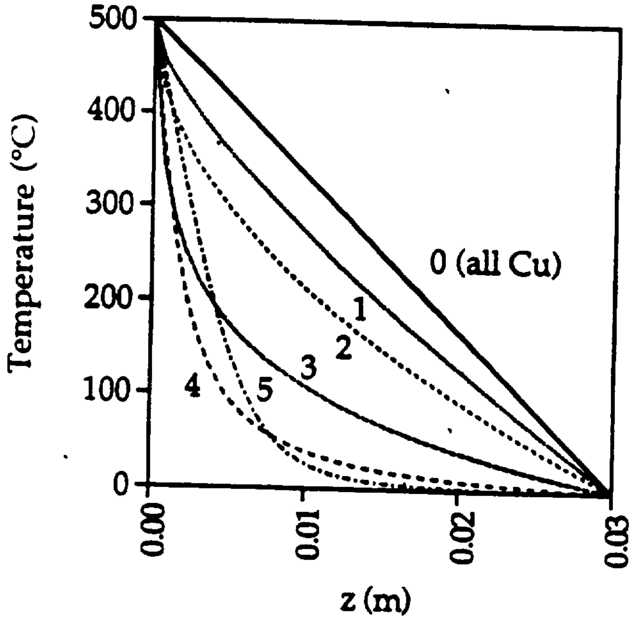
EXAMPLE CASE

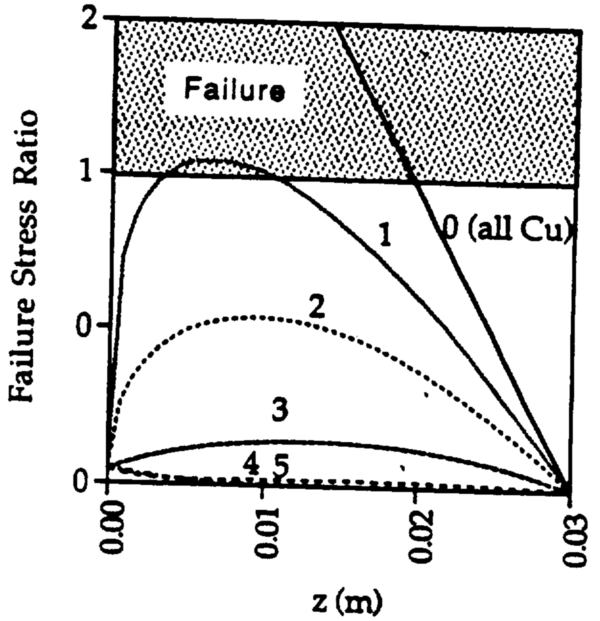


Silica/Copper with Various Gradients



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