Cs Workshop
Fukushima
30 Sept-3 Oct 2013

Quantitative modelling of Cs transfer processes and assessing doses to populations

Ian McKinley & Susie Hardie*

*Currently attached to JAEA

mcm

Contents

- Introduction
- Historical overview of RN (Cs) migration modelling
- Advantages & disadvantages of different approaches
- Concept for tailoring to Fukushima
  - Cs migration
  - Biosphere modelling & dose assessment
- Model verification & validation

mcm

Introduction

- The distribution of artificial radionuclides in the environment has been studied since the middle of the last century – on scales ranging from global (bomb fallout) to very local (soil & sediment profiles)
- Radiocaesium (especially Cs-137) has been a special focus for such work and a range of models have been developed to interpret, interpolate and extrapolate observational data
- In early days a major constraint was the capability of digital computers; requiring great simplifications in representation of system understanding and use of analytical / semi-analytical approaches or even analog models

Starting point: analytical solutions

- Seminal work on bomb fallout in sea sediments: solutions for diffusion developed for standard source terms and geometries that could be applied to model laboratory and field measurements (E.K. Duursma, C. Hoede, Neth. J. Sea Res, 3, 423-457 (1967))

432 E. K. DUURSMA AND C. HOEDE

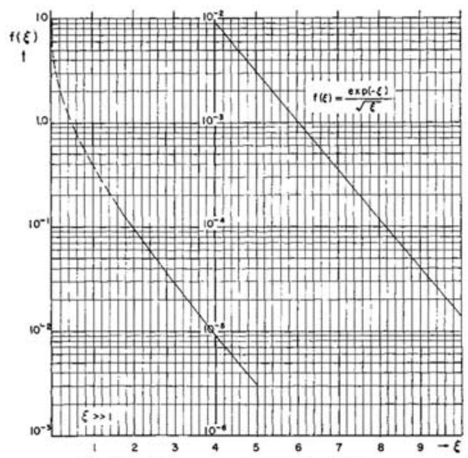


Fig. 3. Graphical representation of the formula (II.5) as: $f(\xi) = \frac{\exp(-\xi)}{\sqrt{\xi}}$

…inherently limited by solvable equations – focus on Kd to describe sorption

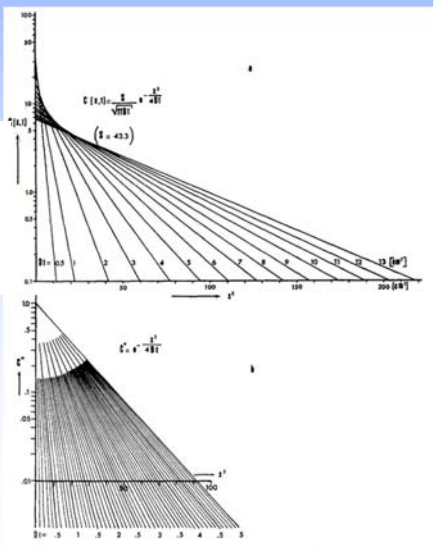


Fig. 4. a. Pattern of theoretical graphs of diffusion from an instant source for different values of Dt.
b. Graph of the slope dependency for different values of Dt. This graph can be used for rapidly finding Dt from an experimental graph by overlapping, if the graphs are of the same scale and graph b is transparent.

Computer models (1)

- In the '60s, '70s and even early '80s, digital computer capabilities constrained all modelling applications
- Simple compartment models could be developed, but run times often very long (hours, days)

…both system and process description had to be greatly simplified

The IBM 1401 in the early 1960's - the first mass-produced digital, all-transistorized, business computer. The basic 1401 came with 4,096 characters of memory; a Storage Expansion Unit expanded this 16K!! Cost was $125,000 – 180,000 with a weight of 1 – 3.5 tons

mcm

Example – late '70s

- Simple box models of Cs migration developed at Glasgow University and run on mainframe
- Used to simulate transport of Cs in a coastal marine environment
- Because of limitations of even a big "mainframe", model calibration with a home-made analog model

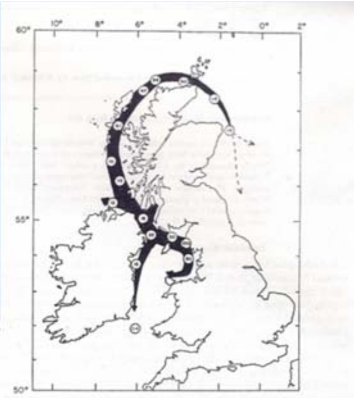


Figure 1. The Windscale radiocaesium plume (after Jefferies et al., 1973). Numbers are ^{137}Cs concentrations in pCi l^{-1} (1972 values).

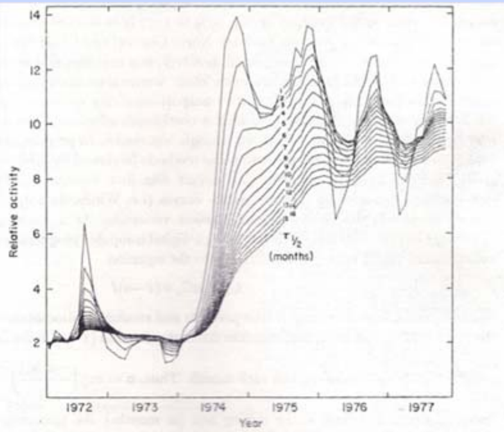


Figure 5. Box model output derived from Windscale source ^{137}Cs curve for water residence half-time between 1 and 16 months.

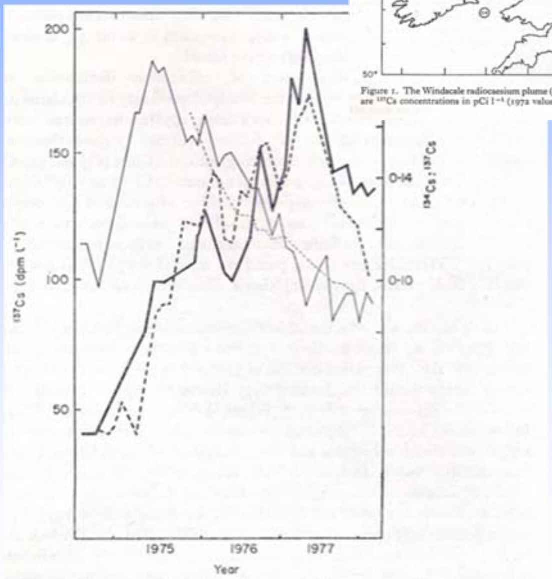
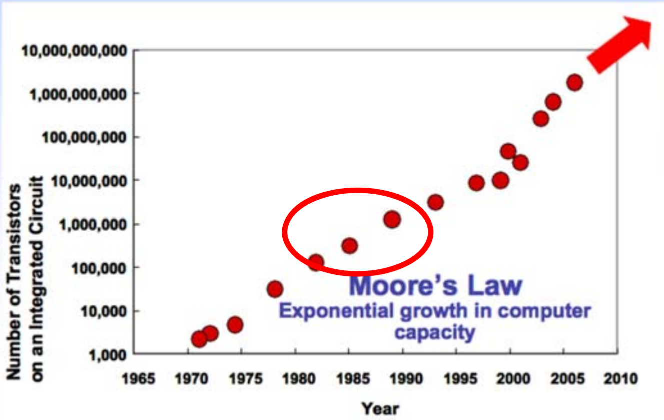


Figure 7. Comparison of observed (——, ^{137}Cs; ——, ratio) and modelled (– – –, ^{137}Cs; – – –, ratio) radiocaesium curves for the Clyde Sea area.

McKinley, I.G., Baxter, M.S., Jack, W., A simple model of radiocaesium transport from Windscale to the Clyde Sea Area, Est. Coast. Shelf Sci., **13**, 59-67, (1981).

Computer models (2)

- From the ‘80s, expanding applications, in particular associated with geological disposal safety assessment
- Semi-analytical models used, using digital computers to solve complex equations numerically
- Growth of finite-element and finite-difference models for engineering and hydrogeological applications (generally 2D)



mcm

Example – ’80s

- Initially, semi-analytical computer models were used for geological disposal PAs (e.g. KBS-3, Project Gewähr, H-3): single fracture flow with matrix diffusion but generally represent sorption only in terms of a Kd
- Some models extended to consider non-linear sorption of Cs – represented by a Freundlich isotherm – but very complex to develop and test (man-years of effort)
- Box model used to verify semi-analytical models including non-linear sorption; in-situ experiments initiated for validation (Nagra/PNC collaboration)

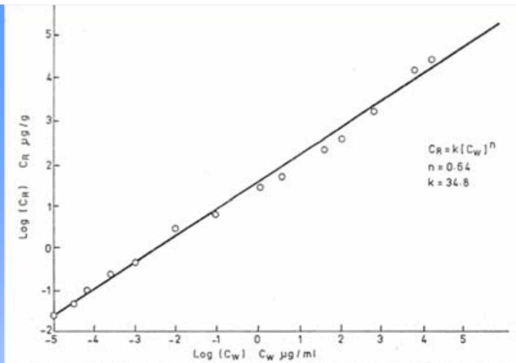


FIG. 1 FREUNDLICH PLOT : ^{137}Cs / ALTNABREAC DEGRADED GRANITE / 25°C.

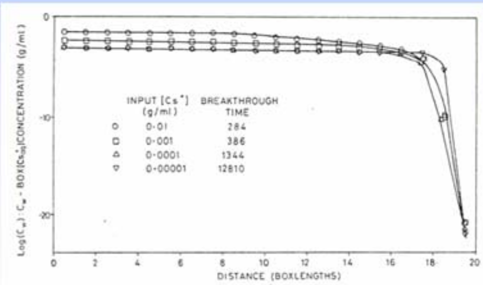


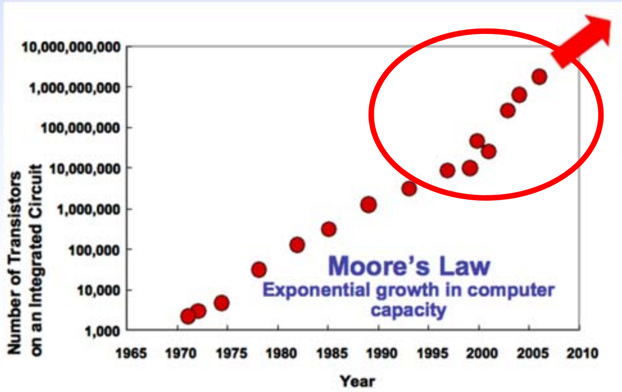
FIG. 2 20 ZONE ^{137}Cs BREAKTHROUGH MODEL :- EFFECT OF INPUT Cs⁺ CONCENTRATION, $C_R = 34{\cdot}8 [C_w]^{0{\cdot}64}$

McKinley, I.G., Prediction of radionuclide retardation during groundwater transport from laboratory sorption data, Proc. IAEA Symp. Migration in the terrestrial environment of long-lived radionuclides from the nuclear fuel cycle, pp. 147-152, (1982).

mcm

Computer models (3)

- From the '90s, wide growth of models in many environmental applications
- Transport models coupled with chemical thermodynamic codes
- Development of coupled T-H-M-C(-B) models
- Finite-element (and other mesh-type) models extended to include solute transport (2D & 3D)
- Exotic model variants to take advantage of parallel computers (e.g. Cellular automata)



mcm

Example: extended box model

- In the late '90s in Switzerland, box model formalised in the SANTA code for handling more realistic representation of Cs migration in-situ (from Grimsel experiments)
- Flexibility further illustrated by incorporation of complex chemistry – SANTA-CHEM (collaboration with JNC)

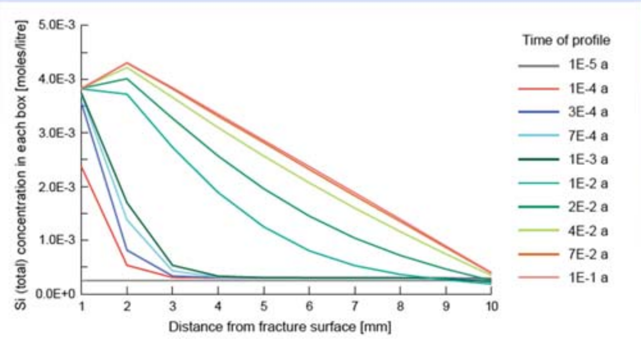


Fig. B2.4: Change in porewater total Si concentration with time through a 10 mm (10 box) section of wall rock adjacent to a fracture filled with portlandite saturated groundwater

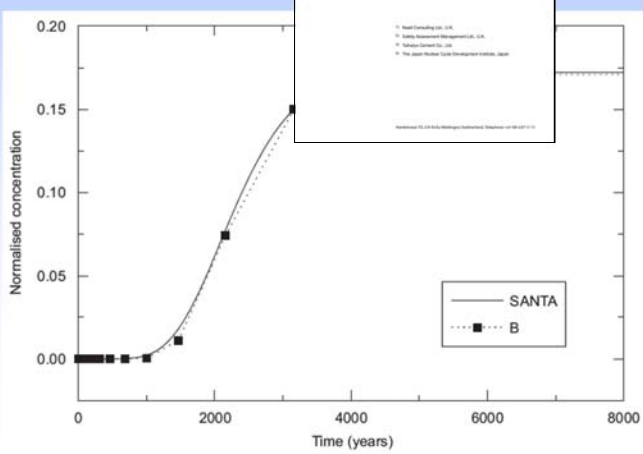


Fig. 7.22: SANTA / PICNIC (B) breakthrough curve including advection, dispersion, sorption and decay

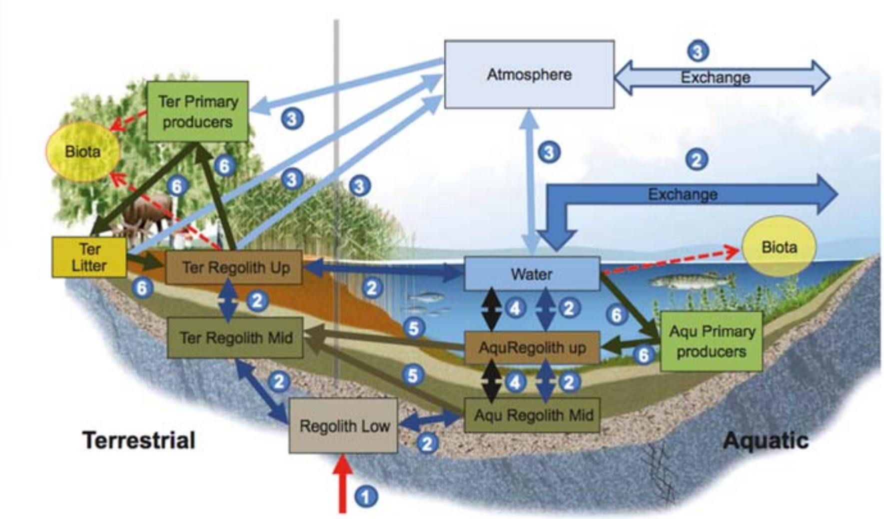
Pros & cons of different approaches

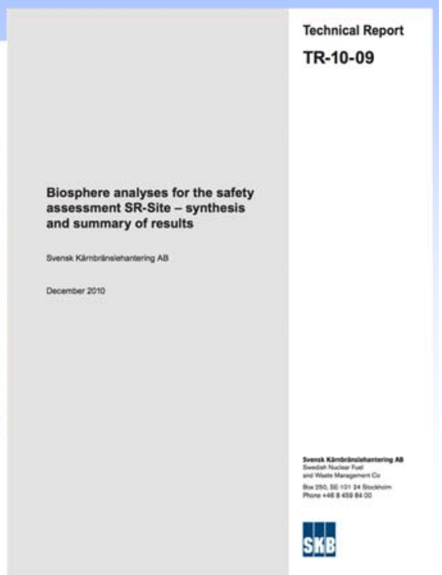
- Analytical models: efficient and academically elegant, but inherently inapplicable to most real environmental cases (exception something like Sr migration in a sand aquifer)
- Semi-analytical numerical models: as above
- Numerical mesh models (FE, FD,…): very powerful but extremely difficult to set up and computationally heavy for regional systems with extensive heterogeneity and variable time constants for different processes. Difficult to develop in a modular fashion.
- Cellular automata: extremely flexible and suited to parallel processing, but little experience for complex, real-world applications
- Box / compartment models: computationally inefficient, but extremely flexible and suited to modular development ➔ recommended approach for F-TRACE

mcm

Additional argument: biosphere models

- Compartment models almost universally used for post-closure performance assessment of the biosphere and other applications quantifying dose from environmental contamination: easy to integrate within a total system box model




Technical Report

TR-10-09

Biosphere analyses for the safety assessment SR-Site – synthesis and summary of results

Svensk Kärnbränslehantering AB

December 2010

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel and Waste Management Co
Box 250, SE 101 24 Stockholm
Phone +46 8 459 84 00

SKB

Fundamentals

- Define properties of system units
- Establish 2 or 3D distribution
- Define transport between boxes and RN processes

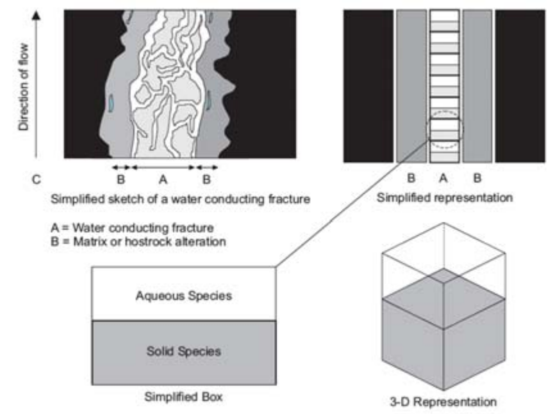


Fig. 2.1: A box derived from a representation of reality

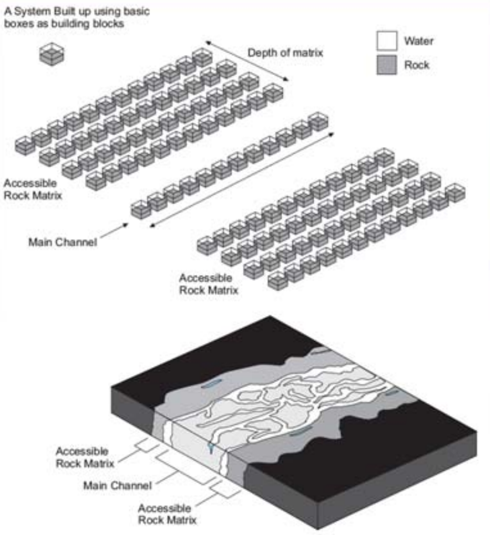


Fig. 2.2: Typical system constructed from boxes and comparative 3-D simplification of reality

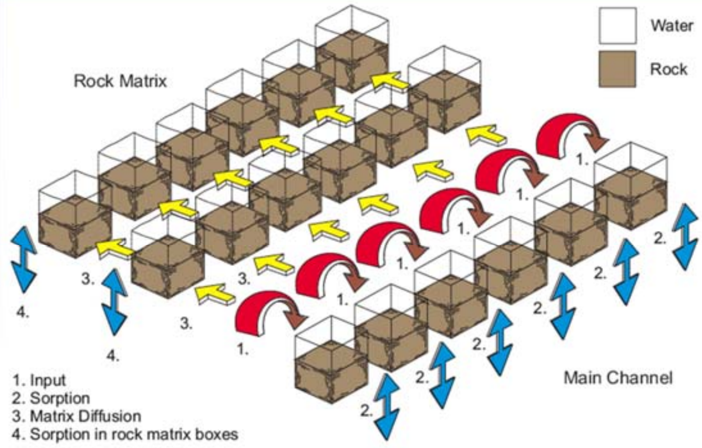


Fig. 5.1: Representation of sorption in the box model

Fukushima modelling

- A critical requirement for F-TRACE is to provide a conceptual model framework that allows radio-Cs measurements to be integrated, interpolated and extrapolated to future times in order to form the basis of assessing current and future doses to populations and the impacts of various measures to control Cs mobilisation
- Although many different approaches exist, the inherent simplicity and flexibility of box-modelling may be appropriate – especially as the power of modern computers compensates for the major disadvantage of this method (computational inefficiency)

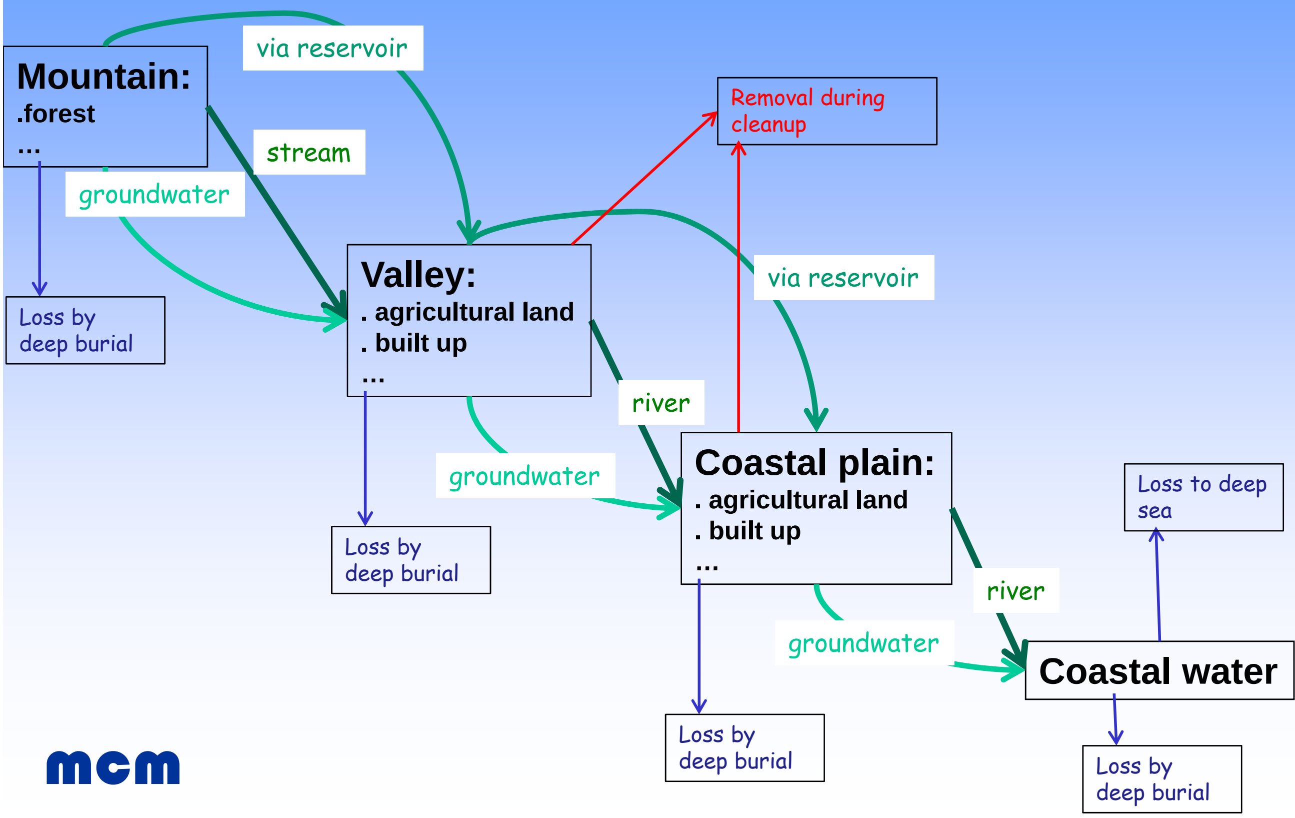
mcm

Application to F-TRACE

- Test model development can run on different scales:
  - Regional scale: quantification of fluxes of Cs from original fallout locations to points of final deposition or loss from the region considered
  - Study area scale: quantification of transport processes between different reservoirs and rate of gain / loss from the area from / to those neighbouring
  - Small scale: quantification of redistribution and gain/loss within a specific local reservoir
- Use of a common model structure facilitates integration within a total system model
- Can be readily extended to include:
  - Population dose assessment
  - Effects of migration counter-measures

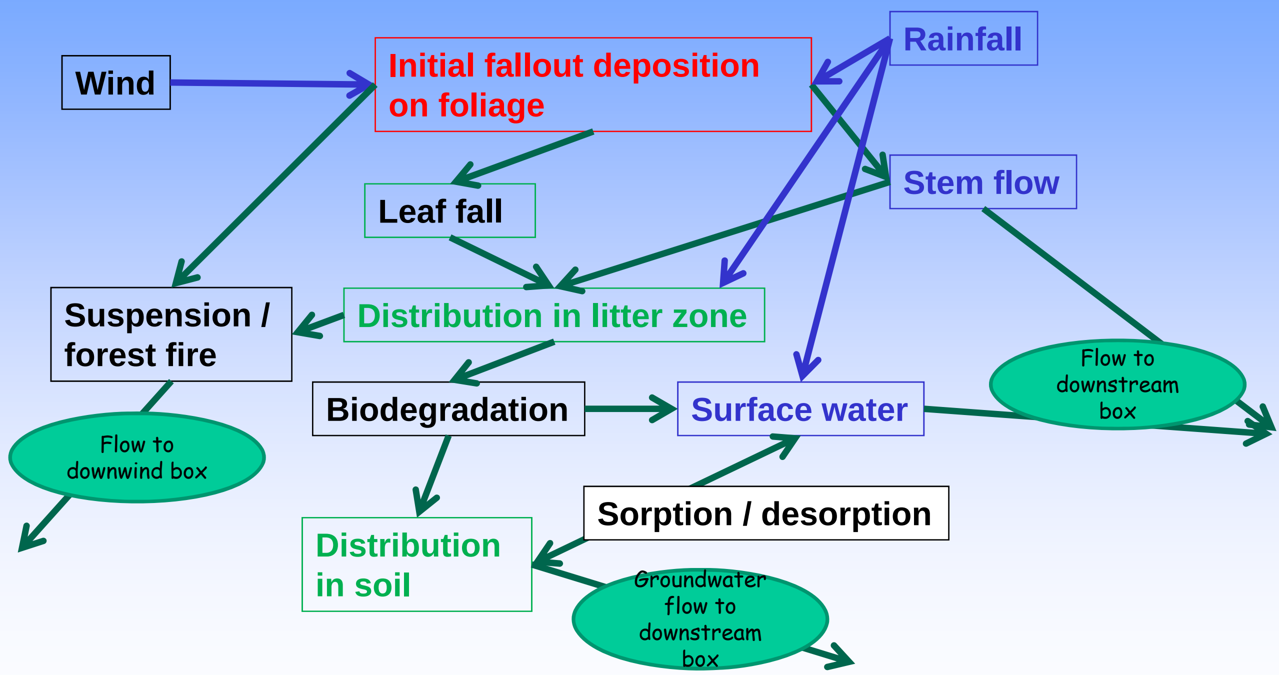
mcm

Outline of regional scale model

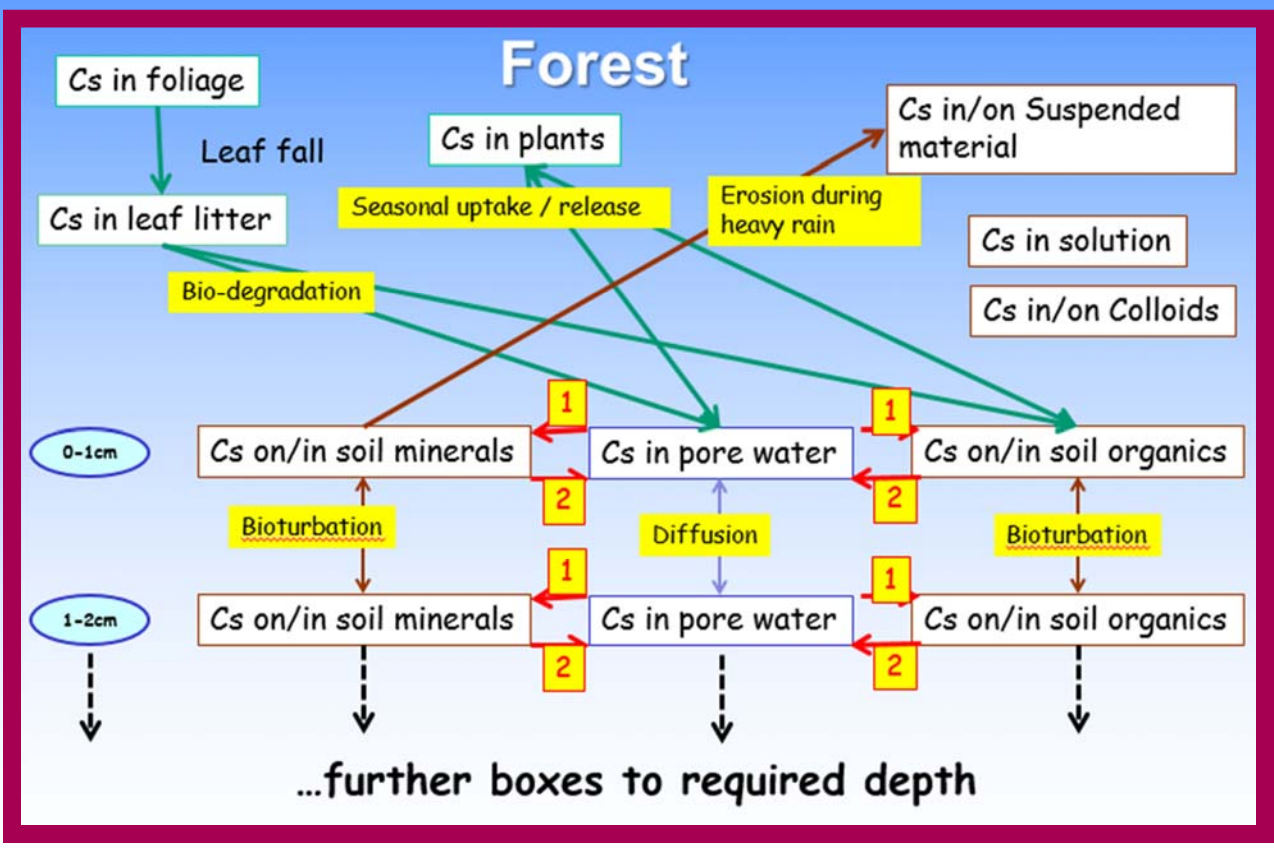


mcm

Outline of study area model: forest



mcm



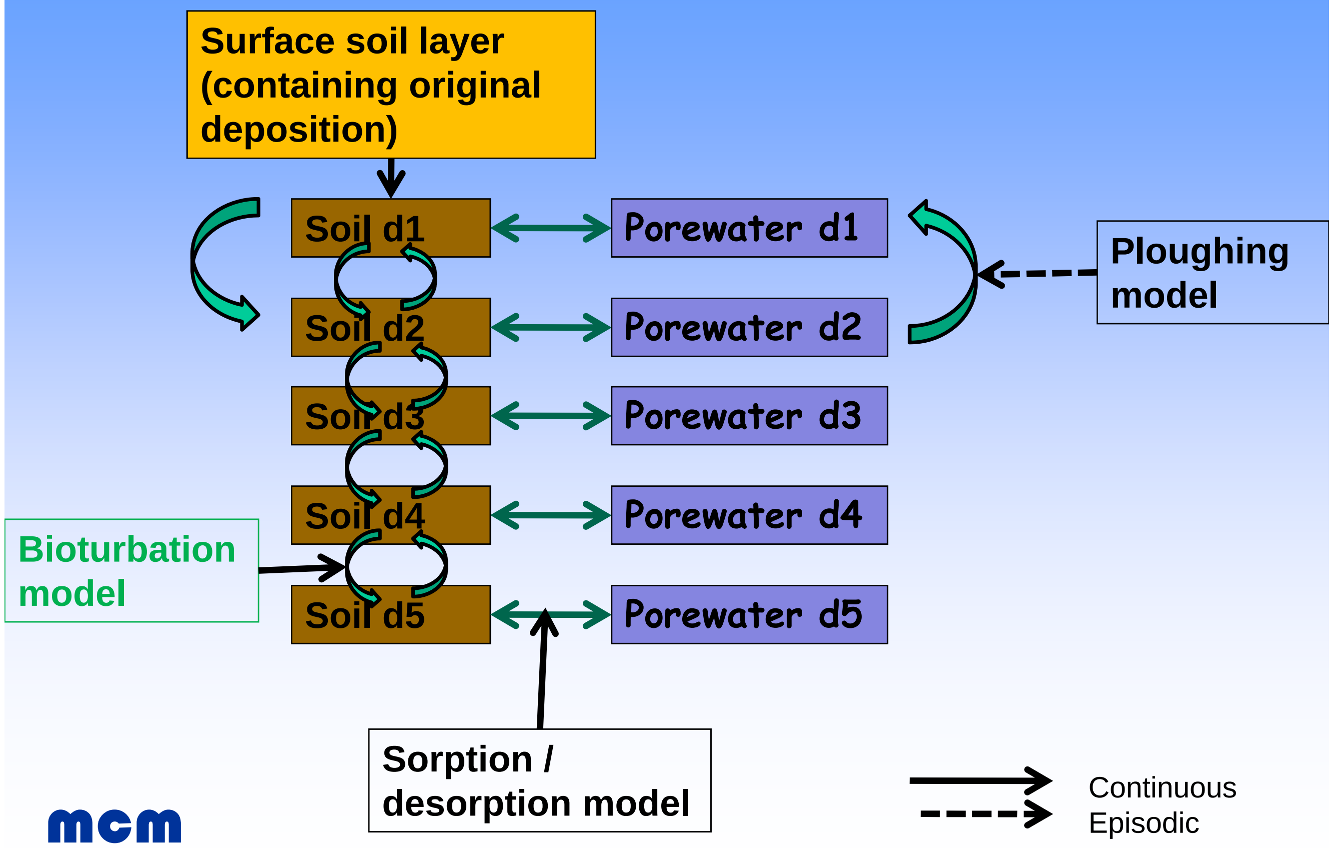
mcm

Capture of system understanding (1)

- Although many Cs models focus on inorganic processes, in a forest system biodegradation of leaf litter plays a very important role after the first wash-off of easily mobilised material (probably within the first few months)
- Combined microbiological / macrobiological processes can play a significant role also in forest soils in terms of both uptake/release and bioturbation
- Important distinction between soil porewater (which may gradually percolate deeper and hence contribute to Cs immobilisation) and surface water (which may transport Cs in dissolved, particulate and "organic" form)

mcm

Small-scale model - soil



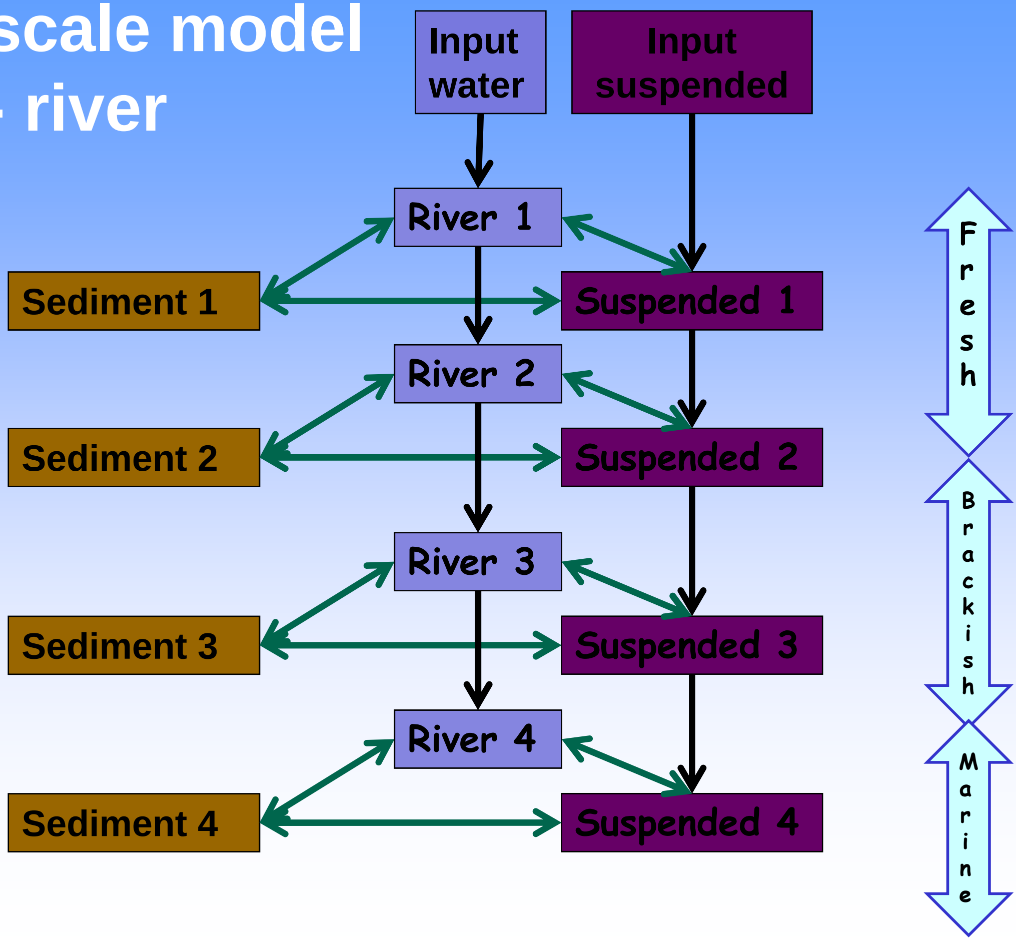
mcm

Capture of system understanding (2)

- Apart from biological and anthropogenic mixing processes, immobilisation by uptake processes onto/into solids and erosion of such solids are critical to understand extent of mobility
- A box model is extremely flexible and can readily include uptake involving:
  - Irreversibility or slow sorption / desorption
  - Concentration-dependent sorption (e.g. described by a Freundlich isotherm)
  - Spatial and temporal variation due to changes / evolution of properties of both solid and solution phase
  - System with more than 2 phases (e.g. including explicit treatment of colloids, microbes)

mcm

Small-scale model - river



mcm

Capture of system understanding (3)

- Transport of Cs in surface waters may include low concentrations in true solution and very variable quantities in either colloidal or suspended solid phase
- Colloid stability may vary along the flow path – especially due to changes in salinity
- Suspended solid sedimentation / re-suspension is very variable in both space and time and may be completely dominated by extreme flow events – e.g. during typhoons. These need to be explicitly represented and cannot be sensibly "averaged" in any way.

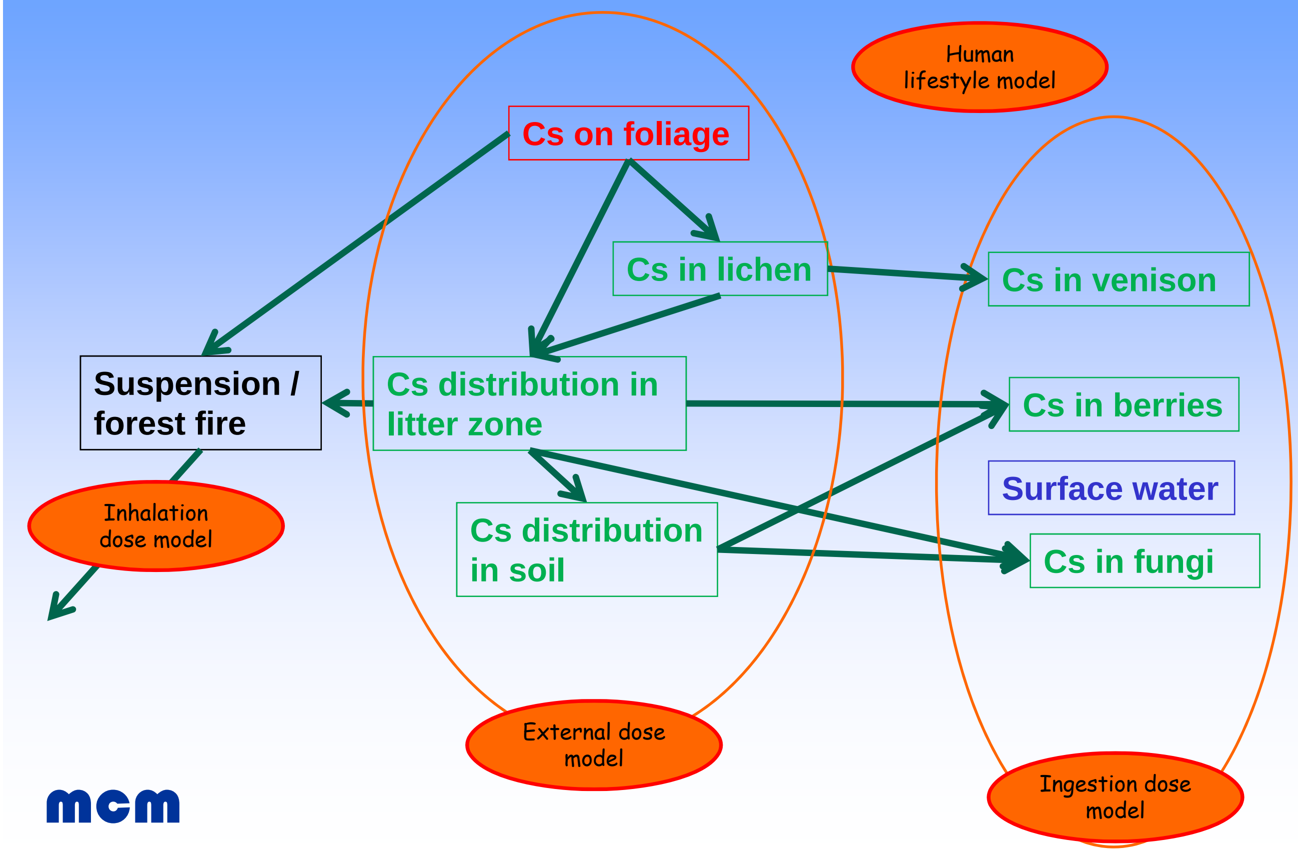
mcm

Biosphere box models

- Can be based on existing biosphere models used by JAEA
- The model has to be modified to couple input on individual geographical units: the main characteristics being soil type, land use and hydrogeology (establishing flows within and between compartments). A further major modification will be to develop simple partitioning models for relevant built-up areas
- Specific Cs partitioning data are derived or extrapolated from existing data, but continually refined by field measurements

mcm

Simple biosphere model - forest



mcm

Capture of system understanding (4)

- To be developed to allow emphasis on real doses rather than simple calculations from local gamma dose rates
- In addition to better representing real health risks, very important for assessing the impact of different management strategies (e.g. limiting access to forests compared to limiting use of forest foodstuffs)
- Although basic model can be readily derived from existing biosphere codes, databases may well be incomplete and need to be expanded by specific data mining / R&D work

mcm

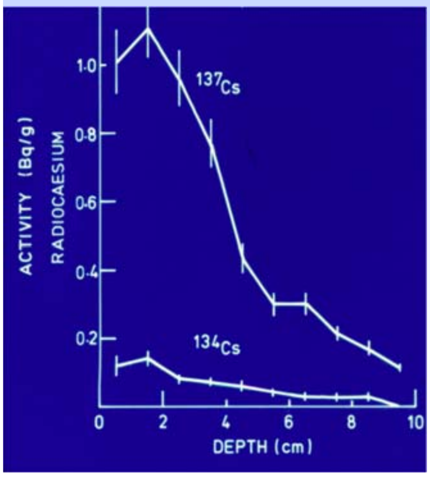
Practicalities

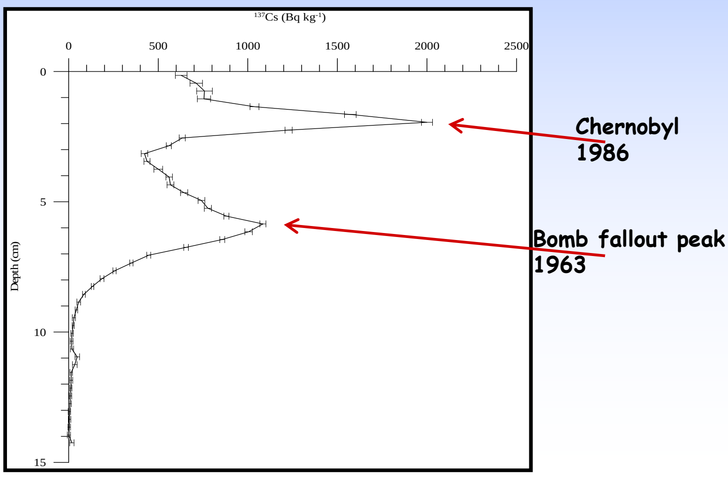
- The first goal will be to establish the basic model and initialise it based on best estimates of the deposition event.
- Redistribution is run forward in time steps, tracing inventories in different compartments. Comparison with measurements allows continuous refinement of the model. The dose calculation models allow impact on local populations to be assessed for various defined lifestyles (which may integrate input from several geographical units)
- For specific sub-components of the model, the impact of various strategies from the remediation tool kit can be assessed.

mcm

Model testing

- The 2 key aspects of model testing are verification and validation.
- Verification involves checking that models are mathematically correct: can be readily done by comparison with other codes / analytical solutions for simple test cases (at least for detailed models)
- Validation is trickier – showing that the model adequately represents reality. This is best done using relevant analogues.





Possible way forward

- Refine concepts with input from this workshop!
- Develop a first simple box model outline for one of the test sites focused on current Cs redistribution in a number of reservoirs
- Run some test cases (timescale ≈ 1-2 years) – check that output is “sensible”
- Set up analogue test case (Scotland) – run for 30-50 year timescale
- Assess output: if reasonable, extend functionality to include biosphere components, possible counter-measures and dose calculations

mcm