Insights into Mathematical Preparation from an Industrial Perspective

Steven J. Weinstein
Department of Chemical Engineering

Nate Barlow
School of Mathematical Sciences

Rochester Institute of Technology (RIT)
THANK YOU!
Outline

• Research Area
  > Introduction to coating
  > Systems engineering approach
  > Theoretical analysis of coating flows: Governing equations
  > Practical limitations of numerical simulation
  > Simplify mathematics using physics: Math Modeling
  > Examples: Modeling of thin film flows
  > Example: Pitfalls in theoretical analysis and role of experiment
  > Summary of engineering approach

• General Principles: Applied mathematics in practice

• Discussion on math preparation
  > Math education vs. research requirements
  > General challenges in math preparation
  > Case Studies: Addressing the challenges

• Summary
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• Summary
Typical Coating Process

Chill Box

Cold Air

Warm Air

Dryer

Coating die (Distributor)

Coating roll

Push-pull grid

Unwinder

Winder

Web Motion
Typical Cross-Section of Multi-Layered Film
Features of Typical Coated Film

• Typical coated wet thickness ~ 100 microns

• Individual wet layers may be 10x thinner

• Typical substrate speeds ~ 1000 ft/min

• Dry thickness ~ 10 microns

• Highly uniform liquid layers: ~ 1% variations
Different Coating Methods

Bead Coating
- Die
- Fluid Inlet
- Bead

Curtain Coating
- Curtain

Weir Coating
- Fluid Inlet

Pan (Dip) Coating
Systems Engineering Approach

- Break process down into fundamental pieces
- Examine physics and mathematics of these pieces
- Assemble pieces to assess interactions
- Reassemble these pieces to develop new and unexpected processes—patents
- I have worked on all of these pieces in my research

Approach is entirely analogous to examining word problems in algebra!
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Theoretical Analysis of Coating Flows

- Liquid layers are simultaneously applied to moving substrate
- Liquid-liquid and air-liquid interfaces present
- Advantages and limitations of process ⇒ Fluid mechanics
- Fluid mechanics embody: Conservation of mass, Newton’s 2^{nd} law, Constraints
- Mathematics is highly complex
General Equations Governing Coating Flows

**Governing Equations:**

**Force Balance:**

\[
\rho_i \left( \frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \right) = -\nabla P_i + \mu_i \nabla^2 \mathbf{u}_i + \rho_i \mathbf{g}
\]

\[\mathbf{u}_i = V_{xi} \hat{x} + V_{yi} \hat{y} + V_{zi} \hat{z}\]

**Mass Balance** \((\rho = \text{constant})\):

\[\nabla \cdot \mathbf{u}_i = 0\]

**Boundary Conditions at Interfaces:**

\((at \ y = h_i(x, z, t))\)

**No Slip:**

\[\mathbf{u}_i \cdot \hat{s} = \mathbf{u}_{i+1} \cdot \hat{s}\]

**Kinematic:**

\[V_{yi} = \frac{\partial h_i}{\partial t} + V_{xi} \frac{\partial h_i}{\partial x} + V_{zi} \frac{\partial h_i}{\partial z}\]

**Dynamic:**

\[(P_i - P_{i+1})\mathbf{n}_i + \mathbf{n}_i \cdot (\mathbf{r}_{i+1} - \mathbf{r}_i) + \nabla_{\parallel} \sigma_i - \frac{\sigma_i \mathbf{n}_i}{R_m} = 0\]

**Additional constraints:** Wall constraints, initial conditions (if transient flow), inflow and outflow boundary conditions…..depend on problem

**Highly Nonlinear System:** Force balance and unknown interface locations

**Numerical Simulation Required:** Solve equations on computer

**SOLUTION NOT GUARANTEED**
Practical Limitations of Numerical Simulation

• Once steady solution obtained, this is only the beginning!

• Engineers need to know how disturbances affect the process!

• Need to do hundreds of computer runs. Could take months or years to examine a process theoretically.

• And, as new disturbances arise, may take months to incorporate and analyze them. Just not practical!

• Justification for all theory is experimental verification ⇒ need to validate at least some of the theoretical results, so have confidence in predictions.
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Simplify Mathematics Using Physics: Math Modeling

• Examine governing equations much more closely

• Examine order of magnitude of terms in equations based on physics (math + physics = simplifications….)

• Often the case that many terms are small

• Once neglected, analytical techniques may be accessible, or numerical implementation is simplified that solutions are more robust, and run times reduced.

• Example: Single runs: 8 hours down to 7 seconds using these techniques (example)

• Solutions may often be implemented in spreadsheets⇒Accessibility of solution regardless of educational background!

• Industry embraces and values this approach: MATH MODELING

• Numerical simulation is approximate, so neglect of terms may incur errors smaller than in the numerical approximation!
Definitions: Problem Solving Approaches

- **Numerical Simulation**: Solve whole set of governing equations on computer
- **Math Modeling**: Solve appropriately simplified set of equations by injecting physics into the math: Solve either by hand or on computer.

Adapted from the modeling cycle used by www.engageny.org
Example: Modeling of Thin Film Flows

In many coating configurations, film thins gradually in direction of flow.

Physical Features:

- Small slope of interface (often with respect to solid surface)
- Many terms in the governing equations are so small they can be neglected
Math Modeling of Thin Film Flows

- Integrate simplified equations across the film—satisfy them on average

- Introduce assumed velocity profile that closely matches nature

- Obtain nonlinear, 1st order ODE to solve for interface location $h(x)$

Math Model

$> \text{Typical form:} \quad \frac{dh}{dx} = \frac{N(h)}{D(h)}$

- Easy to solve, and highly accurate!

Comment: Modeling invariably uses basic techniques learned in previous math courses (High school!)—Integrative in nature
Theoretical Assessment

Models often have high accuracy, and can often replace numerical simulation.

Laminar, Gravitational driven flow of a thin film on a Curved wall; ASME 2003, Steve Weinstein and Kenneth Ruschak
Example: Effect of Angle of Inclination on Interface Shape

Die

Wave

h_{slot}

Flow: q

Flow

<table>
<thead>
<tr>
<th>1 Degree Tilt</th>
<th>1.5 Degree Tilt</th>
<th>2 Degree Tilt</th>
</tr>
</thead>
<tbody>
<tr>
<td>μ = 0.12 Poise</td>
<td>q = 1.7 cm²/s</td>
<td>ρ = 1.1 g/cc</td>
</tr>
<tr>
<td>h_{slot} = 0.015 cm</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Example: Effect of Angle of Inclination on Interface Shape

Math Model Results

\[ h_c = \left( \frac{\mu g}{\rho g} \right)^{1/3} \]
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Pitfalls in Theoretical Analysis

• People are enamored with computer analysis

• Results often are complicated, and often require sophisticated implementation

• People tend to believe results when they are spit out of a computer

• But, computer analysis has assumptions, and just because answer looks complex and has pretty pictures, it may not even agree with what is observed physically!

• Because we solve equations on the computer approximately, the answers we obtain may even be bogus in some cases!

• Need to be very careful….need limiting theoretical cases, and experiments!

Analytical Math Skills Essential!!!
Example: A Pitfall Revealed

Model the following sequence: Assumption, 2-D Flow

- Fill container with a set volume of liquid (Step 1)
- Rotate container slowly (state 2)…simple model works well….
- Go from state 2 to state 3… Math model fails.
- BUT….Numerical simulation fails in this case as well!

WHAT IS GOING ON?
Example: A Pitfall Revealed

Model the following sequence: Assumption, 2-D Flow

- Observations reveal that spin up is 3 dimensional from steps 2 to 3!
- Model assumptions are wrong, even in full computation

Moral: Be careful in trusting theoretical solutions
Experiments are necessary!
Summary of Engineering Approach

Simulation
Modeling
Experiment

= Engineering Solution
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General Principles: Applied Math in Practice
Based on industry/research experience

• You will make math errors, regardless of how good you are mathematically

• The number of math errors increases as the length of an analysis increases—use most efficient technique possible

• Math errors will typically be algebraic, or calculus-type errors, and not occur elsewhere in the application of a sophisticated technique

• In general, the speed at which you obtain a solution is not important. Slow and steady pays off in the long run

• Solution needs to be mathematically correct…Bad engineering can lead to disaster literally!
General Principles: Applied Math in Practice

Question:

How do you know your answer is mathematically correct when you get it?
General Principles: Applied Math in Practice

Answer:

Self consistency checks!!!!!

I view this as the single most important procedure in a math analysis

I spend a lot of time teaching my students this!!!!
How do we do a self-consistency check?

- Verify solution satisfies equation—approach direct for solutions done by hand
- Obtain same solution using a different technique
- Compare with known published literature results
- Numerical simulation is harder to check….

> Numerical simulation of differential equations is an algebraic approximation!

> Verify that algebraic equations you have implemented are satisfied

> Refine accuracy of technique to verify mathematical consistency

> Generate check yourself--typically by hand in a limiting case—verifies that numerical approximations are consistent with physics
General Principles: Applied Math in Practice

How do we find errors once we have done self consistency check?

• Use “opposite” technique: If integrate, differentiate. If multiply, divide; if add, subtract, etc.

• Need to have good paper organization—otherwise, no way to find errors

• Write in pencil, and have an eraser handy (correct the analysis, don’t rewrite)—you don’t want to rewrite hundreds of pages of analysis

• Give yourself a lot of working space!!!!!! (e.g., orient page sideways)
  > More space ⇒ less errors as you are not wrapping large equations
  > More space ⇒ less brain cramps…more room to explore!
  > This has helped me, and my students, immensely!
Question:

Is mathematical consistency alone enough to proclaim an engineering problem solved?
The justification for any theoretical analysis is the agreement between theory and experiment.

So, favorable comparison with experiment is essential!
**General Principles: Applied Math in Practice**

The Process of Solving a Real Problem is Iterative!

- Experimental and theoretical examination of research problems is iterative.

- Often need to do math problems (simulation or modeling) on simplified geometries to understand underlying math structure and physics.

- Increased complexity can be added with subsequent problems.

- Best shot at theory can be compared with experiment, and assumptions in theory adjusted based on outcome—building intuition is essential!

- Simplified experiments can also be developed to elucidate phenomena based on theoretical predictions.

- Agreement between theory and experiment to desired accuracy indicates that model captures physics appropriately for application.
Research Process is not linear: Iterations within and between methods is required to obtain solutions!
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Math Education vs. Research Requirements

- High school/undergraduate testing teaches our students that they must get things right quickly and the first time

- Timed tests often do not lead to time for self consistency checks, which are essential for engineering practice

- It is a necessity to teach the approach of identifying and attempting to solve simple problems on the way to solving bigger problems (word problems are awesome!)

- Research is about getting things “wrong”, probably many times, before a problem is completed, through the iterative problem solving process of theory and experiment

- Significant reorientation in expectations in students is required as students embark on open-ended research, so they do not view themselves as failures
General Challenges in Math Education

- Students (and professionals!) think the calculator and computer can solve anything

- More fundamental mathematics is now being handled on the calculator. Students are unwilling to learn what is resident on the calculator already, as it is sitting right there.  

  ⇒ Do we acknowledge, and alter what we teach (e.g., square roots)?

- Utility of many techniques is not apparent until later in education

- Students do not know how to read math formulas well in general
General Challenges in Math Education (Continued)

- Students are spending more time on the computer, and are not writing enough down, and are thus losing basic organizational skills in solving problems on paper

- Students are losing sight of some basic skills like counting the number of equations in unknowns in systems of algebraic equations, essential for computer implementation (consequence of not writing stuff down)….

- Professors are also getting sloppy in using canned computer codes to solve problems very inefficiently, while simpler techniques are available. Students are mimicking this behavior

  > Simpler techniques often lead to more robust solutions
  > Simple techniques are more accessible to others (e.g., spreadsheet!)
Addressing These Challenges

Problem: Students think the calculator/computer can solve anything

Solution: Show examples where this is not true

Example: Calculators can only handle unique solutions to algebraic systems

So, give students a problem or two that have more than one solution!

\[ 4x + 2y = 1 \]
\[ 8x + 4y = 2 \]

Non-unique solution: Computer will not handle it!
Addressing These Challenges
Problem: Students think the calculator/computer can solve anything
Solution: Show examples where this is not true

Example: Chemical Stoichiometry

Atoms on one side must be same as on the other...find w, x, y, and z:

\[ wCH_4 + xO_2 \rightarrow yCO_2 + zH_2O \]

Equations:

\[
\begin{align*}
C &: w = y \\
H &: 4w = 2z \\
O &: 2x = 2y + z
\end{align*}
\]

Non-unique solution expected!
Computer will not handle it.

Three equations in 4 unknowns!

Many students think that for a problem to be well posed, always need the same number of equations in unknowns (if they think of it)!
Addressing These Challenges

Problem: Students think the calculator/computer can solve anything
Solution: Show examples where this is not true

Example Continued: Chemical Stoichiometry

Atoms on one side must be same as on the other...find \( w, x, y, \) and \( z \):

\[
wCH_4 + xO_2 \rightarrow yCO_2 + zH_2O
\]

Matrix system:

\[
\begin{bmatrix}
1 & 0 & -1 & 0 \\
4 & 0 & 0 & -2 \\
0 & 2 & -2 & -1
\end{bmatrix}
\begin{bmatrix}
w \\
x \\
y \\
z
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}
\]

So, non-unique solution yields:

\[
aCH_4 + 2aO_2 \rightarrow aCO_2 + 2aH_2O
\]

Divide by \( a \) to put in conventional form:

\[
CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O
\]

Result

\( w = a, \ y = a, \ z = 2a, \ x = 2a \)
Addressing These Challenges

Problem: Students think the calculator/computer can solve anything
Solution: Show examples where this is not true

Example: Most calculators/computers do not identify identities, and are subject to overflow errors!

Evaluate: \( y = \frac{\sinh(x)}{\cosh(x)} \) for \( x=1000 \) – Typical calculator will give error!

Reason for error: Calculator evaluates numerator, and then denominator.

Rewrite: \( y = \tanh(x) \), evaluate at \( x=1000 \) – Calculator easily yields \( y=1! \)
Addressing These Challenges

Problem: Students think the calculator/computer can solve anything
Solution: Show examples where this is not true

Example: Most calculators and computers are subject to overflow errors!

Evaluate:
\[
y = \frac{1 + e^{4x}}{2e^{4x}} \quad \text{for } x=1000
\]

Typical calculator will give error!

Reason for error: Calculator evaluates numerator, and then denominator

Rewrite: (Make numerator and denominator bounded)

\[
y = \left( \frac{1 + e^{4x}}{2e^{4x}} \right) \left( \frac{e^{-4x}}{e^{-4x}} \right) = \frac{e^{-4x} + 1}{2} \quad \text{for } x=1000
\]

Calculator easily yields \(y=1/2\)!
Addressing These Challenges

Problem: Utility of technique is not apparent until later in education
Solution: Integrate math topics where possible to demonstrate usefulness

Note: Integration of math topics naturally occurs when students study engineering and science, but even there, we can do better....

Example: Integrate the following

\[ I = \int (e^x \sin x) \, dx \]

Use integration by parts:

\[ u = e^x \quad dv = \sin x \, dx \]
\[ du = e^x \, dx \quad v = -\cos x \]

\[ I = -e^x \cos x + \int (e^x \cos x) \, dx \]

Use integration by parts again:

\[ I_1 = \int (e^x \cos x) \, dx \]

\[ u = e^x \quad dv = \cos x \, dx \]
\[ du = e^x \, dx \quad v = \sin x \]

\[ I_1 = e^x \sin x - \int (e^x \sin x) \, dx \]
Addressing These Challenges

Problem: Utility of technique is not apparent until later in education
Solution: Integrate math topics where possible to demonstrate usefulness

\[ I = -e^x \cos x + I \]
\[
\int (e^x \sin x) \, dx = -e^x \cos x + e^x \sin x - \int e^x \sin x \, dx + C
\]

Combine integrals and divide:
\[
\int (e^x \sin x) \, dx = \frac{1}{2} (e^x \sin x - e^x \cos x) + C
\]
Addressing These Challenges

Problem: Utility of technique is not apparent until later in education
Solution: Integrate math topics where possible to demonstrate usefulness

Example: Integrate the following (Method 2)

\[ I = \int \left( e^x \sin x \right) dx \]

Use complex variables:
\[ \sin x = \frac{1}{2i} \left( e^{ix} - e^{-ix} \right) \]

So:
\[ I = \int e^x \frac{1}{2i} \left( e^{ix} - e^{-ix} \right) dx \]

\[ I = \frac{1}{2i} \int \left( e^{x(1+i)} - e^{x(1-i)} \right) dx \]

\[ I = \frac{1}{2i} \left( \frac{e^{x(1+i)}}{1+i} - \frac{e^{x(1-i)}}{1-i} \right) + C \]

\[ I = \frac{e^x}{2i} \left( \frac{e^{ix}}{1+i} - \frac{e^{-ix}}{1-i} \right) + C \]

Original integral was real, so result must be real. Complex variables introduced to help with math analysis!
Addressing These Challenges

Problem: Utility of technique is not apparent until later in education
Solution: Integrate math topics where possible to demonstrate usefulness

Extract real result:

\[ I = \frac{e^x}{2i} \left( \frac{e^{ix}}{1+i} - \frac{e^{-ix}}{1-i} \right) + C \]

Use polar form:

1 + i = \sqrt{2}e^{i\pi/4}
1 - i = \sqrt{2}e^{-i\pi/4}

So:

\[ I = \frac{e^x}{2i} \left( \frac{e^{ix}}{\sqrt{2}e^{i\pi/4}} - \frac{e^{-ix}}{\sqrt{2}e^{-i\pi/4}} \right) + C \]

Continue simplifying:

\[ I = \frac{e^x}{2i} \left( \frac{e^{i(x-\pi/4)}}{\sqrt{2}} - \frac{e^{-i(x-\pi/4)}}{\sqrt{2}} \right) + C \]

\[ I = \frac{e^x}{\sqrt{2}} \left( e^{i(x-\pi/4)} - e^{-i(x-\pi/4)} \right) + C \]

\[ I = \frac{e^x}{\sqrt{2}} \sin(x - \pi/4) + C \]

After double angle formula, same result as before (more compact!)
Addressing These Challenges

Problem: Utility of technique is not apparent until later in education

Example: Complex roots of a quadratic equation

\[ x^2 + 4 = 0, \text{ Roots: } x = \pm 2i \]

Roots? We say there are two, but none are apparent in plot!
Are there roots, or not?

• All physical problems can have only real roots!
• Imaginary roots are “imaginary”
• Complex variable roots to this problem are used as a means to solve other problems
• Ultimately, structure of any problem using complex variables will lead to real roots (this is why complex conjugates appear—it is only by adding complex conjugates that real solutions can arise!)
Addressing These Challenges

Problem: Students do not know how to read complex math formulas
Solution: Do not assume they can. Be careful to demonstrate

Example: Let’s try one you may not be familiar with and see how it works

Leibnitz’ rule:

\[ \frac{d}{dx} \int_{a(x)}^{b(x)} f(x,t) \, dt = \int_{a(x)}^{b(x)} \frac{\partial f(x,t)}{\partial x} \, dt + \frac{db}{dx} f(x,t = b(x)) - \frac{da}{dx} f(x,t = a(x)) \]

Good approach to figuring out what this beast means and how to use it…..
try it on something you can evaluate not using the rule!

Evaluate:

\[ I = \frac{d}{dx} \int_{x}^{x^2} xt \, dt \]
Addressing These Challenges

Problem: Students do not know how to read complex math formulas

Solution: Do not assume they can. Be careful to demonstrate

Evaluate Directly:

\[ I = \frac{d}{dx} \int_x^{x^2} xtdt \]

\[ I = \frac{d}{dx} \left( x \int_x^{x^2} tdt \right) \]

\[ I = \frac{d}{dx} \left( x \left[ \frac{1}{2} t^2 \right]_{t=x^2} \right) \]

\[ I = \frac{d}{dx} \left( x \left[ \frac{1}{2} x^4 - \frac{1}{2} x^2 \right] \right) \]

\[ I = \frac{d}{dx} \left( \frac{1}{2} x^5 - \frac{1}{2} x^3 \right) \]

\[ I = \frac{5}{2} x^4 - \frac{3}{2} x^2 \]

Solution
**Addressing These Challenges**

**Problem:** Students do not know how to read complex math formulas

**Solution:** Do not assume they can. Be careful to demonstrate

---

**Leibnitz Rule:**

\[
\frac{d}{dx}\int_{a(x)}^{b(x)} f(x, t)dt = \int_{a(x)}^{b(x)} \frac{\partial f(x, t)}{\partial x} dt + \frac{db}{dx} f(x, t = b(x)) - \frac{da}{dx} f(x, t = a(x))
\]

\[
I = \frac{d}{dx} \int_x^{x^2} xtdt\quad \text{Function of } x \text{ only!}
\]

**Identify terms in integral--left hand side:**

\[
f(x, t) = xt, \quad b(x) = x^2, \quad a(x) = x
\]

**Evaluate pieces of formula:**

\[
\frac{\partial f(x, t)}{\partial x} = t, \quad \frac{db}{dx} = 2x, \quad \frac{da}{dx} = 1
\]

\[
f(x, t = b(x)) = xb = x^3
\]

\[
f(x, t = a(x)) = xa = x^2
\]

\[
\int_x^{x^2} \frac{\partial f(x, t)}{\partial x} dt = \int_x^{x^2} t dt = \frac{1}{2} t^2 \Big|_x^{x^2}
\]

\[
\int_x^{x^2} \frac{\partial f(x, t)}{\partial x} dt = \frac{1}{2} (x^4 - x^2)
\]

**Put it all together:**

\[
I = \frac{1}{2} (x^4 - x^2) + (2x)x^3 - (1)x^2
\]

\[
I = \frac{5}{2} x^4 - \frac{3}{2} x^2 \quad \text{Solution (Same!)}
\]
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EXTRA
My Background

- Industry for 18 years (Kodak)
- Joined RIT full time in January 2007
- Expertise: Interfacial fluid dynamics, transport processes, applied mathematics
- Application area: Coating, transport, and physics of thin liquid films in various systems
- Industry interaction: Continuing in coating area with many funded projects
- Teaching experience prior to full time position at RIT: Adjunct professor at University of Rochester, RIT, Cornell (current)
- Courses at RIT
  - Graduate: Math for Engineers I and II, Fluid dynamics
  - Undergraduate: Fluid dynamics, Chemical process analysis, Mass transfer unit operations, Chemical reactor design
- Master’s graduate students: 4
- Designed Chem E curriculum, and appointed head of new department (First recruited freshman class entering in fall of 2009)
Definitions: Theoretical Approach

- **Numerical Simulation**: Solve whole set of governing equations on computer

- **Math Modeling**: Solve appropriately simplified set of equations by injecting physics into the math: Solve either by hand or on computer