Combined Analytical and Numerical Modeling in Industrial Mathematics

by

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Overview

The Mathematical Problems in Industry (MPI) Workshop has been run annually for the past 17 years.

Apart from one year at the University of New Mexico and two years at the University of Delaware, all MPI workshops have been held at Rensselaer.

Partial list of past problems and companies:

- MPI 97 (Rensselaer)
  - Optimization of a Flexible Cable, IBM
  - Bond Default Correlation, Merrill Lynch
  - Gas Concentration Measurements in Underground Waste Storage Tanks, Pacific Northwest Laboratory
  - Kinetic Modelling of Multicomponent Electrowinning, Los Alamos National Laboratory
  - MEMS Diffraction Grating, Interscience
- MPI 98 (Rensselaer)
  - Analysis of Vapor and Liquid Flow in Packed Columns, BOC Gases
  - Thermomechanical Models of Air Gap Nucleation During Pure Metal Solidification on Moving Molds with Periodic Surface Topographies, Alcoa
  - Measurement of Modal Power in Optical Fibers, Corning
  - Reverse Pumping in a Rotary Lip Seal with Microundulations, Rockwell
  - Pressure Drop in Chromatography Columns, BIOGEN

- MPI 99 (Univ. of Delaware)
  - Shape Optimization of the Read Coil Used in Hard Disk Drives, IBM
  - Modeling of Epitaxial Semiconductor Crystal Growth on Patterned, Masked and/or Structured Substrates, AstroPower
  - Interference Filters for Thermophotovoltaic Applications, KAPL
  - The Dynamics of a Roll Press Nip, Albany International
- MPI 2000 (Univ. of Delaware)
  - Options on Baskets, Numerix
  - Inverse Problems for Optical Fiber Device Measurements and Design, Corning
  - A Water-Wave Interaction Problem, Vehicle Research
- MPI 2001 (Rensselaer)
  - Boundary Layers and Material Deformation in Fiber Drawing, Corning
  - Symmetry Breaking in Jetting, Xerox
  - Multi-name Credit Derivatives, Nomura
  - Shape Optimization of Pressurized Air Bearings, IBM
- MPI 2002 (Rensselaer, June 3–7)

MPI Web Site

`http://www.math.rpi.edu/Faculty/Schwendeman/Workshop/MPI2001/home.html`

Workshop Problems

A typical workshop problem involves a combination of modeling, analysis and computation. (The role of computations during the workshop has increased significantly over the past 10 years.)

In some cases the workshop problems involve an analysis of existing model equations, and in other cases the problems involve building model equations from first principles given a description of the physical system.

An effective approach to these problems has been a combination of analytical and numerical techniques.

Two Sample Problems

1. Light-off behavior of automotive catalytic converters (Allied Signal)

2. Two-phase flow modeling and computations in a roll press nip (Albany International)

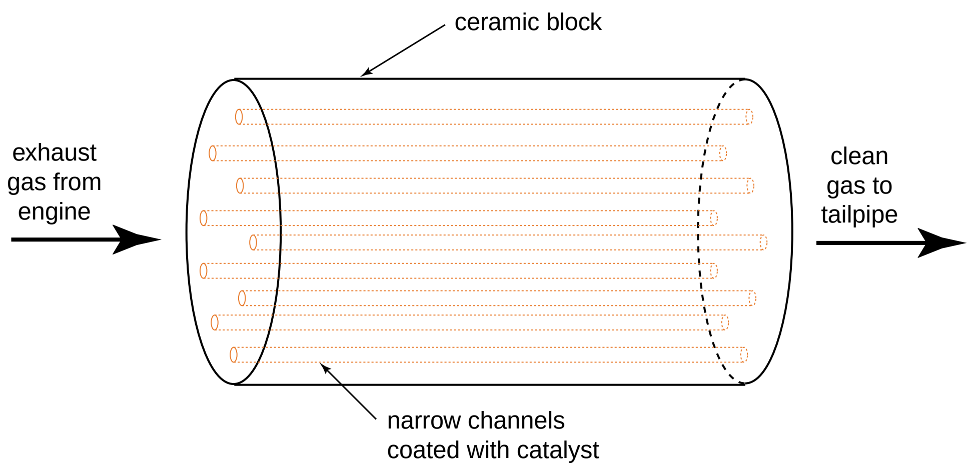
These problems are representative of the two cases described above.

Light-off Behavior of Automotive Catalytic Converters

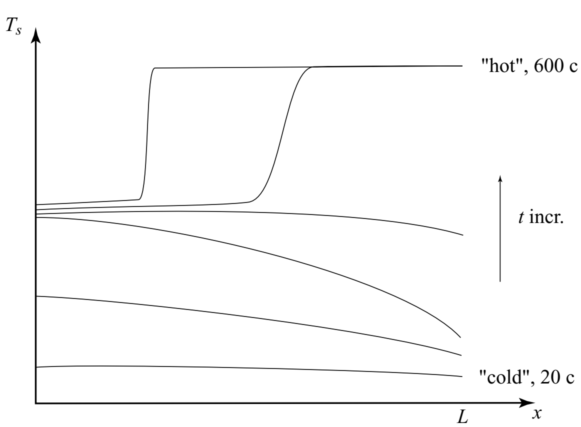
Contributors...

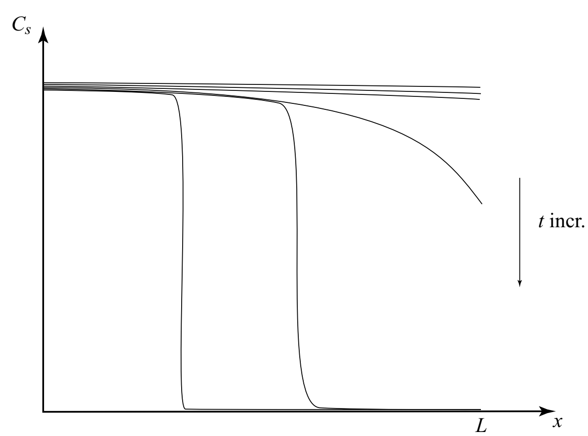
Pat Hagan (LANL), Colin Please (Southampton), DWS (RPI), and a cast of thousands...

Catalytic converter basics...



Warm-up & light-off behavior...





Existing Model Equations (Oh & Cavendish)

Gas flow: (conservation of species and heat)

$$\epsilon\frac{\partial C_{g,i}}{\partial t} + v\frac{\partial C_{g,i}}{\partial x} = k_i Q\left(C_{s,i} - C_{g,i}\right), \qquad i = 1, \ldots, 5$$

$$\rho_g c_g \left(\epsilon\frac{\partial T_g}{\partial t} + v\frac{\partial T_g}{\partial x}\right) = hQ\left(T_s - T_g\right)$$

where

$C_{g,i}$, $C_{s,i}$ = gas, surface concentrations

$$\left.\begin{array}{rcl} i = 1 & \Rightarrow & \mathrm{CO} \\ 2 & \Rightarrow & \mathrm{C_3H_6} \\ 3 & \Rightarrow & \mathrm{CH_4} \\ 4 & \Rightarrow & \mathrm{H_2} \end{array}\right\} \text{oxidants}$$

$$\begin{array}{rcl} 5 & \Rightarrow & \mathrm{O_2} \end{array}$$

T_g, T_s = gas, solid temperatures

and

ϵ	=	open frontal area fraction
v	=	gas velocity
k_i, h	=	mass, heat transfer coefficients
Q	=	catalyst surface area per unit converter volume
ρ_g, c_g	=	density and specific heat of the gas

Solid surface/substrate: (surface reaction, heat flow)

$$a(x)R_i(C_{s,j},T_s) = \rho_s k_i Q\left(C_{g,i} - C_{s,i}\right), \qquad i = 1,\ldots,5$$

$$(1-\epsilon)\rho_s c_s \frac{\partial T_s}{\partial t} = (1-\epsilon)K_s \frac{\partial^2 T_s}{\partial x^2} + hQ(T_g - T_s) + a(x)\sum_{i=1}^{4}\left(-\Delta H_i\right)R_i(C_{s,j},T_s)$$

where

$a(x)$	$=$	local surface area of catalyst per unit converter volume
R_i	$=$	reaction rate for species i (Arrhenius-type)
ρ_s, c_s	$=$	density and specific heat of the solid
K_s	$=$	thermal conductivity of solid
$-\Delta H_i$	$=$	heat of reaction of oxidant species i

Basic Problems (Allied Signal)

1. The numerical method for the existing “full” model equations was time consuming and in some cases did not converge.

   Are there simpler models suitable for analysis that are good approximations of the full equations?

   Such simpler models could be used to test various design parameters and to check various numerical approaches to the full equations.

2. Also, would like to predict the time to light-off based on the parameters of the device.

   Ideally, the designer would like to choose parameters for the converter to minimize the time to light-off.

Single Oxidant Model

Observations:

Carbon monoxide is the most abundant oxidant species and the main source of heat in the system.

Modeling simplification:

Model the behavior of CO only and regard the other oxidant species as fixed in concentration (at their inlet values say).

Assume an abundance of oxygen in the system and take its concentration as fixed. (Not difficult to include the effects of a variable oxygen concentration.)

Dimensionless variables:

$$x' = \frac{x}{L}, \qquad t' = \frac{t}{t_{\text{ref}}}, \qquad C_g' = \frac{C_g}{C_{g,\text{in}}}, \qquad C_s' = \frac{C_s}{C_{s,\text{in}}}$$

$$T_g' = \frac{T_g - T_{g,\text{in}}}{\Delta T}, \qquad T_s' = \frac{T_s - T_{g,\text{in}}}{\Delta T}$$

where

$$t_{\text{ref}} = \frac{(1-\epsilon)\rho_s c_s L}{\rho_g c_g v_{\text{avg}}} \simeq 14\,\text{sec} \qquad \left(\begin{array}{c} \text{time scale for heat transfer} \\ \text{from hot gas to cold solid} \end{array} \right)$$

$$\Delta T = \frac{(-\Delta H)\, C_{g,\text{in}}}{c_g} \simeq 300^\circ\,\text{C} \qquad (\text{ adiabatic temperature rise })$$

Model equations: (dimensionless, drop primes)

$$\begin{aligned}
\mu \frac{\partial C_g}{\partial t} + v \frac{\partial C_g}{\partial x} &= \alpha \left(C_s - C_g\right) \\
\mu \frac{\partial T_g}{\partial t} + v \frac{\partial T_g}{\partial x} &= \beta \left(T_s - T_g\right) \\
aR(C_s, T_s) &= C_g - C_s \\
\frac{\partial T_s}{\partial t} &= \delta \frac{\partial^2 T_s}{\partial x^2} + \beta \left(T_g - T_s\right) + \alpha a R(C_s, T_s)
\end{aligned}$$

Dimensionless parameters:

μ	=	convection time/t_{ref}	$\simeq$	.0005
α	=	dimensionless mass transfer coefficient	=	$O(1)$
β	=	dimensionless heat transfer coefficient	=	$O(1)$
v	=	$v(t)$, scaled gas velocity	=	$O(1)$
a	=	$a(x)$, scaled catalyst surface conc.	=	$O(1)$
δ	=	dimensionless diffusivity	$\simeq$	.001
R	=	dimensionless reaction rate	=	sensitive func. of T_s

Dimensionless reaction rate: (*highly simplified*)

$$R(C_s, T_s) = \frac{A}{\gamma} C_s e^{\gamma T_s}$$

A	=	rate constant	=	$O(1)$
γ	=	activation energy	$\simeq$	10

Initial and boundary conditions:

$$T_s(x, 0) = T_{s,\text{cold}}, \qquad T_g(0, t) = T_{g,\text{in}}, \qquad C_g(0, t) = C_{g,\text{in}}$$

$$\frac{\partial T_s}{\partial x}(0, t) = \frac{\partial T_s}{\partial x}(1, t) = 0$$

Asymptotic Analysis

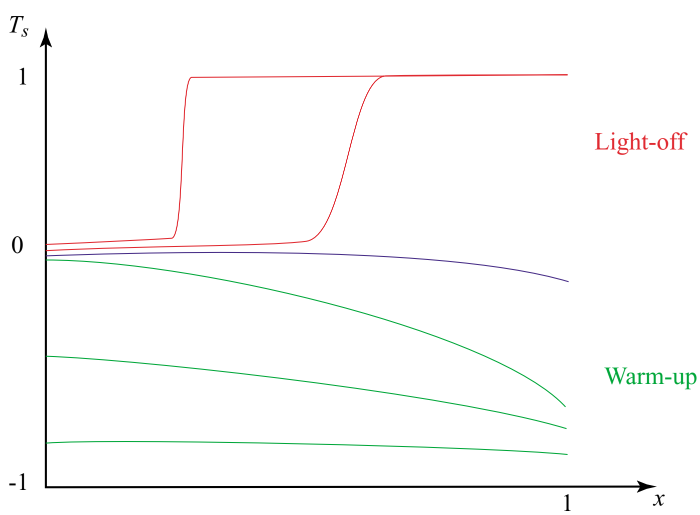
Assume:

$$\begin{aligned} \delta &\ll 1 \quad \text{(small diffusion)} \\ \mu &= 0 \quad \text{(fast convection time)} \\ v &= \text{constant} \quad \text{(gas velocity)} \\ a &= \text{constant} \quad \text{(local catalyst surface conc.)} \end{aligned}$$

Two-stage structure:

(1) Warm-up $\Rightarrow$ gentle heating with small reaction and negligible diffusion

(2) Light-off $\Rightarrow$ steady state heat transfer separated by slow moving diffusion layer



(1) Warm-Up

Leading order equations: (negligible diffusion)

$$v\frac{\partial C_g}{\partial x} = \alpha\,(C_s - C_g)$$

$$v\frac{\partial T_g}{\partial x} = \beta\,(T_s - T_g)$$

$$aR(C_s, T_s) = C_g - C_s$$

$$\frac{\partial T_s}{\partial t} = \beta\,(T_g - T_s) + \alpha a R(C_s, T_s)$$

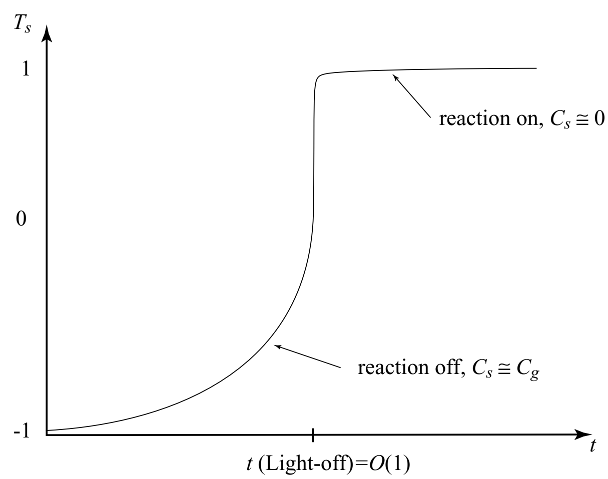
with

$$C_g(0,t) = C_{g,\text{in}}, \qquad T_g(0,t) = T_{g,\text{in}}, \qquad T_s(x,0) = T_{s,\text{cold}}$$

No analytical solution (due to nonlinear reaction rate term), only numerical solution.

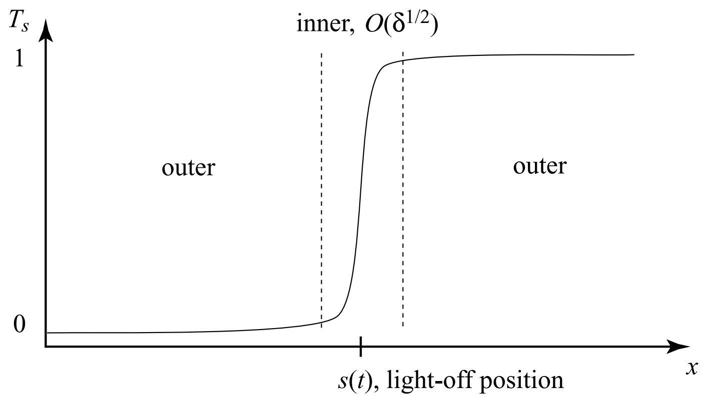
Basic structure of the solution:

$$\frac{\partial T_s}{\partial t} = \left(\begin{array}{c} \text{source of heat due to} \\ \text{heat transfer from hot gas} \end{array} \right) + a\alpha\frac{A}{\gamma}C_s e^{\gamma T_s}$$



(2) Light-Off

Seek layer-type solution:



Outer equations:

$$v\frac{\partial C_g}{\partial x} = \alpha\,(C_s - C_g)$$

$$v\frac{\partial T_g}{\partial x} = \beta\,(T_s - T_g)$$

$$aR(C_s, T_s) = C_g - C_s$$

$$0 = \beta\,(T_g - T_s) + \alpha a R(C_s, T_s)$$

with

$$C_g(0,t) = C_{g,\text{in}}, \qquad T_g(0,t) = T_{g,\text{in}}$$

Heat/Mass transfer balance:

$$C_g + T_g = C_{g,\text{in}} + T_{g,\text{in}}$$

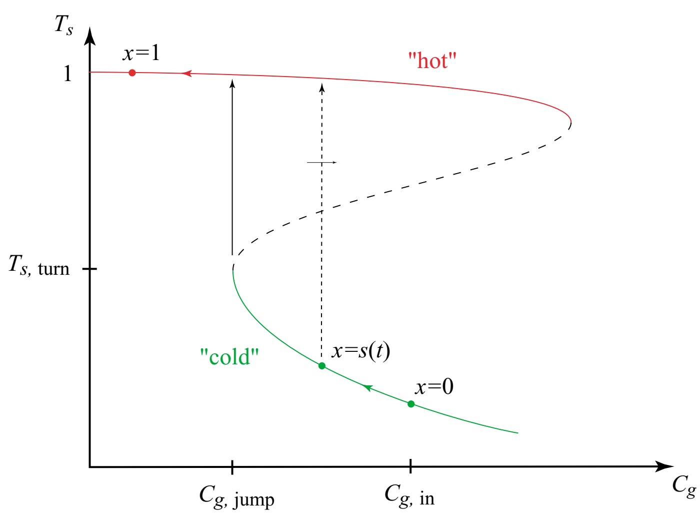
Eliminate T_g:

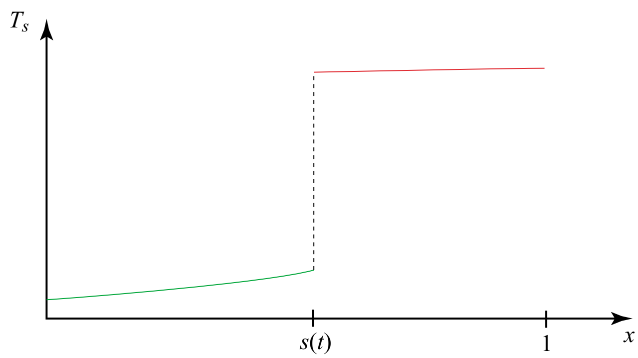
$$v\frac{\partial C_g}{\partial x} = -\alpha a\frac{A}{\gamma}C_s e^{\gamma T_s}, \qquad C_g(0,t) = C_{g,\text{in}}$$

with

$$C_g = C_s\left(1+\frac{aA}{\gamma}e^{\gamma T_s}\right) = \frac{\left(C_{g,\text{in}}+T_{g,\text{in}}-T_s\right)\left(1+\frac{aA}{\gamma}e^{\gamma T_s}\right)}{1+\left(1-\frac{\alpha}{\beta}\right)\frac{aA}{\gamma}e^{\gamma T_s}}$$

Outer solution behavior:





Inner equations:

$$
\begin{aligned}
C_g &= C_{g,\text{jump}} + o(1) \\
T_g &= T_{g,\text{in}} + C_{g,\text{in}} - C_{g,\text{jump}} + o(1) \\
C_s &= \frac{C_{g,\text{jump}}}{1 + \frac{aA}{\gamma} e^{\gamma T_s}}
\end{aligned}
$$

and

$$
-\frac{ds}{d\tau}\frac{\partial T_s}{\partial \xi} = \frac{\partial^2 T_s}{\partial \xi^2} + \beta\left(C_{g,\text{in}} + T_{g,\text{in}} - C_{g,\text{jump}} - T_s\right) + \alpha\left(C_{g,\text{jump}} - C_s\right)
$$

where

$$
\xi = \frac{x - s(t)}{\delta^{1/2}}, \qquad \tau = \delta^{1/2} t
$$

Eigenvalue problem:

For a given value of $C_{g,\text{jump}}$ from the outer problem, find the value of $\lambda = -ds/d\tau$ such that the solution for T_s matches with the corresponding values from the outer problem as $\xi \to \pm\infty$.

Since $C_{g,\text{jump}}$ depends on s, the solution of the eigenvalue problem gives

$$
-\frac{ds}{d\tau} = \lambda(s)
$$

which may be integrated (numerically) to determine the path of the light-off front.

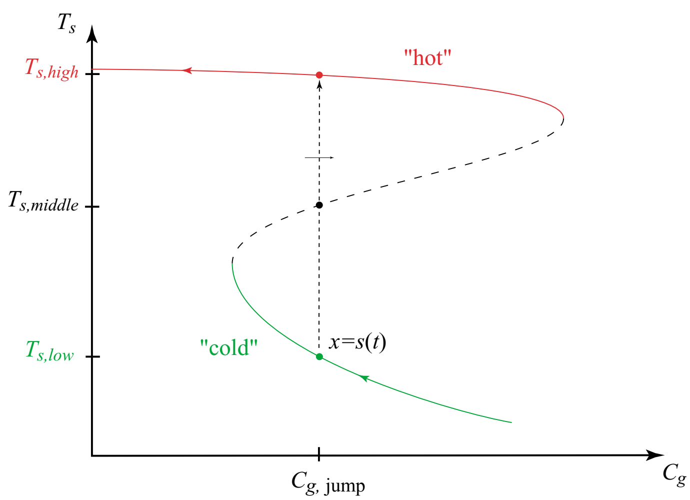
Phase plane:

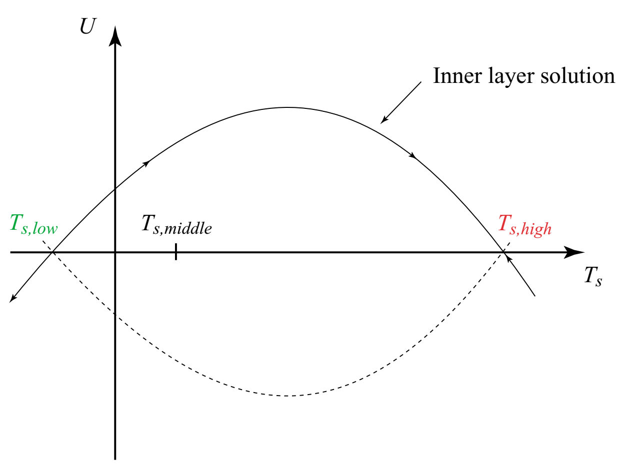
$$\left.\begin{aligned} T_s' &= U \\ U' &= \lambda U - S(T_s) \end{aligned}\right\}$$

where

$$S(T_s) = \beta\left(C_{g,\text{in}} + T_{g,\text{in}} - C_{g,\text{jump}} - T_s\right) + \alpha\left(C_{g,\text{jump}} - C_s\right)$$

Inner solution behavior:





Numerical Analysis

Single oxidant model, full equations: ($\mu = 0$)

$$\begin{aligned} v(t)\frac{\partial C_g}{\partial x} &= \alpha\,(C_s - C_g) \\ v(t)\frac{\partial T_g}{\partial x} &= \beta\,(T_s - T_g) \\ a(x)R(C_s, T_s) &= C_g - C_s \end{aligned}$$

$$\frac{\partial T_s}{\partial t} = \delta\frac{\partial^2 T_s}{\partial x^2} + \beta\,(T_g - T_s) + \alpha a(x) R(C_s, T_s)$$

with

$$T_s(x,0) = T_{s,\text{cold}}, \qquad T_g(0,t) = T_{g,\text{in}}, \qquad C_g(0,t) = C_{g,\text{in}}$$

$$\frac{\partial T_s}{\partial x}(0,t) = \frac{\partial T_s}{\partial x}(1,t) = 0$$

Numerical approach:

- Suppose T_s is known at a fixed time t:

$$\begin{aligned} C_g &= C_{g,\text{in}}\,\exp\left\{-\frac{\alpha}{v(t)}\int_0^x \frac{a(x')Ae^{\gamma T_s}}{\gamma + a(x')Ae^{\gamma T_s}}\,dx'\right\} \\ T_g &= T_{g,\text{in}}\,e^{-\beta x/v(t)} + \frac{\beta}{v(t)}\int_0^x T_s e^{-\beta(x-x')/v(t)}\,dx' \\ C_s &= \frac{C_g}{1 + \frac{a(x)A}{\gamma}e^{\gamma T_s}} \end{aligned}$$

- Equation for T_s:

$$\frac{\partial T_s}{\partial t} = \delta \frac{\partial^2 T_s}{\partial x^2} + G(T_s)$$

Spatial discretization, numerical quadrature $\Rightarrow$

$$\frac{d}{dt} T_s = F(T_s), \qquad T_s = T_{s,\text{cold}} \text{ at } t = 0$$

Solve ODE.s using a second-order Runge-Kutta scheme.

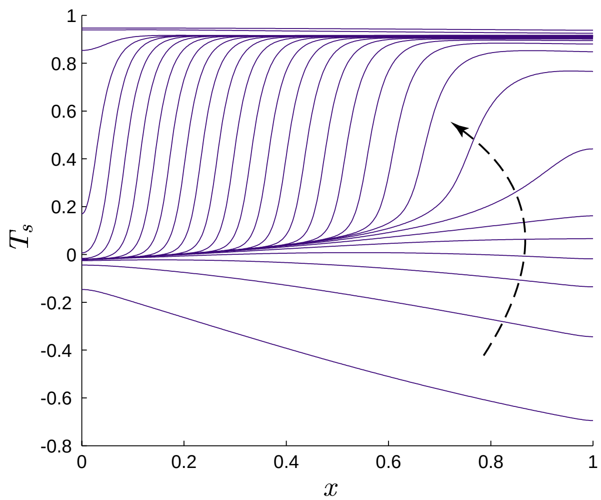
Numerical results:

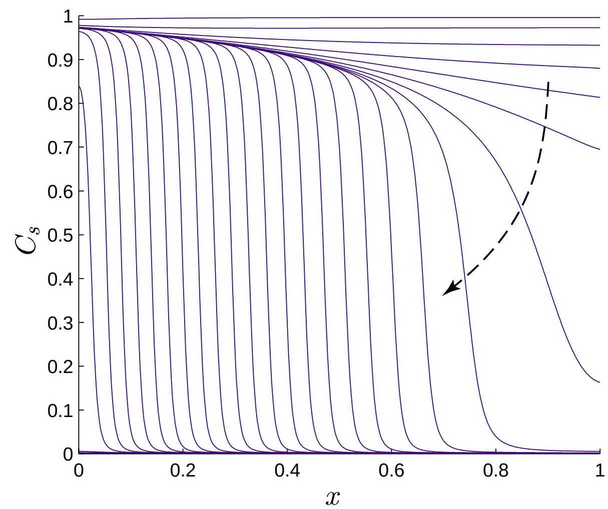
Parameter values ...

$$\alpha = \beta = 3, \qquad \delta = .001, \qquad A = .35, \qquad \gamma = 10$$

$$C_{g,\text{in}} = 1, \qquad T_{g,\text{in}} = -.05, \qquad T_{s,\text{cold}} = -1$$

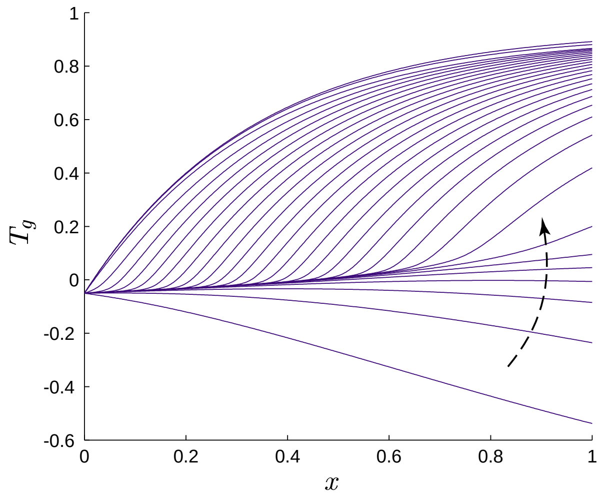
Behavior of T_s and C_s ...

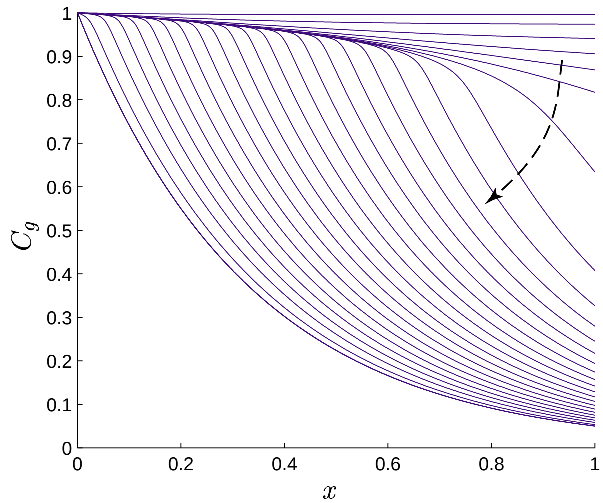




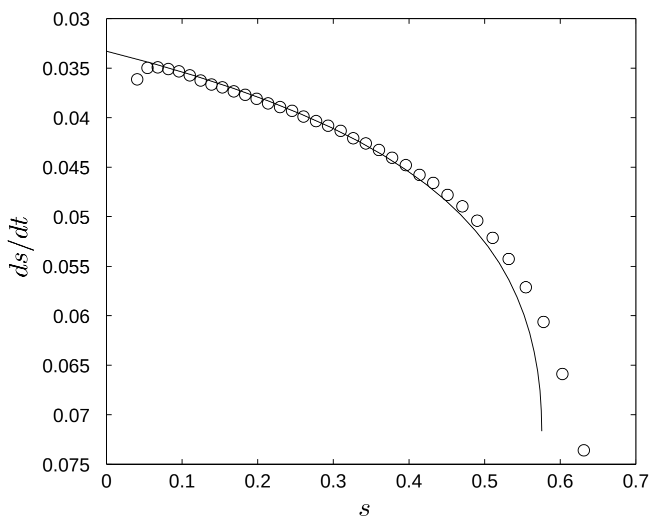
(Arrows indicate increasing time.)

Behavior of T_g and C_g ...





Comparison of light-front speed ...



Solid curve is an asymptotic result ($\delta \ll 1$) and the marks are from the numerical solution of the model equations.

Extensions of the Analysis

An asymptotic analysis of the single-oxidant model in the small diffusivity limit ($\delta \ll 1$) describes the two-stage structure of the solution and the motion of the light-off front.

The asymptotic equations still require a numerical treatment.

A further asymptotic analysis can be done for large activation energy ($\gamma \gg 1$), but the "small" parameter becomes $(1/\ln\gamma)$ which is not very small so that the formulas give only qualitative information.

Extensions of the Model

The single-oxidant model provides a basic model on which various extensions could be included. For example ...

- include oxygen concentration in the gas and on the catalyst surface in order to consider the possibly of oxygen deprivation,

- include more complex (realistic) reaction models and correspondingly more oxidant species,

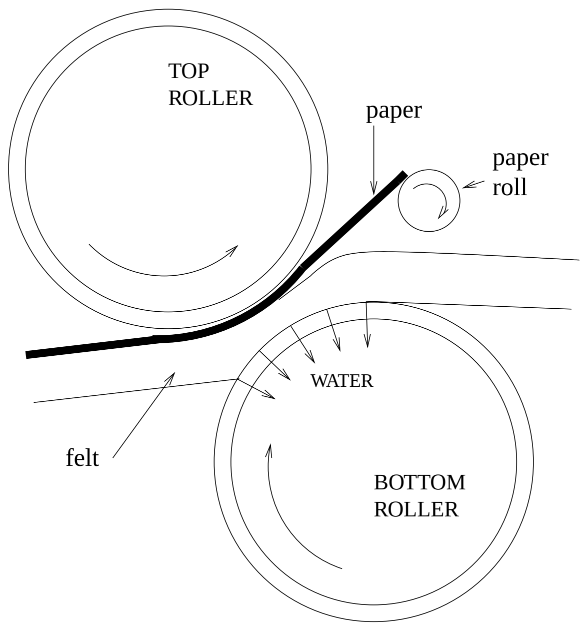
- include spatial variation in the cross-flow directions.

Multiphase Flow in a Roll Press Nip

Contributors...

A. Fitt (Southampton), P. Howell (Oxford), DWS (RPI),
J. King (Nottingham), C. Please (Southampton),
and a cast of thousands...

Roll press nip geometry...



Parameters...

diameter of rollers = 1 m
thickness of paper layer = 0.5 mm
thickness of felt carrier = 3 mm
solid volume fraction in felt = 0.5 − 0.8
velocity of the felt = 20 m/s
peak pressure in the nip = 10 MPa

Modeling Objectives

Albany International manufactures the felt material used in the pressing step. In order to optimize the design of the felt material, they suggested a number of modeling objectives...

- Propose a general theoretical framework in which to study the behavior of the flow in the nip.

- Determine the flow of water in the felt and relate this flow to the details of air flow in the felt and the deformation of the felt.

- Obtain reduced equations and exact solutions if possible by exploiting the geometry of the nip.

The modeling results in a system of nonlinear PDEs for the three-phase flow of air, liquid (water), and solids (felt) in the nip.

The layer of paper that lies on top of the felt is relatively thin and is neglected in the present model. It could be added later as a source of liquid at the surface.

Multiphase Flow Model

Let α_i, $i = a$, ℓ, and f be the volume fractions of air, water, and felt, respectively, so that

$$\alpha_a + \alpha_\ell + \alpha_f = 1$$

Model equations: (dimensionless)

$$\nabla \cdot (\alpha_i \mathbf{q}_i) = 0, \qquad i = a,\ \ell,\ f$$

$$\begin{aligned} 0 &= -\alpha_a \nabla p \\ 0 &= -\alpha_\ell \nabla p + K\mathbf{D}_{\ell f} \\ 0 &= -\alpha_f \nabla p + \nabla \cdot \tau_f - K\mathbf{D}_{\ell f} \end{aligned}$$

where

$$\begin{aligned} p &= \text{pressure} \\ \mathbf{q}_i &= \text{velocity for phase } i \\ \tau_f &= \text{stress tensor for the felt} \\ K &= \text{ratio of viscous and elastic forces} \\ \mathbf{D}_{\ell f} &= \text{drag on the liquid due to the felt} \end{aligned}$$

Drag model: (Darcy-type)

$$\mathbf{D}_{\ell f} = -\frac{\alpha_\ell(\mathbf{q}_\ell - \mathbf{q}_f)}{k(\alpha_\ell)}, \qquad k(\alpha_\ell) = \text{permeability}$$

Stress model: (mattress)

$$\tau_{f_{zz}} = \mathcal{F}(\alpha_f), \qquad \text{only transverse displacement of felt}$$

Air phase decouples:

$$0 = -\alpha_a \nabla p \quad \Rightarrow \quad \begin{cases} \alpha_a = 0, & \text{saturated flow} \\ \alpha_a \neq 0, & \text{unsaturated flow } (p = \text{const.}) \end{cases}$$

Thin-Layer Approximation

Geometric parameters:

$$\epsilon = \frac{1}{2}\sqrt{\frac{H}{R}} \simeq 0.04 \ll 1, \qquad \eta = \text{compression ratio} \simeq 0.5$$

Re-scale:

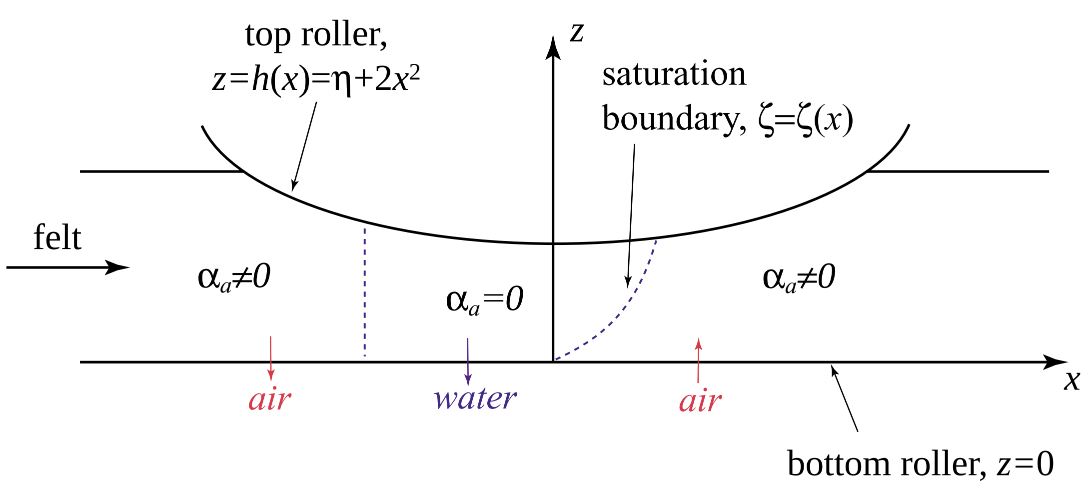
$$\mathbf{x} = (x/\epsilon, z), \qquad \mathbf{q}_i = (u_i, \epsilon w_i), \qquad K = \kappa/\epsilon$$

Leading order equations: $(\epsilon \ll 1,\ u_i = 1)$

$$\alpha_{ix} + (\alpha_i w_i)_z = 0, \qquad i = \ell \text{ or } f$$

$$p = \text{constant } (\alpha_a \neq 0) \quad \text{or} \quad \alpha_\ell + \alpha_f = 1 \ (\alpha_a = 0)$$
$$w_\ell = w_f - k(\alpha_\ell) p_z/\kappa$$
$$\mathcal{F}(\alpha_f) = p_z$$

Solution structure:



Inlet unsaturated region:

Exact solution:

$$\alpha_\ell = \frac{\alpha_{\ell,\text{in}}}{h(x)}, \qquad \alpha_f = \frac{\alpha_{f,\text{in}}}{h(x)},$$

$$p = 0, \qquad w_\ell = w_f = \frac{zh'(x)}{h(x)},$$

$$h(x) = \eta + 2x^2$$

Flow becomes saturated at $x = x_1$ when $\alpha_\ell + \alpha_f = 1$:

$$\Rightarrow \quad x_1 = -\sqrt{\frac{\alpha_{\ell,\text{in}} + \alpha_{f,\text{in}} - \eta}{2}}$$

If $\alpha_{\ell,\text{in}} + \alpha_{f,\text{in}} < \eta$, then the flow never becomes saturated and no water is squeezed out.

Central saturated region:

Equations:

$$\alpha_{ix} + (\alpha_i w_i)_z = 0, \qquad i = \ell \text{ or } f$$
$$\alpha_\ell + \alpha_f = 1$$
$$w_\ell = w_f - k(\alpha_\ell) p_z/\kappa$$
$$\mathcal{F}(\alpha_f)_z = p_z$$

Let $\alpha = \alpha_\ell$. Summing the continuity equations leads to

$$\alpha w_\ell + (1-\alpha) w_f = h'(x)$$

Eliminate w_f:

$$w_\ell = h' + \left[\frac{(1-\alpha)k(\alpha)\mathcal{F}'(1-\alpha)}{\kappa}\right] \alpha_z$$

Continuity of water: (parabolic)

$$\alpha_x + (\alpha w_\ell)_z = 0$$

Initial conditions:

$$\alpha = \frac{\alpha_{\ell,\text{in}}}{\alpha_{\ell,\text{in}} + \alpha_{f,\text{in}}} \quad \text{at } x = x_1$$

Boundary conditions: $x_1 < x < 0$

$$\alpha k(\alpha)\mathcal{F}'(1-\alpha)\alpha_z = \kappa h'(x), \quad \text{at } z = 0 \ (w_f = 0)$$

$$\alpha_z = 0, \quad \text{at } z = h(x) \ (w_\ell = w_f = h')$$

Boundary conditions: $0 < x < x_s$

$$\left.\begin{aligned} \alpha_z &= 0 \\ (1-\alpha)h'(x) &= \alpha_x \zeta(x) \end{aligned}\right\} \quad \text{at } z = \zeta(x) \text{ (continuity of } \alpha_i \text{ and stress)}$$

$$\alpha_z = 0, \quad \text{at } z = h(x) \; (w_\ell = w_f = h')$$

A numerical method of solution is required to solve the nonlinear diffusion equation for $\alpha = \alpha_\ell$ and to determine the saturation boundary $\zeta = \zeta(x)$.

Outlet unsaturated region:

The felt is unstressed ($p = 0$), so that

$$w_\ell = w_f = -\frac{zg'(x)}{g(x)}, \qquad \alpha_f = g(x)$$

where

$$g(x) = \begin{cases} 1 - \alpha(x, \zeta(x)) & \text{for } 0 < x < x_s \\ \dfrac{\alpha_{f,\text{in}}}{h(x)} & \text{for } x > x_s \end{cases}$$

Continuity of Water: (hyperbolic)

$$\alpha_x + (w_\ell \alpha)_z = 0$$

Initial conditions:

$$\alpha = \alpha(x, \zeta(x)), \quad \text{on saturation boundary}$$

A numerical method is needed to continue the solution from the saturation boundary into the unsaturated region.

Numerical Method

Let $y = z/h(x)$. Continuity of water becomes

$$(\alpha h)_x + \left[\alpha\left(w_\ell - yh'\right)\right]_y = 0$$

where

$$w_\ell = \begin{cases} h' + \left[\dfrac{(1-\alpha)k(\alpha)\mathcal{F}'(1-\alpha)}{\kappa}\right]\alpha_z & \text{saturated} \\ -\dfrac{zg'(x)}{g(x)} & \text{unsaturated} \end{cases}$$

Conservative finite-volume discretization:

$$\frac{U_j(x+\Delta x) - U_j(x)}{\Delta x} + \frac{F_j(x) - F_{j-1}(x)}{\Delta y} = 0$$

where

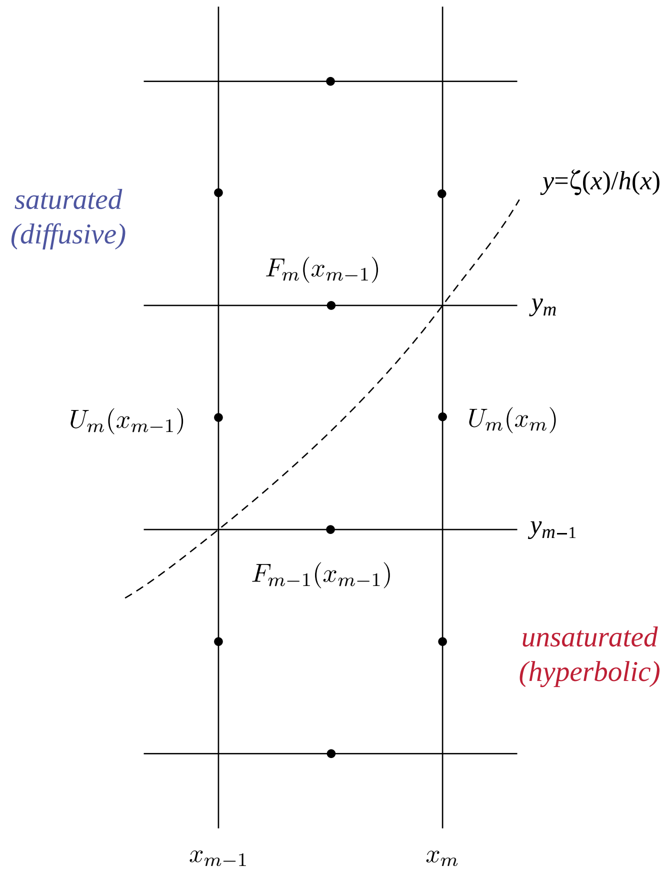
$$U_j(x) = \frac{1}{\Delta y}\int_{y_{j-1}}^{y_j} \alpha h \, dy$$

$$F_j(x) = \frac{1}{\Delta x}\int_x^{x+\Delta x} \left[\alpha(w_\ell - yh')\right]\Big|_{y=y_j} dx$$

Approximate F_j using suitable numerical quadrature formulas depending on whether the region is saturated (parabolic) or unsaturated (hyperbolic).

In the saturated region, the discretization becomes an implicit Crank-Nicolson method, and in the unsaturated region, it becomes an explicit Lax-Wendroff method.

Numerical treatment of the saturation boundary:



with $\Delta x_m = x_m - x_{m-1}$ chosen so that the (numerical) saturation boundary aligns itself with the grid.

Integral conservation:

$$\sum_{j=1}^{n} U_j(x)\Delta y = \int_0^{h(x)} \alpha\, dz = \begin{cases} h(x) - \alpha_{f,\mathrm{in}} & \text{for } x < 0 \\ \eta - \alpha_{f,\mathrm{in}} & \text{for } x > 0 \end{cases}$$