What is Mathematical Modelling?

John Stockie

CFD Research Group Meeting

http://www.math.sfu.ca/~stockie/research/cfdgroup.html

May 21, 2014

Outline

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What is a "model"?

- The word **model** has many different meanings:

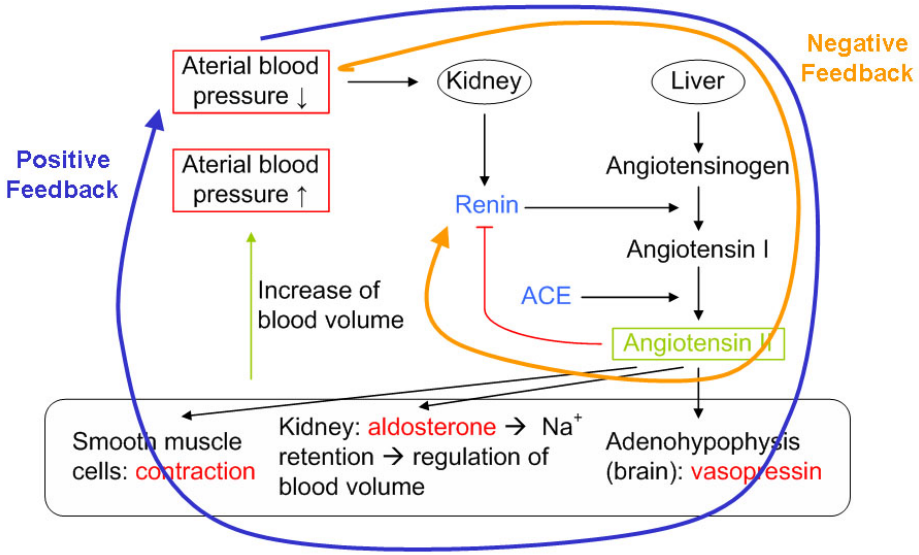
mod·el (mŏd′l)
n.

1. A small object, usually built to scale, that represents in detail another, often larger object.
2.
a. A preliminary work or construction that serves as a plan from which a final product is to be made: *a clay model ready for casting.*
b. Such a work or construction used in testing or perfecting a final product: *a test model of a solar-powered vehicle.*
3. A schematic description of a system, theory, or phenomenon that accounts for its known or inferred properties and may be used for further study of its characteristics: *a model of generative grammar; a model of an atom; an economic model.*
4. A style or design of an item: *My car is last year's model.*
5. One serving as an example to be imitated or compared: *a model of decorum.* See Synonyms at ideal.
6. One that serves as the subject for an artist, especially a person employed to pose for a painter, sculptor, or photographer.
7. A person employed to display merchandise, such as clothing or cosmetics.
8. *Zoology* An animal whose appearance is copied by a mimic.

- Even when restricted to the scientific endeavour (#3) the number of shades of meaning is *huge*, which can lead to confusion!
- In the literature, the use of "model" varies greatly depending on discipline . . .

Model for an experimentalist (biologist, chemist, . . .)

conceptual or biological or chemical model $\Longrightarrow$ hypothesis or picture (to explain experimental observations)



doi:10.2136/sssaj1984.03615995004800040015x

A Chemical Model of Phosphate Adsorption by Soils: I. Reference Oxide Minerals

Sabine Goldberg and Garrison Sposito

Abstract

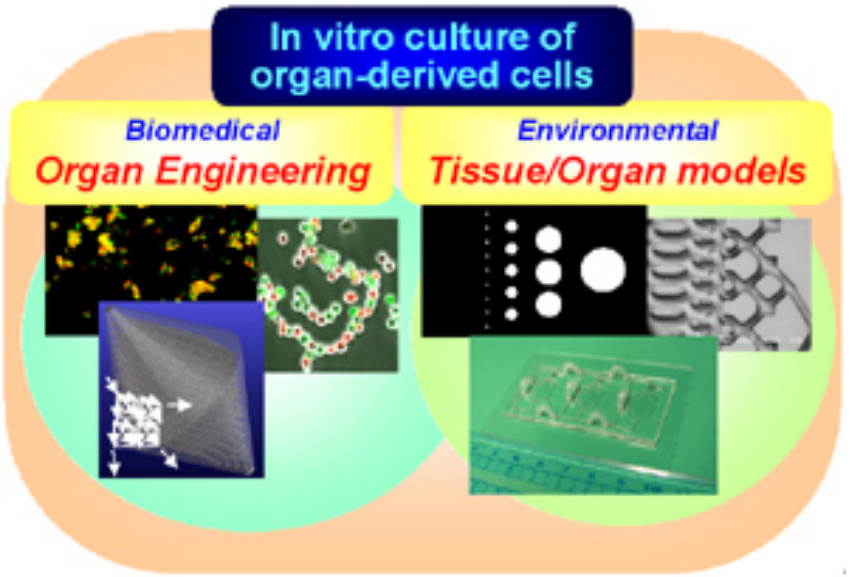
The Constant Capacitance model is shown to provide a quantitative description of *o*-phosphate adsorption by a variety of aluminum and iron hydrous oxides, including the effect of varying pH values. This model, based on a ligand exchange mechanism for *o*-phosphate adsorption, comprises six adjustable parameters: two surface protonation-dissociation constants, three *o*-phosphate surface complexation constants, and a capacitance density parameter. The five surface equilibrium constants can be obtained from potentiometric titration data and *o*-phosphate adsorption data. These constants are independent of pH but, in principle, can depend on the composition of the background electrolyte solution. The capacitance density parameter cannot be obtained directly from experiment. A working value can be chosen on the basis of previous applications of the Constant Capacitance model and other model parameters are not sensitive to this choice.

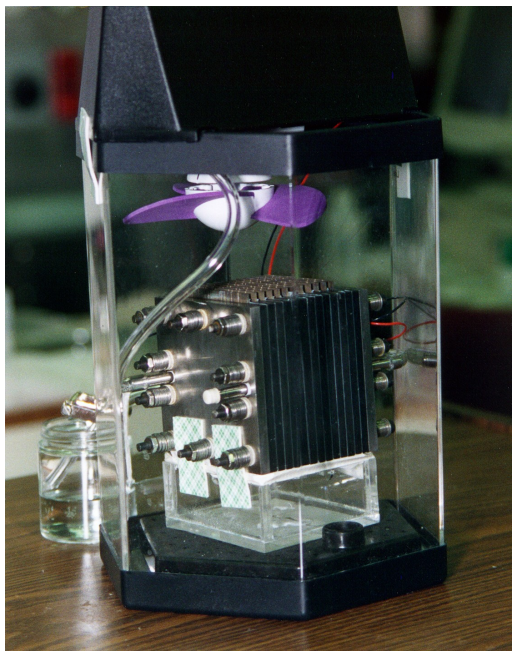
Model for (some) engineers

experimental or engineering model or system

$\Longrightarrow$

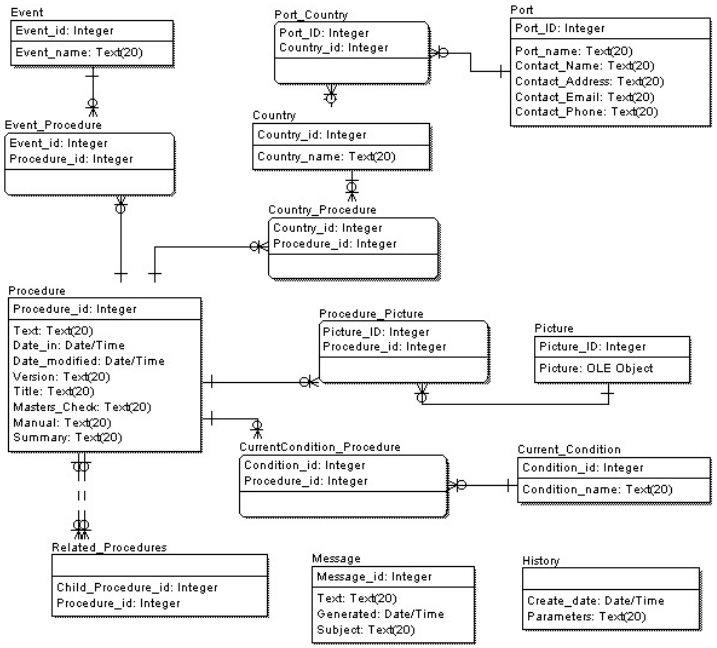
device that mimics a more complex one





Model for a software engineer

software model $\Longrightarrow$ system description via modelling language, diagrams or graphs (model theory)



What is a Model?

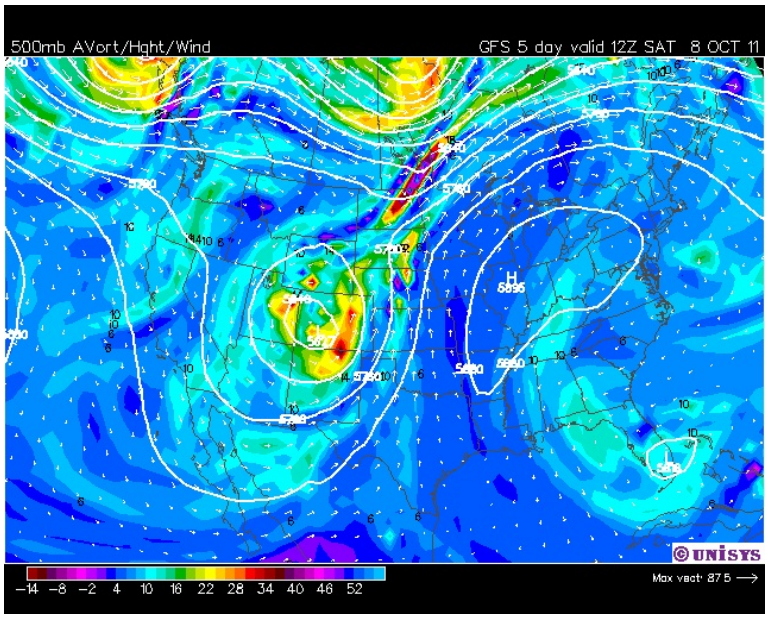
Thomas Kühne[1]

Darmstadt University of Technology, Darmstadt, Germany
kuehne@informatik.tu-darmstadt.de

Abstract. With the recent trend to model driven development a commonly agreed notion of "model" becomes a pivotal issue. However, currently there is little consensus about what exactly a model is and what it is not. Furthermore, basic terms such as "metamodel" are far from being understood in the same way by all members of the modeling community. This article attempts to start establishing a consensus about generally acceptable terminology. Its main contribution is the distinction between two fundamentally different kinds of models, i.e. "type model" versus "token model". The recognition of the fundamental difference in these two kinds of models is crucial to avoid misunderstandings and unnecessary disputes among members of the modeling community.

Model for a computational scientist/engineer

numerical or computational model $\Longrightarrow$ computer code that simulates a real system



Chemical Engineering Science
Volume 54, Issues 13–14, July 1999, Pages 2217–2226
ELSEVIER

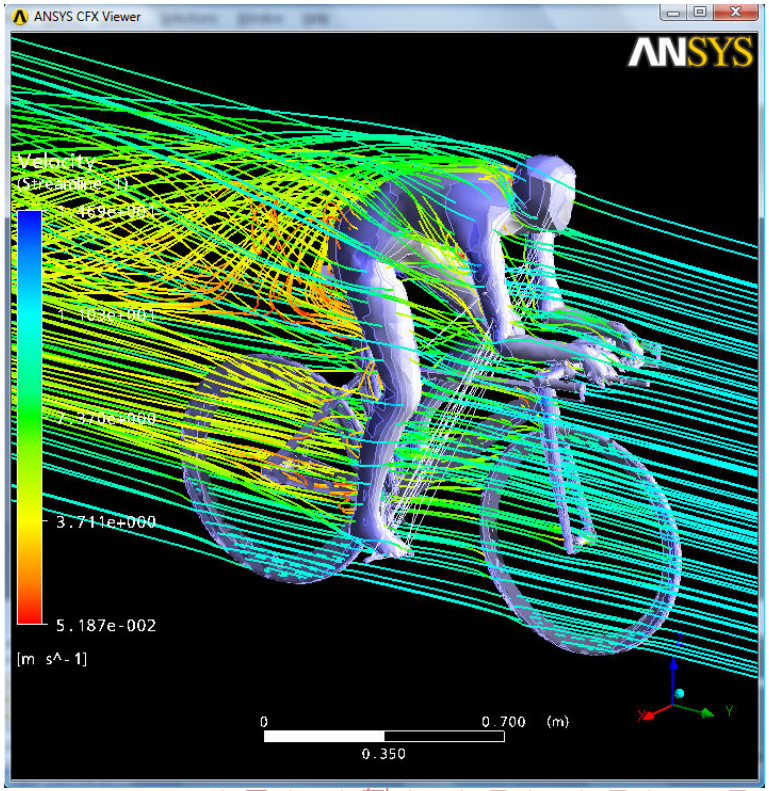
A three-dimensional CFD model for gas–liquid bubble columns

E. Delnoij, J.A.M. Kuipers, W.P.M. van Swaaij
Department of Chemical Engineering, Twente University, P.O. Box 217, 7500 AE Enschede, Netherlands

Numerical or computational models:

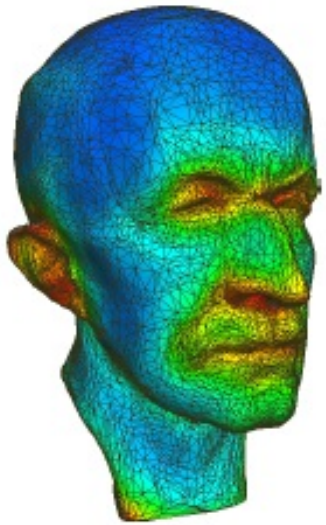
- Similar to mathematical models in that they are based on mathematical equations implemented in code.
- Focus is much more on expert use of code, understanding assumptions and limitations, and fiddling with parameters.

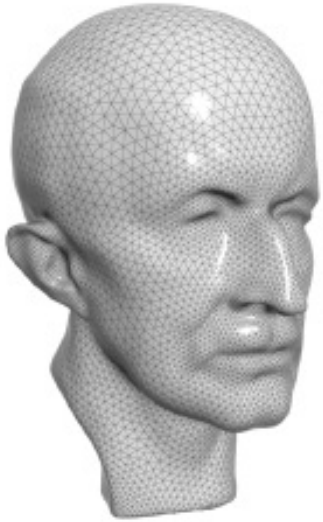
Example (CFD modelling): Running a commercial CFD code involves defining problem geometry (CAD) and selecting physical and numerical parameters. The underlying equations are well-known.



Model for a computer graphics or animation expert

3D model or graphical model $\Longrightarrow$ mathematical representation of a 3D surface or object





Model for a statistician

statistical model $\Longrightarrow$ fitting to a curve or distribution, parameter estimation

IEEE SIGNAL PROCESSING LETTERS, VOL. 6, NO. 1, JANUARY 1999 1

A Statistical Model-Based Voice Activity Detection

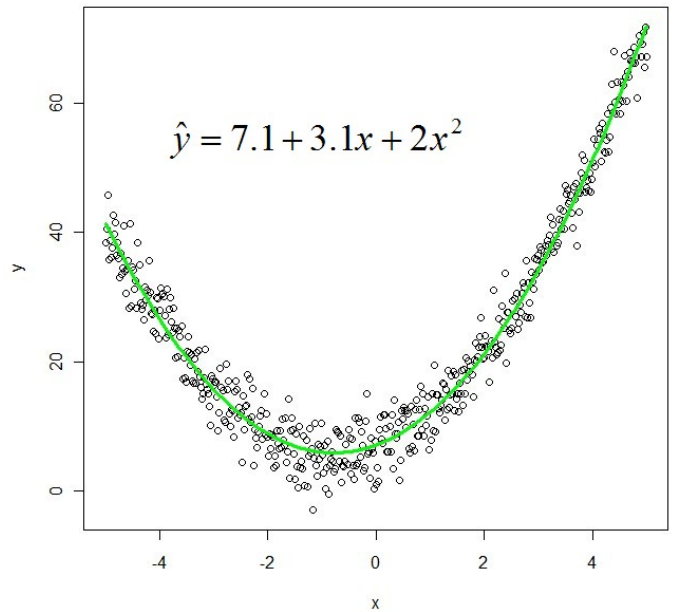
Jongseo Sohn, *Student Member, IEEE,* Nam Soo Kim, *Member, IEEE,* and Wonyong Sung

***Abstract*— In this letter, we develop a robust voice activity detector (VAD) for the application to variable-rate speech coding. The developed VAD employs the decision-directed parameter estimation method for the likelihood ratio test. In addition, we propose an effective hang-over scheme which considers the previous observations by a first-order Markov process modeling of speech occurrences. According to our simulation results, the proposed VAD shows significantly better performances than the G.729B VAD in low signal-to-noise ratio (SNR) and vehicular noise environments.**

***Index Terms*— Decision-directed estimation, hidden Markov model, likelihood ratio test, voice activity detection.**

where $\mathbf{S}$, $\mathbf{N}$, and $\mathbf{X}$ are L dimensional discrete Fourier transform (DFT) coefficient vectors of speech, noise, and noisy speech with their kth elements S_k, N_k, and X_k, respectively. We adopt the Gaussian statistical model that the DFT coefficients of each process are asymptotically independent Gaussian random variables [3]. Then the probability density functions conditioned on H_0 and H_1 are given by

$$p(\mathbf{X}|H_0) = \prod_{k=0}^{L-1} \frac{1}{\pi\lambda_N(k)} \exp\left\{-\frac{|X_k|^2}{\lambda_N(k)}\right\} \quad (1)$$



Other uses of the word model

- Theoretical model = hypothesis
- Data model = data structure (in computer science)
- Climate model = massive climate code (in geosciences)
- Other (non-scientific) uses listed in Wikipedia:
  - Mental model
  - Metaphysical model
  - Logical model
  - Epistemlological model
  - etc.

Painfully overloaded use of "model"

In a paper by McCray, Nieber, Poeter (2008), the word model is used in so many different ways it's confusing and even painful!

- "An analytical model is a closed form mathematical solution" (approximate solution to PDE)
- "Conceptual model for the analytical solution" (a figure)
- "Numerical models discretize the flow domain into subdomains of space and time" (discretized PDE)
- "The errors associated with theoretical considerations of an analytical model described previously, however, are probably less severe than errors associated with using incorrect values for hydraulic conductivity in the analytical model" (yikes)

tool = solution = model ?

8. Groundwater Mounding in the Vadose Zone from On-Site Wastewater Systems: Analytical and Numerical Tools.

By: McCray, John E.; Nieber, John; Poeter, Eileen P. ***Journal of Hydrologic Engineering***. Aug2008, Vol. 13 Issue 8, p710–719. 10p. 3 Diagrams, 1 Chart, 6 Graphs. DOI: 10.1061/(ASCE)1084–0699(2008)13:8(710).

Outline

What is a mathematical model?

There are many, many definitions of mathematical model:

- Wikipedia: *"A description of a system using mathematical concepts and language."* **(too vague)**
- Vahid Dabbaghian (2013): *"A principled activity that has both principles behind it and methods that can be successfully applied."* **(Huh?)**
- Rutherford Aris (1978): *"Any complete and consistent set of mathematical equations which is thought to correspond to some other entity, its prototype."* **(fantastic book!)**
- Jeremy Gunawardena (2014): *"A logical machine for converting assumptions into conclusions."*
- Gerda de Vries (2001, paraphrased): *"The use of mathematics to describe and explain real-world phenomena, investigate important questions about the observed world, test ideas, and make predictions."*

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What is a mathematical model?

There is no perfect definition of "mathematical model" but . . .

My choice:

"A well-posed system of equations that describes a real system."

Quotes

- George Box (1987): *"The fact that [the model] is an approximation does not necessarily detract from its usefulness because models are approximations. All models are wrong, but some are useful."*
- J.R. Philip (1966): *"A model is a useful (and often indispensible) framework on which to organize our knowledge about a phenomenon . . . It must not be overlooked that the quantitative consequences of any model can be no more reliable than the a priori agreement between the assumptions of the model and the known facts about the real phenomenon. When the model is known to diverge significantly from the facts, it is self-deceiving to claim quantitative usefulness for it by appeal to agreement between a prediction of the model and observation."*
- David Levermore (PIMS-CSC seminar, 2014): *"A model can be viewed as a form of data compression, and simulation is a method for decompressing or unpacking the data."*

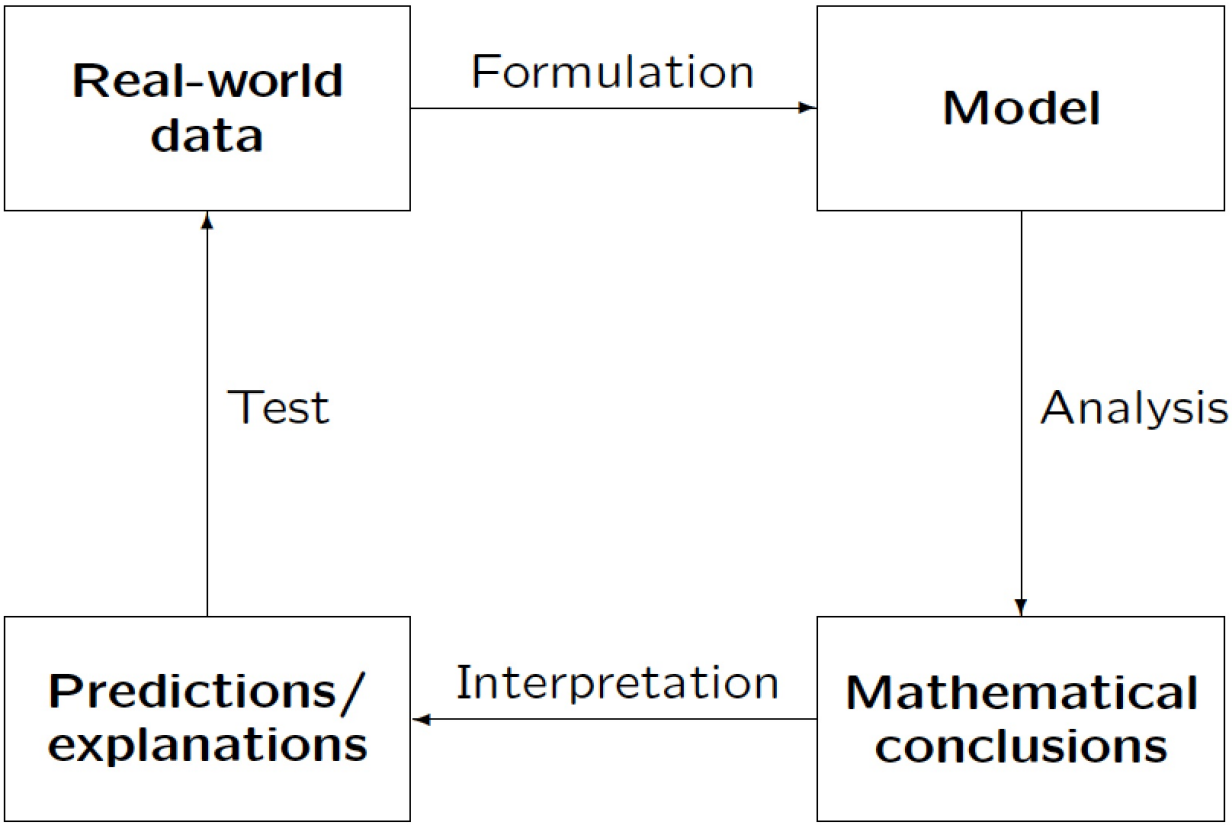
More quotes

- Gerda de Vries (2001): *"A modeller undertakes experiments on mathematical representations of the real world."*
- Howard Emmons: *The challenge in mathematical modelling is "not to produce the most comprehensive descriptive model but to produce the simplest possible model that incorporates the major features of the phenomenon of interest."* **(see Gunawardena)**
- Reinhard Illner et al. (2005): *"Mathematical modelling is a subject without boundaries in every conceivable sense."*
- Andrew Fowler (1997): *"Mathematical modelling is a subject that is difficult to teach . . . one learns it by practice: There are no set rules, and an understanding of the 'right' way to model can only be reached by familiarity with a wealth of examples."*

Fowler's modelling process

1. Problem identification
2. Model formulation
3. Analysis
4. Computation
5. Model validation

Process of mathematical modelling



Source: de Vries (2001)

A better process diagram

A more philosophical view of modelling

- A mathematical model is the mathematical structure that ties the specific situation back into a more general theory
- Its validity as an "explanation" of what is going on in the given situation rests on the tripod of:
  1. the adequacy of its representation of the situation
  2. its internal correctness
  3. the acceptability of the general theory which is involved

Source: Aris and Penn, "The mere notion of a model" *Mathematical Modelling*, 1:1-12, 1980.

Outline

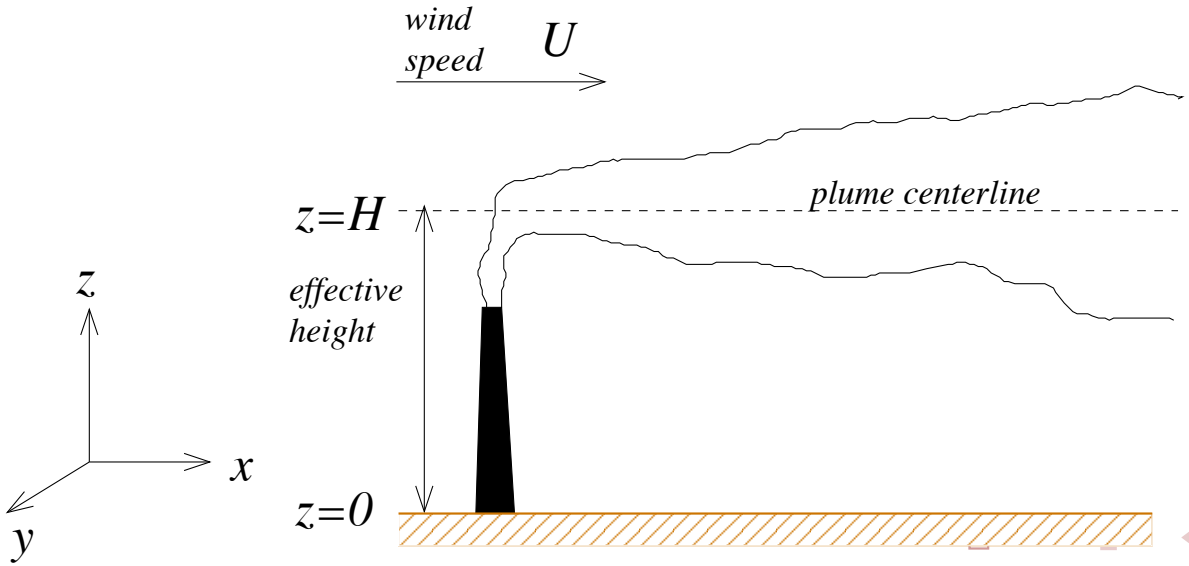
Example 1: Atmospheric dispersion modelling

- Transport of a contaminant by advection and diffusion.
- Governing equations are very well-understood:

$$\vec{u} \cdot \nabla C = \nabla \cdot (K \nabla C) + Q\,\delta(x)\,\delta(y)\,\delta(z - H)$$

- Gaussian plume solution:

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]$$



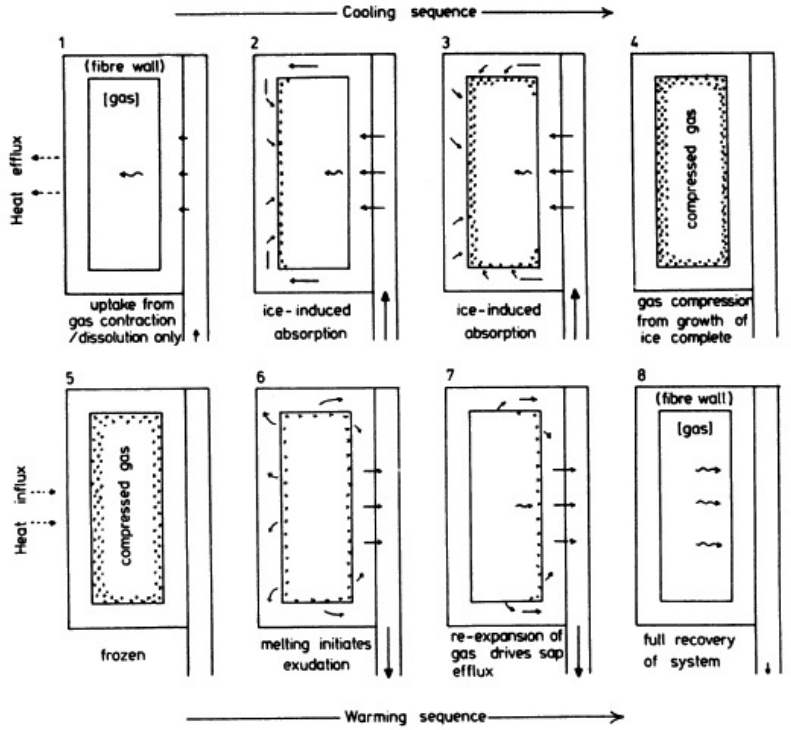
Example 1: Atmospheric dispersion modelling

Aim: Given measurements of C, find Q.

- We used the Gaussian plume solution to develop a very efficient inverse solver.
- Most effort was expended initially in fitting parameters.
- Our results were in excellent agreement with current emission estimates.
- Currently developing a much more accurate and robust inversion approach (Bamdad).

Example 2: Maple sap exudation

- **Mystery:** Maple trees exude sap in winter with no leaves or root uptake.
- Leading hypothesis due to Milburn-O'Malley assumes a combination of:
  - multiphase flow of liquid and gas
  - freezing and thawing sap (Stefan problem)
  - dissolving gas (Henry's law)
  - porous flow through cell walls (Darcy's Law)
  - osmotic pressure across selectively permeable membranes



Example 2: Maple sap exudation

- Writing down a consistent set of equations for the freezing process alone took Maurizio and I almost a full year!
- Tyree's challenge (1983): *"There is insufficient quantitative information to set up a system of physical equations."* **(wrong)**
- Indeed, we had to introduce several corrections/additions to the Milburn-O'Malley hypothesis to get things to work

$\Longrightarrow$ this is the real value of a mathematical model!

Outline

Conclusions

- Be careful how you use the word model, paying attention to your audience.
- If you want to succeed at modelling, then you should:
  1. absorb as much mathematics as you can;
  2. step outside your comfort zone and become an expert on non-math subject(s), or at least collaborate with such an expert.
- Being a mathematical generalist affords you valuable opportunities to study an enormous variety of physical and biological problems.
- Remember that no model is perfect, so always be critical of your assumptions and carefully validate them.

What next?

In a few weeks, I'll get deeper into the topic of mathematical modelling with

Challenges and Opportunities in
"Mathematics For Industry"

(lecture at CAIMS meeting)

Closing remarks

Aris and Penn (1980) on modelling as craftsmanship:

What goes on in the modeller's head is not purely formalizable . . . Nor is it purely subjective . . . It has structure, it has techniques that can be taught and learned, but involves also a personal touch, not only in trivialities (such as the choice of notation) but in deeper considerations of skill and suitability. It also involves an element of risk, since a wrong turn in the development of a model may lead to its complete stultification. Like the furniture maker, the mathematical modeller shapes the several parts of his work and fits them together. If one is marred or misshapen it must be reworked or even discarded and replaced."

Aris was a true master of the English language, and is a real joy to read!

stul·ti·fy (stŭl′tə-fī′)
tr.v. **stul·ti·fied, stul·ti·fy·ing, stul·ti·fies**
1. To render useless or ineffectual; cripple.
2. To cause to appear stupid, inconsistent, or ridiculous.
3. *Law* To allege or prove insane and so not legally responsible.

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