‘MODELLING FOR GEOCHEMISTS’
EVERYTHING YOU ALWAYS WANTED TO KNOW ABOUT MODELLING, BUT WERE AFRAID TO ASK!

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INTRODUCTION

During previous SWIM’s, we noted some of the modellers lacked the knowledge to fully appreciate the papers of the chemists and the other way round. To make the papers of the other ‘root’ of our work better understandable, the 17th SWIM included two parallel lectures. In this one, the practise of modelling will be explained to those usually concerned with chemistry. The other course explains the basics of hydrogeochemical studies to the modellers.

This is not a ‘regular’ paper. Instead of writing text, I preferred to hand in my presentation sheets as a paper. This paper should give a refreshing view on the subject. In my opinion, this time sheets are better than words. No bullshit and to the (power)point!! I hope anyone who reads this, will know the ins and outs of groundwater modelling.

Modelling for Chemists

• Modelling protocol
• Discretisation Partial Differential Equation (PDE)
• Groundwater flow: MODFLOW
• Solute transport: MOC3D

Difficult to determine target group for this lecture
No density differences considered
I like equations, so don’t be shocked by the PDEs
45 min.: not enough to understand it all completely
These sheets will be available

The Hydrological Circle

Ten steps of the Modelling Protocol
1. Problem definition
2. Purpose definition
3. Conceptualisation
4. Selection computer code
5. Model design
6. Calibration
7. Verification
8. Simulation
9. Presentation
10. Postaudit
MODELLING PROTOCOL

Why numerical modelling?

+: • cheaper than scale models
  • analysis of very complex systems is possible
  • a model can be used as a database

-: • simplification of the reality
  • only a tool, no purpose on itself
  • garbage in = garbage out: (field)data important
  • perfect fit measurement and simulation is suspicious

Modelling protocol

IMPORTANT

3. Conceptualisation (I)

Model is only a schematisation of the reality

Which hydro(geo)logical processes are relevant?

Which processes can be neglected?

Boundary conditions

Variables and parameters:
  • subsoil parameters
  • fluxes in and out
  • initial conditions
  • geochemical data

Mathematical equations

3. Concept (II): example of salt water intrusion

Relevant processes:
  • groundwater flow in a heterogeneous porous medium
  • solute transport
  • variable density flow
  • natural recharge
  • extraction of groundwater

Negligible processes:
  • heat flow
  • swelling of clayey aquitard
  • non-steady groundwater flow

Boundary conditions
  • no flow at bottom
  • flux in dune area
  • constant head in polder area

4. Selection computer code

There are numerous good groundwater computer codes!

See internet, e.g.:

USGS: water.usgs.gov/nrp/gwsoftware/

Scientific Software Group: www.scisoftware.com/

Groundwater computer codes

Mathematical models
  • Scale model
  • Analog model
  • Discrete fracture model
  • Dual porosity model

Physical models
  • Two or more fluids
  • Solute transport
  • Heat transport
  • Salt water

Mathematical models
  • Deterministic
  • Stochastic

Direct computation
  • Inverse modelling

Saturated flow
  • Unsaturated flow
  • Coupled models

One fluid
  • Two or more fluids

Steady-state
  • Transient

1D
  • 2D
  • 3D

Only groundwater flow
  • Dissolved solutes
  • Heat transport

Porous media
  • Fractured rocks

5. Model design (I)

Choice grid $\Delta x$:
  • depends on natural variation in the groundwater system
  • concept model
  • data collection

Choice time step $\Delta t$:

Conditions:
  • initial conditions
  • boundary conditions:
    1. Dirichlet: head
    2. Neumann: flux, e.g., no flow
    3. Cauchy: mixed boundary condition
5. Model design (II): example

Geometry, subsurface parameters, boundary conditions

- Sand dunes
- Holocene aquitard
- Middle aquifer
- Phreatic aquifer
- Deep aquifer
- No flow boundary

Length of the geohydrologic system, [m]

- Depth with respect to N.A.P., [m]
- Sand dunes
- Holocene aquitard
- Middle aquifer
- Phreatic aquifer
- Deep aquifer
- No flow boundary

1000 1500 2000 2500 3000 3500 4000 4500 5000

6. Calibration (I)

Fitting the groundwater model: is your model okay?

- Trial and error
- Automatic parameter estimation/inverse modelling (PEST, UCODE)

6. Calibration (II): example

Measured and computed freshwater heads

- Measured freshwater head [m]
- Computed freshwater head [m]

7. Verification: testing the calibrated model

Verification problem: there is always a lack of data

8. Simulation

Simulation of scenarios

- Computation time depends on:
  - Computer speed
  - Size model
  - Efficiency compiler
  - Output format

9. Presentation

10. Postaudit

Postaudit: analysing model results after a long time

Anderson & Woessner (1992): four postaudits from the 1960s

Errors in model results are mainly caused by:
- Wrong concept
- Wrong scenarios
**DISCRETIZATION PDE**

I. Darcy’s law (1856)

\[
\Delta \phi = \frac{Q}{L} \left( \phi_2 - \phi_1 \right)
\]

Reference level \( Q \)

**Discretisation PDE**

\[ Q \propto \phi - \phi_i, \quad Q = \frac{1}{L}, \quad Q \propto A \Delta \phi \]

\( Q = KA \frac{\Delta \phi}{L} \) where \( K \) is hydraulic conductivity \([L/T]\)

II. Darcy’s Law

\[
q_i = -K \frac{\partial \phi}{\partial x}, \quad q_j = -K \frac{\partial \phi}{\partial y}, \quad q_k = -K \frac{\partial \phi}{\partial z}
\]

**Discretisation PDE**

Discretisation - PDE

**Continuity equation**: steady state

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho \frac{\partial q}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho \frac{\partial q}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho \frac{\partial q}{\partial z} \right) = 0
\]

**Discretisation PDE**

**Analogy physical processes**

- Groundwater flow: Darcy’s law
- Heat conduction: Fourier law
- Electrodynamic: Ohm’s law

**Discretisation PDE**

**Taylor series development**: steady state

Best estimate of \( \phi_{i+1} \) is based on \( \phi_i \)

\[
\phi_{i+1} = \phi_i + \Delta \phi \frac{\partial \phi}{\partial x} \left( \frac{1}{2} \frac{\partial \phi_{i+1}}{\partial x} + \frac{1}{6} \frac{\partial^3 \phi_{i+1}}{\partial x^3} + \frac{1}{12} \frac{\partial^3 \phi_{i+1}}{\partial x^2 \partial y} \right) + K
\]

If \( K \) is constant and \( \rho \) is constant then:

\[
\frac{\partial^2 \phi}{\partial x^2} = 0 \quad \text{Laplace equation}
\]

\[
\nabla^2 \phi = 0
\]
Groundwater flow equation = Flow equation (Darcy’s Law) Multiply with constant thickness D of the aquifer gives:

\[ \psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j} + \psi_{i+1,j-1} + \psi_{i+1,j+1} + \psi_{i-1,j+1} = \frac{1}{12}\Delta x^2 \frac{\Delta x^2}{\Delta x^2} \frac{\Delta x^2}{\Delta x^2} + K \]

**Fivepoint operator: constant head example (I)**

\[ \phi_{i,j} = \phi_{i-1,j} + \phi_{i+1,j} + \phi_{i,j-1} + \phi_{i,j+1} \]

**Fivepoint operator: example (II)**

\[ \phi_{i,j} = \phi_{i-1,j} + \phi_{i+1,j} + \phi_{i,j-1} + \phi_{i,j+1} \]

**Fivepoint operator: No-flow example (I)**

\[ \phi_{i,j} = \phi_{i-1,j} + \phi_{i+1,j} + \phi_{i,j-1} + \phi_{i,j+1} \]

**Non steady state groundwater flow equation**

Flow equation (Darcy’s Law) Non steady state continuity equation =

Groundwater flow equation

Multiply with constant thickness D of the aquifer gives:

\[ \psi_{i,j} = \psi_{i-1,j} + \psi_{i+1,j} + \psi_{i,j-1} + \psi_{i,j+1} \]

\[ W = \text{specific storage coefficient [} L^2 \text{]} \]

\[ W = \text{source-term} \]

\[ \text{Horizontal no-flow boundary} \]

**Boundary conditions**

BOUNDARY 1: no-flow near the mountains
BOUNDARY 2: linear from 100 m (near mountains) to 0 m (near sea)
BOUNDARY 3: constant seawater level of 0 m
BOUNDARY 4: no-flow

**Laplace equation in 2D**

\[ \nabla^2 \phi = 0 \Rightarrow \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \]

**Discretisation in x-direction (i)**

\[ \frac{\partial^2 \phi_{i,j}}{\partial x^2} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} \]

**Discretisation in y-direction (j)**

\[ \frac{\partial^2 \phi_{i,j}}{\partial y^2} = \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} \]

**If \( \Delta x \times \Delta y \)** then:

\[ \phi_{i+1,j} + \phi_{i-1,j} + \phi_{i+1,j+1} + \phi_{i+1,j-1} - \phi_{i,j} = 0 \]

\[ \phi_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1}}{4} \]

**Explicit numerical 1D solution**

One-dimensional non steady state groundwater flow equation:

\[ \frac{\partial^2 \psi}{\partial t^2} + \frac{\partial^2 \psi}{\partial x^2} = 0 \]

\[ q = -k \frac{\partial \psi}{\partial x} = 0 \]

\[ q = \frac{W}{S} \]

\[ W = \text{flow transmissivity} \left( \frac{L^2}{T} \right) \]

Properties:

- Direct solution
- Can be numerical instable
**MODFLOW**

**IMPORTANT**

**MODFLOW**

a modular 3D finite-difference ground-water flow model
(M.G. McDonald & A.W. Harbaugh, from 1983 on)
- USGS, 'public domain'
- non steady state
- heterogeneous porous medium
- anisotropy
- coupled to reactive solute transport
MOCE (Konikow et al, 1996)
MT3D, MT3DMS (Zheng, 1990)
RT3D
- easy to use due to numerous Graphical User Interfaces (GUI’s)
   - PMWIN, GMS, Visual Modflow, Argus One, Groundwater Vistas, etc.

**Nomenclature MODFLOW element**

- row \( i \)
- column \( j \)
- layer \( k \)
- \( NCOL \)
- \( NROW \)
- \( NLAY \)
- \( \Delta x \)
- \( \Delta y \)
- \( \Delta z \)
- \( \Delta x \) row direction
- \( \Delta y \) column direction
- \( \Delta x \) layer direction

**MODFLOW: start with water balance of one element \([i,j,k]\)**

**Continuity equation (I)**

\[
\sum Q_i = S_i \frac{\Delta \phi}{\Delta V}
\]

\(\text{In - Out = Storage}\)

\[
\frac{\partial}{\partial t} \left( k \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial \phi}{\partial z} \right) - W = S \frac{\partial \phi}{\partial t}
\]

\[
\sum Q_i = S_i \frac{\Delta \phi}{\Delta V}
\]

**Flow equation (Darcy’s Law)**

\[
Q = \text{surface} \times q = \text{surface} \times k \frac{\partial \phi}{\partial x}
\]

\[
Q_{i+1/2,j,k} = k_{i+1/2,j,k} \Delta V \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{\Delta x}
\]

where \( CR_{i+1/2,j,k} \) is the conductance \([L^2/T]\)
Groundwater flow equation

\[ Q_{i,j,k} = CR_{i,j,k} (\phi_{i-1/2,j,k} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} = CR_{i,j,k} (\phi_{i-1/2,j,k} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} = CC_{i,j,k} (\phi_{i,j-1/2} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} = CC_{i,j,k} (\phi_{i,j-1/2} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} = CV_{i,j,k} (\phi_{i,j,k-1/2} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} = CV_{i,j,k} (\phi_{i,j,k-1/2} - \phi_{i,j,k}) \]

\[ Q_{i,j,k} + Q_{i+1/2,j,k} + Q_{i,j+1/2,k} + Q_{i,j-1/2,k} + Q_{i,j,k+1/2} + Q_{i,j,k-1/2} = SS_{i,j,k} \frac{\phi_{i,j,k} - \phi_{i,j,k}^\prime}{\Delta V} \]

Boundary conditions in MODFLOW (I)

Example of a system with three types of boundary conditions

area where heads vary with time

aquifer boundary

area of constant head

Boundary conditions in MODFLOW (II)

For a constant head condition: IBOUND=0

For a no flow condition: IBOUND=0

For a variable head: IBOUND=0

Packages in MODFLOW

1. Well package
2. River package
3. Recharge package
4. Drain package
5. Evaporation package
6. General head package

Example of a system with three types of boundary conditions

1. Well package

\[ Q_{well} = Q_{i,j,k} \]

Example: an extraction of 10 m³ per day should be inserted in an element as

\[ Q_{ext} = -10 \]

(\( \text{in} = \text{positive} \))

2. River package (I)

river loses water

\[ Q_{riv} = KLW \left( \frac{\phi_{i,j,k} - \phi_{i,j,k}^\prime}{M} \right) \]

\[ Q_{riv} = KLW \left( \frac{\phi_{i,j,k} - \phi_{i,j,k}^\prime}{M} \right) \]

\[ Q_{riv} = KLW \left( \frac{\phi_{i,j,k} - \phi_{i,j,k}^\prime}{M} \right) \]

river gains water

2. River package (II)

Determine the conductance of the river in one element:

\[ C_{riv} = \frac{KLW}{M} \]

where \( C_{riv} \) is the conductance [L²/T] of the river
2. River package (III)

Leakage to the groundwater system

Special case:
if \( \phi_{i,j,k} < \text{RBOT} \), then 
\[ Q = C_m (\phi_{i,j,k} - \text{RBOT}) \]

3. Recharge package

\[ Q_{\text{rec}} = I \Delta x \Delta y \]

4. Drain package

\[ Q_{\text{drn}} = C_{\text{drn}} (\phi_{i,j,k} - d) \]

Special case:
if \( \phi_{i,j,k} + d \) then \( Q_{\text{drn}} = 0 \)

5. Evapotranspiration package

Evapotranspiration rate

\[ \text{ET rate} = 0 \]

Maximum ET rate

Evapotranspiration (ET)

6. General head boundary package

\[ Q_{\text{ghb}} = C_{\text{ghb}} (\phi_{i,j,k} - \phi_{\text{ghb}}) \]

Time indication MODFLOW

\[ \text{ITMUNI} = \begin{cases} 1: \text{second} \\ 2: \text{minute} \\ 3: \text{hour} \\ 4: \text{day} \\ 5: \text{year} \end{cases} \]
MOC3D

Solute transport equation

Partial differential equation (PDE):

\[ R_d \frac{\partial C}{\partial t} = D_{ij} \frac{\partial}{\partial x_i} \left( \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( CV_j \right) + \frac{(C-C_0)W}{Re} - R_d \lambda C \]

- change in concentration
- dispersion
- advection
- source/sink
- decay

- \( D_{ij} \): hydrodynamic dispersion \([L^2T^{-1}]\)
- \( R_d \): retardation factor \([-\] \)
- \( \lambda \): decay-term \([T^{-1}]\)

Solute transport equation: column test (I):

Pollutant distribution at \( t=0 \)

Solute transport equation: column test (II):

Pollutant distribution at \( t>0 \)

Solute transport equation: column test (III):

Advection-diffusion-dispersion-retardation

Hydrodynamic dispersion

\[
D_{ij} = \text{hydrodynamic dispersion} = \text{mechanical dispersion} + \text{diffusion}
\]

- mechanical dispersion:
  - tensor
  - velocity dependent

- diffusion:
  - molecular process
  - solutes spread due to concentration differences

Mechanical dispersion

Differences in velocity in the pore
Differences in velocity due to variation in pore-dimension
Differences in velocity due to variation in velocity direction
Method of Characteristics (MOC)

Solve the advection-dispersion equation (ADE)

\[
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( C V_j \right) + \frac{\partial}{\partial x_j} \left( \frac{C - C_0}{\rho} \right)
\]

Lagrangian approach:
Splitting up the advection part and the dispersion/source part:
- advection by means of a particle tracking technique
- dispersion/source by means of the finite difference method

Advantage of the approach of MOC?

It is difficult to solve the whole advection-dispersion equation in one step, because the so-called Peclet-number is high in most groundwater flow/solute transport problems.

(history form of the equation is dominant)

The Peclet number stands for the ratio between advection and dispersion

Procedure of MOC: advective transport by particle tracking

- Place a number of particles in each element
- Determine the effective velocity of each particle by (bi)linear interpolation of the velocity field which is derived from MODFLOW
- Move particles during one solute time step \( \Delta t_{\text{solute}} \)
- Average values of all particles in an element to one node value
- Calculate the change in concentration in all nodes due to advective transport
- Add this result to dispersive/source changes of solute transport

Steps in MOC-procedure

1. Determine concentration gradients at old timestep \( k-1 \)
2. Move particles to model advective transport
3. Concentration of particles to concentration in element node
4. Determine concentration gradients on new timestep \( k^* \)
5. Determine concentration in element node after advective, dispersive/source transport on timestep \( k \)

Causes of errors in MOC-procedure

1. Concentration gradients
2. Average from particles to node element, and visa versa
3. Concentration of sources/sinks to entire element
4. Empty elements
5. No-flow boundary: reflection in boundary

Stability criteria (I)

Stability criteria are necessary because the ADE is solved explicitly

1. Neumann criterion:

\[
\frac{D_{zz} \Delta t}{\Delta z^2} + \frac{D_{yy} \Delta t}{\Delta y^2} + \frac{D_{xx} \Delta t}{\Delta x^2} \leq 0.5
\]

\[
\Delta t \leq \frac{0.5}{\frac{D_{xx}}{\Delta x^2} + \frac{D_{yy}}{\Delta y^2} + \frac{D_{zz}}{\Delta z^2}}
\]

Reflection in boundary

2. Mixing criterion

Change in concentration in element is not allowed to larger than the difference between the present concentration in the element and the concentration in the source

\[
\Delta t \leq \frac{n b_{ij,k}}{Q_{ij,k}}
\]
3. Courant criterion

\[
0 < \frac{\Delta t}{\max} \leq \frac{\Delta x}{V_x}, \quad 0 \leq \frac{\Delta t}{\max} \leq \frac{\Delta y}{V_y}, \quad -1 \leq \frac{\Delta t}{\max} \leq \frac{\Delta z}{V_z}
\]

Additional information (good documentation):

MODFLOW: http://water.usgs.gov/nrp/gwsoftware/modflow.html
MODFLOW: http://water.usgs.gov/nrp/gwsoftware/moc3d/moc3d.html

FILES

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NUMERICAL DISPERSION

Numerical dispersion and oscillation

Derivation of numerical dispersion: 1D (I)
\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x}
\]
Discretisation: backwards in space, backwards in time

By means of Taylor series development:
\[
\frac{C_i^t - C_i^{t-1}}{\Delta t} = D \frac{C_{i+1}^t - 2C_i^t + C_{i-1}^t}{\Delta x^2} - V \frac{C_i^{t+1} - C_i^t}{\Delta x}
\]

Derivation of numerical dispersion: 1D (II)

Now Taylor series development with truncation errors:
\[
\frac{C_i^t - C_i^{t-1}}{\Delta t} = \frac{\partial C}{\partial t} - \frac{\partial^2 C}{\partial x^2} + O(\Delta t^2)
\]
\[
\frac{C_i^t - C_i^{t-1}}{\Delta x} = \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} + O(\Delta x^2)
\]
\[
\frac{C_i^t - 2C_i^{t+1} + C_{i+1}^t}{\Delta x^2} = \frac{\partial^2 C}{\partial x^2} + O(\Delta x^4)
\]

Neglect 3rd and 4th order terms:
\[
\frac{\partial C}{\partial t} - \frac{\partial^2 C}{\partial x^2} - V \left( \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right)
\]
Derivation of numerical dispersion: 1D (IV)

Rewriting term: \[ \frac{\partial^2 C}{\partial t^2} \]

\[ \frac{\partial^2 C}{\partial t^2} = \frac{\partial^2 C}{\partial x^2} - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) \]

\[ \frac{\partial^2 C}{\partial t^2} = \frac{\partial^2 C}{\partial x^2} - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) + V^2 \frac{\partial^2 C}{\partial x^2} \]

Derivation of numerical dispersion: 1D (V)

Rewrite all extra terms:

\[ \frac{\partial C}{\partial t} - \frac{\Delta t}{2} \frac{\partial^2 C}{\partial x^2} = D \left( \frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x} \frac{\partial^2 C}{\partial x^2} \right) - V \left( \frac{\partial C}{\partial x} - \frac{\Delta t}{2} \frac{\partial^2 C}{\partial x^2} \right) \]

\[ \frac{\partial C}{\partial t} - \frac{\Delta t}{2} \frac{\partial^2 C}{\partial x^2} = \frac{\partial^2 C}{\partial x^2} - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) - \frac{\partial}{\partial x} \left( \frac{D}{\partial x} \frac{\partial C}{\partial x} - \frac{\partial^2 C}{\partial x^2} \right) + V^2 \frac{\partial^2 C}{\partial x^2} \]

\[ \frac{\partial C}{\partial t} = \left( D + \frac{\Delta t}{2} \frac{\partial^2 C}{\partial x^2} \right) \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + V^2 \frac{\partial^2 C}{\partial x^2} \]

**IMPORTANT**

Derivation of numerical dispersion: 1D (VI)

Numerical dispersion:

\[ D = D_{\text{real}} + V \frac{\Delta t}{2} + \frac{\Delta x}{2} \]

Remedy to reduce numerical dispersion:

1. \( \Delta x \) en \( \Delta t \) smaller
2. Use a different numeric scheme (Crank-Nicolson)
3. Use a smaller \( D_{\text{real}} \)

**EVERYTHING YOU ALWAYS WANTED TO KNOW**

Modelling for Chemists

1. Everything you always wanted to know about modelling, and now you know it?
2. Everything you always wanted to know about modelling, and now you are definitely afraid to ask?

Additional information:


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