MATHEMATICAL MODELLING
-a different course

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SIAM report on *Mathematics in Industry* (http://www.siam.org/mii):

- Most needed skill:
  - *mathematical formulation of problems*
  - *modelling and simulation*
- Most important lesson:
  ”*Problems never come formulated as mathematical problems*”



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MATHEMATICAL MODELLING - *OBJECTIVES*

The main objectives of the course should be to teach the students

- a professional attitude towards problem solving using methods requiring insight
- how to ask colleagues the right questions, - questions that force *them* to think again about what is really the problem!
- simple techniques to check model consistency and do the important primary analysis

The *real* challenge:
To teach the student to think before (and while) they compute!



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“There are no general recipes which can be taught in lectures for direct applications to different classes of modelling problems”

F. Y. M. Wan: *Mathematical Models and Their Analysis*, Harper and Row Publ. 1989.



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THREE GENERIC TOOLS OF MATHEMATICAL MODELLING

Technique	Importance	Related mathematical techniques
Dimensional analysis • reduce the number of parameters • check whether a model is appropriate	• lab. work • experimental design • numerical experiments • data analysis	
Scaling • systematic model analysis • basis for perturbation methods	• forces the modeler to think!	• perturbation/multiple scale/asymptotic techniques • selection of numerical techniques
Conservation laws • basic requirement of models!	• models conform to nature • develop numerical models • understand shock behavior	• hyperbolic PDEs • diffusion equations • shock tracking num. schemes

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DIMENSIONAL ANALYSIS

- is a basic law in physics!
- requires all valid relations to be unit independent
- gives a minimal number of parameters to be used in experimental and numerical work
- may prove that a suggested model is impossible
- suggests suitable dimensionless parameters

There are phenomena in nature where dimensional analysis gives information we have not yet been able to explain directly!



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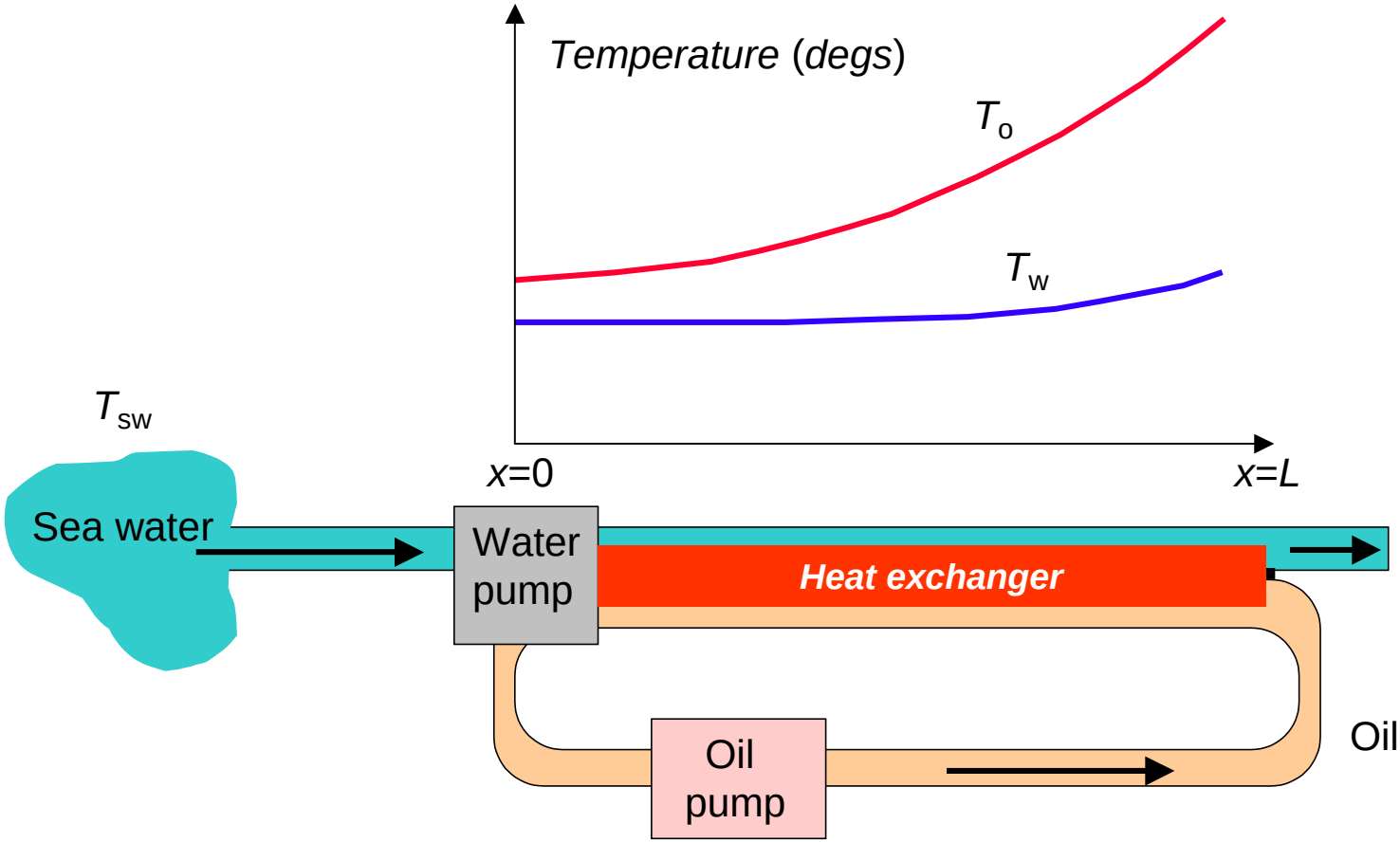
SCALING

- The scale is a "natural measuring stick" for the variable
- Scaling forces problem insight!
- Scaled equations show what is important and what is not
- Scaled equations are important for revealing the behaviour of numerical algorithms
- No scales? - similarity solutions!



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OIL COOLING OF A WATER PUMP



What determines the maximum oil temperature?

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VARIABLES AND PARAMETERS

x	*position*
t	*time*
$T_{o,w}$	*oil/water temperatures*
L	*length of heat exchanger*
T_{sw}	*sea water temperature*
$c_{o,w}$	*oil, water specific heats*
$A_{o,w}$	*oil, water cross sections*
$\rho_{o,w}$	*oil, water densities*
$k_{o,w}$	*oil/water turbulent heat diffusivities*
W	*water velocity*
U	*oil velocity*
α	*heat exchange coefficient*
Q	*heat production in the water pump*

4 variables and 14 parameters !



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After scaling and showing that turbulent heat diffusion is negligible, we end up with a *linear* system and 3 dimensionless parameters for the stationary temperature distribution:

$$\frac{dT_o}{dx} = \mu(T_o - T_w)$$

$$\frac{dT_w}{dx} = \varepsilon\mu(T_o - T_w)$$

$$T_w(1) = \varepsilon\Delta T,\ T_w(0) = 0$$

$$\Delta T = T_o(1) - T_o(0)$$

$$\mu = \frac{\alpha L}{A_o U \rho_o c_o}$$

$$\varepsilon = \frac{A_o U \rho_o c_o}{A_w W \rho_w c_w}$$

$$\Delta T = \frac{Q}{A_o U \rho_o c_o}$$

Exact solution:

$$T_o(1) = \frac{e^{\mu(1-\varepsilon)} - \varepsilon}{e^{\mu(1-\varepsilon)} - 1}\Delta T$$



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More subtle aspects of scaling:

Lack of scales leads to similarity solutions, - and *almost* lack of scales leads to solutions *close* to similarity solutions:

Intermediate Asymptotics

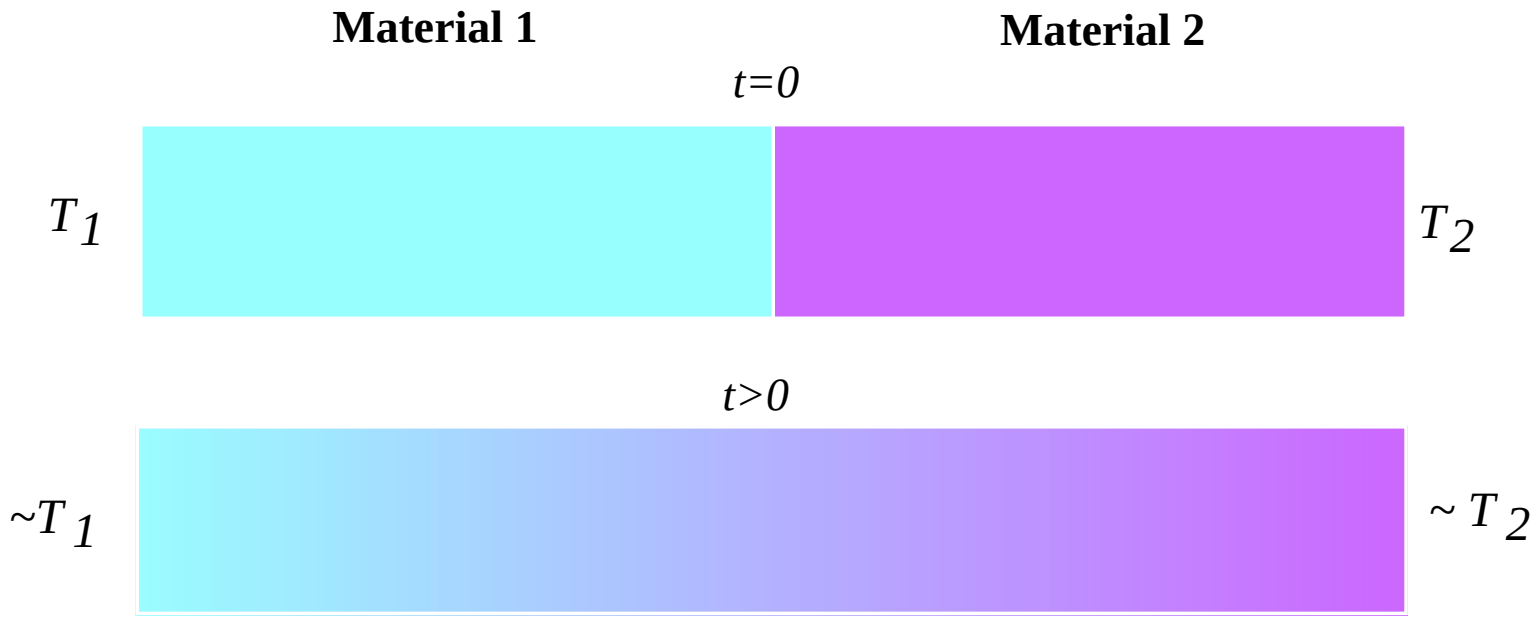
- the fundamental solution of the heat equation is the intermediate asymptotic solution for all localized initial data.
- the first eigen-function dominates away from the initial condition
- stable front solutions of e.g. Burgers equation.

Simple and idealized analytic solutions have a broader range of applicability than often recognized.



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- Two ”infinite” slabs with different, but constant temperatures are brought into contact:



What is the temperature for $T > 0$, in particular at the interface?

No separate scales for x and $t \Rightarrow$

$$T = T_1 + (T_2 - T_1)\tau$$

$$\tau = \tau(x, t, \rho_1, c_1, k_1, \rho_2, c_2, k_2) = \tau_0(\eta, a, b),$$

$$\eta = \frac{x}{\sqrt{\kappa_1 t}}, \quad \kappa_i = \frac{k_i}{c_i \rho_i}$$

$$a = \frac{k_2}{k_1}, \quad b = \frac{\kappa_2}{\kappa_1}$$



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1. Temperature at the interface: $\tau(0,t) = \tau_0(0,a,b)$ = *constant!*

2. The partial heat diffusion equations reduce to ordinary differential equations, e.g.,

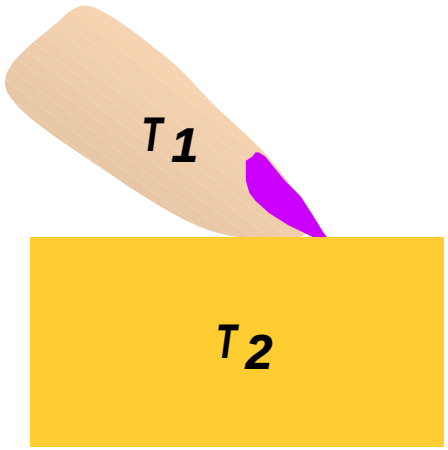
$$\frac{\partial \tau}{\partial t} = \kappa_1 \frac{\partial^2 \tau}{\partial x^2} \quad \Rightarrow \quad -\frac{1}{2}\eta \frac{d\tau_0}{d\eta} = \frac{d^2\tau_0}{d\eta^2}$$

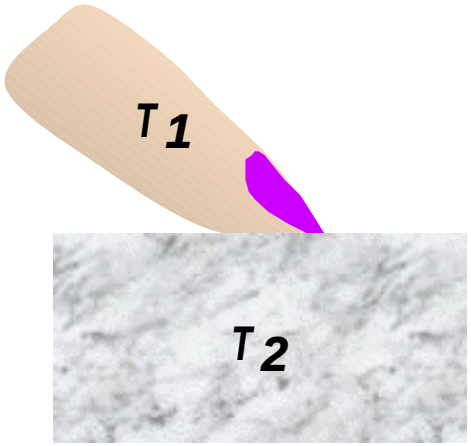
3. It follows from the solution that

$$T(0,t) = \frac{T_1 w_1 + T_2 w_2}{w_1 + w_2}, \quad w_i = \sqrt{\rho_i c_i k_i}$$



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Wood

Metal

$$w_1 >> w_2$$
$$T(0,t) \approx T_1$$

$$w_1 << w_2$$
$$T(0,t) \approx T_2$$

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WALKING ON BURNING COAL

	ρ[kg/m3]	c [J/kgK]	k [W/mK]	T [°C]	w [m2Ks.5]
Foot	1000	4000	.6	37	1550
Burning coal	150	800	.04	600	70

Contact temperature:

$$T_k = \frac{37°C \times 1550 + 600°C \times 70}{1550 + 70} = 62°C\,!$$

How long can we rely on the similarity solution ?

Time scale:

$$S = \frac{L_{skin}^{\ 2}}{\kappa_{foot}} = \frac{\rho_{foot} c_{foot}}{k_{foot}} L_{skin}^{\ 2} = \frac{1000 \times 4000}{0.6} \left(.5 \times 10^{-3}\right)^2 s = 1.6s$$

KEEP WALKING!

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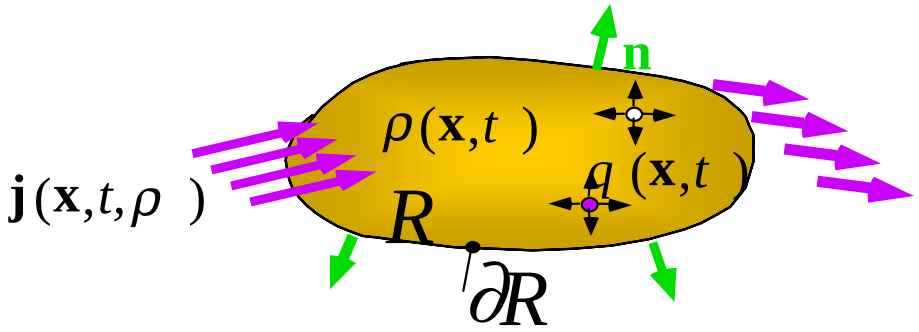
THE UNIVERSAL CONSERVATION LAW

$$\frac{d}{dt}\int_R \rho(\mathbf{x},t)\,dV + \int_{\partial R} \mathbf{j}(\mathbf{x},t,\rho)\cdot\mathbf{n}\,d\sigma = \int_R q(\mathbf{x},t)\,dV$$

Change of content in control volume

Transport across the boundary

Production ($q>0$) or destruction ($q<0$)



1. Identify what is density, flux, and sources

2. Use Reynold's Transport Theorem to transform the first term when necessary.

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INTEGRAL FORM

DIFFERENTIAL FORM

Gauss' theorem etc.

$$\frac{d}{dt}\int_R \rho(\mathbf{x},t)\,dV + \int_{\partial R} \mathbf{j}(\mathbf{x},t,\rho)\cdot\mathbf{n}\,d\sigma = \int_R q(\mathbf{x},t,\rho)\,dV \quad \Rightarrow \quad \frac{\partial \rho(\mathbf{x},t)}{\partial t} + \nabla\cdot\mathbf{j}(\mathbf{x},t,\rho) = q(\mathbf{x},t,\rho)$$

- independent of coordinate system
- direct connection to physics
- required for discontinuous solutions
- basis for conservative numerical schemes

- classic theory of differential equations (analytical solutions, series expansions, integral transforms, perturbation techniques)
- conventional numerical algorithms
- cannot treat discontinuous solutions properly

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THE MATHEMATICAL MODELLING COURSE AT NTNU

- 4. year students from the Industrial Mathematics program.
- Ph.d. students from other faculties.
- No advanced background in PDEs.

- Focus on generic tools with applications to case studies

- Introductory book: *Lin and Segel*.

- Case studies from from *Fowkes and Mahoney*, *Logan*, *Fowler* etc., and specially prepared material.

- A two week modelling seminar (Similar form as the ECMI Modelling Week, but less requirement for reporting)



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POPULATION MODELS

(Based on material from Robert M. May)

- the basic models (logistic, Lotka-Volterra…)
- logistic model with delay
- fish harvesting
- moose hunting
- whales and krill, inclusive whale hunting
- species having mutual dependence

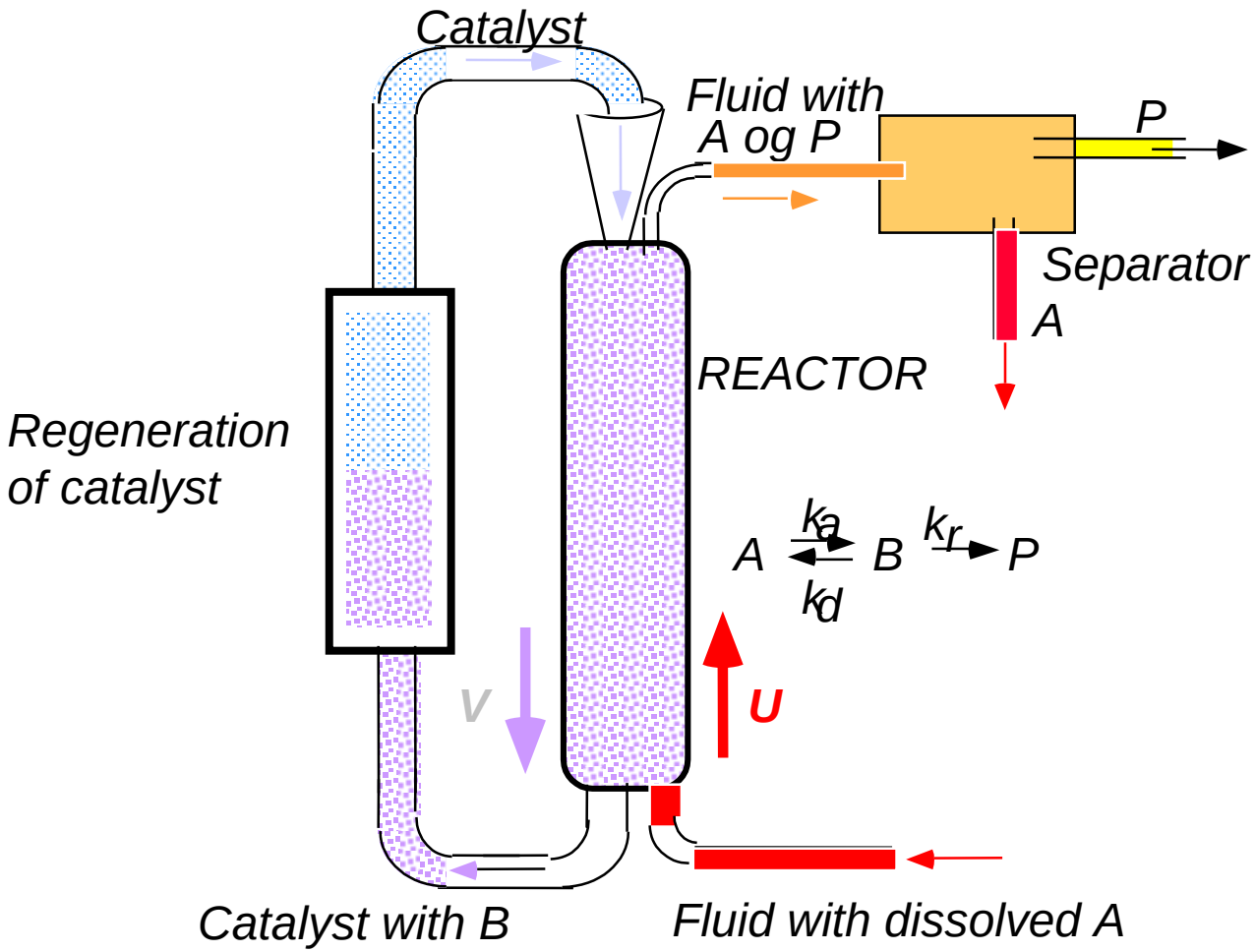
Nice field, interesting results, easy to do numerical experiments



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THE COUNTER-FLOWING CATALYCTIC REACTOR

(Adapted from R. Aris: *Mathematical modelling Techniques*, Dover)



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Differential equations:

$$\frac{\partial a^*}{\partial t^*} + U\frac{\partial a^*}{\partial x^*} - \frac{\partial}{\partial x^*}\sigma_a \frac{\partial a^*}{\partial x^*} = -k_a a^*(B_0 - b^*) + k_d b^*$$

$$\frac{\partial b^*}{\partial t^*} - V\frac{\partial b^*}{\partial x^*} - \frac{\partial}{\partial x^*}\sigma_b \frac{\partial b^*}{\partial x^*} = +k_a a^*(B_0 - b^*) - k_d b^* - k_r b^*$$

$$\frac{\partial p^*}{\partial t^*} + U\frac{\partial p^*}{\partial x^*} - \frac{\partial}{\partial x^*}\sigma_p \frac{\partial p^*}{\partial x^*} = k_r b^*, \quad a^*(0, t^*) = a_0.$$

Scales:

For *a** : $a_0\ ,\ k_d / k_a$

For *b** : $B_0\ , a_0$

Length scales: $L\ , k_r / U\ , \sqrt{\sigma_a (L/U)}, \cdots$

Time scales: $1/k_r\ , 1/\ B_0 k_a\ , L/U, L/V, \cdots$



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SOME SPECIAL CASES:

Well-mixed reactor:

- ordinary DEs in time
- linearization, phase plane analysis

Stationary flow:

- ordinary DE in space. Special initial conditions
- possibility for shock solutions

Reaction equilibrium:

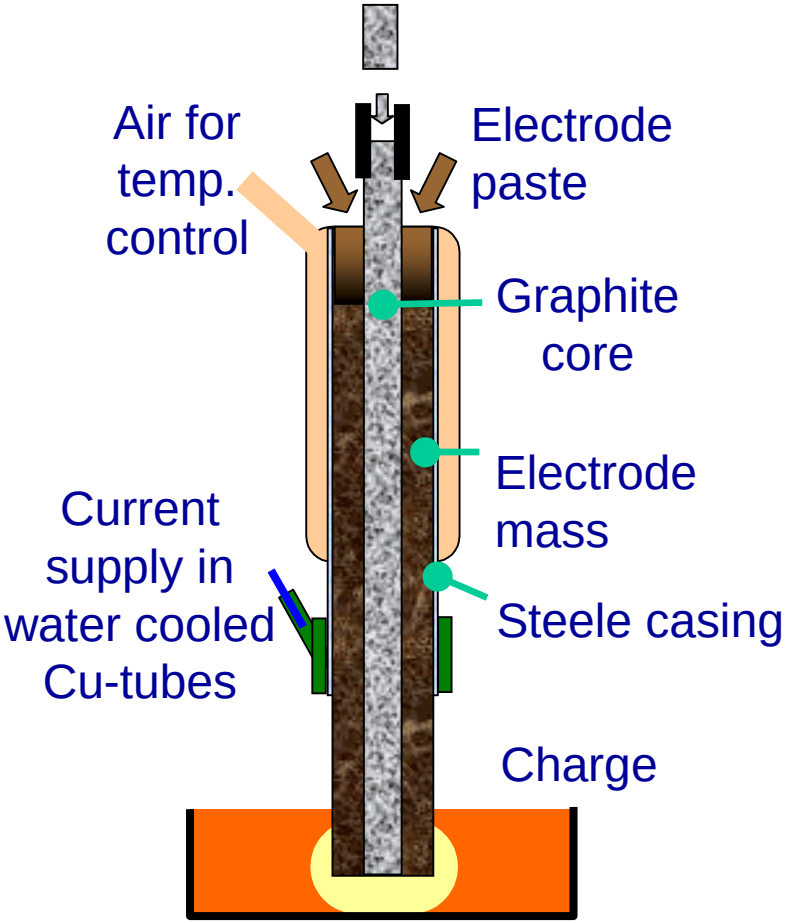
- first order PDE. Characteristics, shocks
- singular perturbatjons

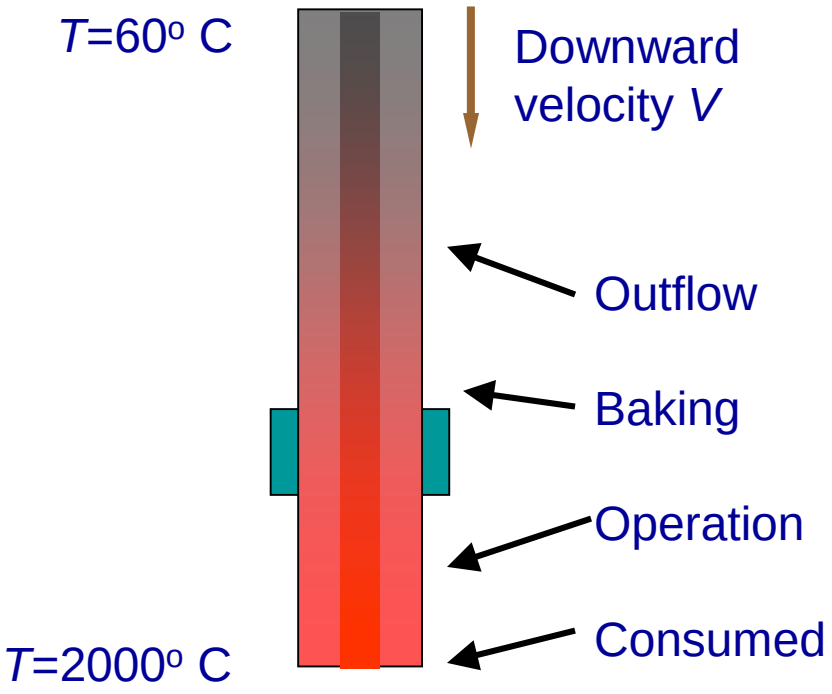


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THE SELF-BAKING ELECTRODE

(Provided by *Elkem Research, Norway)*





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Elkem asked us to consider the following two main problems:

(A) How can we “shape” the temperature isotherms in the upper region of the electrode when the slip velocity, *V*, and the temperature on the circulating air change?



(B) The current is entered radially into the electrode. Since the electric conductivity of the electrode paste is strongly temperature dependent, is it possible that this arrangement becomes unstable, that is, that one develops hot and cold regions in the electrode?

(For more info: See the *Proc. ECMI Modelling Week 2000* from Lund)

THE STUDENTS' EXPERIENCE:

Mathematics: Difficult methods applied to simple problems!

Modelling: Simple methods applied to difficult problems!

The future challenge is:

- *To teach the students to think before (and while) they compute!*

- *To teach the students to use the computer tools in a meaningful way ("The numerical laboratory")*

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