Dispersion modelling: ERICA methodology and optional alternatives

1. Dispersion models: why are they required

Dispersion models are mathematical simulations of how pollutants spread through environmental pathways. Depending on the environment considered they are classified into atmospheric, aquatic (freshwater, river or marine) or terrestrial models. The modelling is performed with computer programs or spreadsheets that solve the (often complex) mathematical equations which simulate the pollutant dispersion. They can be used to estimate or predict the concentration of pollutants emitted from industrial sources at a point removed from the location of the pollutant emmission.

In an assessment of radiation dose to non-human biota, often the receptor is not at a point of emission but is linked to it via an environmental pathway where dilution occurs. There is a need to deduce media concentrations when adequate data are not available. This is particularly critical when conducting authorisation-based assessments for the protection and conservation of species such as those listed under the EC Birds and Habitats Directives. For this reason, dispersion models often need to be employed in an assessment.

The ERICA tool provides a basic set of dispersion models which have been coded from the IAEA SRS-19 report on Generic Models for Use in Assessing the Impact of Discharges of Radioactive Substances to the Environment. The following transport models are available: Small lake (<400 km2); Large lake (≥ 400 km^2); Estuarine; River; Coastal and Air. It is not the purpose of these notes to give a description of the models; this is amply given in the accompanying IAEA publication (www-pub.iaea.org/MTCD/publications/PDF/Pub1103_scr.pdf). Suffices to say that the SRS 19 models are considered to be the simplest, linear compartment models capable of carrying out a simple screening approach, robust but conservative. They assume a default discharge period of 30-years, as an approximation to the lifetime of a facility, with doses being estimated for the 30th year of discharge.

The SRS 19 models suffer from limitations in their applicability. For example, the aerial model includes only one wind direction. The coastal dispersion model not intended for open waters e.g. oil/gas marine platform discharges. The various surface water models assume geometry (e.g. river cross-section) and flow characteristics (e.g. velocity, water depth) that do not change significantly with distance / time, as well as steady-state partitioning of radionuclides between water/sediment K_d. None of the models can be used for long source-receptor distances. This is considered to be an acceptable price to pay for models that are designed to minimize under-prediction (conservative generic assessment) and that use the minimum possible number of parameters. If more realistic simulations are required, this goes beyond the specifications of the ERICA tool, and the user needs to apply more advanced methods. These notes cover the issues of applicability, advantages & disadvantages as well as limitations of the SRS 19 models and some of their common alternatives.

2. Atmospheric dispersion modelling

2.1 Approach used in ERICA and its limitations

The SRS 19 Air Transport Model is a Gaussian plume approach to assess the dispersion of long term atmospheric releases; this model is widely accepted for use in radiological assessment activities. The basic equation for a Gaussian plume model for an elevated release is as follows:

$$C(x,y,z)=\frac{Q}{2\pi u_{10}\sigma_z\sigma_y}\exp\left[-\frac{y^2}{2\sigma_y^2}-\frac{(z-H_s)^2}{2\sigma_z^2}\right]$$

Where C = the air concentration (Bq/m^3) or its time integral Bq.s/m^3
Q = release rate (Bq/s) or total amount released (Bq)
u_{10} = wind speed at 10 m above the ground (m/s)
σ_z = standard deviation of the vertical Gaussian distribution (m)
σ_y = standard deviation of the horizontal Gaussian distribution (m)
H_S = effective release height (m)
x, y, z = rectilinear co-ordinates of the receptors

The use of the Gaussian model requires the specification of plume spread rates in the horizontal direction (σ_y) and in the vertical direction (σ_z). Numerical values of σ_y and σ_z are obtained from experimental data or any one of a number of different mathematical methods. Additionally, the plume height (h) and a wind speed, usually at a height of 10 m, u_{10}, also need to be specified.

The SRS 19 model calculations depend on the relationship between building height, HB and cross-sectional area of the building influencing flow, AB. Assumed are a predominant wind direction and neutral stability class. The key inputs are discharge rate Q & location of source / receptor points (H, HB, AB and x).

The model is considered appropriate for representing the dispersion of either continuous or long-term intermittent releases within a distance of a few kilometres from source. The model should not be used to calculate radionuclide concentrations in air resulting from short-term releases (e.g. short duration, accidental releases). It should also be noted that the Gaussian plume model is not generally applicable at $x > 20$ km. As a result, it is recommended that any receptors of concern that are beyond 20 km from the release point should be considered to be at $x = 20$ km for generic assessment purposes.

Owing to the model's limitations, the uncertainty associated with the application of a Gaussian plume model for continuous releases from a single source is about a factor of 4 or 10 for a flat and complex terrain respectively. At distances less than 2.5 times the square root of the frontal area of the building, the model provides generally conservative results, whereas for distances of about 2.5 the square root of the front area, the model tends to underpredict the real concentrations for wind speeds above 5-m s^{-1}. However, for the purpose of the assessment tool, the exact simulation of the influence of the building is relatively unimportant and not likely to be the most contentious issue.

2.2 Alternatives for aerial modelling

The stand-alone code PC-CREAM (see below) also uses a Gaussian dispersion model – the radial grid 'R-91' atmospheric dispersion model (PLUME). This is still a Gaussian dispersion model, unsuitable for long distances (though it has been wrongly used in that way), and also assumes constant meteorological conditions. It does not correct for plume filling the boundary layer. Consequently, this is not much of an improvement on the SRS 19 approach.

The "next generation" models, the more advanced models to calculate plume dispersion, go beyond the Gaussian (or normal) distribution of the SRS 19 methodology, by providing more advanced methods of calculating the dispersion parameters (σ_y and σ_z) and the plume height, h. Such models are Gaussian in stable and neutral conditions but non-Gaussian (skewed) in unstable conditions. They use continuous turbulence data rather than simplified stability categories to define boundary layer. They also include the effects on dispersion from buildings, complex terrain & coastal regions, allowing a more accurate calculation.

One of the most common "off-the-shelf" alternatives is the Atmospheric Dispersion Modelling System (UK-ADMS) (Carruthers *et al.*, 1994), essentially a modified Gaussian plume model, i.e. it still assumes a Gaussian distribution of concentration in the horizontal cross-wind direction. The vertical air concentration distribution is assumed to be Gaussian in stable and neutral conditions; however, the distribution is skewed (not symmetric) in the vertical in unstable meteorological conditions, as stated previously. UK ADMS incorporates improved physical modelling of the atmosphere, particularly in convective (unstable) conditions. Instead of using the Pasquill-Gifford stability classes, A to G, the stability is characterised by the boundary layer height and a scaling parameter of turbulence, known as the Monin-Obukhov length (a length scale based on frictional and buoyancy forces).

In ADMS, plume spread depends on local wind speed and turbulence and thus on plume height. This is in contrast to the simple SRS 19 aerial model, which assumes that plume spread is independent of height. A separate meteorological module is usually used to calculate the required boundary layer parameters. The plume-spread parameters (σ_y and σ_z) are then calculated directly from boundary layer variables. Moreover, ADMS is capable of including (though not always simultaneously) the effects on dispersion from complex terrain, building structures and coastal regions.

Anther 'next generation' model is the US EPA model AERMOD, which is widely used in the US. As with UK-ADMS, AERMOD utilises the 'Monin-Obukhov length' to describe stability (rather than discrete Pasquill-Gifford stability categories). It also includes complex effects such as topography.

Other types of models used in different situations include fine scale street canyon models (often semi-empirical) and heavy gas modelling, a modelling method to simulate condensed gases / gases with a high molecular weight. Probabilistic modelling and Monte Carlo models can also be found, but these are highly sophisticated applications.

3. Marine dispersion modelling

3.1 Approach used in ERICA and its limitations

The generic SRS 19 methodology is based on analytical solutions to advection–diffusion equations describing radionuclide transport in surface waters with steady state uniform flow conditions. Radionuclides may become adsorbed onto sediments in water, and this is simplified by using a steady-state distribution coefficient Kd (L kg^{-1}). Radionuclide releases are assumed along the bank/shore, thus restricting any mixing which might occur.

The key limitation of the SRS 19 model is that it is not designed for modelling large source-receptor distances, so for example it cannot be used for the assessment of doses to biota in an offshore oil platform. For this, it is necessary to use a long-range marine dispersion model to calculate concentrations in water and sediment, using the output values as input to ERICA which can then carry out the rest of the assessment.

3.2 Alternatives for marine modelling

3.2.1 Improved stand-alone alternative: the PC CREAM code

PC CREAM (Consequences of Releases to the Environment Assessment Methodology) is a suite of codes comprising models and data which can be used to perform the radiological impact assessments of routine and continuous discharges from virtually any type of installation including nuclear power plants and nuclear fuel cycling facilities. It was developed for the European Union but parts of the system have been used throughout the world. The methodology provides a suite of models and data for performing radiological impact assessments of routine and continuous discharges.

The marine model used by PC-CREAM is a Compartmental model for European waters (DORIS), based on the assumption of continuous discharge. Instantaneous mixing is assumed with transfer between compartments being proportional to the inventory of material in the source compartment (2D compartmental model, depth averaged, first-order differential equations). This model is an improvement to SRS 19 in that it has long-range geographical resolution, thus allowing for offshore scenarios e.g. marine platform discharges. Sedimentation processes are also represented in the model: settling of particles (modelled using K_ds, sedimentation rates and suspended sediment loads), diffusion and bioturbation, the latter two being treated as diffusive processes. The functionality of the marine modelling part of PC CREAM is very similar to POSEIDON, the code developed by the CEPN (Centre d'Étude pour la Protection Nucléaire, France) and validated by the EC MARINA project.

The PC CREAM marine model is adequate for assessing the consequences of continuous discharges. The use of annually averaged data for water flow parameters is considered suitable for assessments on an annual basis or integrated over a longer time-scale. The model can only calculate mean annual concentrations following a continuous release at an annual rate specified by the user. Thus, this model is not appropriate for short-term releases or for deriving information on concentrations over short times (e.g. less than one year).

3.2.2 Further approaches to marine modelling

With radionuclides, a vast range of both time and space scales can be relevant. The complexity of the representation varies with the type of model and can range from simple 'compartmental models' that shift volumes of water between boxes representing different parts of the ocean on an annual basis, and those which include full 3D tidal simulations. What is desirable in either case is geographically resolving models that allow for nonequilibrium situations, e.g. acute release into protected site.

The advantage of this type of model is that the code resolves into a large geographical range and, hence, the results are more accurate (if properly calibrated). The key disadvantages are that such models are CPU- and data-hungry (Bathymetry, wind fields, tidal velocities, sediment distributions, source term are all required). Small time step and grid sizes demand more computer resources. Additionally, the run time is dependent on grid size and time step, and the model requires a more specialised type of user. Moreover, some data post-processing is required for dose calculation (to adapt for use as input to ERICA).

The choice of model depends on the aims of the assessment and this should be considered at the outset. Model suitability is decided by model type (grid or box model), the time and grid scale, dynamic processes (tides, wind effects, sediment transport, etc.) and chemical processes (e.g. radioactive decay, biodegradation).

Roughly speaking there are two types of marine model:

- Short-range (usually 'finite elements'). In finite element models, the variables are integrated over finite volumes. The grid representing these volumes usually shows triangular shapes of finite elements. The main advantage of this type of model is that the variability of the grid scale is suitable for complicated coastlines as the finer grid near the coast gives a better resolution.
- Long-range (usually compartmental). Compartmental models give average solutions in compartments connected by fluxes. These models often appear to be more suitable for covering large areas, unlike finite element models, which give a better representation of the processes at a smaller scale.

3.2.3 Examples of short-range models

An example of a finite difference grid model is the DHI (2001) MIKE21 model, a generic two-dimensional horizontal model using a separated approach. The term generic means that it is not attached to any specific geographical area. Therefore, its grid size and timescale are adaptable to the requirements of the assessment and the model domain. The model is suitable for short-term assessments. The model package contains different modules that can compute the hydrodynamics and the advection/dispersion of conservative and non-conservative tracers. Another example of a finite elements grid model is the TELEMAC code.

3.2.4 Examples of long range models

The most readily available model is POSEIDON, designed for modelling the dispersion and transfer of radionuclides in European continental shelf waters. In POSEIDON, the area of interest is divided into large area boxes and transfer at boundaries depends on the parameters in the adjacent boxes. POSEIDON contains the sediment transport developed in project MARINA. It is simple, quick, easy to use and includes time variable discharges and continuous leaching of an immersed solid material. The post-processing for annual dose to humans is intrinsic, hence only minor coding required for determination of dose to biota. Further information on POSEIDON can be found in Lepicard *et al*. (1998).

Another long-range type of model is MEAD, the standard marine model for dose assessments for Sellafield, developed at the former Westlakes Research Institute (UK). This model has been extensively validated for radionuclides in the Cumbrian coast. It covers the Irish Sea area and it has enhanced process representation, particularly regarding sediment interactions. It uses a separate approach to compute the suspended sediment distribution, the activity concentration in the Irish Sea, the transfer of activity to biota and sediment, and the dose to critical groups. Because of the timescale, the variables are averaged over a time step of one year. The velocity field uses residual flow that has been averaged over a one-year simulation of the hydrodynamics, including tides and wind effects. The hydrodynamics is therefore pre-defined as an input condition. The grid is also pre-defined, with a regular interval of 2 km.

4. River/estuary/lake dispersion modelling

4.1 Approach used in ERICA and its limitations

The SRS 19 river/estuary/lake model present in ERICA is similar to the coastal model in that it also uses simplified analytical solutions to the basic advection–diffusion equations. For rivers, it is assumed that radionuclides are discharged in some of the banks, not in the midstream. As stated previously, values for flow rates, current velocity and water depth are representative of the lowest annual average conditions occurring over a period of 30 years. The estuary model considers an average speed of the current representative of the behaviour of the tides. In all cases, the concentrations are provided for the centre of the line of the plume, which will give the highest concentration within the plume.

The small lakes and reservoirs model is extremely simple in that it assumes a homogeneous concentration throughout the water body, and expected lifetime of facility is required as input.

4.2 Alternative approaches to river and estuary modelling

PC CREAM also uses a semi-empirical river model, the simplest approach that will provide the necessary degree of predictive. The model used is an extension of the algorithm developed by Schaeffer (1975), but an effluent plume model in PC CREAM has replaced the assumption of instantaneous dilution. In addition to bed sediment transport, the latest version in PC CREAM incorporates a river-beach or riverbank compartment.

There are more advanced river and estuary models but these have large input requirements: bathymetry, rainfall and catchment data, sediment properties, network mapping, and source term. The output is usually activity concentration in water and sediment, or hydrodynamic data for rivers. All use the same advection/dispersion equations as marine but differences exist in boundary conditions. Generally, models solve equations to give water depth and velocity over the model domain and to calculate dilution of a tracer.

Commonly river / estuary models can be ‘1D’, ‘2D’ or ‘3D’, depending on whether the river or estuary is represented by a line in downstream direction, a two-dimensional representation or the above plus a depth profile. Mostly at the present level of assessment only 1D models are used; 2D models have some use where extra detail is required but 3D models are rarely used unless very detailed process representation is needed.

Most applied ‘off-the-shelf’ models are the MIKE11 model developed by the DHI (Industry standard code representing the river as a line in downstream direction), Water and Environment (1D model); VERSE (developed by WSC); MOIRA (Delft Hydraulics) and, on the more research side, PRAIRIE (AEA Technology), RIVTOX & LAKECO (RODOS PV6 package).

4.3 Modelling transfer through the terrestrial food chain

The uptake of radioactivity *via* terrestrial pathways from aerial radionuclide releases may require consideration of the whole hydrogeological cycle. It is necessary to perform catchment modelling, i.e. convert rainfall over the catchment to river flow out of the catchment zone. ERICA does not include a catchment model, but the user should know that there are two possible approaches: A simple “black box”-type model, such as empirical relationship from rainfall to runoff (cannot be used to simulate changing conditions), or complex physically based models where all processes are explicitly represented. An example of the latter is the DHI MIKE SHE model (Graham and Butts, 2005). This is one of the more widely used models, in which an integrated groundwater - surface water solution is provided through an advanced rainfall runoff model with extensive process representation. MIKE SHE is a good choice when the close linkage of surface water and ground water is important to the study. On the minus side, such an approach has an intense parameter demand.

5. Conclusions

ERICA uses the IAEA SRS 19 dispersion models to work out a simple, conservative source - receptor interactions. However, SRS 19 have some shortcomings. PC-CREAM can be used as an alternative suite of marine and river dispersion models but there are further off-the-shelf models performing radiological impact assessments of routine and continuous discharges ranging from simple to complex. The key criteria in choosing one of these models to assess dispersion are simplicity of use and number of parameters required, as well as the availability of input data and CPU resources. There is no point in running a sophisticated dispersion model requiring a large amount of input data if the conditions of the assessment are such that very limited information is available. This balance between the accuracy of the model (which comes at the price of higher complexity and input requirements) on the one hand, and the availability of input data on the other, should always be borne in mind by the assessor.

6. References

Carruthers, D.J., Holroyd, R.J., Hunt, J.C.R., Weng, W.-S., Robins, A.G., Apsley, D.D., Thompson, D.J. and Smith, F.B. (1994). UK-ADMS: A new approach to modelling dispersion in the earth's atmospheric boundary layer. *Journal of Wind Engineering and Industrial Aerodynamic*s, **52**, 139-153.

DHI (2001). MIKE21 Environmental Hydraulics - User Guide. *DHI Water and Environment. Denmark.*

Lepicard S, Raffestin D and Rancillac F (1998). POSEIDON: A dispersion computer code for assessing radiological impacts in a European sea water environment. *Radiation Protection Dosimetry*, **74(1-4)**, 79-83.

Graham, D.N. and M. B. Butts (2005) Flexible, integrated watershed modelling with MIKE SHE. In Watershed Models, Eds. V.P. Singh & D.K. Frevert Pages 245-272, CRC Press. ISBN: 0849336090.

Schaeffer, R. (1975). Consequences du deplacement des sediments sur la dispersion des radionuclides. In: *Proceedings of the Conference on Impacts of Nuclear Releases into the Aquatic Environment*, Otaniemi 1975. IAEA-SM 198/4. International Atomic Energy Agency, Vienna.