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WORKSHOP ON "MODELLING REAL SYSTEMS: A HANDS-ON FIRST ENCOUNTER WITH INDUSTRIAL MATHEMATICS

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"How To Solve Industrial Mathematics Problems"

presented by:

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HOW TO SOLVE INDUSTRIAL MATHEMATICS PROBLEMS

A Completely biased view by..........

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Industrial Mathematics is booming in Europe. But what is the true nature of industrial mathematics?

It can mean many different things to many different people.

Here are some of the things that it does NOT mean to me:

1. EXPERIMENTS

When an industry comes to a mathematician with a problem, the answer is almost never to tell them to carry out experiments. Normally they have already considered this, and carried them out or rejected the idea. The problem with experiments is that they are often:

- Expensive
- Dangerous
- Impossible
- Time-consuming
- Ill-conceived
- Useless to add basic understanding

Of course previous experimental results may guide us and our work may eventually suggest the *best* experiments to do.

2. LITERATURE SURVEY

Well of course this has to be done, but normally it's already been carried out by the time the problem arrives.

Most industries are fairly sophisticated these days. If the problem has been done before then they usually know about it.

Of course, someone may have specialist knowledge (working papers, theses etc.)

But all in all the number of problems that can be totally solved by just looking them up in the literature is small.

3. NUMERICAL CALCULATIONS

Sometimes (often!) industry have carried these out. But the trouble with a numerical-based study is that:

- Pages of numbers are hard to interpret
- Often they've solved the wrong problem
- How can we trust the numerics?
- Cannot provide *basic understanding*
- Rarely highlights *mechanisms*
- Can contain many fiddle factors
- Pretty pictures can hide falsehoods

Of course, *after* the modelling process has been completed we may well want to do numerical calculations, but then at least we have a good chance of solving the right problem and knowing what we are doing.....

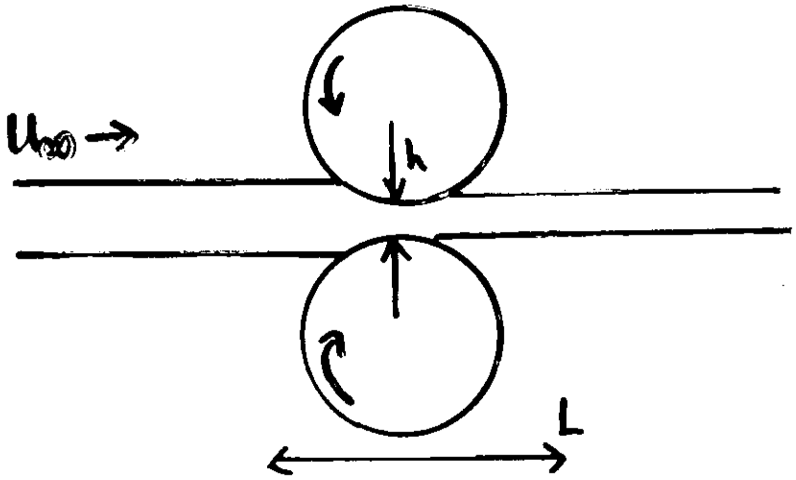
HOW DO DO IT

We will illustrate the general process with an example: some bits of it are made up for the purposes of the lecture, but much of the processes involved are real.

EXAMPLE: PROPELLANT ROLLING

Gun (or if you like air bag) propellant comes in many forms. One important form is "flake" propellant which is made by rolling a plastic-type mixture to thin it.

The basic idea is shown below. (Assume symmetry)



OBSERVATIONS:

- The top roller tends to get hot
- The propellant can flow
- Chemical reactions may take place in the propellant
- The roller speed and pressure are known
- Conditions at the entrance to the roller are known

QUESTIONS:

- What size reduction is reasonable?
- What are the key non-dimensional parameters in the problem?
- What is the maximum U_∞ allowed which ensures $T < T_{max}$?
- What roller pressure will be required?
- Would it help to cool the roller?
- What changes when the propellant type changes?

OK, so let's write down the equations. We have:

(MASS)

$$\rho_t + \nabla.(\rho \boldsymbol{q}) = 0$$

(MOMENTUM)

$$\rho(\boldsymbol{q}_t + (\boldsymbol{q}.\nabla)\boldsymbol{q}) = \nabla.\boldsymbol{\tau} + \boldsymbol{b}$$

(ENERGY)

$$\rho c_p(T_t + (\boldsymbol{q}.\nabla)T) = k\nabla^2 T + \Phi + G + C$$

Where:

ρ = propellant density

$\boldsymbol{q}$ = propellant velocity

$\boldsymbol{\tau}$ = propellant stress tensor

$\boldsymbol{b}$ = body force

c_p = propellant specific heat

k = propellant thermal conductivity

T = propellant temperature

Φ = viscous dissipation

G = compressible energy terms

C = chemical reaction terms

THIS IS A *NORMAL MODELLING PROBLEM*: Its easy to write down the general equations, but of course they're too awful to do anything with. So HOW CAN WE PROCEED?

(Note: If we go to the computer at this stage then we can expect SEVERE TROUBLE!)

ANSWER: The skill lies in the modelling assumptions!

We have to be very clear what we have assumed and how these assumptions would change if circumstances were different.......

NOTE: we are NOT just "approximating". Eventually we will deal in proper asymptotic expansions. We will be able to say how big the likely errors are and go to the next term if need be.

This problem provides a GOOD ILLUSTRATION of how we have to "pick off" the modelling assumptions one by one. *discussing each as we go* (preferably with the person from the industry).

SO HERE WE GO with all the modelling assumptions:

(1) We work in 2-D (x, z) since the rollers are VERY wide. (Edge effect problems may have to be done separately.)

(2) We assume that the FLOW IS INCOMPRESSIBLE (to check this we can check the Mach number and many other things after we have solved the problem).

(3) We will assume that the FLOW IS STEADY so that nothing depends explicitly on time. (There is also a "start-up" problem that could be done where things to depend on time, but steady operation is our main interest).

(4) We will assume that SUITABLE BOUNDARY CONDITIONS are known. (This sounds obvious, but often it turns out that nobody knows the boundary conditions!)

(5) We will assume that the fluid is a LINEAR VISCOUS FLUID. (Again, should all be checked when we have finished).

(6) We will assume that the fluid has a CONSTANT VISCOSITY μ (NOTE: this is almost certainly NOT TRUE!).

(7) We will assume that the ONLY BODY FORCE is GRAVITY.

Hmmmm 7 major assumptions already! - what does this give?

THE ANSWER: still a horrid mess. We have

$$\nabla.\boldsymbol{q} = 0$$

$$\rho(\boldsymbol{q}.\nabla)\boldsymbol{q} = \nabla.\boldsymbol{\tau} - \rho\boldsymbol{g}$$

$$\rho c_p(\boldsymbol{q}.\nabla)T = k\nabla^2 T + \mu d_{ij}d_{ij} + C$$

$$d_{ij} = \frac{1}{2}\left(\frac{\partial q_i}{\partial x_j} + \frac{\partial q_j}{\partial x_i}\right)$$

.....But at least we've done some
INITIAL MODELLING.

NOW we need to know how BIG things are.

Are some terms more important than others?

Can some of the terms in these equations be ignored?

(After all, where's the relativity?!!)

To find this out we need to NON-DIMENSIONALIZE

NON-DIMENSIONALIZATION

We want to scale everything with its typical size.

All variables with a bar will be NON-DIMENSIONAL

Obviously we put $x = L\bar{x}$, $z = h\bar{z}$.

To preserve continuity, put
$u = U_\infty \bar{u}$, $w = \epsilon U_\infty \bar{w}$ where $\epsilon = h/L$.

We don't know a scale for p yet so put $p = P\bar{p}$

Let T_0 = temperature of oncoming propellant
T_1 = temperature of top roller (assume that we can control this: of course, we can't!)

So put $T = (T_1 - T_0)\bar{T} + T_0$

NOTE: $\bar{T} > 0$ but maybe $\bar{T} > 1$ as well!

Also for the chemistry put $C = C_0\bar{C}$

When we write the equations out in component form, we get

(subscripts indicate differentiation)

$$u_x + w_z = 0$$

$$uu_x + wu_z = -\frac{p_x}{\rho} + \nu(u_{xx} + u_{zz})$$

$$uw_x + ww_z = -\frac{p_z}{\rho} + \nu(w_{xx} + w_{zz}) - g$$

$$\rho c_p(uT_x + wT_z) = k(T_{xx} + T_{zz}) + \mu(u_x^2 + w_z^2 + u_z w_x + \frac{1}{2}u_z^2 + \frac{1}{2}w_x^2) + C$$

Now let's transform all of this to barred variables:

$$\bar{u}_{\bar{x}} + \bar{w}_{\bar{z}} = 0$$

$$\bar{u}\bar{u}_{\bar{x}} + \bar{w}\bar{u}_{\bar{z}} = -\frac{P}{\rho U_\infty^2}\bar{p}_{\bar{x}} + \frac{\nu}{LU_\infty}(\bar{u}_{\bar{x}\bar{x}} + \frac{1}{\epsilon^2}\bar{u}_{\bar{z}\bar{z}})$$

$$\bar{u}\bar{w}_{\bar{x}} + \bar{w}\bar{w}_{\bar{z}} = -\frac{P}{\rho U_\infty^2 \epsilon^2}\bar{p}_{\bar{z}} + \frac{\nu}{LU_\infty}(\bar{w}_{\bar{x}\bar{x}} + \frac{1}{\epsilon^2}\bar{w}_{\bar{z}\bar{z}}) - \frac{gL}{\epsilon U_\infty^2}$$

$$\bar{u}\bar{T}_{\bar{x}} + \bar{w}\bar{T}_{\bar{z}} = \frac{\nu k}{LU_\infty \mu c_p}\left(\bar{T}_{\bar{x}\bar{x}} + \frac{1}{\epsilon^2}\bar{T}_{\bar{z}\bar{z}}\right) +$$

$$\frac{\mu U_\infty}{\rho L c_p(T_1 - T_0)}\left(\bar{u}_{\bar{x}}^2 + \bar{w}_{\bar{z}}^2 + \bar{u}_{\bar{z}}\bar{w}_{\bar{x}} + \frac{1}{2\epsilon^2}\bar{u}_{\bar{z}}^2 + \frac{1}{2}\epsilon^2\bar{w}_{\bar{x}}^2\right) + \frac{LC_0}{\rho c_p U_\infty(T_1 - T_0)}\bar{C}$$

Now everything is multiplied by 1 except for the terms that are multiplied by the non-dimensional combinations

$$\frac{P}{\rho U_\infty^2}, \quad \frac{\nu}{LU_\infty} \quad \frac{\nu}{LU_\infty \epsilon^2}$$

$$\frac{P}{\rho U_\infty^2 \epsilon^2}, \quad \frac{gL}{\epsilon U_\infty^2}$$

$$\frac{\nu k}{\mu U_\infty L c_p}, \quad \frac{\nu k}{\mu U_\infty L c_p \epsilon^2} \quad \frac{\mu U_\infty}{L \rho c_p (T_1 - T_0)}$$

$$\frac{\mu U_\infty \epsilon^2}{L \rho c_p (T_1 - T_0)} \quad \frac{\mu U_\infty}{L \rho c_p (T_1 - T_0) \epsilon^2}, \quad \frac{C_0 L}{\rho c_p U_\infty (T_1 - T_0)}$$

Now we have to make a key observation:

We MUST keep the pressure in as it is the main physical mechanism!

So we have to choose

$$P = \frac{\mu U_\infty}{L \epsilon^2}$$

OK, so here are some typical sizes of things:

(NOTE: industrial input is *crucial* here. Also - we might have to guess some of them.)

$L \sim 0.5\text{m}$

$h \sim 0.001\text{m}$

$U_\infty \sim 0.2\text{m/s}$

$\rho \sim 200\text{kg/m}^3$

$\mu \sim 1000\text{kg/m/s}$

$k \sim 4\text{J/s/m/K}$

$c_p \sim 2000\text{J/kg/K}$

$T_0 \sim 300\text{K}, \qquad T_1 \sim 310\text{K}$

$C_0 \sim 4 \times 10^8$

Now we will identify the sizes of each term:

$$\overset{1}{\boxed{\bar u_{\bar x}}} + \overset{1}{\boxed{\bar w_{\bar z}}} = 0$$

$$\overset{1}{\boxed{\bar u \bar u_{\bar x} + \bar w \bar u_{\bar z}}} = -\overset{10^{6}}{\boxed{\frac{P}{\rho U_\infty^2}}}\bar p_{\bar x} + \frac{\nu}{LU_\infty}\left(\overset{10^{3}}{\boxed{\bar u_{\bar x\bar x}}} + \overset{10^{6}}{\boxed{\frac{1}{\epsilon^2}}}\bar u_{\bar z\bar z}\right)$$

$$\overset{1}{\boxed{\bar u\bar w_{\bar x}+\bar w\bar w_{\bar z}}} = -\overset{10^{13}}{\boxed{\frac{P}{\rho U_\infty^2\epsilon^2}}}\bar p_{\bar z} + \frac{\nu}{LU_\infty}\left(\overset{10^{3}}{\boxed{\bar w_{\bar x\bar x}}} + \overset{10^{6}}{\boxed{\frac{1}{\epsilon^2}}}\bar w_{\bar z\bar z}\right) - \overset{10^{5}}{\boxed{\frac{gL}{\epsilon U_\infty^2}}}$$

$$\overset{1}{\boxed{\bar u\bar T_{\bar x}+\bar w\bar T_{\bar z}}} = \frac{\nu k}{LU_\infty \mu c_p}\left(\bar T_{\bar x\bar x} + \overset{25}{\boxed{\frac{1}{\epsilon^2}}}\bar T_{\bar z\bar z}\right) +$$

$$\frac{\mu U_\infty}{\rho L c_p(T_1-T_0)}\left(\bar u_{\bar x}^2+\bar w_{\bar z}^2+\bar u_{\bar z}\bar w_{\bar x}+\underset{25}{\boxed{\frac{1}{2\epsilon^2}\bar u_{\bar z}^2}}+\frac{1}{2}\epsilon^2\bar w_{\bar x}^2\right)+\underset{25}{\boxed{\frac{LC_0}{\rho c_p U_\infty(T_1-T_0)}}}\bar C$$

To leading order the governing equations are therefore

$$u_x + w_z = 0$$

$$p_x = \mu u_{zz}$$

$$p_z = 0$$

$$0 = kT_{zz} + \frac{\mu}{2} u_z^2 + C$$

(redimensional)

Hooray ! we now have some "working equations":

Of course, we need some boundary conditions too:

Suppose the top roller is $z = h(x)$

$$w(x,0) = 0, \qquad u_z(x,0) = 0$$

$$u(x, h(x)) = U_r, \qquad w(x, h(x)) = U_r h'$$

$$T_z(x,0) = 0, \qquad T(x, h(x)) = T_1$$

Actually we can make *substantial* progress with these equations, but before we even solve anything.......

LOOK at all the things that we now know about this problem *WITHOUT EVEN TOUCHING A COMPUTER!*

We know that:

- Inertia is irrelevant.
- We can *say* how small the inertial effects are.
- Convection of heat is irrelevant.
- The pressure is only a function of z.
- The only important momentum balance is between the pressure and the viscous effects
- We know the order of magnitude of the pressure forces.
- We know exactly how the process speed enters into the problem.
- The flow problem may be solved independent of the temperature problem.

- There will be boundary layers at the entrance at the exit of the rollers.
- We know the thickness of the inertial entry boundary layer.
- We know the thickness of the thermal entry boundary layer.
- Gravity is totally irrelevant.
- The key heat balance is between diffusion, viscous dissipation, and the chemical reaction term.
- We know *exactly* how important the chemical reaction is.
- We have a heat scale for the problem
- We have identified the mechanisms that might heat up the top roller.

This is "good business" for a few minutes work.....

Although hopefully the point has been made, it seems a shame not to go on and integrate the equations.....!

Using elementary methods we find that

$$u = U_r + \frac{z^2 - h^2}{2\mu} p_x$$

$$w = \frac{z}{2\mu} \left(2hh_x p_x - (z^2/3 - h^2)p_{xx}\right)$$

Where the pressure $p(x)$ satisfies a second-order ODE (whose boundary conditions we have to think a bit carefully about),

Some other things need to be thought about as well now, for we do not yet know how much the propellant thins or where it leaves the top roller.

There are many other details to be cleared up, but basically we *understand* the flow problem.

What about T? well T satisfies the equation

$$0 = kT_{zz} + \frac{\mu}{2}u_z^2 + C$$

where u is now known. We must say something about C.

Simplest:

$$C = C_0 \exp(-E/RT)$$

where $R =$ gas constant, $E =$ activation energy.

This then gives a nonlinear PDE for the temperature

Now *this* could be solved numerically (using MAPLE, for example).

NOTE: In reality, we might expect the reactions to be complicated. There are probably multiple reactions.

General observations:

(i) The gas constant R and the activation energy E are in most books.

(ii) Nobody in the world EVER knows C_0!

NOW would be a good time to do some numerical calculations.

Using an off-the-shelf CFD code, we could try to confirm

(i) the parabolic velocity profile

(ii) pressure is constant across the gap between the two rollers.

(iii) how the roller shape affects the results.

(iv) etc. etc. etc.

Of course, once this was all clear we could put in things like

(a) multiple chemical reactions

(b) complicated constitutive laws

(c) temperature-dependent viscosity

(d) temperature-dependent k and c_p

We could also now try to interpret the results of any experiments that have been carried out.

Again, we could look for general similarites in the predicted flow behaviour.

Also, since we now know *all* of the important non-dimensional parameters we could try to collapse the results on to one graph.

Knowing the non-dimensional parameters can also be VERY useful when it comes to interpreting the numerics.

In a few problems we have been able to dramatically cut down the number of numerical runs needed in this way.

Now that we **understand** the problem, we can also start to think about some extensions that will add to the realism in the modelling. For example:

- Almost certainly $\mu = \mu(T)$. We could find a suitable law for μ and drive the problem with a variable viscosity.
- The assumption of linear viscous flow is dubious. Experimental data suggests that viscoelastic flow may be more appropriate.
- The pressure boundary conditions need to be carefully thought about. (This comment applies to numerical calculations as well).
- We need more details of the chemical reaction.
- It may be necessary to solve a heat conduction problem in the roller.
- It may be necessary to introduce a free boundary that marks where the material starts to flow.
- Do we have to worry about the trapping of air where the propellant leaves the roller?