MODELLING & ASSESSMENT



Why?

Modelling

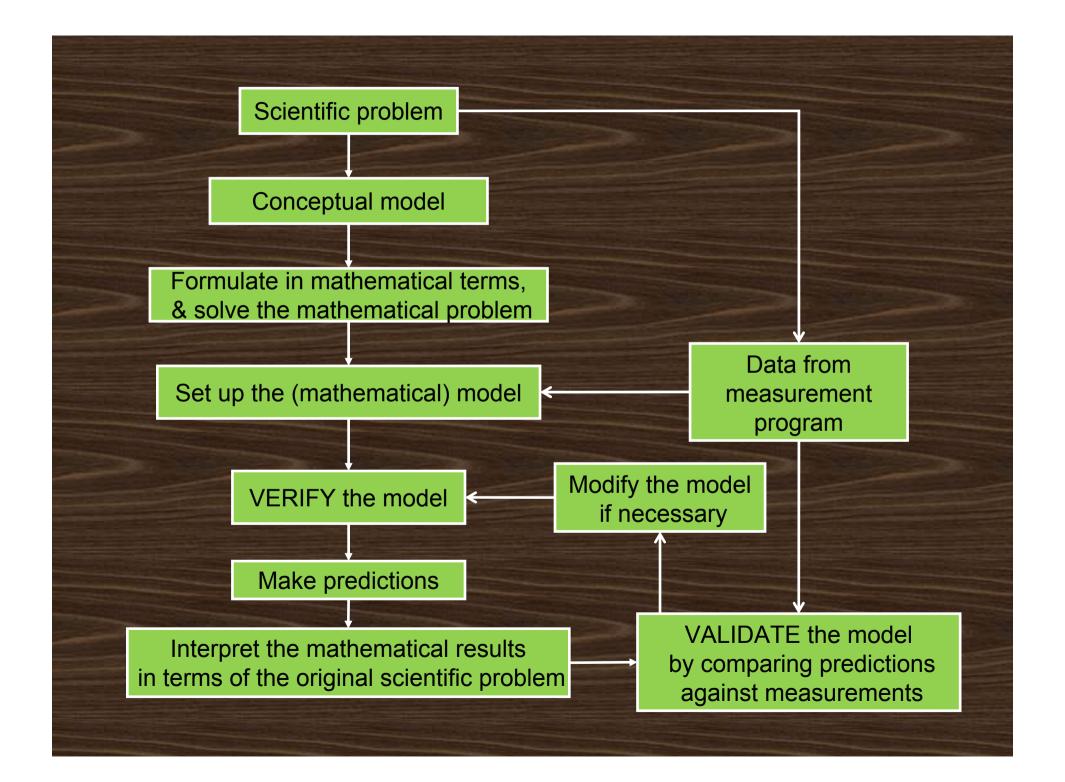
- Can't measure everything
- Need to make predictions when designing new facilities
- Assessment
 - Waste management and disposal
 - Compliance with regulatory requirements
 - Testing remediation strategies
 - Testing the design of new facilities

Problems

- Internal dosimetry
- Atmospheric dispersion
- Tailings dams
- General waste management strategies
- Waste repositories/dumps
- Landfill
- Discharges to lakes, rivers, ocean
- Legacy sites
- Planning/designing of new facilities

Mathematical modelling

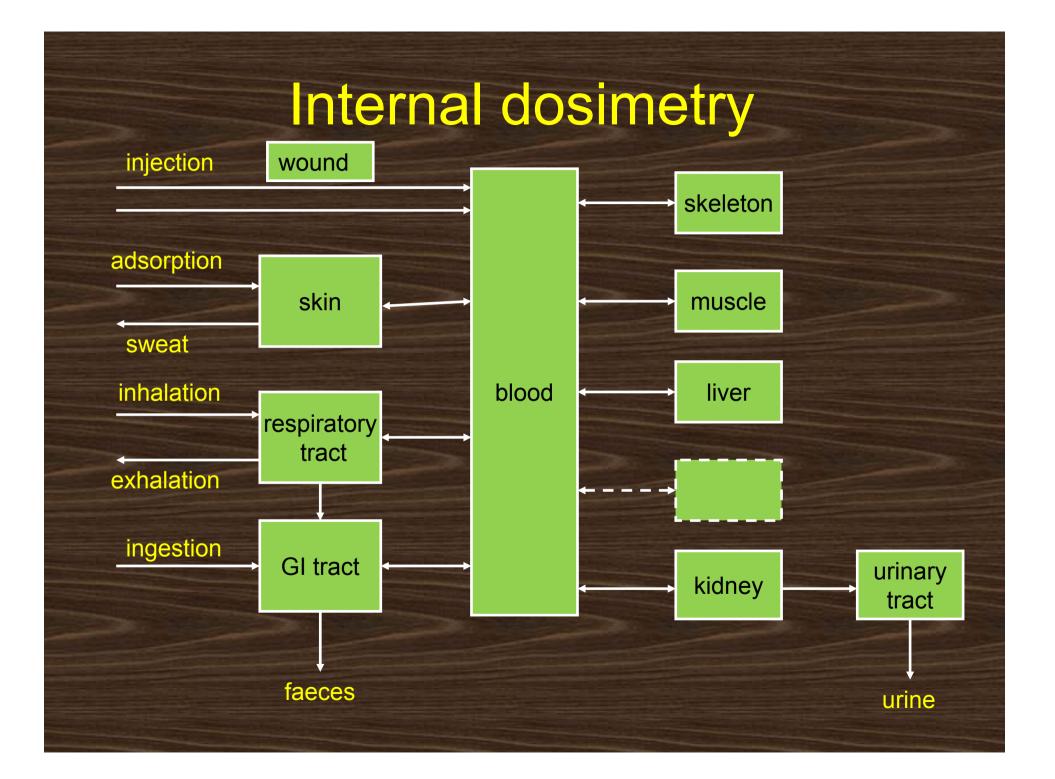
- Mathematics is a scientific discipline in its own right
- It is also an extremely useful tool for developing theories and models because it allows us to express ideas in very precise and concise terms, and because once the problem is formulated in mathematical terms all the power of the mathematics becomes available
- Once the mathematical problem is solved the results have to be converted back into the language of the original problem



Conceptual model

- Which processes to include (assumptions)
- Which processes to exclude (assumptions)
- Flow diagram

 Each assumption places some restrictions on the use of the model or on the interpretation of the model predictions



Compartment models

 For first-order, linear transfer between compartments, a compartment model for a single radionuclide can be described by the matrix-vector equation

$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{A}\mathbf{X} + \mathbf{P}$$

The general solution of this equation is

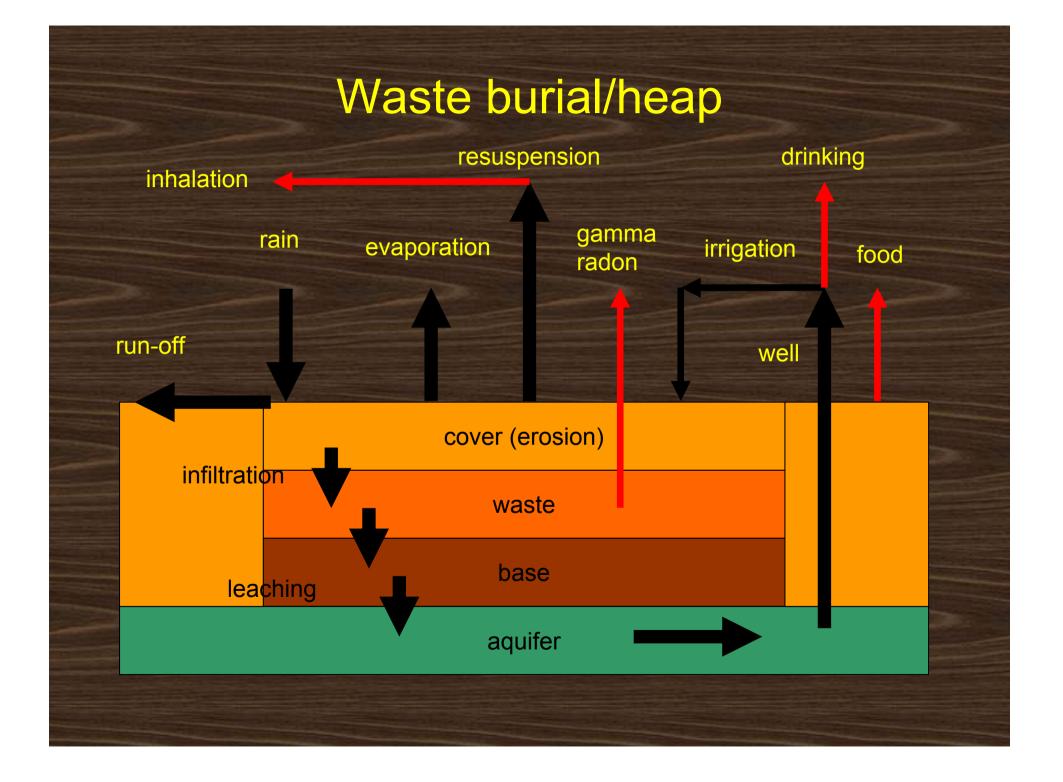
$$\mathbf{X}(t) = \mathbf{e}^{\mathbf{A}t} \mathbf{X}(0) + \left(\mathbf{e}^{\mathbf{A}t} - \mathbf{I}\right) \mathbf{P}$$

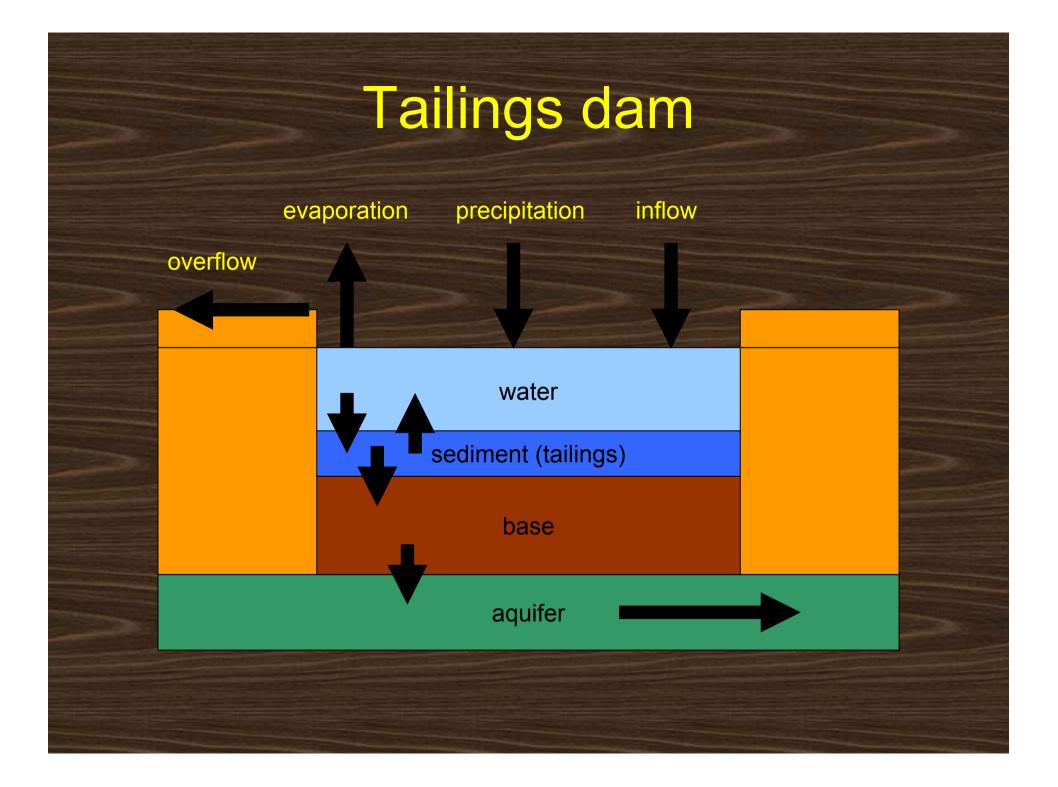
Mathematical problem: Serial decay chain of length N

Chain (non-branching) with different biokinetics

$$\frac{\partial}{dt} \begin{bmatrix} \mathbf{X}_{1} \\ \mathbf{X}_{2} \\ . \\ . \\ . \\ \mathbf{X}_{N} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \lambda_{1}\mathbf{I} & \mathbf{A}_{2} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \lambda_{2}\mathbf{I} & \mathbf{A}_{3} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & . & . & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & . & \lambda_{N-1}\mathbf{I} & \mathbf{A}_{N} \end{bmatrix} \begin{bmatrix} \mathbf{X}_{1} \\ \mathbf{X}_{2} \\ . \\ . \\ . \\ \mathbf{X}_{N} \end{bmatrix} + \begin{bmatrix} \mathbf{P}_{1} \\ \mathbf{P}_{2} \\ . \\ . \\ \mathbf{P}_{N} \end{bmatrix}$$

 This is actually the same equation as before, but written to show the relationship between the members of the decay chain





Fluid mechanics

General conservation equation

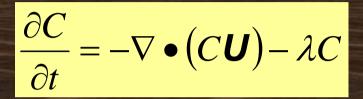
In any region the rate of change of a quantity (mass, momentum, angular momentum, energy) that can be considered to be conserved is given by an expression of the form

Rate of change in region = + rate of flow into region

+ rate of flow into region
- rate of flow out of region
+ rate of generation/loss within region by non-flow processes (chemistry, radioactive decay)

This approach is valid for both microscopic situations (e.g. the equations of classical fluid mechanics) or macroscopic situations (e.g. estimating radionuclide concentrations inside large slabs of material)

 Flow equation for a one-constituent fluid (conservation of mass)



Flow equation for a radioactive contaminant in a fluid

$$\frac{\partial C_a}{\partial t} = -\nabla \bullet \left(C_a \boldsymbol{U}_a \right) - \lambda_a C_a$$

• Fick's law (derived from experiment) states that

$$C_a \left(\boldsymbol{U}_{a} - \boldsymbol{U} \right) = -K_a \nabla C_a$$

The conservation of mass equation now becomes

$$\frac{\partial C_a}{\partial t} = -\nabla \bullet \left(C_a \boldsymbol{U} \right) + \nabla \bullet \left(K \nabla C_a \right) - \lambda C_a$$

This is a form of the diffusion equation

A more familiar form is

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} (UC) + \frac{\partial}{\partial y} (VC) + \frac{\partial}{\partial z} (WC) = \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right) - \lambda C$$

 If the fluid is homogeneous, and the coordinate system is oriented so that the fluid is flowing in the x-direction, then

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} + K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} - \lambda C$$

If the fluid is isotropic then

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K \frac{\partial^2 C}{\partial x^2} + K \frac{\partial^2 C}{\partial y^2} + K \frac{\partial^2 C}{\partial z^2} - \lambda C$$

- This equation can be used as the basis of models of atmospheric dispersion
 - Power stations
 - Ventilation shafts
- It can also be used for area sources

Porous media

• Put
$$C_{tot} = \varepsilon C + (\varepsilon' - \varepsilon)C_t + (1 - \varepsilon')C_s$$

- where
- ε' = total porosity (pore space/total space)
- ε = effective porosity (connected pore space/total space)
- C_{tot} = total concentration of contaminant
- C = concentration of contaminant in connected pores
- C_s = concentration of contaminant on pore surfaces
- C_t = concentration of contaminant in unconnected pores

Flow equation for a contaminant in a porous medium (the same balance approach as before) is

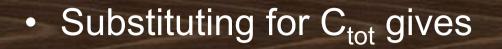
Rate of increase in a small volume ΔV = net rate at which flowing water brings contaminant into ΔV

- + net rate at which contaminant diffuses into ΔV
- rate at which contaminant decays in ΔV

This leads to

$$\frac{\partial C_{tot}}{\partial t} + U \frac{\partial (\varepsilon C)}{\partial x} = K_x \frac{\partial^2 (\varepsilon C)}{\partial x^2} + K_y \frac{\partial^2 (\varepsilon C)}{\partial y^2} + K_z \frac{\partial^2 (\varepsilon C)}{\partial z^2} - \lambda C_{tot}$$

which is the starting point for the discussion of groundwater transport of contaminants



$$\frac{\partial (\varepsilon C + (\varepsilon' - \varepsilon)C_t + (1 - \varepsilon')C_s)}{\partial t} + U \frac{\partial (\varepsilon C)}{\partial x}$$
$$= K_x \frac{\partial^2 (\varepsilon C)}{\partial x^2} + K_y \frac{\partial^2 (\varepsilon C)}{\partial y^2} + K_z \frac{\partial^2 (\varepsilon C)}{\partial z^2} - \lambda (\varepsilon C + (\varepsilon' - \varepsilon)C_t + (1 - \varepsilon')C_s)$$

- Assume that $C_t = C$
- This gives

$$\frac{\partial \left(\varepsilon'C + (1 - \varepsilon')C_{s}\right)}{\partial t} + U \frac{\partial (\varepsilon C)}{\partial x}$$
$$= K_{x} \frac{\partial^{2} \left(\varepsilon C\right)}{\partial x^{2}} + K_{y} \frac{\partial^{2} \left(\varepsilon C\right)}{\partial y^{2}} + K_{z} \frac{\partial^{2} \left(\varepsilon C\right)}{\partial z^{2}} - \lambda \left(\varepsilon'C + (1 - \varepsilon')C_{s}\right)$$

Partition coefficient K_d (the ratio of the concentration of contaminant on the pore surfaces to the concentration of contaminant in solution)

 $C_{s} = K_{d}C$

$$\frac{\partial \left(\varepsilon'C + (1 - \varepsilon')K_{d}C\right)}{\partial t} + U\frac{\partial (\varepsilon C)}{\partial x}$$
$$= K_{x}\frac{\partial^{2}(\varepsilon C)}{\partial x^{2}} + K_{y}\frac{\partial^{2}(\varepsilon C)}{\partial y^{2}} + K_{z}\frac{\partial^{2}(\varepsilon C)}{\partial z^{2}} - \lambda(\varepsilon'C + (1 - \varepsilon')K_{d}C)$$

Final step – retardation factor Put

$$\varepsilon' + (1 - \varepsilon')K_d = \varepsilon R$$

• Then

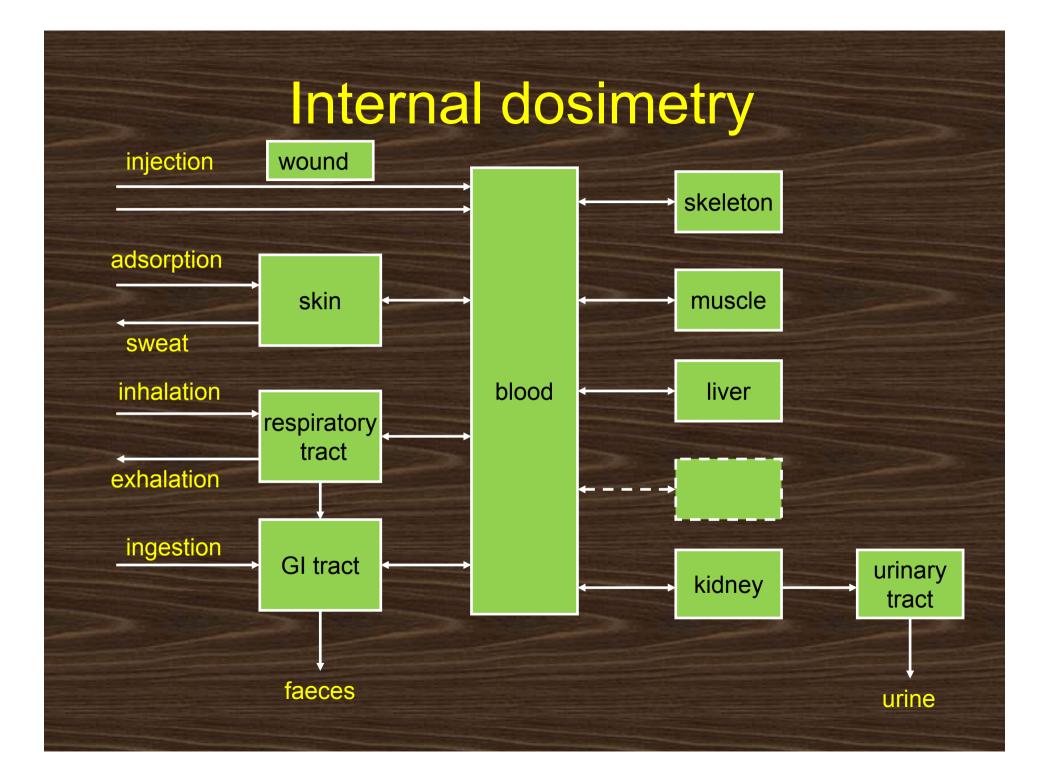
 $\frac{\partial C}{\partial t} + \frac{U}{R}\frac{\partial C}{\partial x} = \frac{K_x}{R}\frac{\partial^2 C}{\partial x^2} + \frac{K_y}{R}\frac{\partial^2 C}{\partial y^2} + \frac{K_z}{R}\frac{\partial^2 C}{\partial z^2} - \lambda C$

 $\frac{\partial C}{\partial t} + \frac{U}{R}\frac{\partial C}{\partial x} = \frac{K_x}{R}\frac{\partial^2 C}{\partial x^2} + \frac{K_y}{R}\frac{\partial^2 C}{\partial v^2} + \frac{K_z}{R}\frac{\partial^2 C}{\partial z^2} - \lambda C$

- This equation has exactly the same form as the atmospheric diffusion (fluid flow) equation - this means that the mathematical solutions of the porous medium equation have the same general form as those for the atmospheric diffusion equation
- For most radionuclides K_d >>1 and therefore R >> 1 which implies that the water moves through the porous medium much faster than the contaminant – again this is confirmed by measurement

ASSESSMENT

- Internal dosimetry
 - Dose calculations
 - Bioassay interpretation
 - Hiroshima, Maralinga
- Environmental impact assessment
 - Check on existing facilities
 - Design of new facilities
 - Checking waste management strategies
 - Checking remediation strategies for legacy sites
 - Hiroshima, Maralinga



Examples

- Consumption of sea-food containing Po-210
- Po-210 poisoning (London)
- Pu fabrication plant accident

Context (Po-210)

 The dose per unit intake for ingestion of Po-210 is approximate 1.2 µSv/Bq

 To get a dose of 1 Sv would require an intake of approximately 1 MBq

 The half-life of Po-210 is 138.4 days, so 1 MBq corresponds to 6 nano grams

Environmental impact assessment - context

- Only interested in the incremental dose resulting from the operation being considered
- Natural background is variable, on all scales
- Most (if not all) the models used for this work do not require any knowledge of the background levels

Assessment – near surface disposal of NORM waste • NORM – naturally occurring radioactive material

Hypothetical scenario

Issues that make NORM modelling complex

- Radionuclides
 - Very long-lived radionuclides
 - Long radioactive decay chains

Materials

- Large variations in the volume of material
- Wide range of radionuclide concentrations
- Many different types of material
 - Waste rock
 - Tailings
 - Sludges
 - Waste water

Issues that make NORM modelling complex

- Wide range of residues (phosphogypsum, red mud, fly ash, scales, uranium tailings...)
 - Low concentration, very large volume (mining)
 - High concentration, small volume (oil & gas)
- Wide range of situations for just one type of residue
 - Geography and geology, hydrogeology are highly variable from one site to another
- Wide range of sites
 - Operational sites
 - Legacy sites
- Recycling of NORM residues
 - Large volumes of material with low to intermediate radionuclide concentrations means that recycling is a potential disposal/management option in many cases

RESRAD

- RESRAD uses the Gaussian form of the analytical solution to the diffusion equation
 The flux core a curfore for a unit
- The flux across a surface for a unit concentration is calculated
- The actual flux can then be calculated for any concentration

Limitations (Assumptions)

- homogeneous fluid
- "slow" flow no turbulence
- very rapid adsorption-desorption (fine pores)

What RESRAD can do

- Buried (solid) waste
- Land fill (solid) waste
- Effects of surface water bodies
- Effects of groundwater flow
- Effects of irrigation
- Effects of barriers
- Radionuclide concentration calculations
- Dose calculations
- Assessment of existing situations
- Planning of remediation strategies for existing situations
- Planning for new waste repositories

What RESRAD cannot do

- Liquid wastes
- Tailings dams
- Lake sediment transfers (check)
- River sediment transfers (check)
- Highly irregular geometries

Setting up

 Work systematically through the input screens when first setting up a problem

Output files

Report form or graphical form
Data for graphs can be exported to EXCEL

File transfer

 Both RESRAD v6.3 and RESRAD-OFFSITE use a single file (.RAD and .ROF) for their input data – this makes it easy to send the input data to a colleague when problems are encountered.

Data required for radiological assessment

- Residue characteristics
 - Radionuclide concentrations on-site
 - "stack/source" dimensions
 - Distribution coefficients (K_d) for radionuclides in local soils and rocks
- Meteorological data
 - Wind speed and direction (annual)
 - Rainfall (annual)
- Radionuclide concentrations off-site (validation)
 - Drinking water, foodstuffs, soil, air.....

Data required for radiological assessment

- Hydrogeology saturated zone
 - Depth and thickness of aquifer
 - Type of material (gravel, sand, loam,....)
 - Hydraulic conductivity/Darcy velocity
 - Hydraulic gradient
 - K_d values
- Hydrogeology unsaturated zone
 - Depth and thickness of unsaturated zone there may be more than one
 - Type of material (gravel, sand, loam,....)
 - Hydraulic conductivity
 - K_d values

Data required for radiological assessment

Land use – present and future

- residential
- industrial
- agricultural
- recreational

Transfer factors

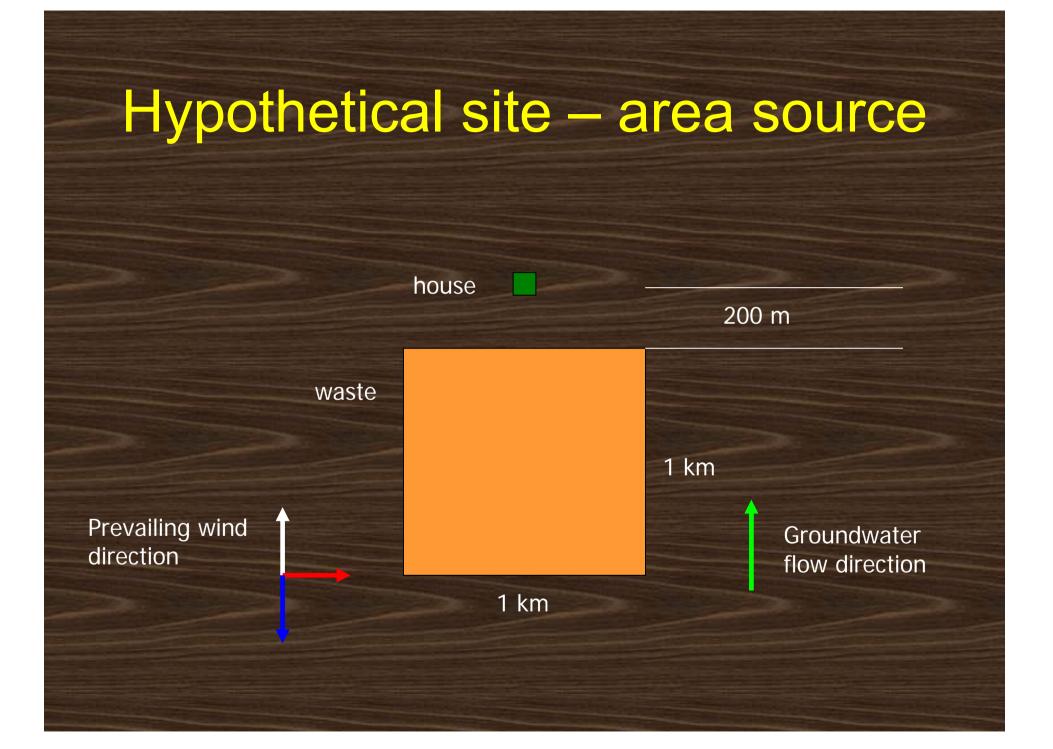
- soil/sediment/water to plant
- soil/sediment/water to animal/fish....
- plant to animal/fish....

Location of dwellings

- Dietary data for local inhabitants and regular visitors
- Time use data for local inhabitants and regular visitors

Water use

- Surface water
- Groundwater
- Irrigation
- Radionuclide concentrations in water



Vertical profile

cover (2m, "clean" soil)

waste (10m, clay)

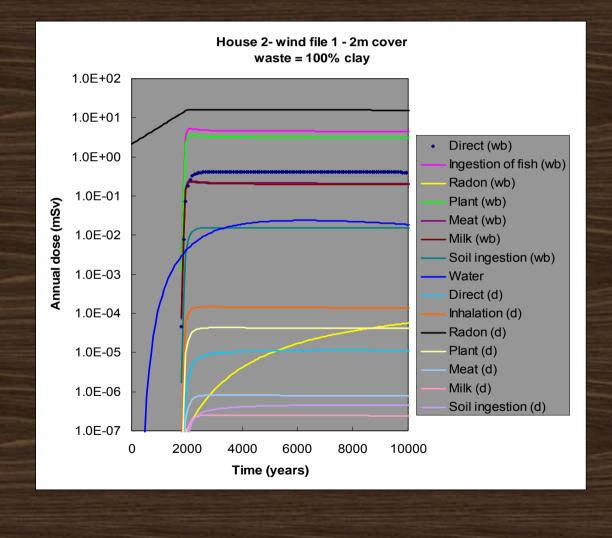
base (3m, 80% sand + 20% clay)

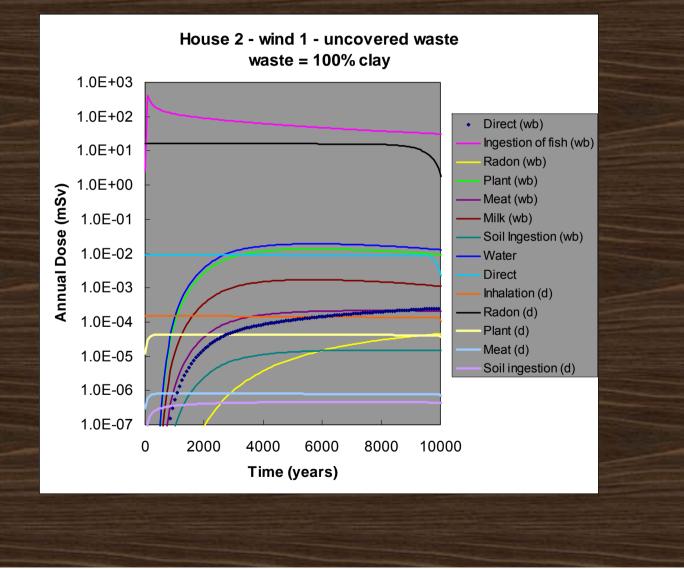
aquifer (15m, sand)

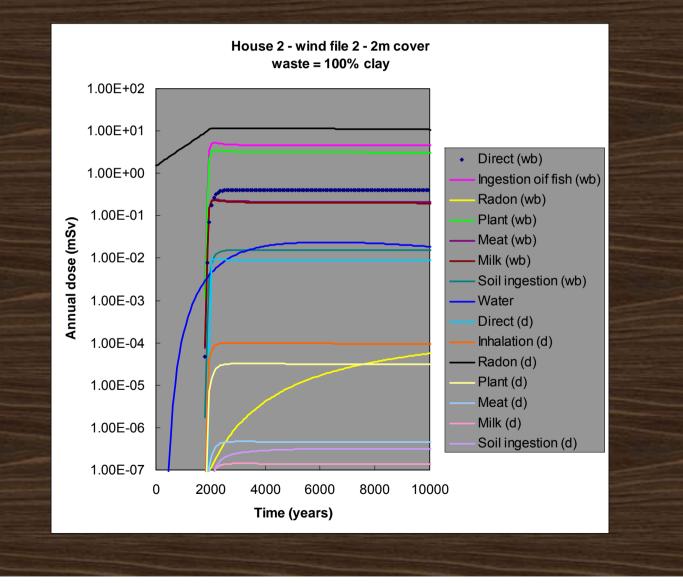
groundwater flow

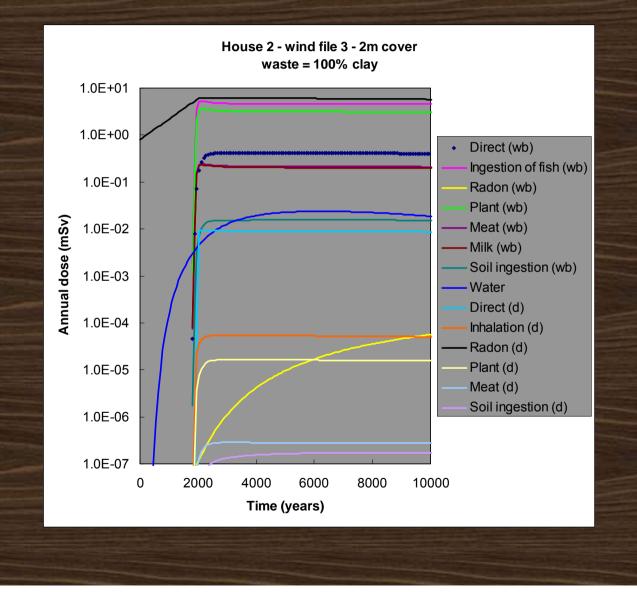


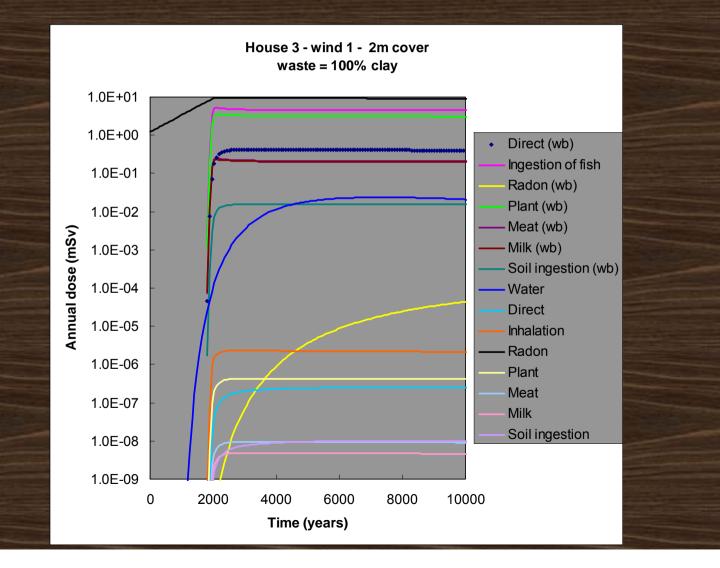
bedrock



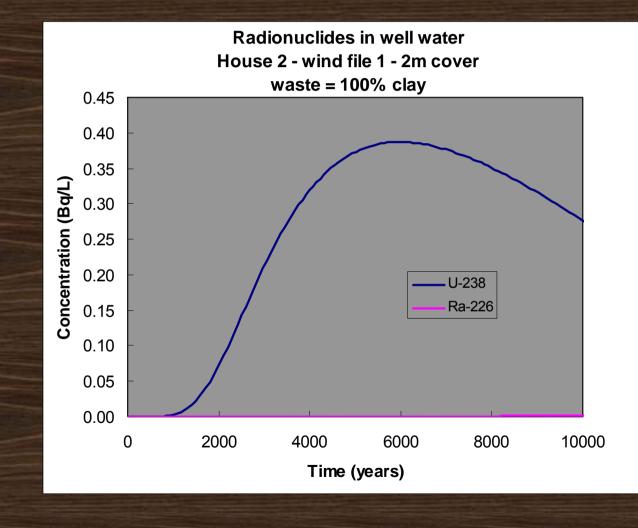




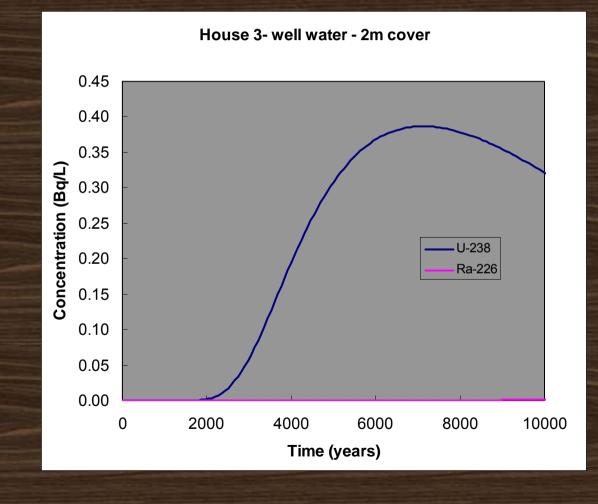


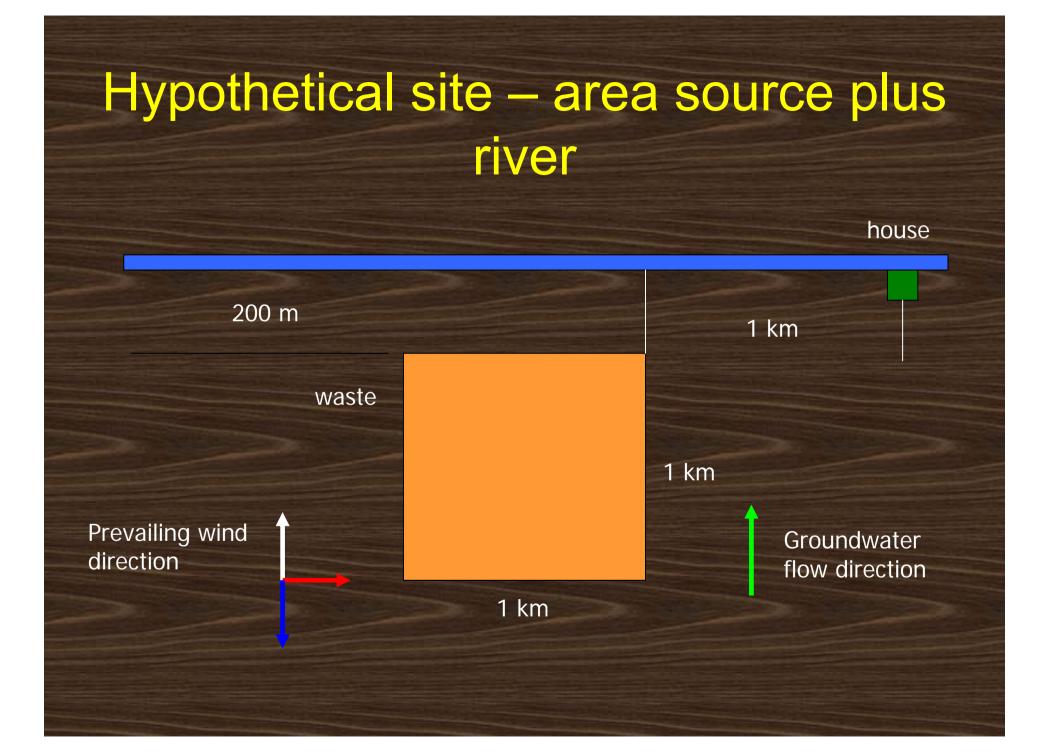


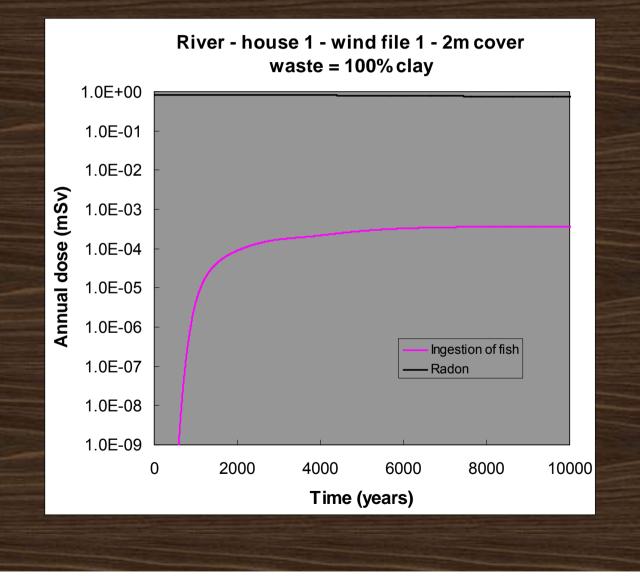
Radionuclides in well water – covered waste

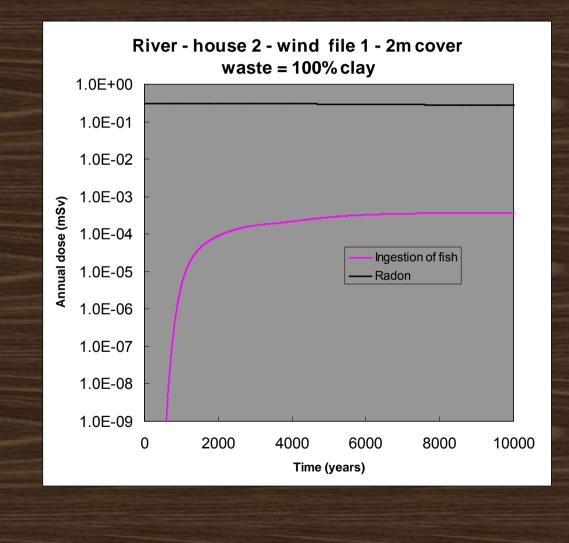


Radionuclides in well water – covered waste

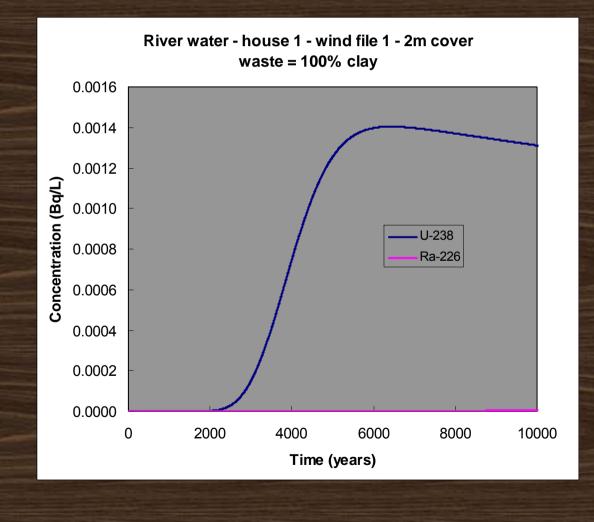








Radionuclides in river water



Applications

- Health and environmental impact assessment, safety assessment
 - Modelling the health and environmental impact of an existing operational site
 - Assessing the effect of proposed remediation work on a legacy site
- Developing strategies for residue management, storage and disposal for a proposed site
 - The basic scenarios can be used as a starting point for a range of studies
 - Generic models are applicable at the planning stage
 - As a project develops and more data become available the model(s) should become more site specific
- Testing remediation strategies for a contaminated (legacy) site