NUMERICAL MODELING OF THERMAL PROCESSES IN COMPLICATED REGIONS WITH LARGE CHANGES IN MATERIAL CHARACTERISTICS AND PROPERTIES

YOGESH JALURIA

Department of Mechanical and Aerospace Engineering

Rutgers, the State University of New Jersey

New Brunswick, NJ 08903

2004 IMECE, Anaheim, CA

rutgers ENGINEERING

Topics Considered

- Modeling and Simulation
- Material Properties, Complex Domains
- Polymer Processing
- Optical Fiber Drawing and Coating
- Solidification and Other Processes
- Validation
- Enclosure Fires, Electronic Systems
- Conclusions and Future Research Needs

Different Approaches

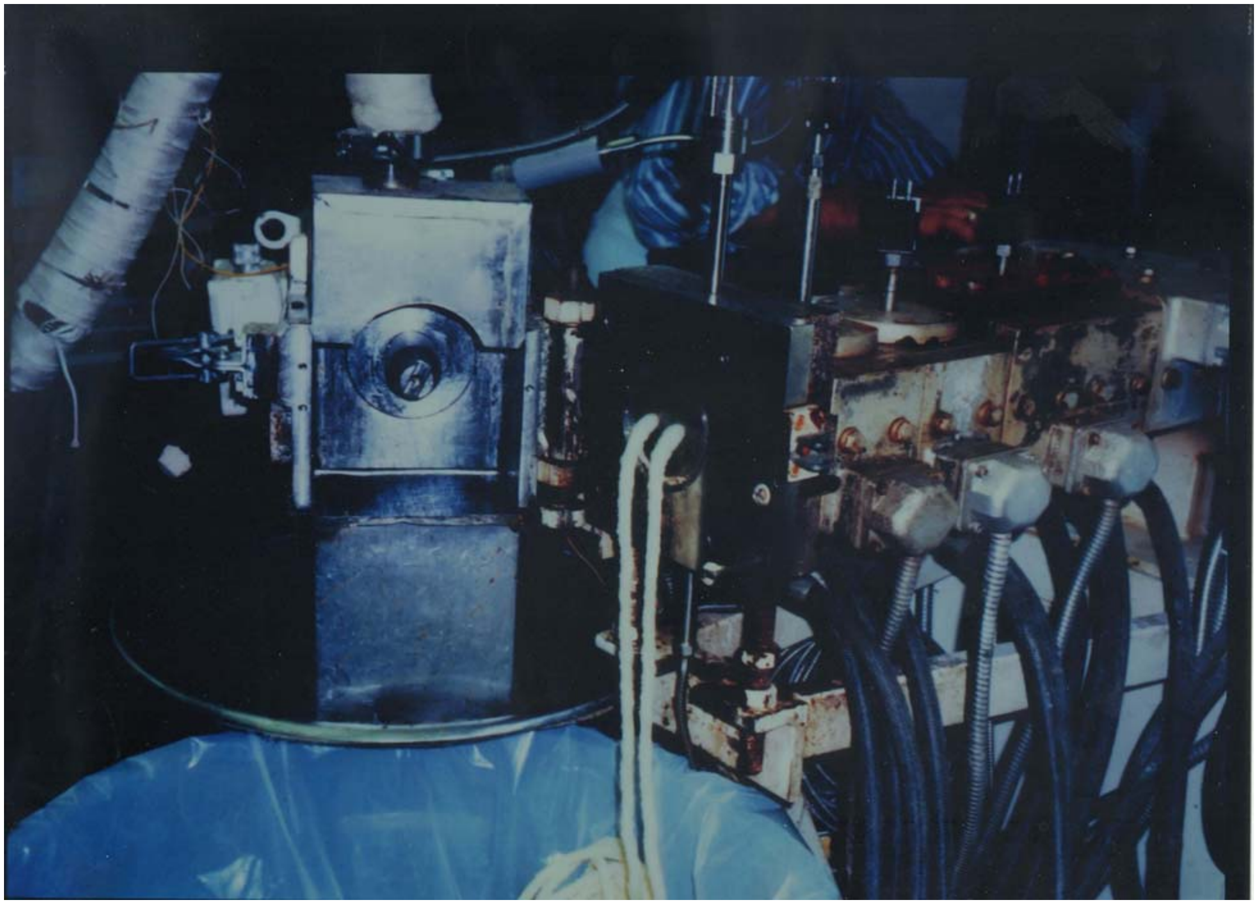
COMPLICATED GEOMETRY

- Transformed Domain:. Simple Grids for FDM and FVM
- Physical Domain: Complex, Arbitrary Discretization for FEM, FVM

VARIABLE MATERIAL PROPERTIES

- Properties at Previous Time Step or Iteration
- Extrapolated Values
- Iterative Property Correction

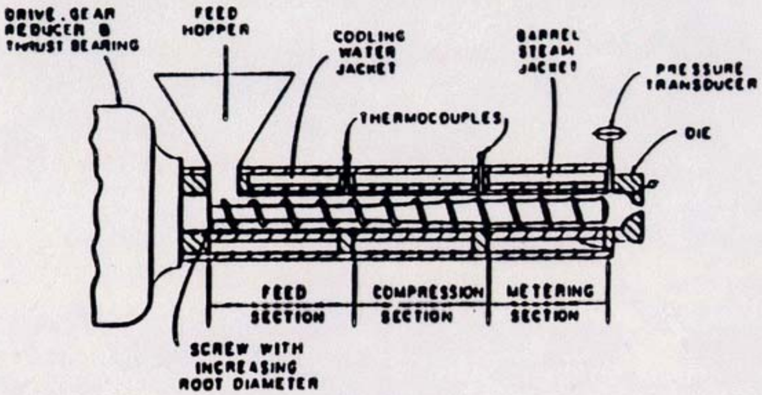
Twin-Screw Food Extruder



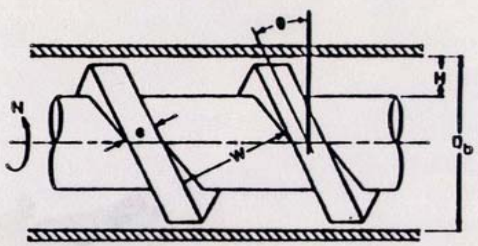
- Feed Hopper
- Rotating Screw
- Extruder Channel
- Heating/Cooling Arrangement
- Die

Extruder geometries

Schematic of a single screw extruder

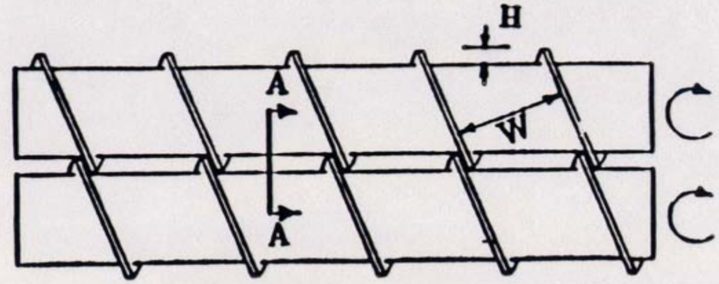


Schematic of a single screw with shallow rectangular channel

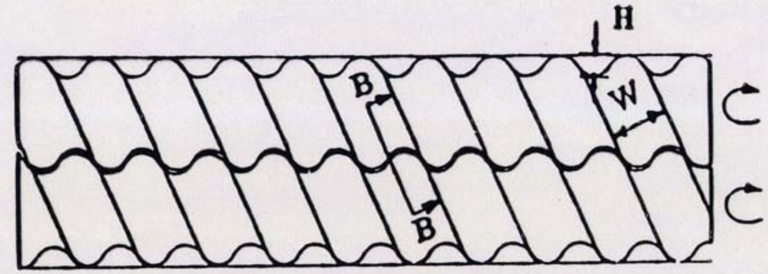


Schematic of a single screw with curved channel

Schematic of twin-screw geometries

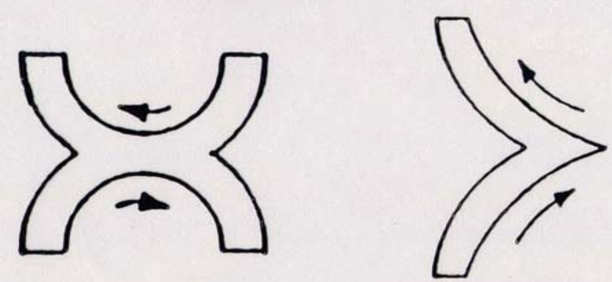


Tangential (finite gap between screws)



Self-wiping (no gap between screws)

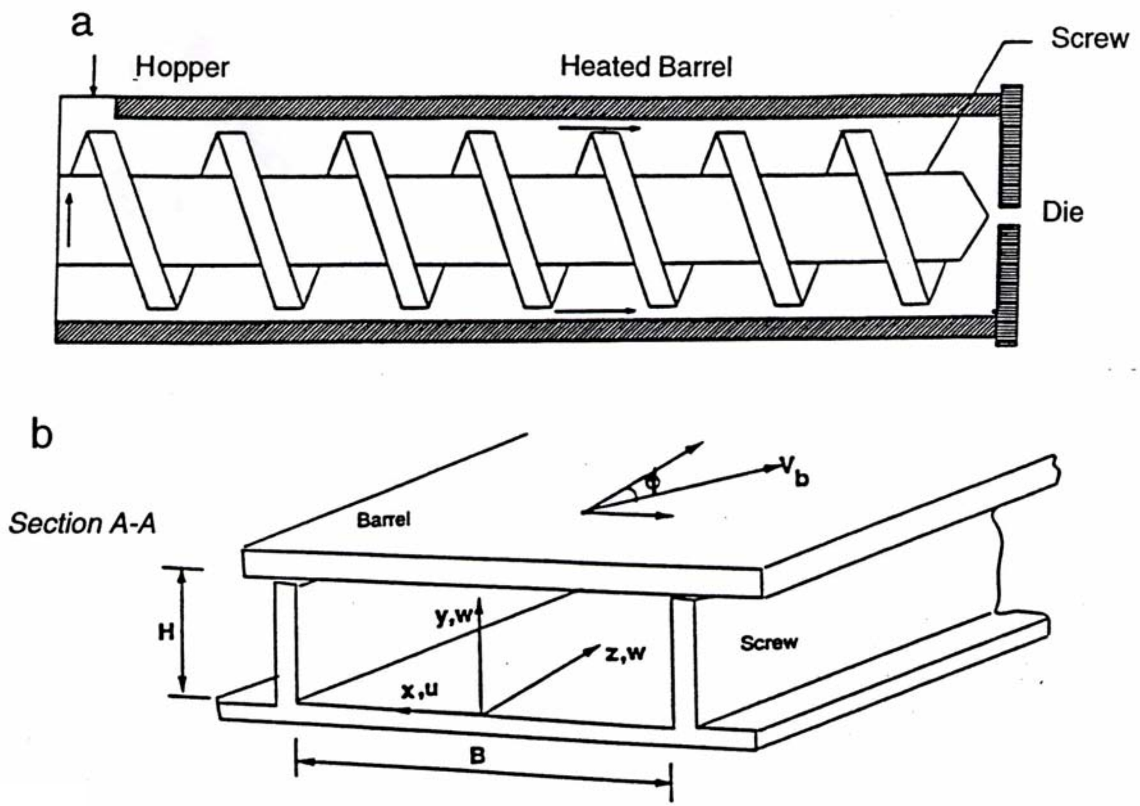
Cross Sections



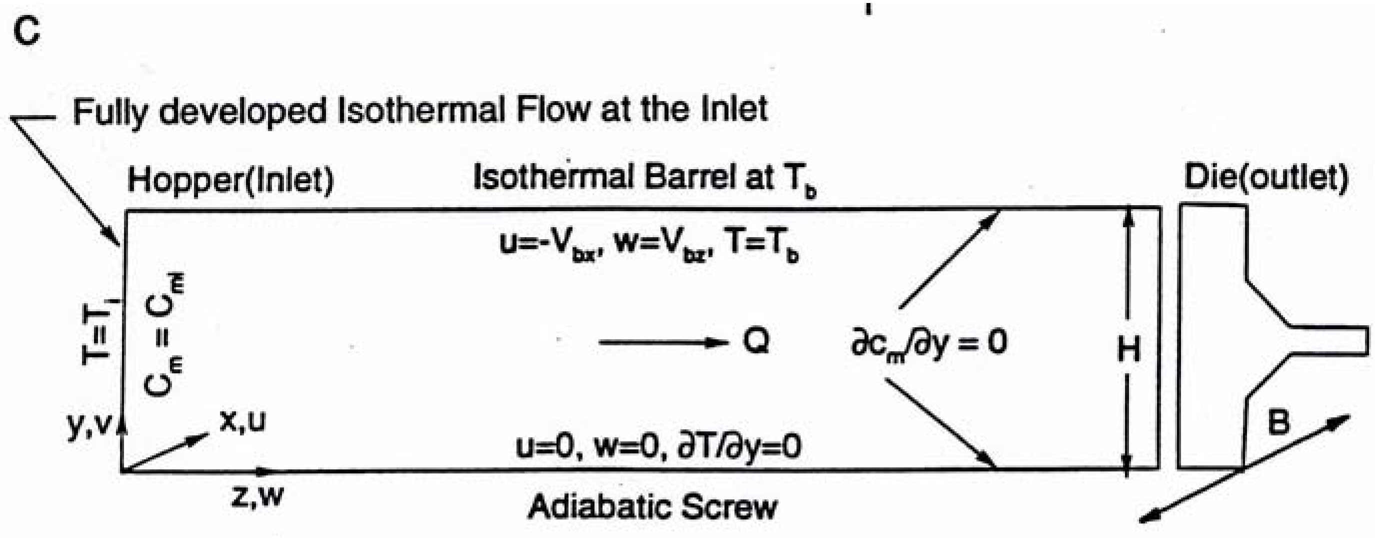
A-A

B-B

Sketch of Single-Screw Polymer Extruder



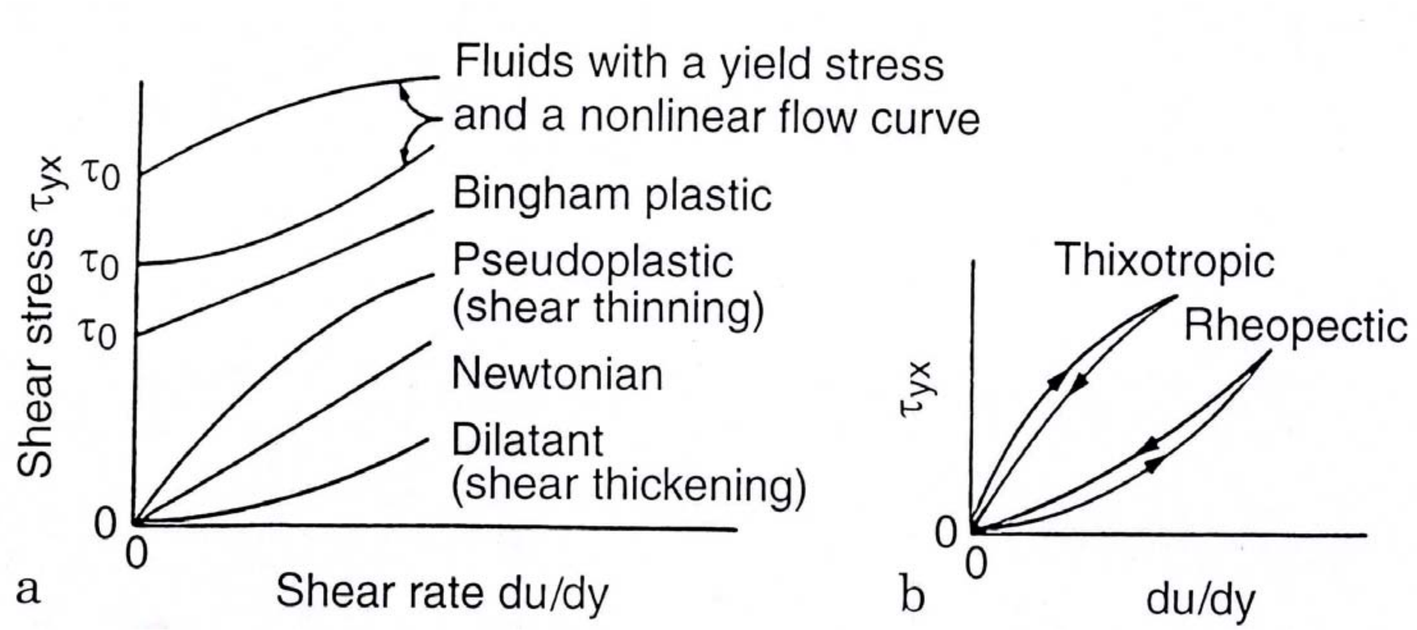
Model of Single-Screw Polymer Extruder



Material Properties

- *Accurate Data on Material Properties*
- *Material Property Variations with Temperature, Shear Rate, Concentration, Pressure, etc.*
- *Link Between Properties and Process*

Material Properties: Shear Stress Versus Shear Rate



Material Properties: Viscosity Variation

GLASS

$\nu = 4545.45 \exp [\, 32\, (T_{melt}/\mathbf{T} - 1)\,]$

POLYMER

$\mu = \mu_o\, (\dot{\gamma}/\dot{\gamma}_o)^{n-1} \exp (\, b\, /T\,)$

REACTIVE POLYMER

$\mu = \mu_o\, (\dot{\gamma}/\dot{\gamma}_o)^{n-1} \exp [\, -b\, (T - T_o)] \exp [\, -b_m\, (C - C_o)]$

Chemical Kinetics

FOOD

$$d[(1-X)]/dt = -K\,(1 - X)^m$$

with $K = K_T + K_S$

where $K_T = K_{To} \exp(-E_T / RT)$

$K_S = K_{So} \exp(-E_S / \tau\, \eta)$

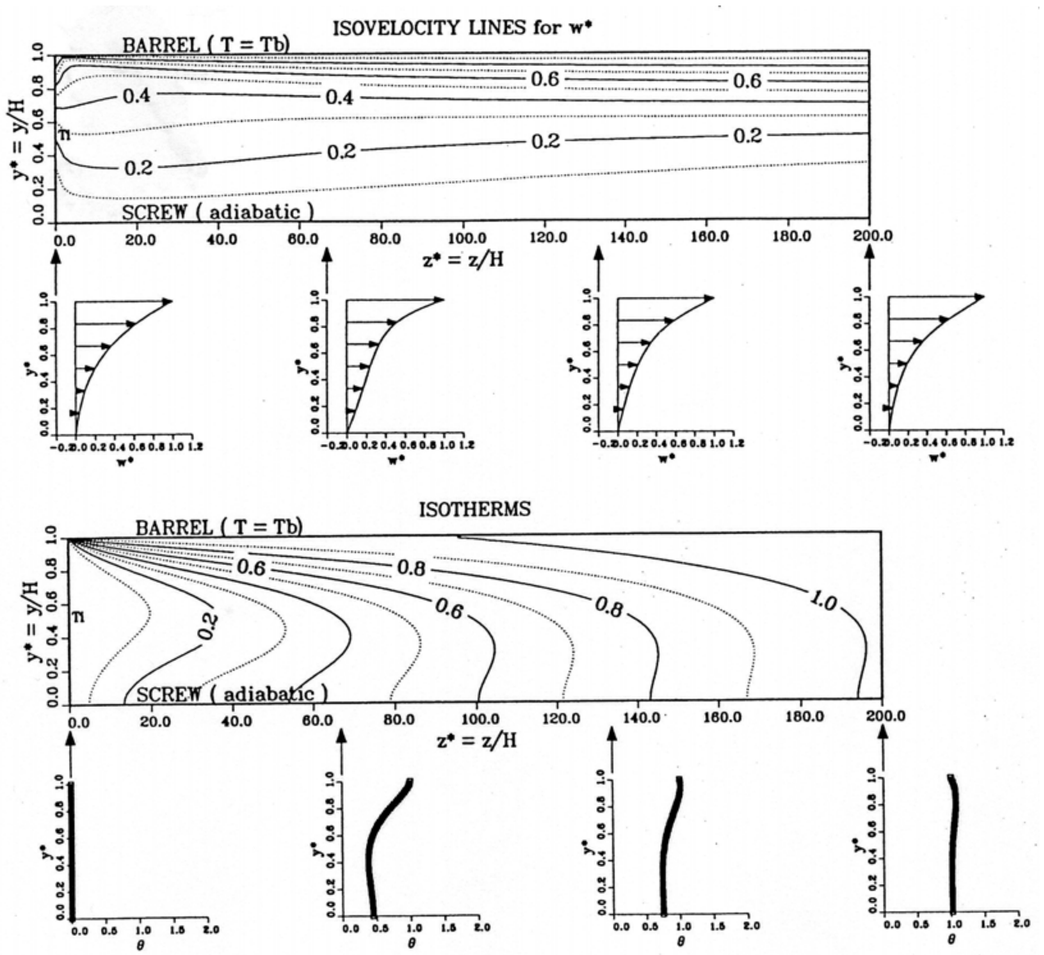
X: Degree of Conversion

CVD

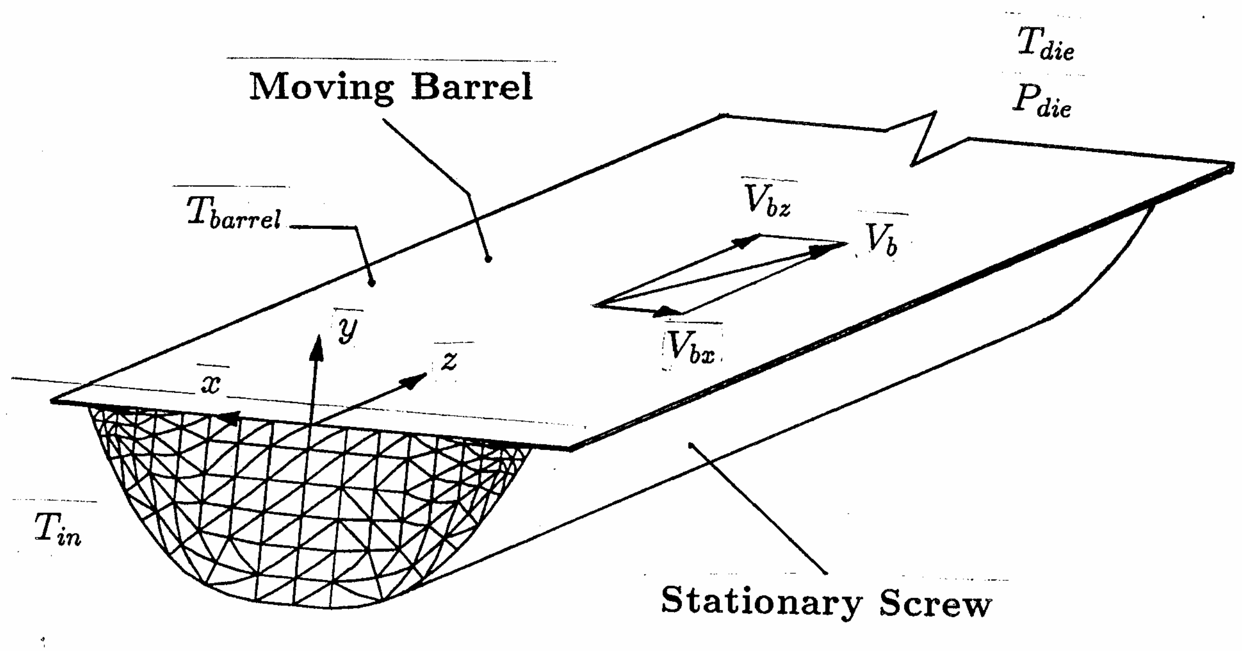
$$K = K_o p_{SiH4}/[1 + K_1 p_{H2} + K_2 p_{SiH4}]$$

rutgers ENGINEERING

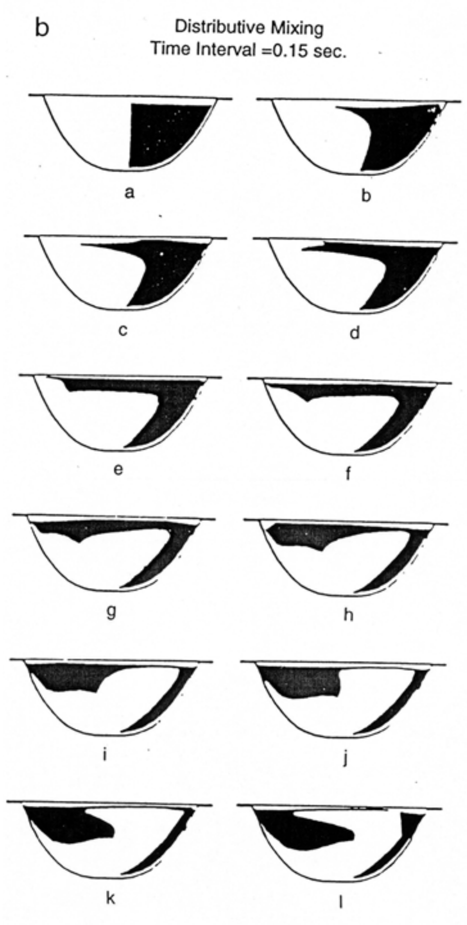
Transport in the Channel of a Single-Screw Polymer Extruder



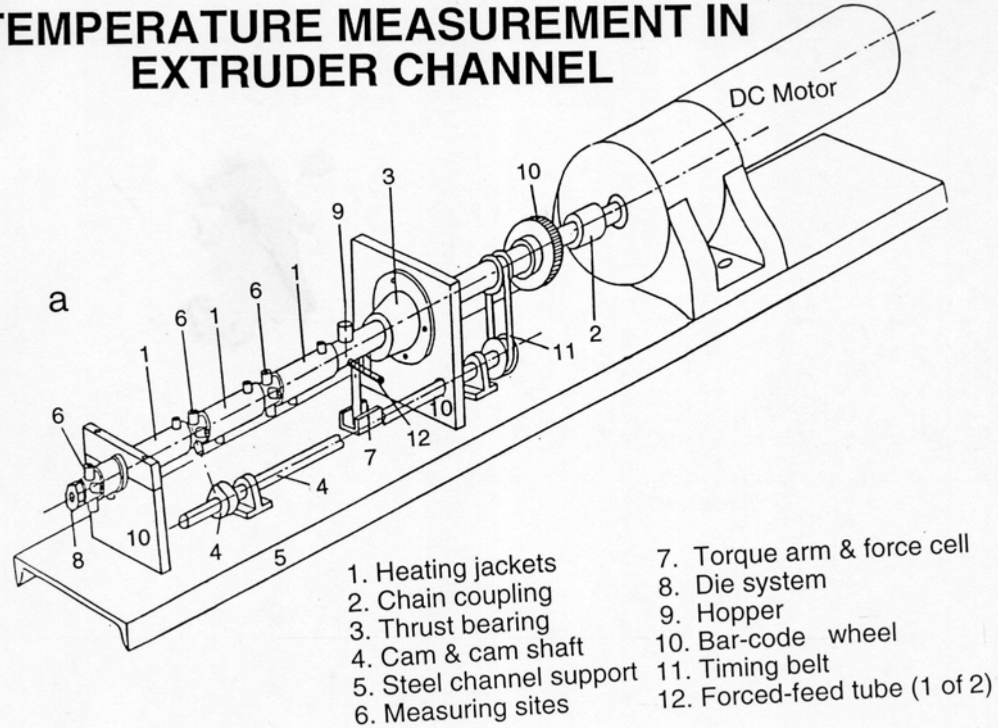
Model of Extruder with Arbitrary Screw Profile

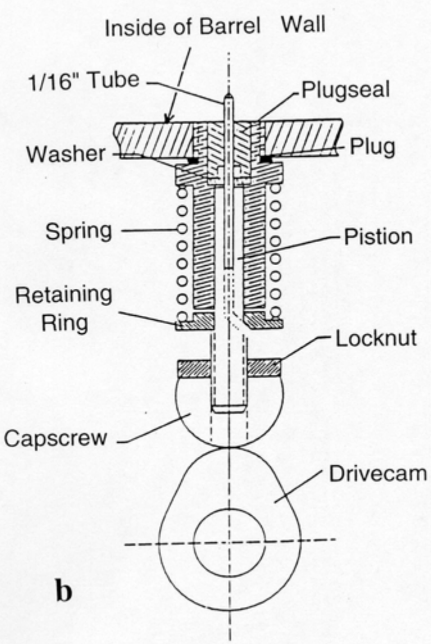


Distributive Mixing in Extruder Channel

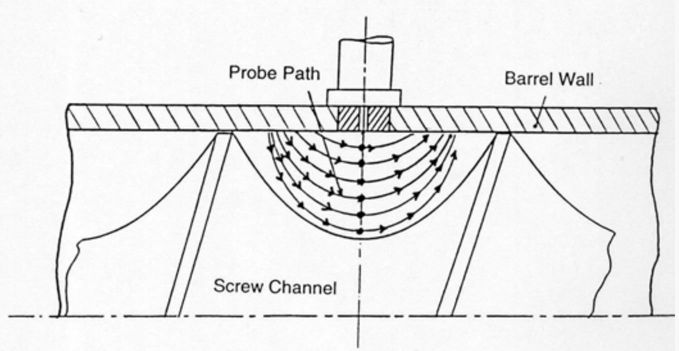


TEMPERATURE MEASUREMENT IN EXTRUDER CHANNEL



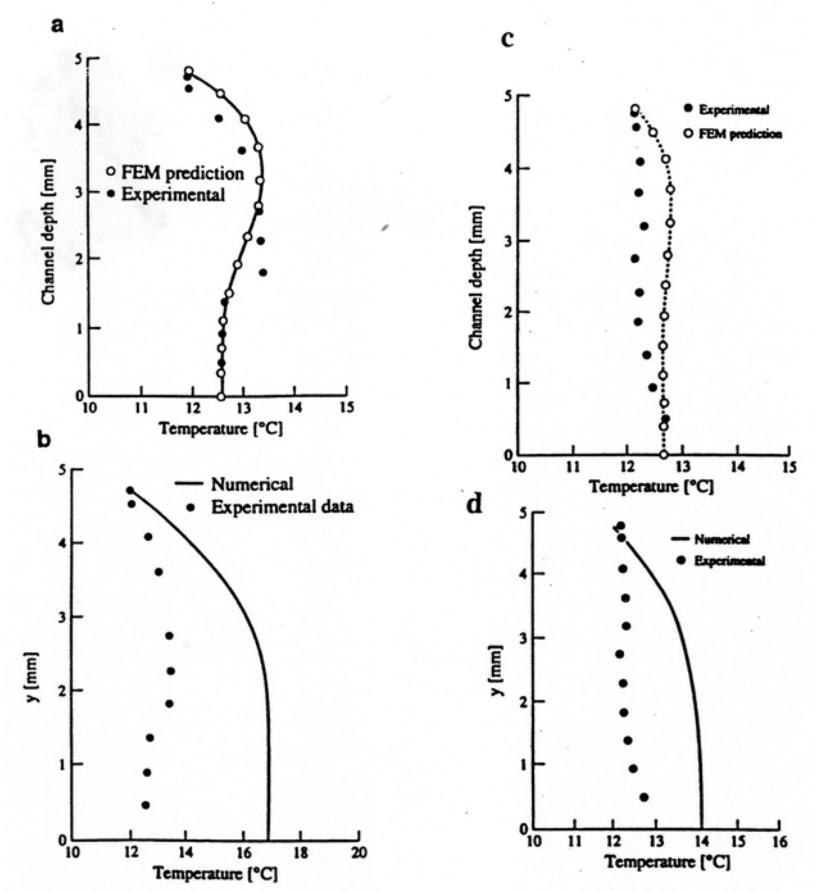


b



c

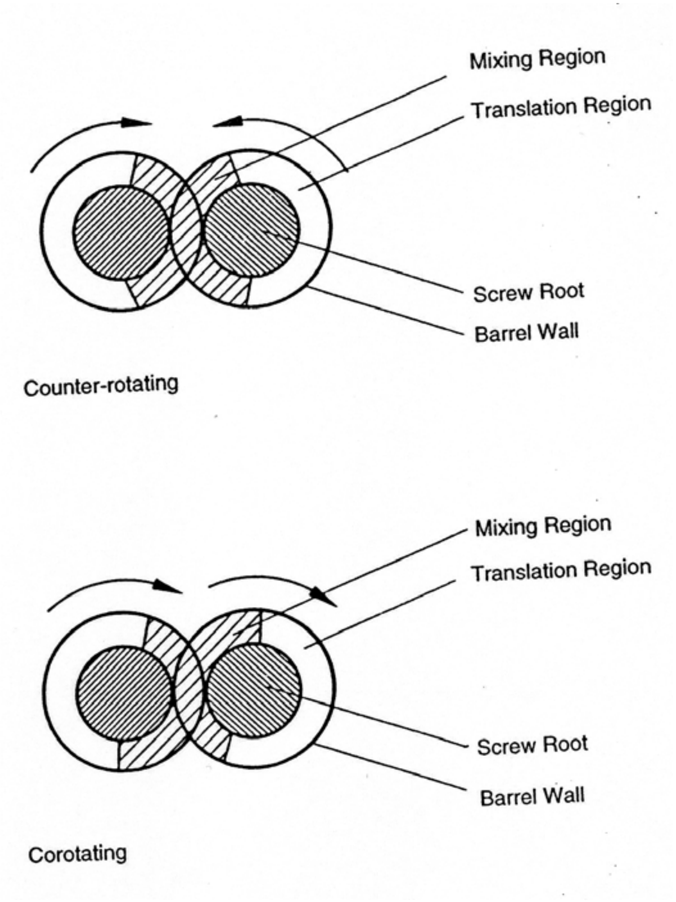
Measured and Calculated Temperature Profiles in Single-Screw Extruder



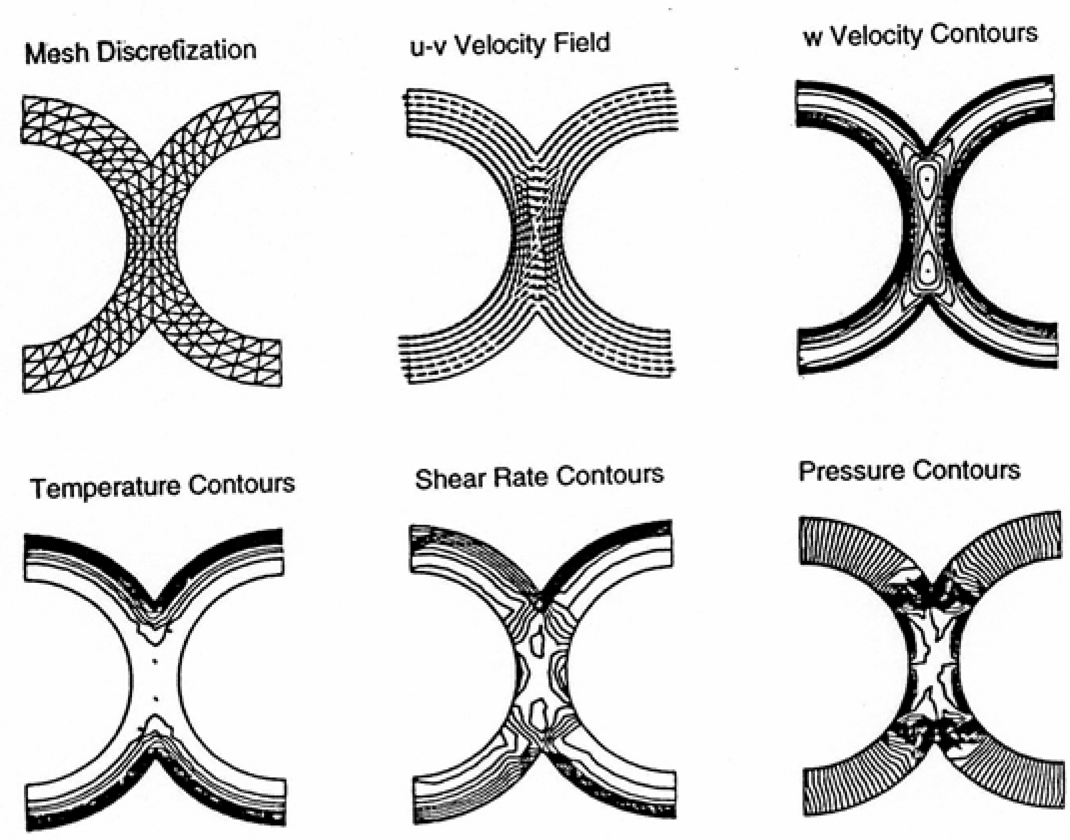
3D (FEM)

2D (FDM)

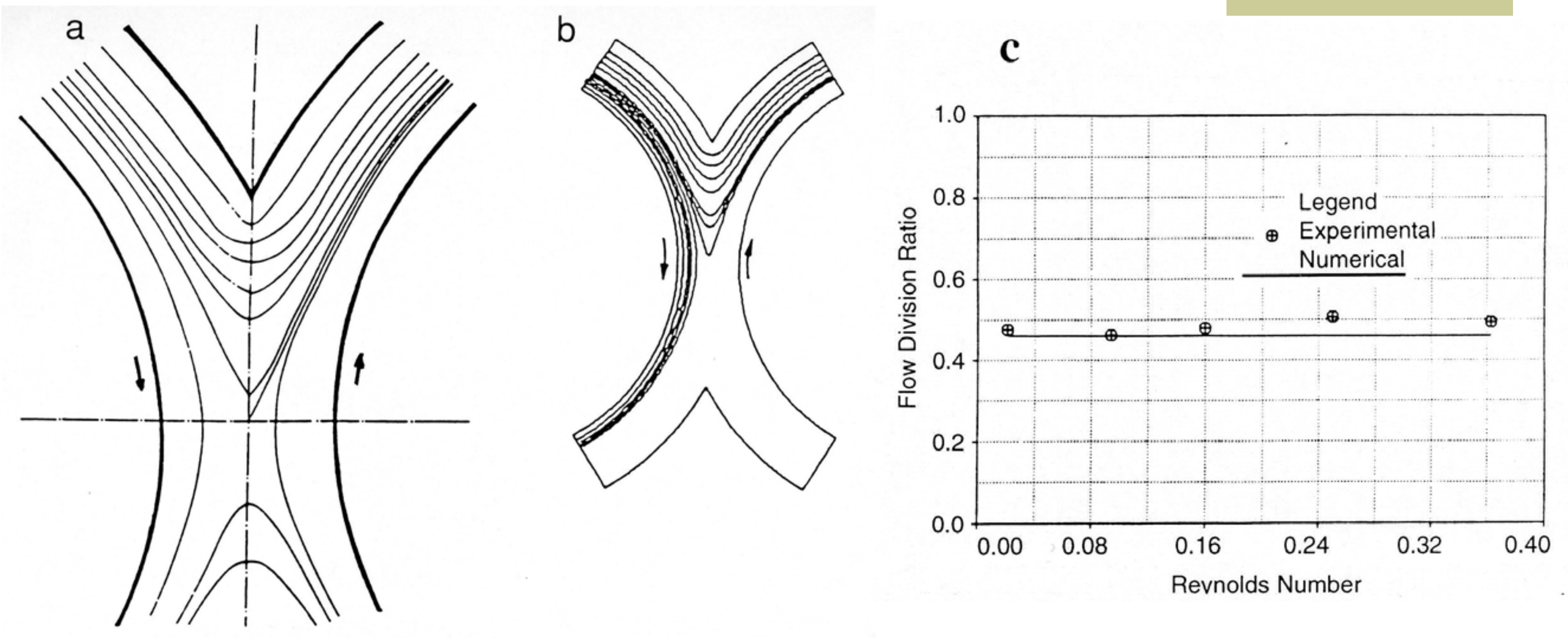
Modeling of Twin-Screw Polymer Extruder



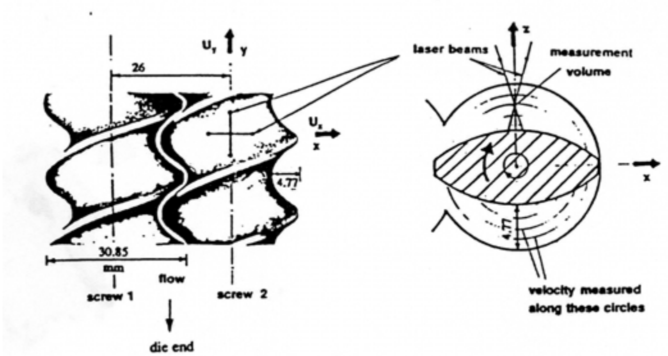
Flow in NIP Region of Twin-Screw Extruder



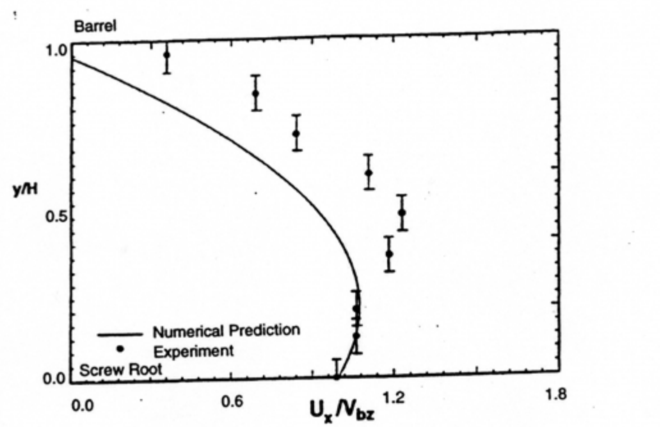
Flow in the Region Between Two Co-Rotating Cylinders



Measured and Calculated Velocity Profiles in Polymer Extrusion

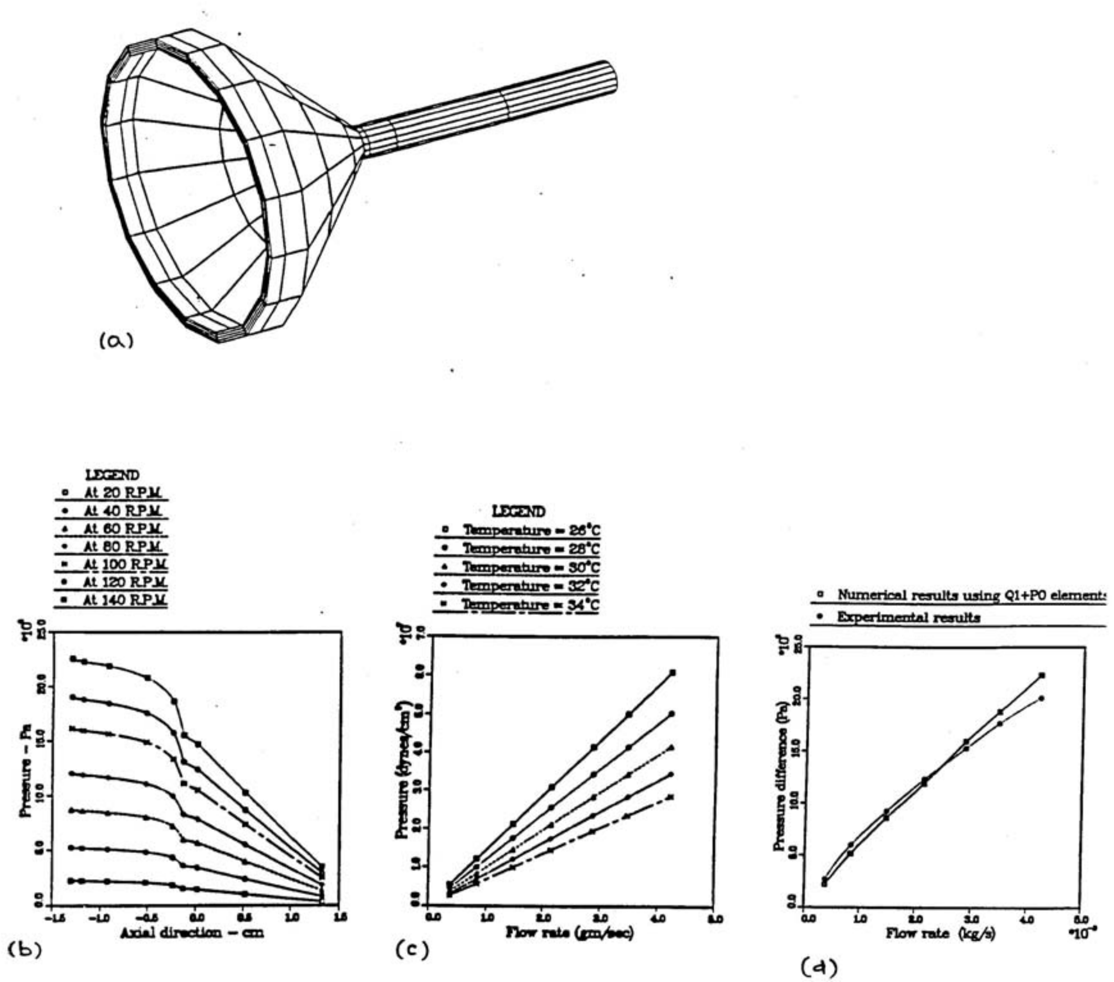


(a)



(b)

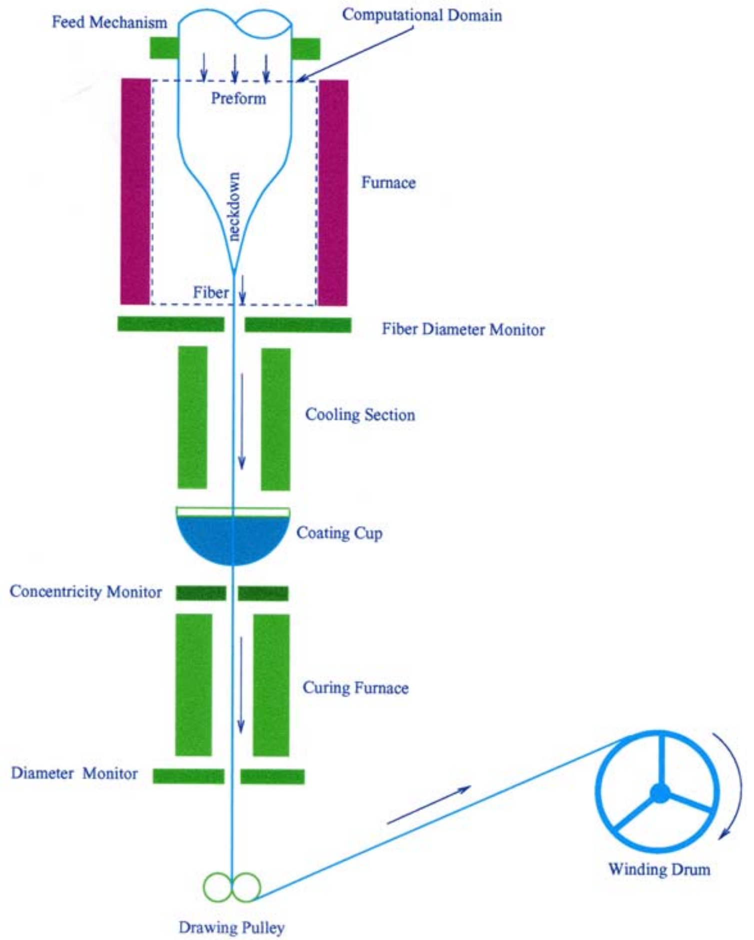
Modeling of Flow through Extrusion Dies



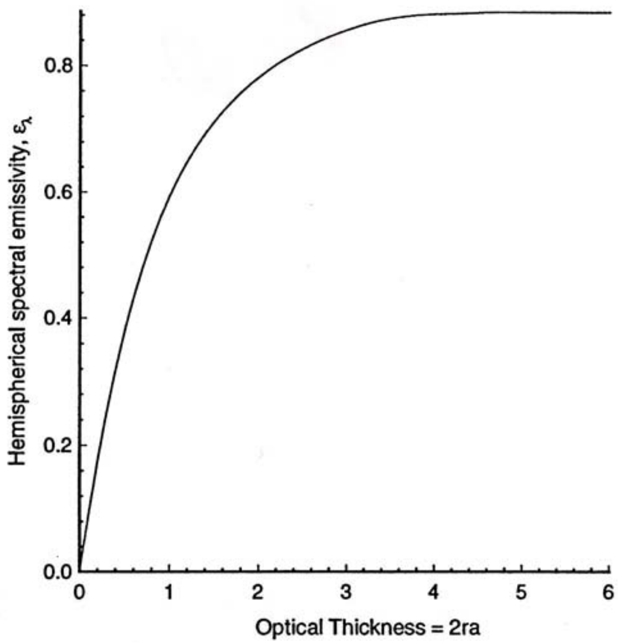
Optical Fiber Drawing System

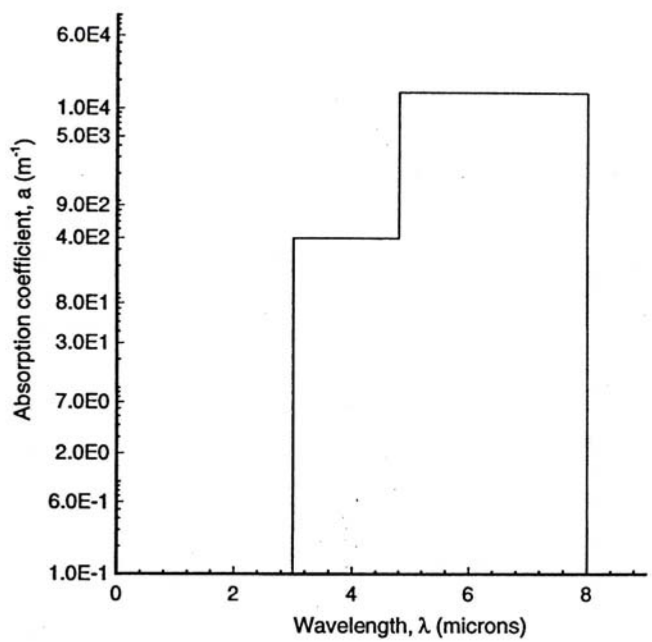
- Drawing Furnace
- Fiber Cooling
- Coating
- Curing
- Take-Up

Sketch of Optical Fiber Drawing System

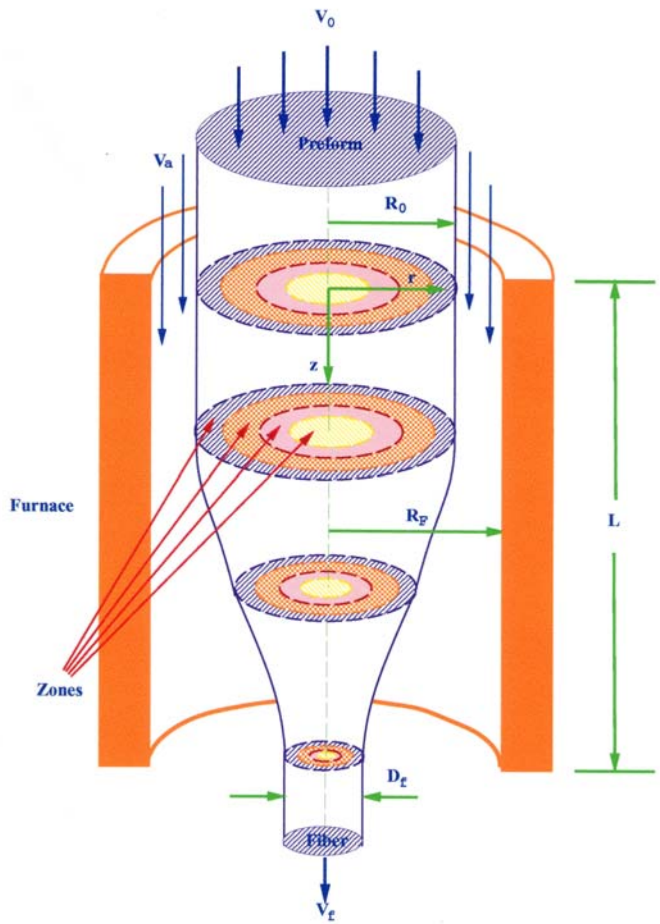


Material properties:
Radiation Properties of Silica Glass





Cylindrical Draw Furnace and Finite Zones For Radiation Analysis



The Governing Equations for Glass and Inert Gas

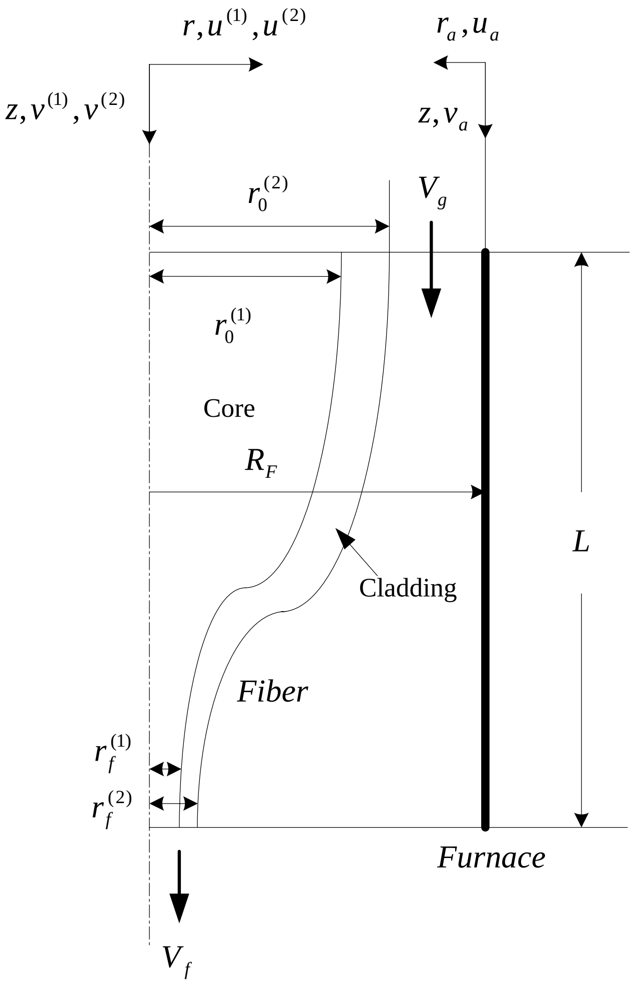
$$\frac{\partial v}{\partial z}+\frac{1}{r}\frac{\partial (ru)}{\partial r}=0 \tag{1}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial r}+v\frac{\partial v}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial z}+\frac{1}{r}\frac{\partial}{\partial r}\left[r\upsilon\left(\frac{\partial v}{\partial r}+\frac{\partial u}{\partial z}\right)\right]+2\frac{\partial}{\partial z}\left(\upsilon\frac{\partial v}{\partial z}\right) \tag{2}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+v\frac{\partial u}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial r}+\frac{2}{r}\frac{\partial}{\partial r}\left(r\upsilon\frac{\partial u}{\partial r}\right)+\frac{\partial}{\partial z}\left[\upsilon\left(\frac{\partial v}{\partial r}+\frac{\partial u}{\partial z}\right)\right]-\frac{2\upsilon u}{r^2} \tag{3}$$

$$\rho C_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial r}+v\frac{\partial T}{\partial z}\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(rK\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right)+\Phi \tag{4}$$

Schematic Diagram of Double-layer Optical Fiber

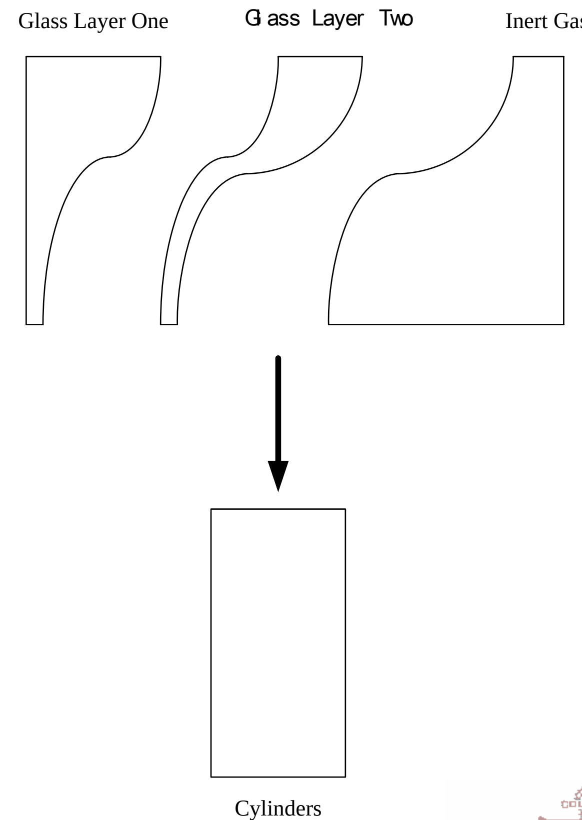


Landau's Transformations

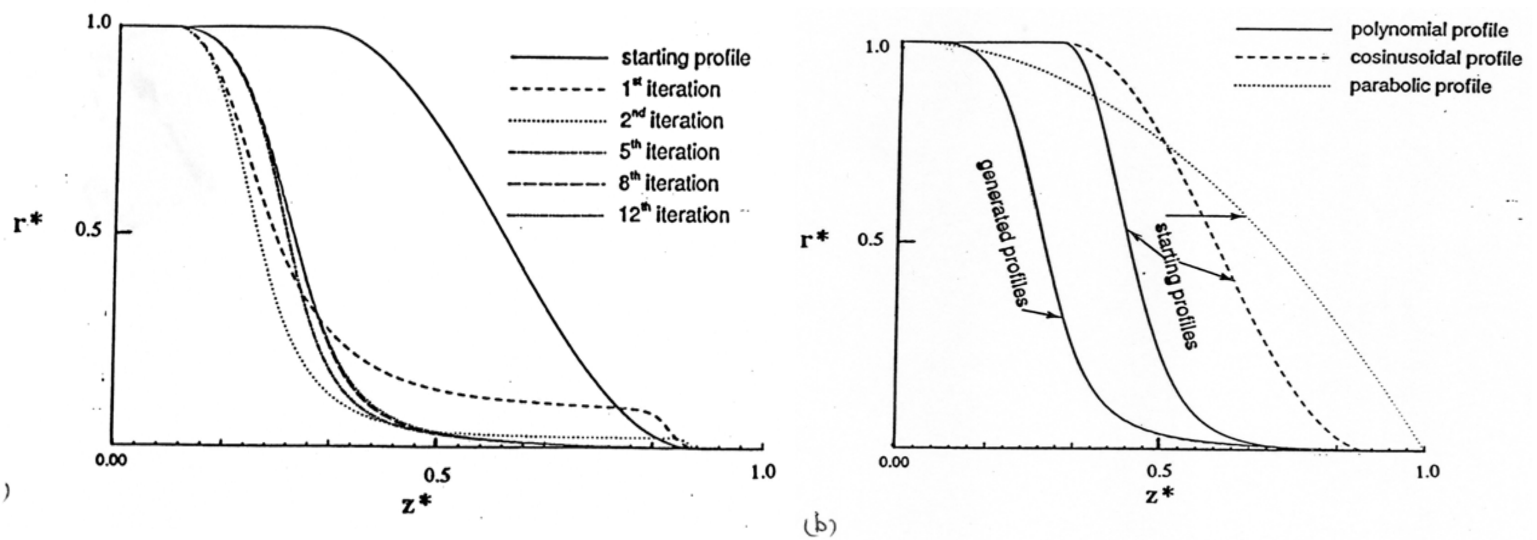
$$\eta^{(1)} = \frac{r^{(1)}}{R^{(1)}(z)}, \quad \beta = \frac{z}{L}$$

$$\eta^{(2)} = \frac{r^{(2)} - R^{(1)}(z)}{R^{(2)}(z) - R^{(1)}(z)}, \quad \beta = \frac{z}{L}$$

$$\eta_a = \frac{r_a}{R_F - R^{(2)}(z)}, \quad \beta = \frac{z}{L}$$

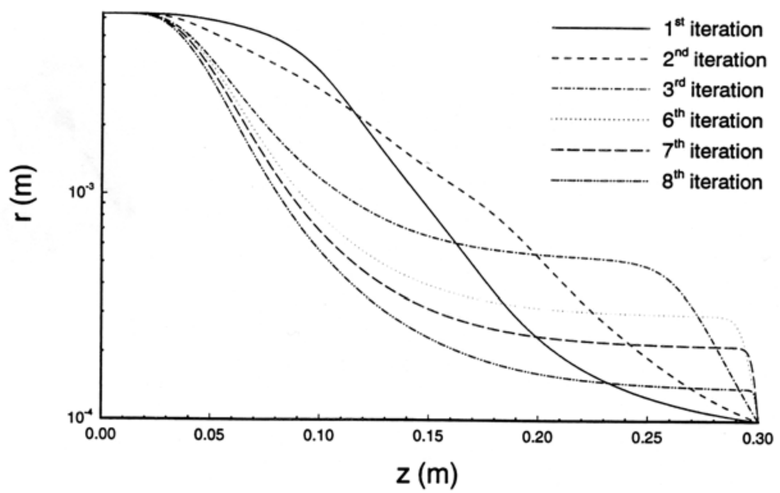


Generation of Neck-Down Profile

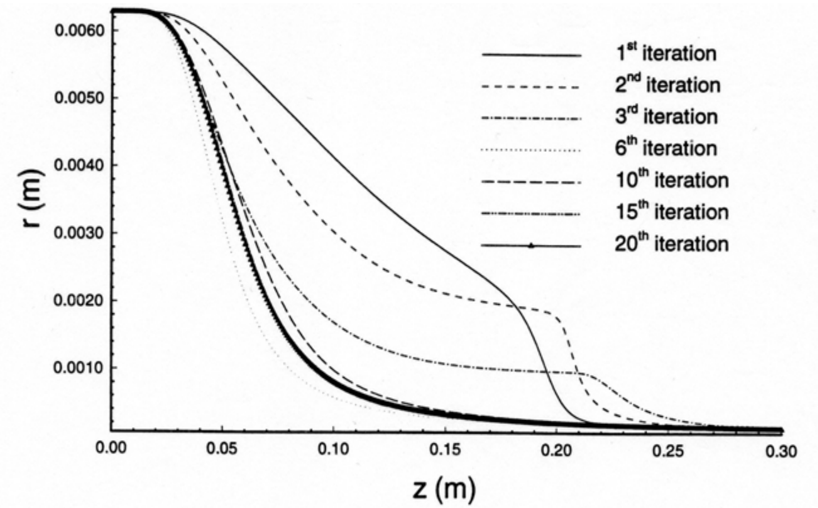


(a) (b)

Iterative Convergence Of Neck-Down Profile

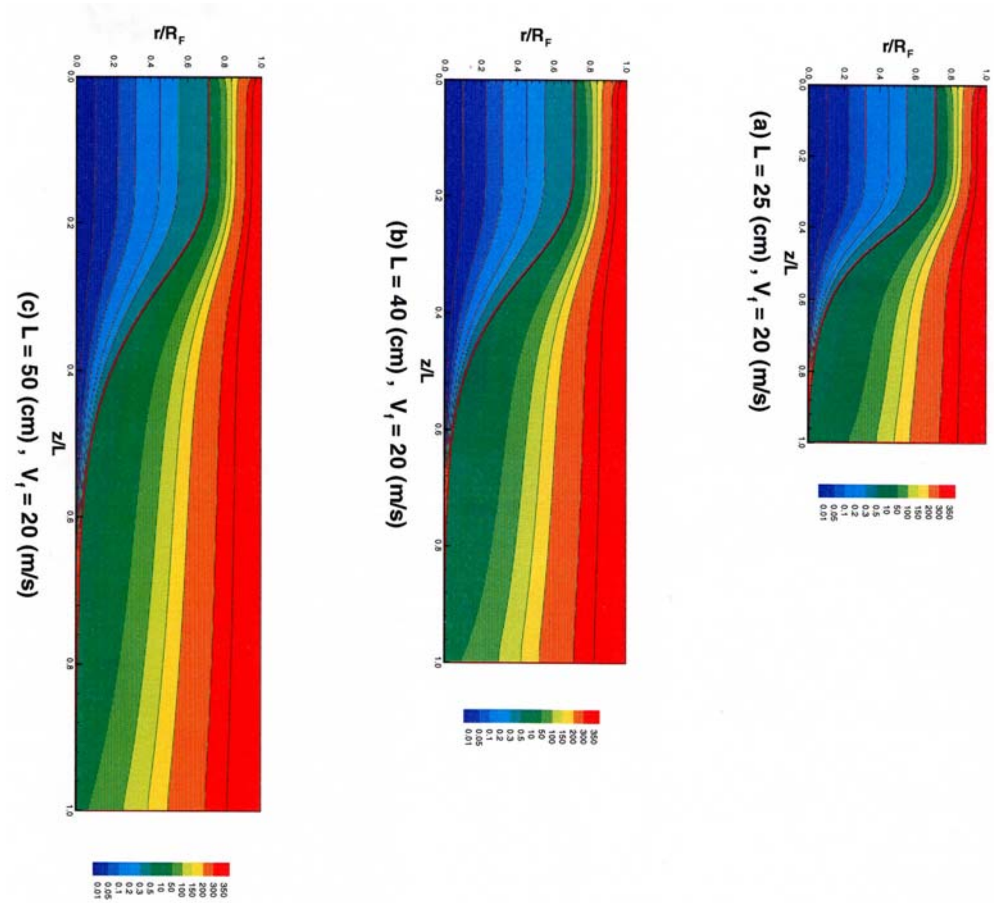


(a) R_f =100 μm (inability to converge)

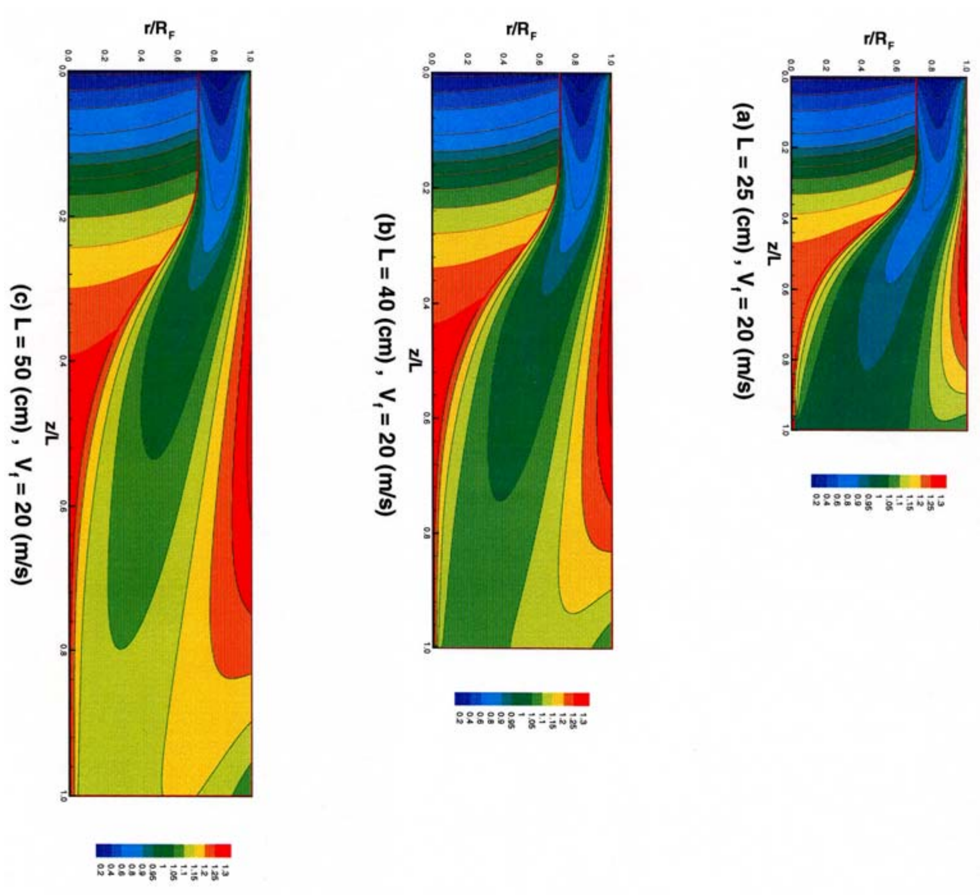


(b) R_f =125 μm (iterative convergence)

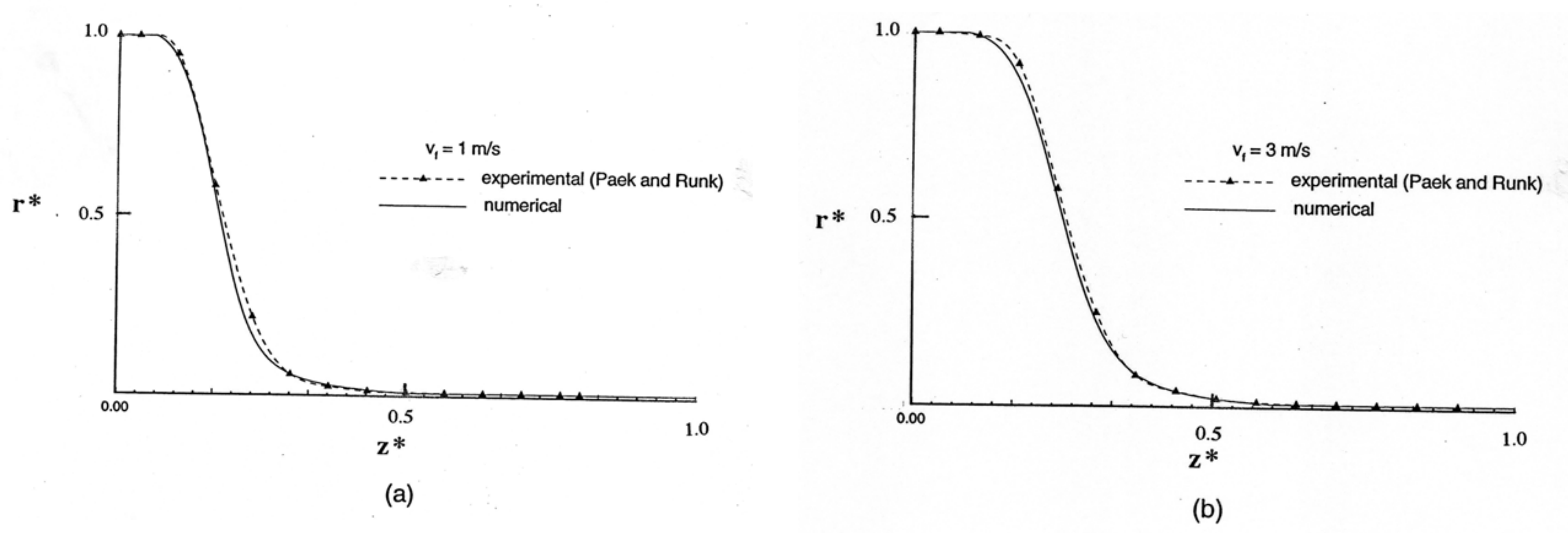
Streamlines in Optical Fiber Drawing



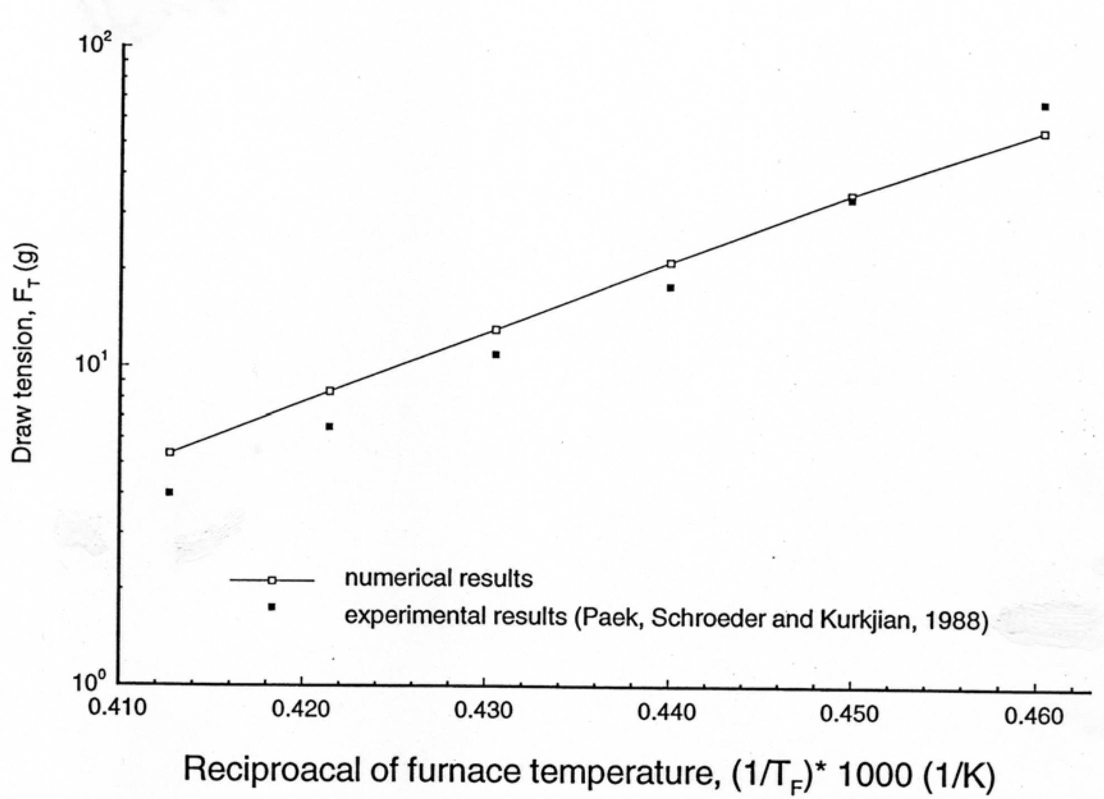
Isotherms in Optical Fiber Drawing



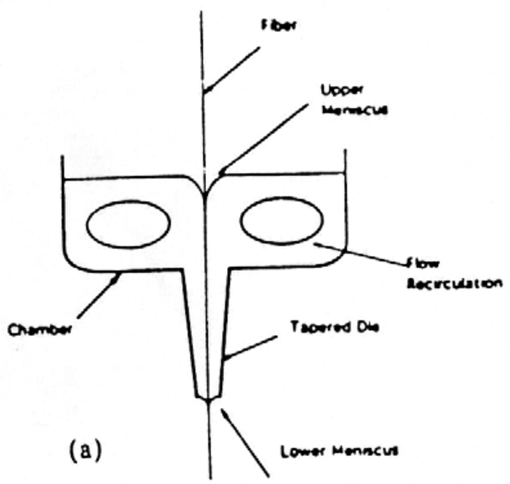
Neck-Down Profile from Numerical Simulation and Experimentation



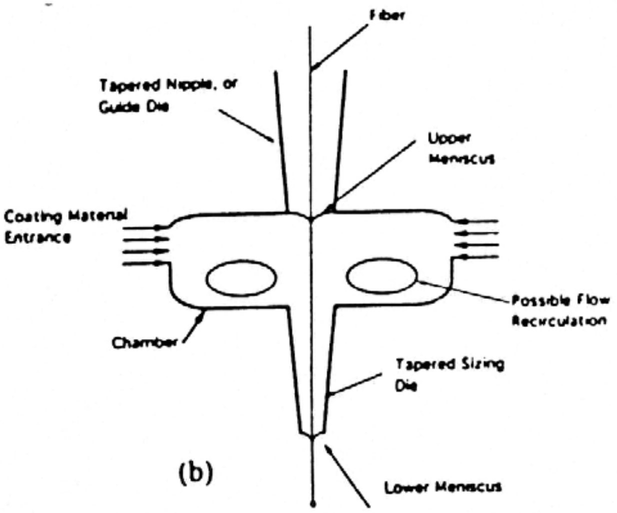
Calculated Versus Measured Tension in Optical Fiber Drawing



Flow in Fiber Coating Process

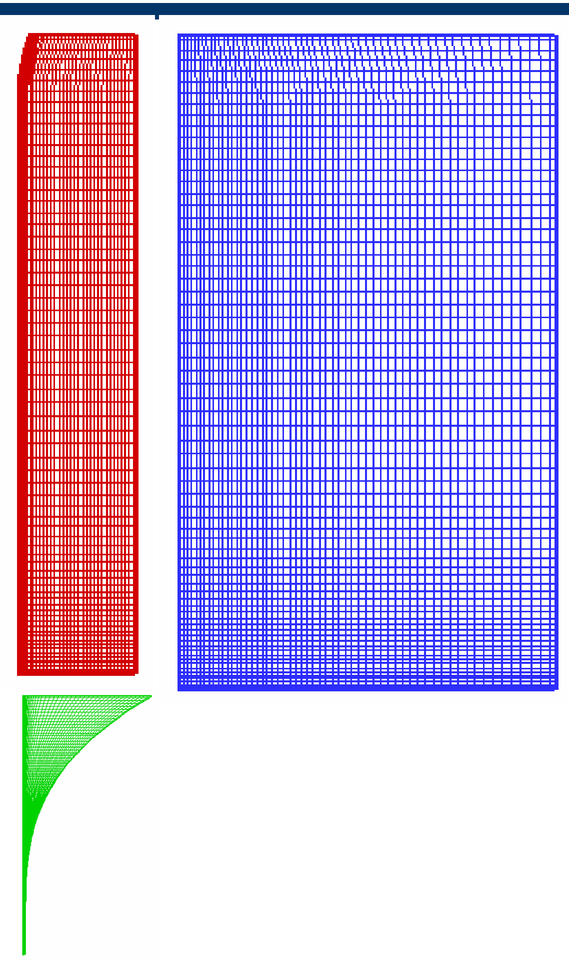


Open-Cup

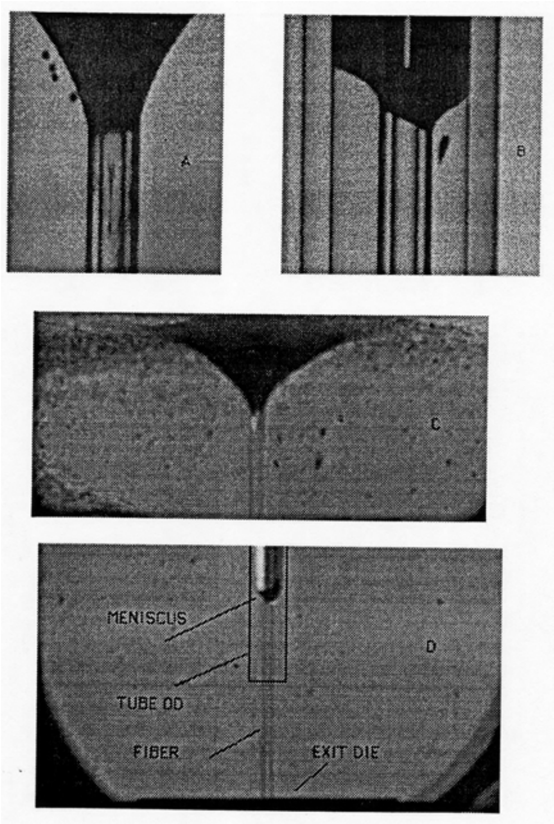


Pressurized

Grid Generation in the Fiber Coating Process



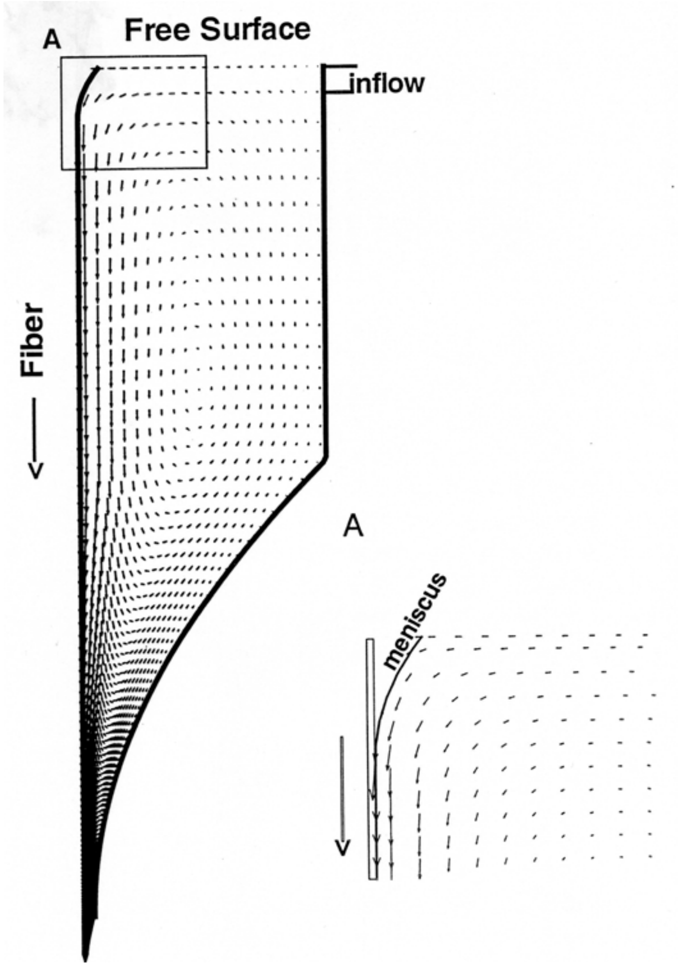
Meniscus in Fiber Coating Process



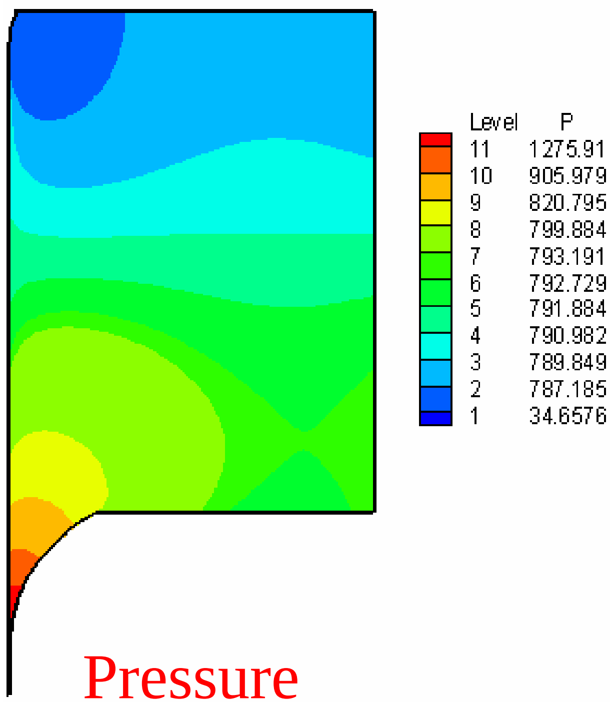
A, C: Unpressurized

B, D: Pressurized

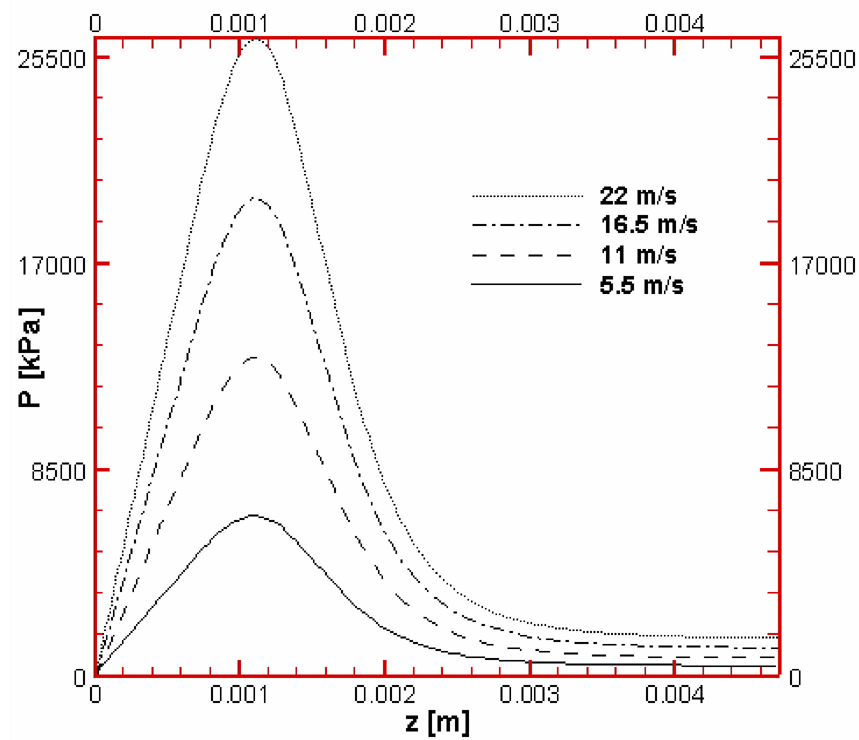
Effect of Meniscus



Pressure Distributions in Coating Die



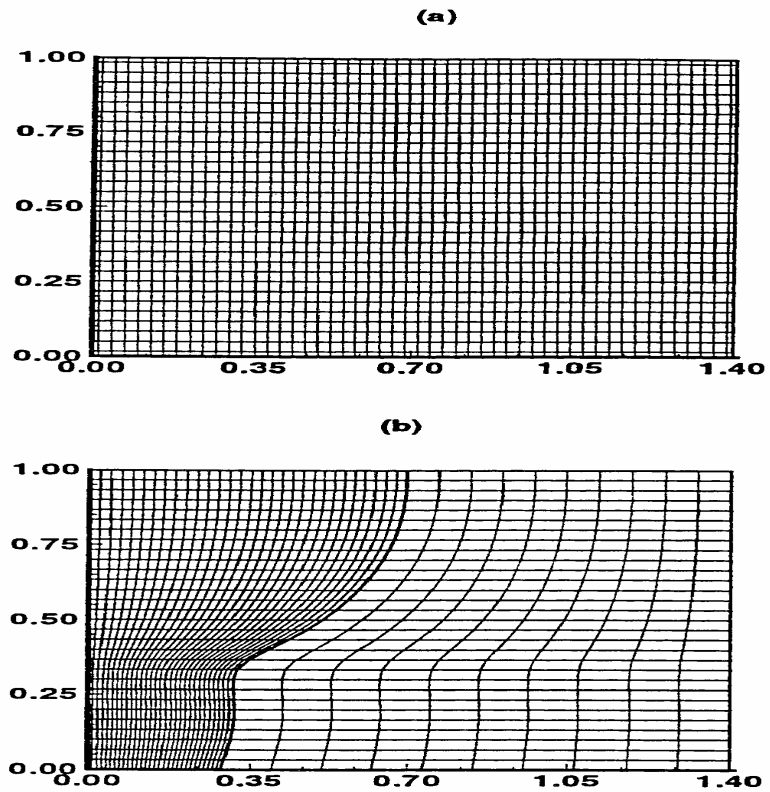
Pressure contours for v_f=11 m/s



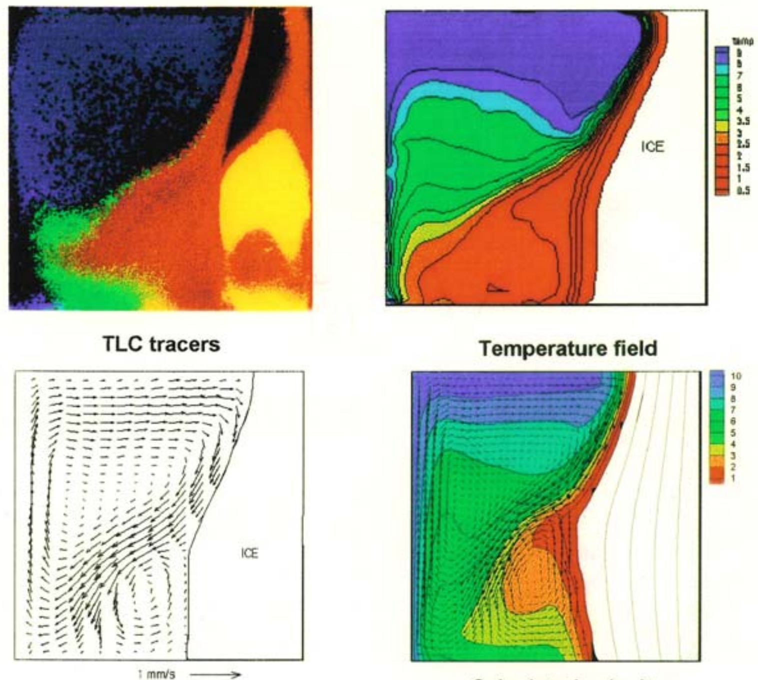
Pressure distributions along the die wall for various fiber speeds

rutgers ENGINEERING

Melting in Enclosed Region



Solidification of Water in an Enclosure with Conjugate Effects



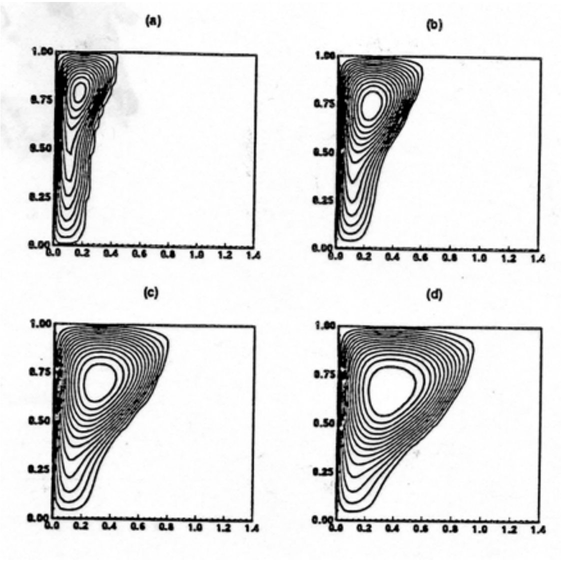
TLC tracers

Temperature field

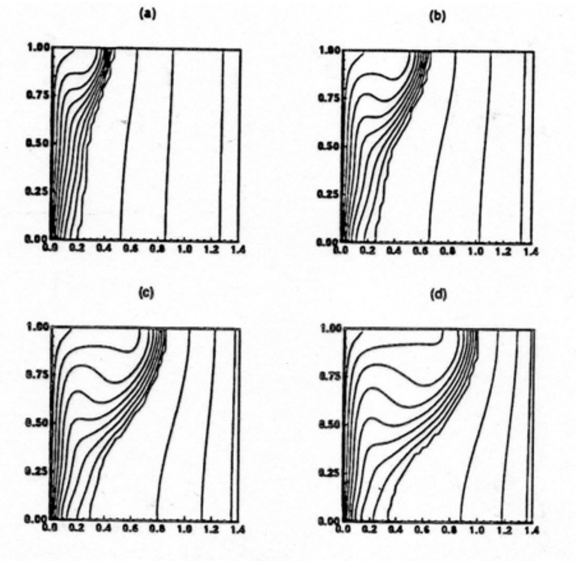
Evaluated velocity

Calculated velocity and temperature fields

Melting of Gallium in Enclosed Region

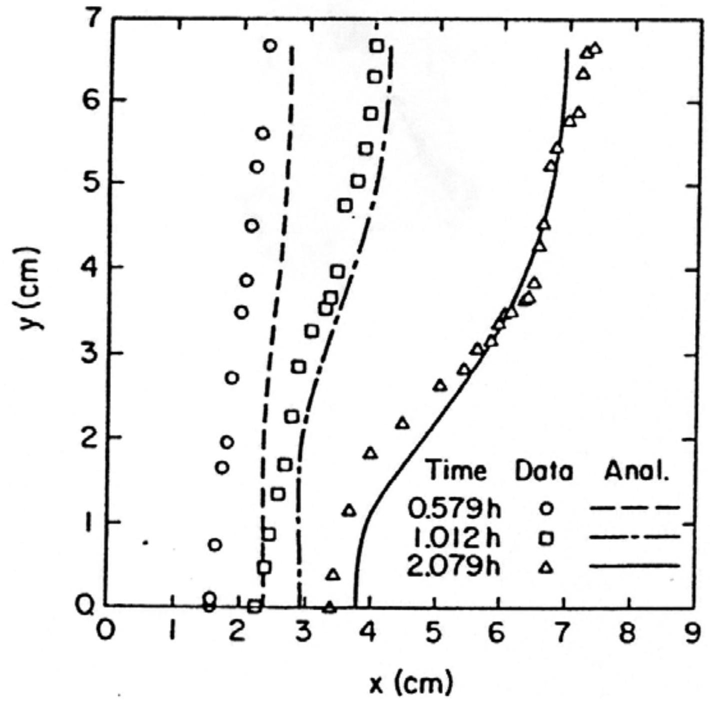


Streamlines

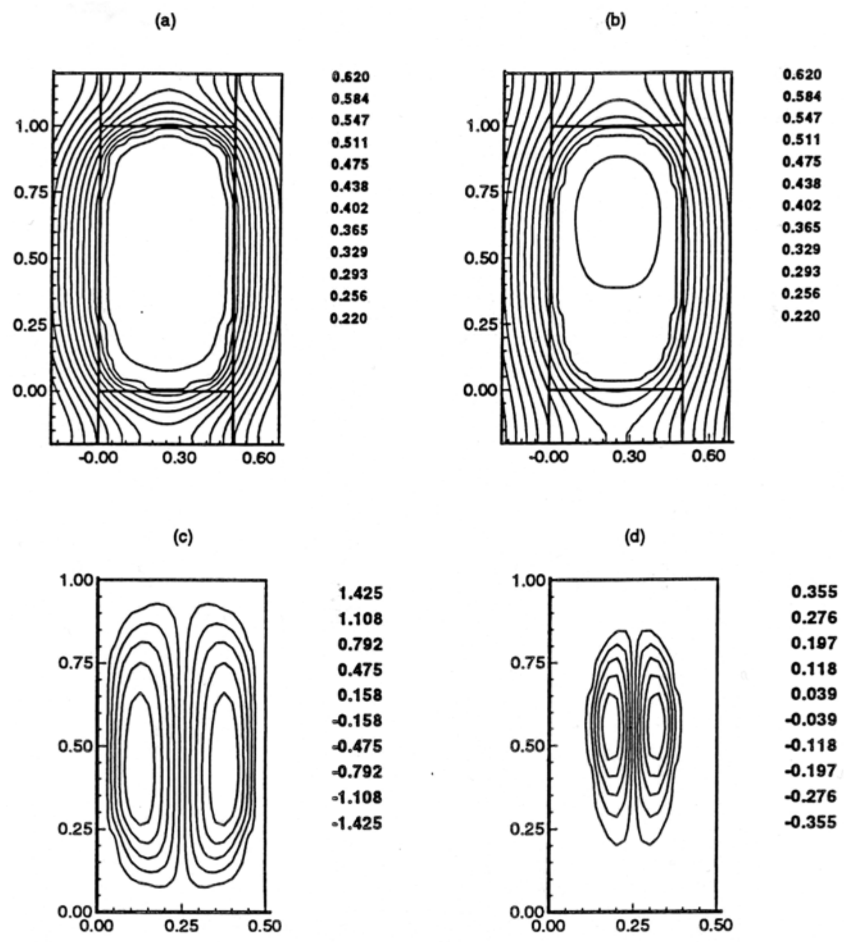


Isotherms

Measured Versus Calculated Solid-Liquid Interface in Solidification



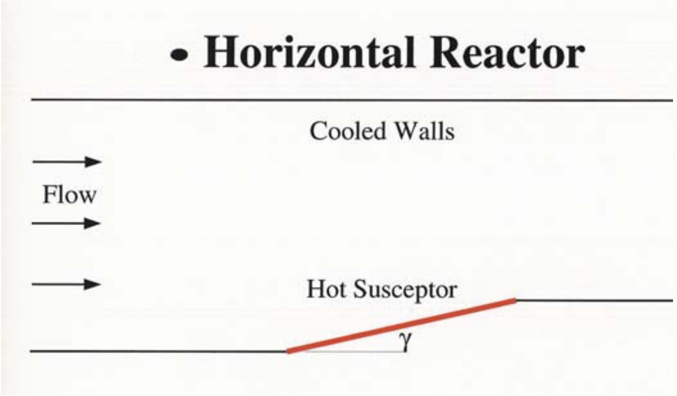
Solidification with Conjugate Transport at the Wall

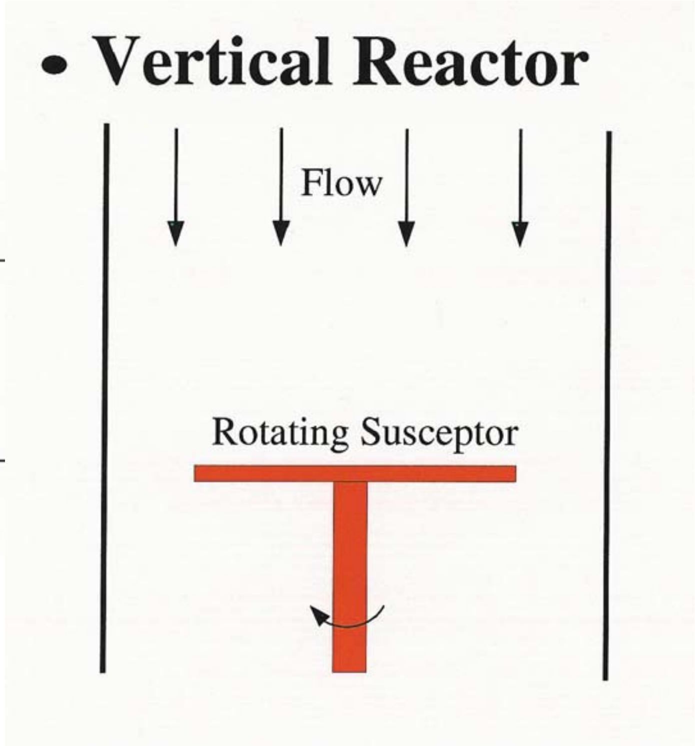


Isotherms

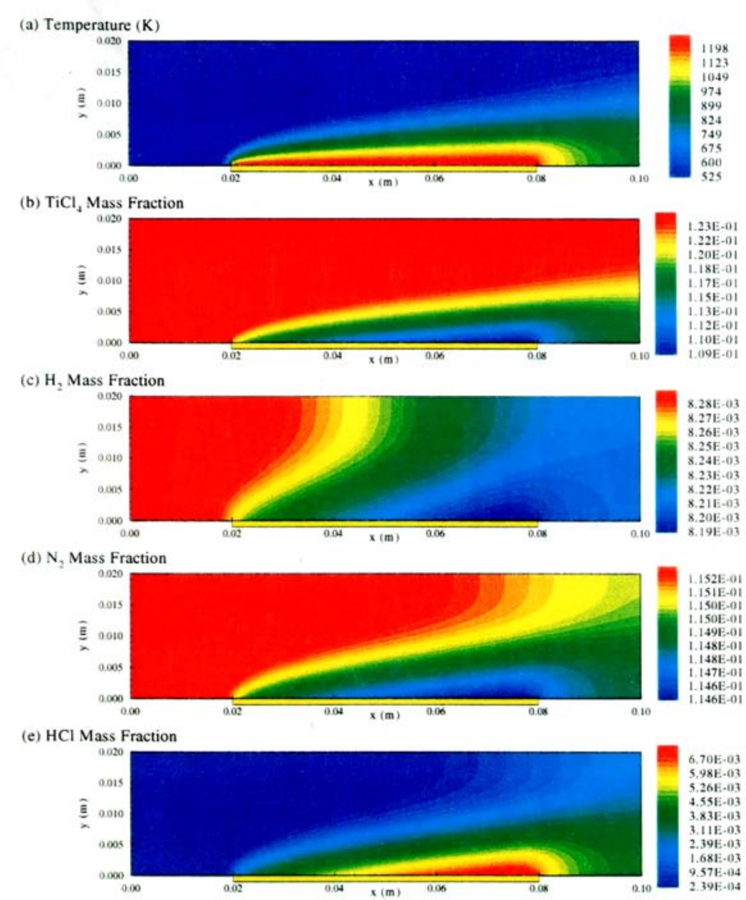
Streamlines

Chemical Vapor Deposition

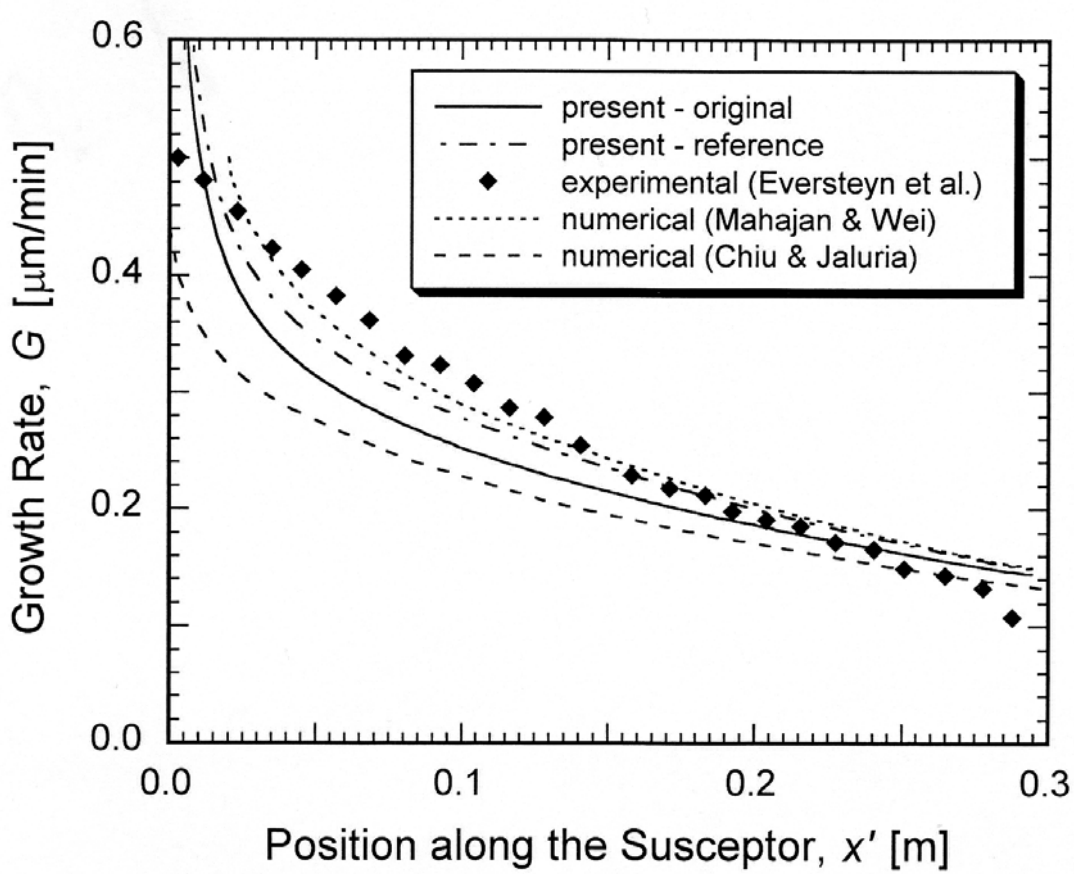




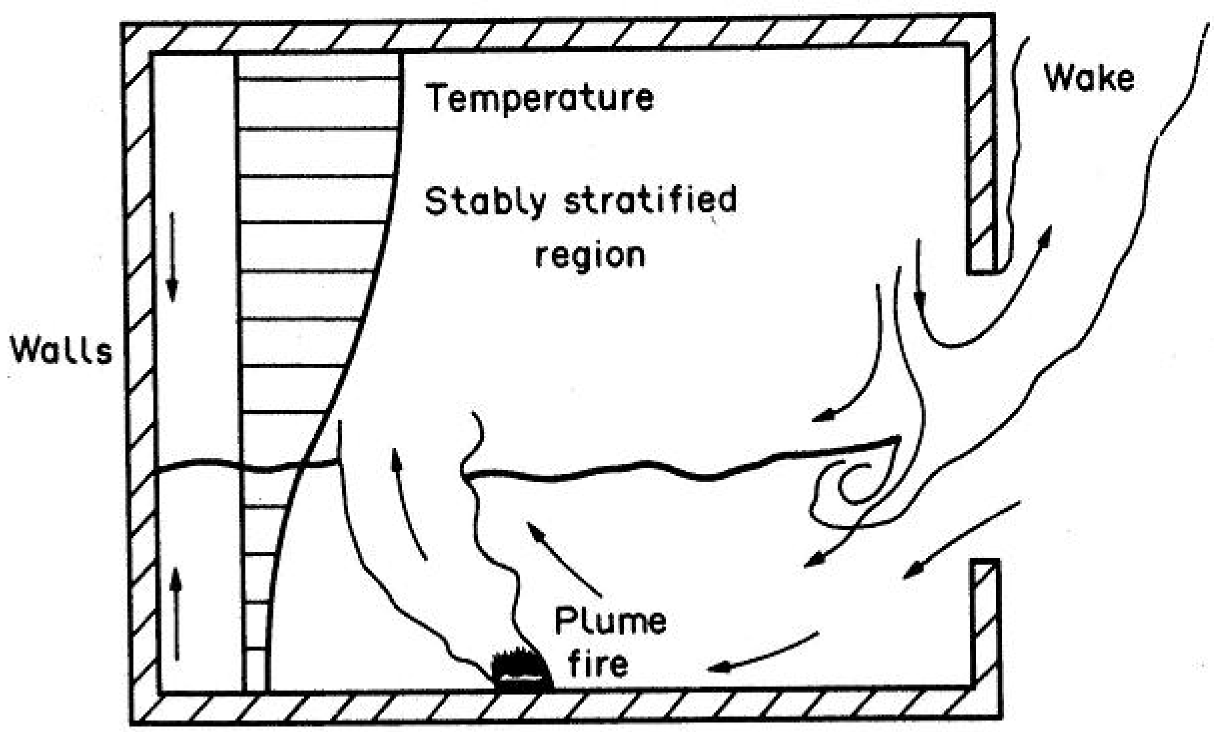
Contours in Horizontal TiN CVD Reactor



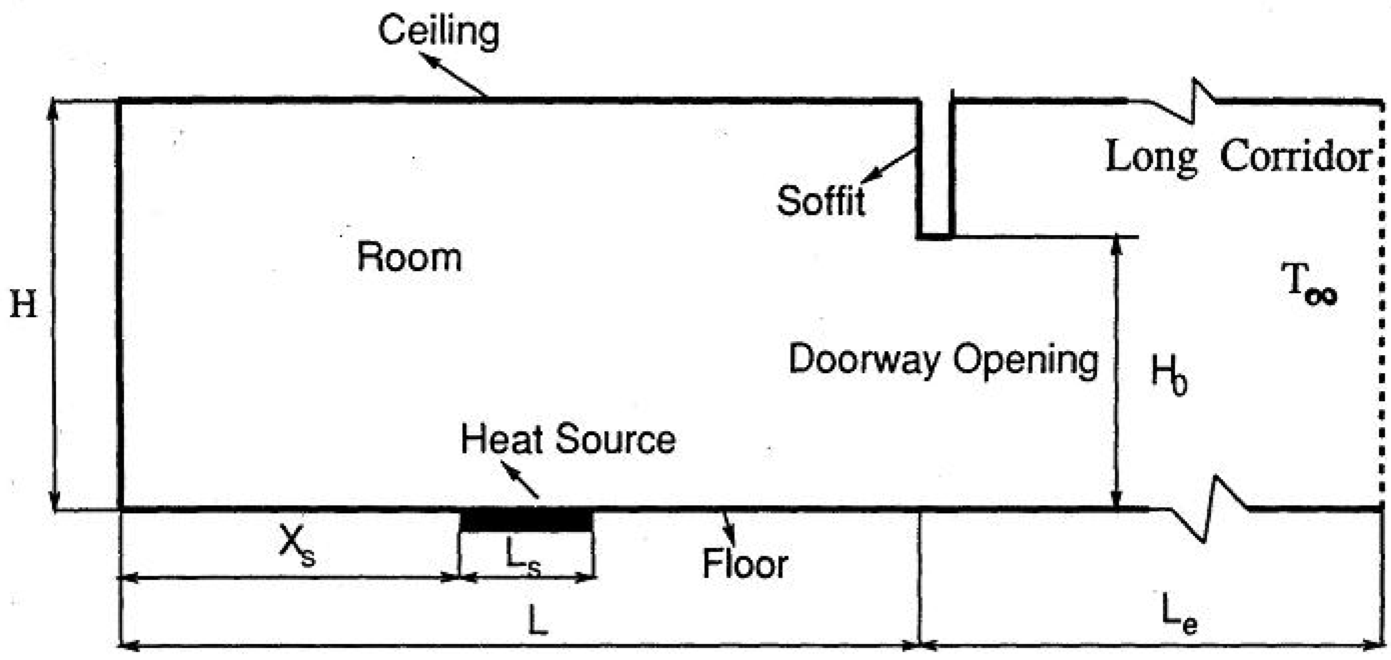
Film Growth in a Horizontal CVD Reactor



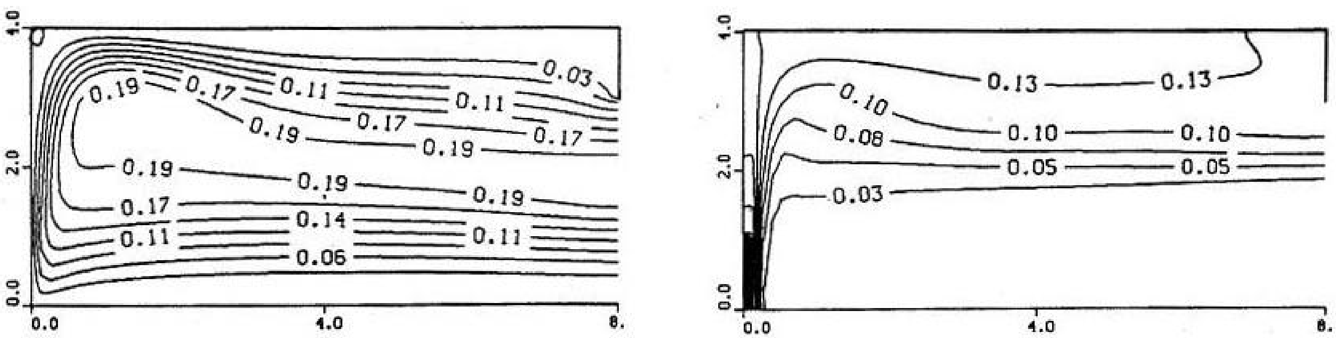
A Typical Room Fire



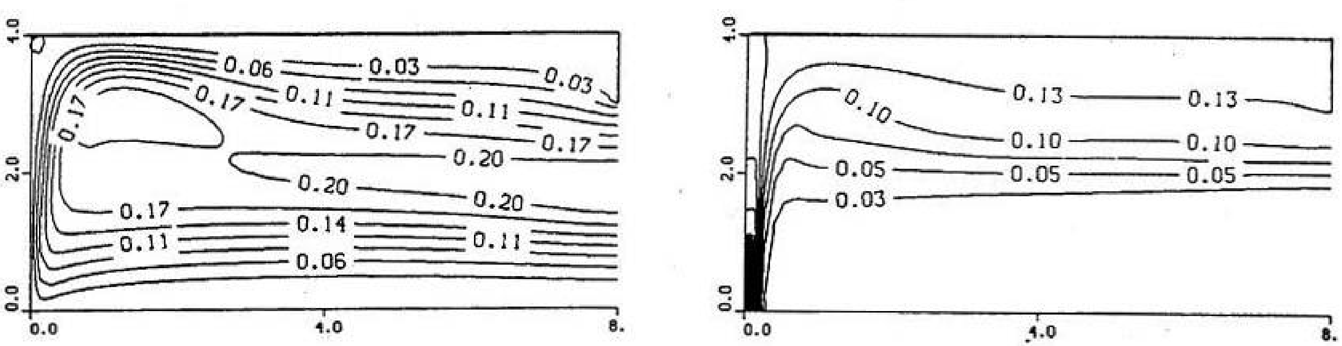
Room & Corridor System



Laminar Flow Generated by a Fire in a Room with an Opening



(a)

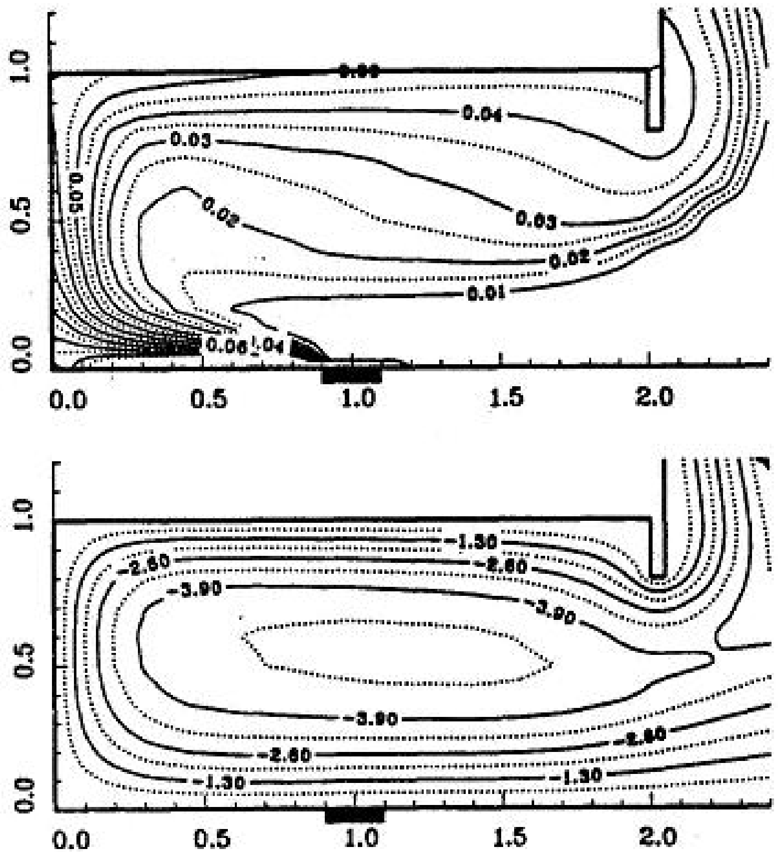


(b)

Flow and Thermal Fields for Turbulent Flow

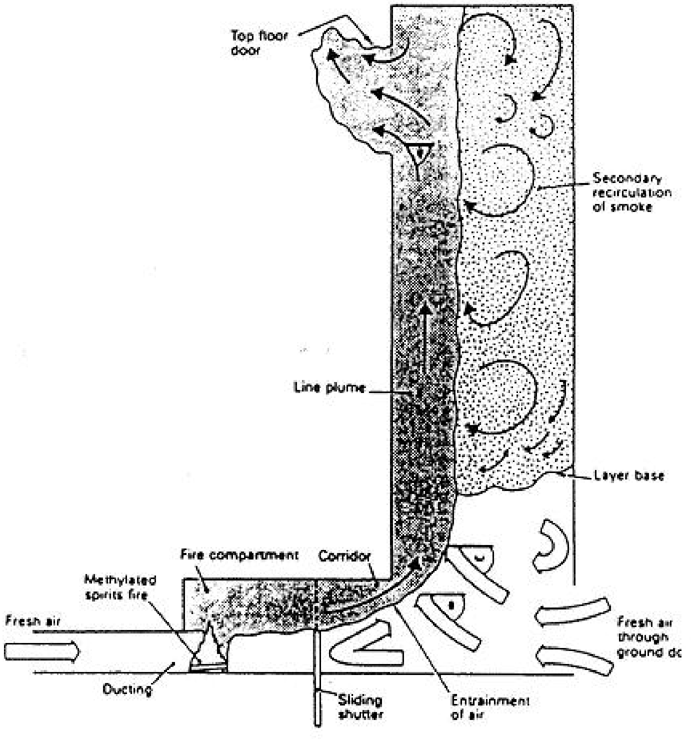
(a)

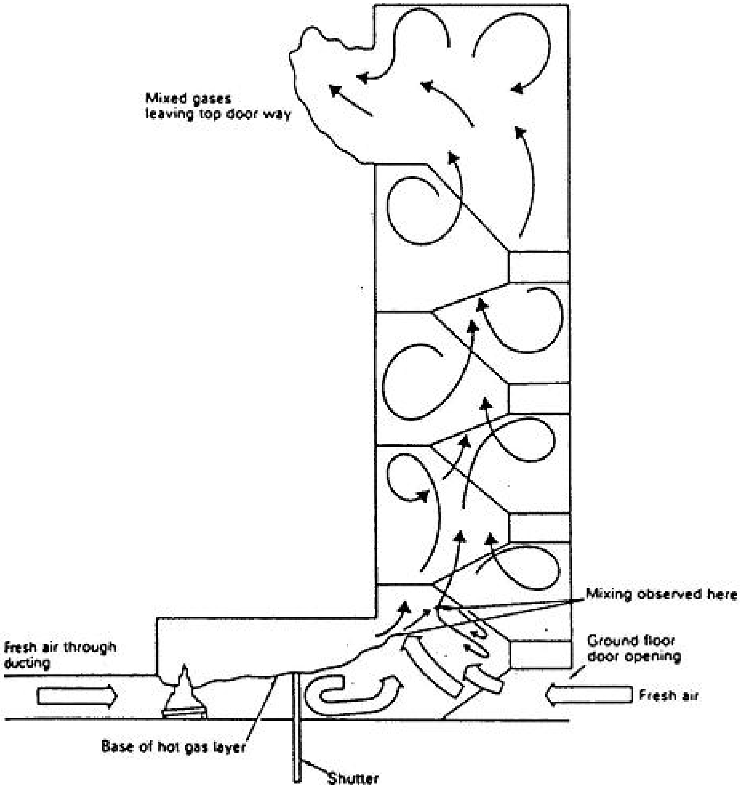
(b)



Steady state flow and thermal Field, (a) Isotherms and (b) Streamlines.

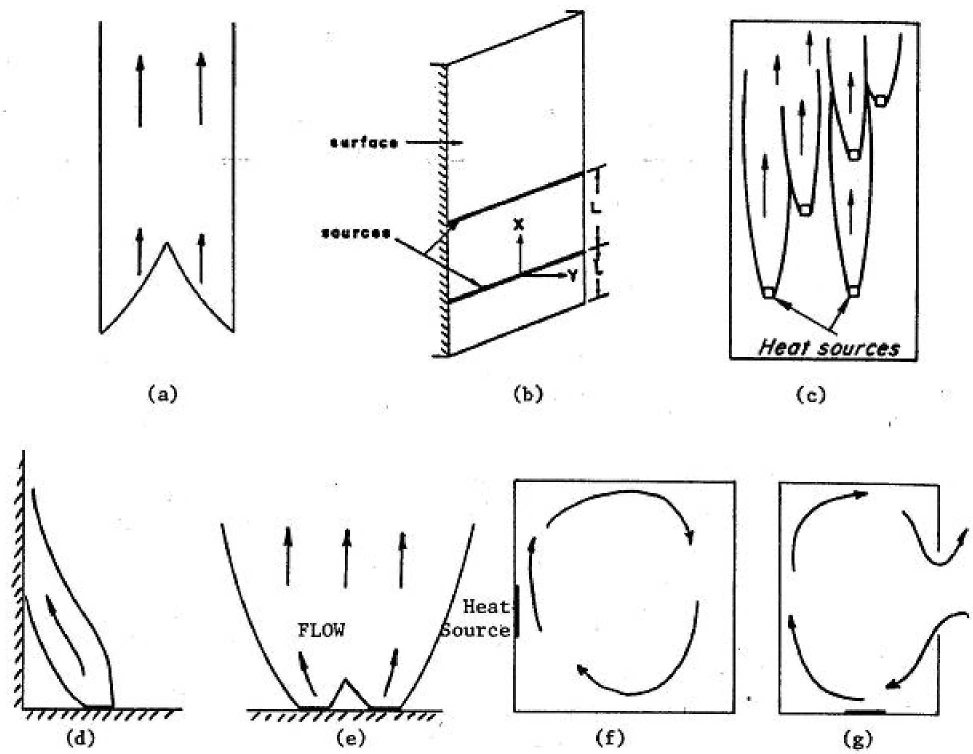
Flows in a Vertical Elevator Shaft and in a Stairwell

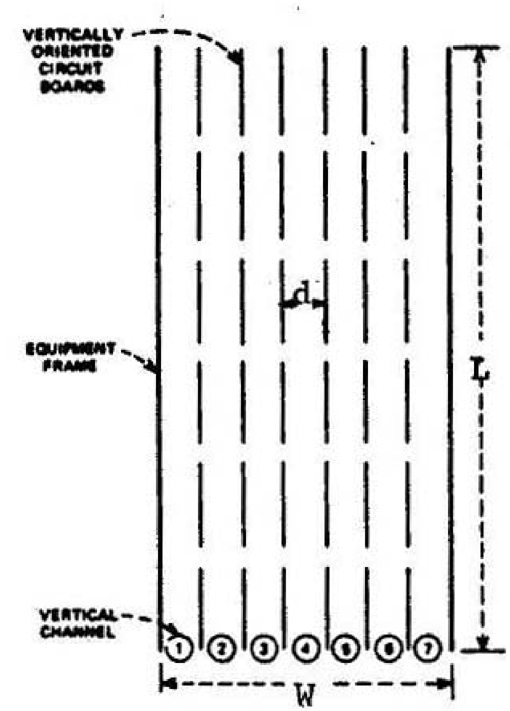




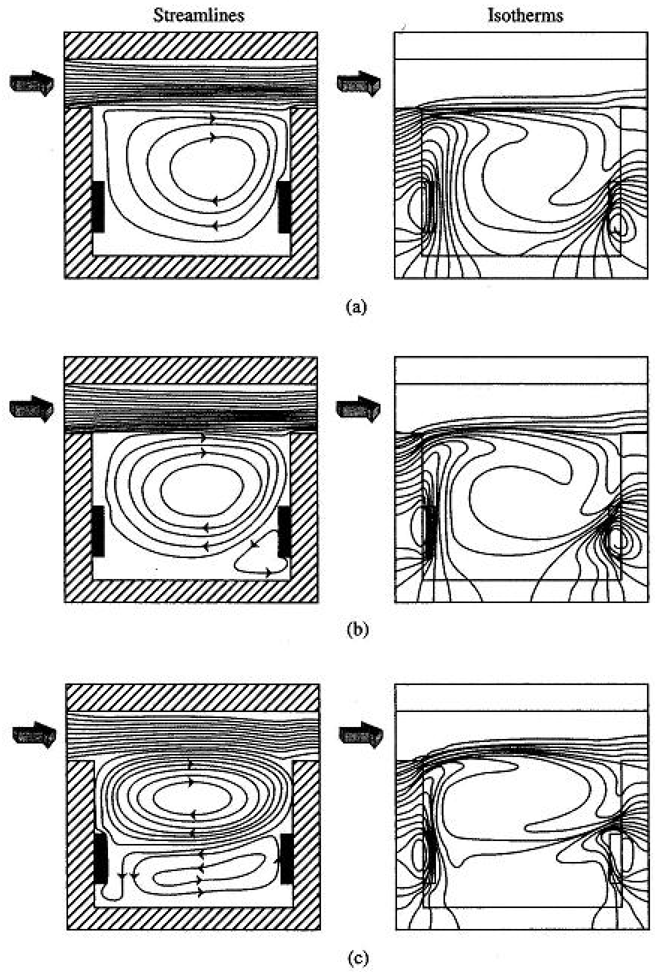
From Marshall (1986)

Natural Convective Cooling of Electronic Equipment





Flow in an Enclosure due to Isolated Heat Sources



Governing Equations with Variable Properties

Dimensionless Property Coefficients[1]

$$\rho = \frac{\hat{\rho}}{\hat{\rho}_0} = \frac{1}{\theta\epsilon + 1}$$

$$c_p = \frac{\hat{c}_p}{\hat{c}_{p0}} = (\theta\epsilon + 1)^{0.104}$$

$$\mu = \frac{\hat{\mu}}{\hat{\mu}_0} = (\theta\epsilon + 1)^{0.65}$$

$$k = \frac{\hat{k}}{\hat{k}_0} = (\theta\epsilon + 1)^{0.79}$$

[1] based on the power law correlation for air given by Fotiadis et al. (1990).

Governing Equations with Variable Properties

Dimensionless Governing Equations

$$\frac{\partial \rho}{\partial \tau} + \frac{\partial (\rho u_j)}{\partial x_j} = 0$$

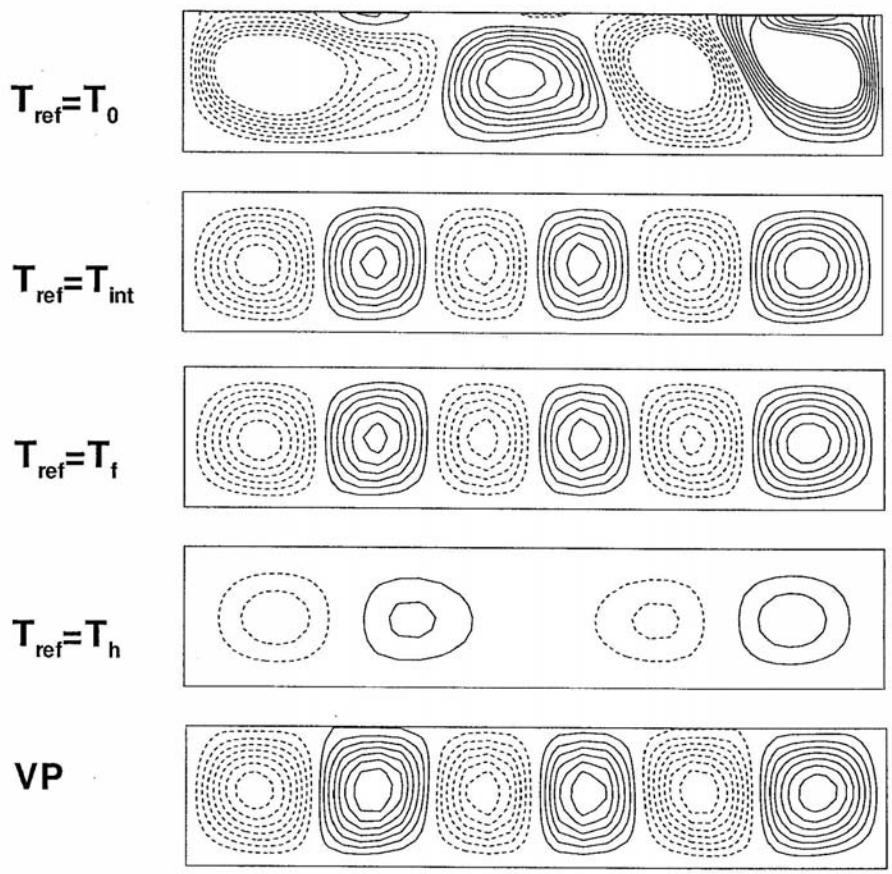
$$\frac{\partial (\rho u_i)}{\partial \tau} + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(\Gamma_v \frac{\partial u_i}{\partial x_j})$$
$$+\frac{\partial}{\partial x_j}(\Gamma_v \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\Gamma_v \frac{\partial u_k}{\partial x_k}) + \frac{Gr}{Re^2}\frac{\rho}{\epsilon}\eta_i$$

$$\frac{\partial (\rho \theta)}{\partial \tau} + \frac{\partial}{\partial x_j}(\rho u_j \theta) = \frac{\partial}{\partial x_j}(\Gamma_\theta \frac{\partial \theta}{\partial x_j}) + \frac{1}{PrRe}\frac{k}{c_p^2}\frac{\partial \theta}{\partial x_j}\frac{\partial c_p}{\partial x_j}$$

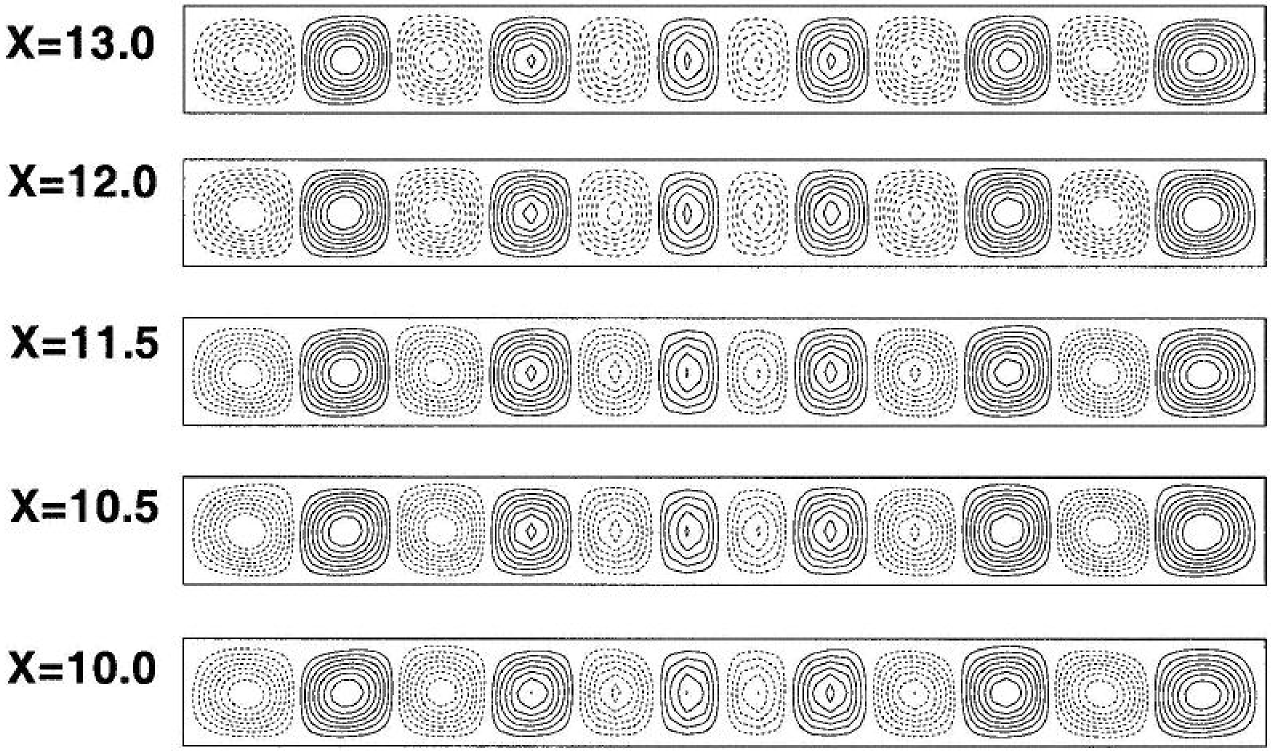
with

$$\Gamma_v = \frac{\mu}{Re}$$
$$\Gamma_\theta = \frac{k}{c_p}\frac{1}{PrRe}$$

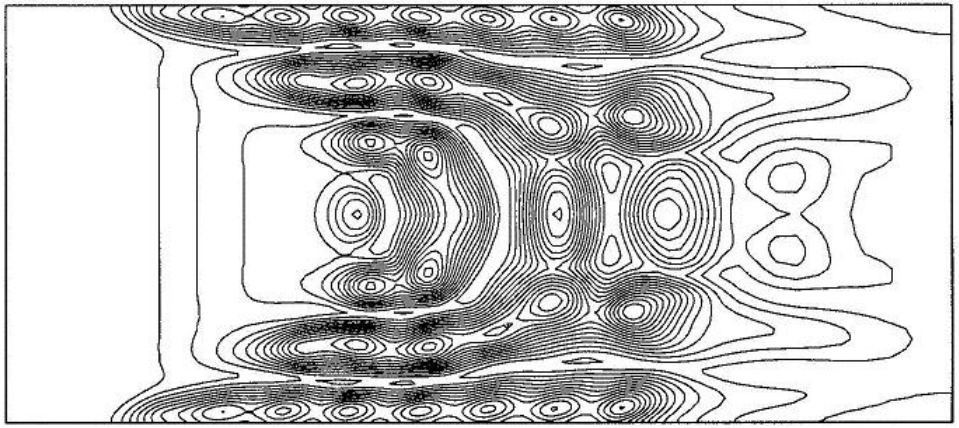
Governing Equations with Variable Properties

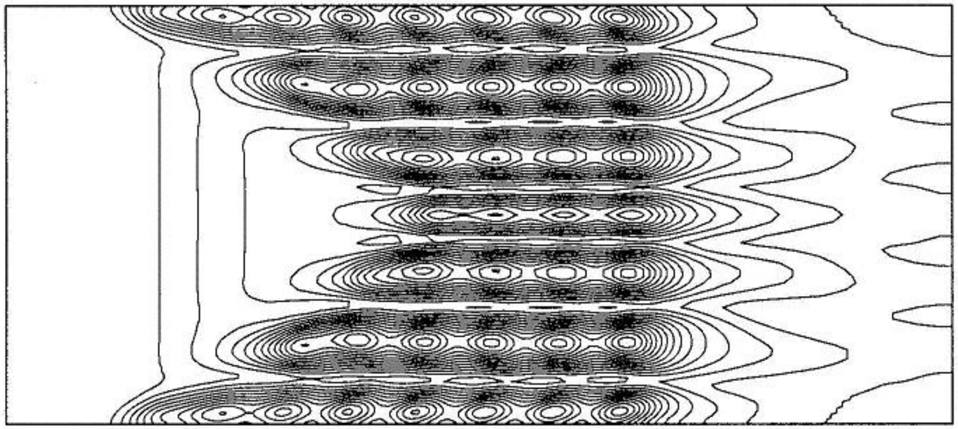


Steady Streamlines on Y-Z Planes for 3D Flow in a Channel



Isotherms on the Horizontal Midplane at τ=8.0 (Top Figure) and τ=24 (Bottom Figure) for Re=20, Gr=10000 and Ar=10.0





Conclusions

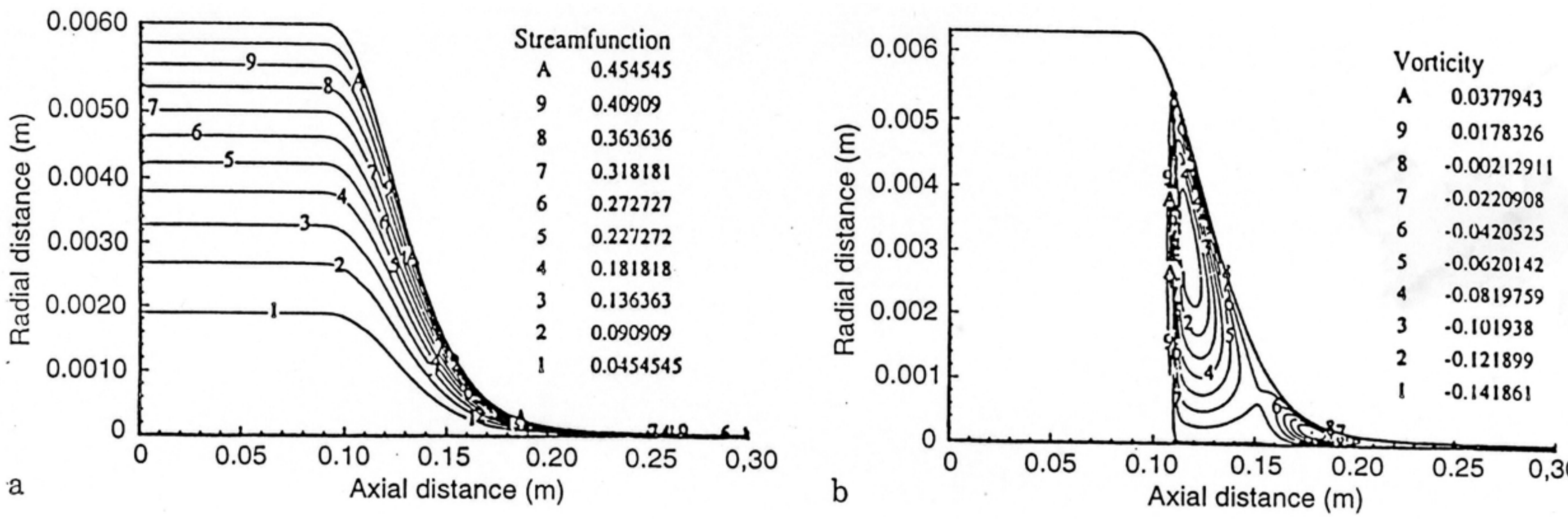
- Strong Need for Material Properties
- Must Model Changing Material Characteristics
- Use of Properties at Previous Time or Iteration Convenient
- Improved Accuracy and Convergence with Extrapolated Property Values
- Transformations, FEM, other Approaches for Complex

  Geometry

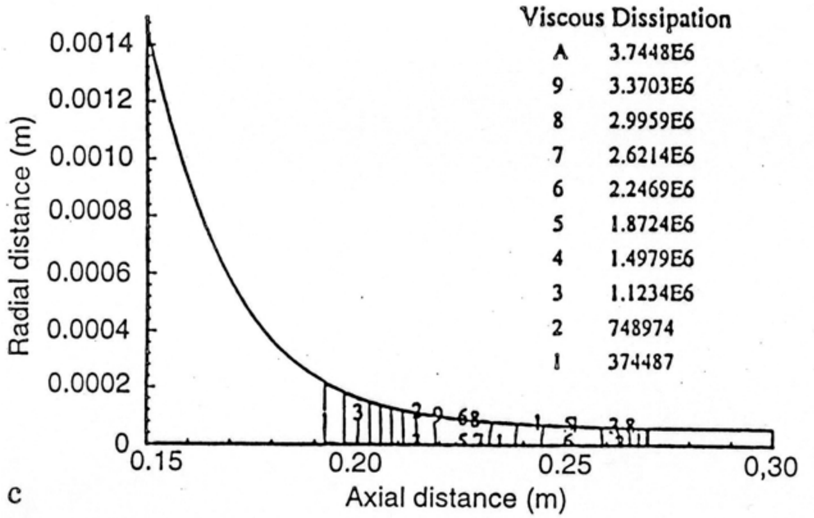
Conclusions (Contd.)

- Important to Employ Suitably Grid
- Critical to Represent Boundary Conditions Correctly
- Convergence Characteristics Strong Functions of Numerical Scheme
- Experimentation for Validation and Insight

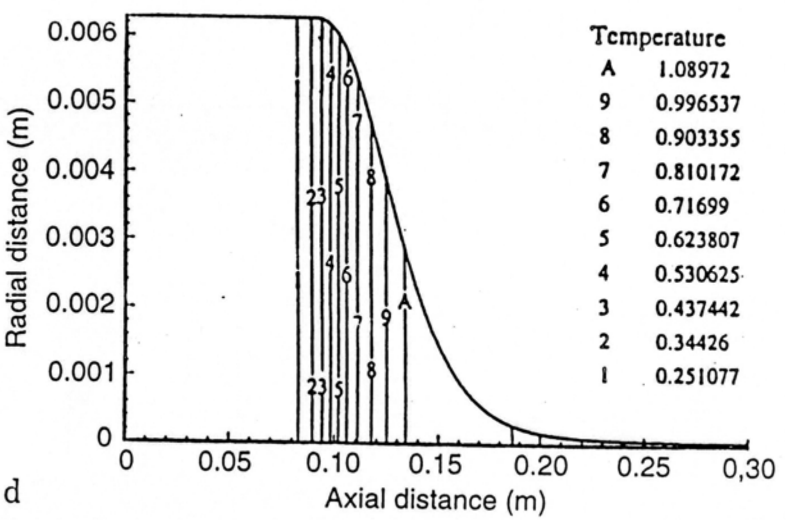
Flow in Neck-Down Region During Optical Fiber Drawing



Viscous Dissipation and Temperature in Neck-Down Region During Optical Fiber Drawing

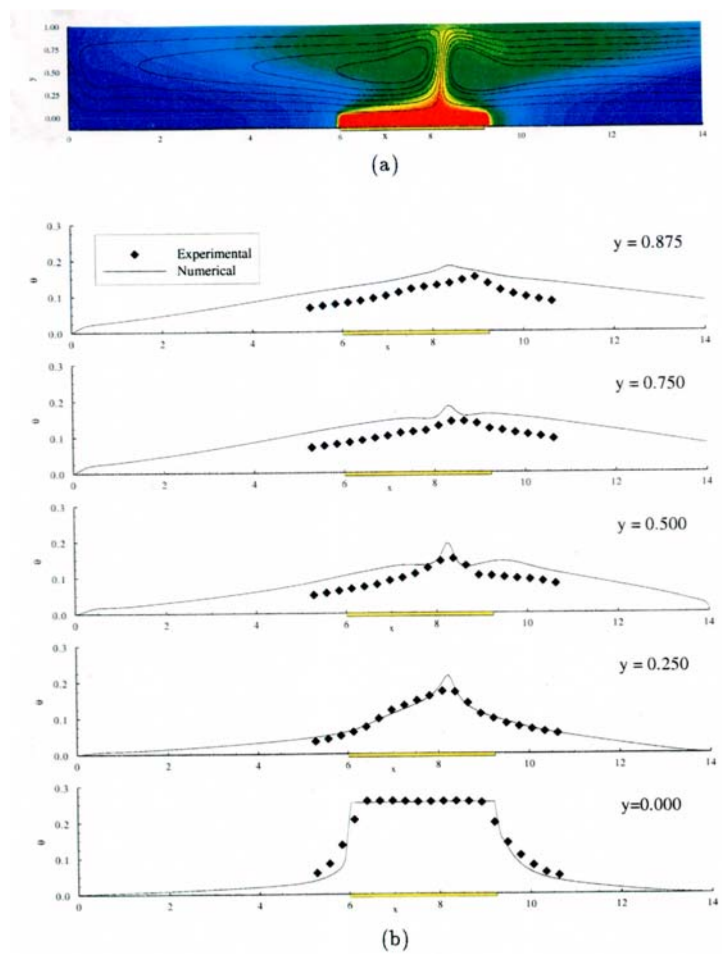


c



d

Flow and Temperature Fields in a Horizontal CVD System



Experimental and Numerical Results on Horizontal Channel Flow for CVD