APPRAISE II: Review of Aquatic Dispersion Models

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The report was commissioned as part of the development for the prototype BPEO tool, APPRAISE. It is a working document to consider the feasibility and scope of dispersion models to assess the consequences of discharges from prescribed processes to aquatic media. The information within this document is meant for the use by EA staff and others involved in IPC regulatory development.

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EXECUTIVE SUMMARY

This report is concerned with a review of models which can be applied to contaminant dispersion in estuarine and freshwater environments. The suitability and complexity of these models have been viewed from the perspective of the prototype system. Ultimately the review has been aimed at evaluating the models' suitability for use in assessing the consequences of process discharges to the aquatic environment within the constraints of a national regulatory decision support system.

A key consideration in the aquatic environment is the way that contaminant transport in water and on sedimentary material are modelled on the spatial and temporal scales of interest. This requires a robust water flow model and an understanding of the partitioning of contaminants between the solid and aqueous phases. Failure to scope the partitioning could introduce large uncertainties in the concentration predictions, particularly in depositional environments such as estuaries. In such depositional environments storativity (i.e. accumulation) is important and subsequent re-suspension can clearly affect both solid and aqueous phase concentrations.

When modelling discharges to the environment, there must be an understanding of the importance and interaction of processes such as:

- dilution and dispersion;
- delays and storativity;
- potential chemical transformations.

However, representing all these processes explicitly, or even implicitly, for a region may not be practical when faced with problems such as availability of national data. Ultimately the practicality of application has to be considered within a regulatory decision making framework. As well as the sparsity of data, other constraints need to be considered, such as ease of use and the uncertainty associated with the model outputs, relative to regulatory criteria and their inherent uncertainty. There is a practical limitation to the resolution levels when deriving concentrations in order to avoid complication of the system. Users must understand the relative robustness of derived concentration measures such as averages and percentiles and make decisions in the presence of their inherent variable uncertainty. For example, an estimate of average water concentration may be within 30% of the true value, whereas a 95%tile prediction may be incorrect by at least 100%. These inherent uncertainties must be considered when they are compared to the relevant regulatory criteria.

When incrementally developing a regulatory prototype system, improvements have to be engineered within a finite project budget and at each step there must be an attempt to identify the most cost-effective return. This alone can lead to inconsistencies of system complexity as some features, events and processes will naturally be easier to model. Some releases naturally may need to be modelled at a higher resolution due to the immediacy of their impact. This should also have implications for the resolution of the required measurements or data.

The main conclusions drawn from the aquatic model review are:

- The current Integrated Pollution Control (IPC) methodology, which adopts the Integrated Environmental Index (IEI), requires that all uncertainties in media concentration predictions are investigated and minimised wherever possible;

- The existing representation of the aquatic environment in APPRAISE is fit for purpose and from a cost-benefit perspective refinements could be made to the existing model, e.g. extrapolation and re-calibration of the flow model on a national scale.

- Potentially, a major limiting factor to the incorporation of more complex aquatic models within a national decision support system is the availability of appropriate data.

- A simple estuarine scoping model should be introduced into APPRAISE. It will calculate average and maximum concentrations by estimating average and minimum compartmental volumes and freshwater flow and contaminant input.

- The soil system is a complex environment and storativity and retardation effects introduce great uncertainties into temporal concentration predictions and estimates of soil-to-water transfers. This component is a weak link in the system and requires further consideration.

- The conceptual representation of media features and processes is primarily a function of the IPC methodology, the regulatory decision support system and the chosen environmental models.

- The current inconsistency in complexity of modelling features and processes in different media in APPRAISE is scientifically acceptable, as well as from a cost-benefit viewpoint.

Areas where there would appear to be most scope for development of the aquatic modelling include:

- Investigation of the potential extension of the water flow model to the whole of England and Wales, using extrapolation for relatively small ungauged areas, or adapting other ungauged catchment models;
- Detailed specification, calibration and validation of a simple estuarine scoping model with more detailed hydrodynamic and water quality studies;
- A detailed investigation into uncertainties and how they affect the regulatory decision process on different spatial and temporal scales;
- Further investigation into soil modelling and resolving soil-to-water transfers.

  The Environment Agency uses, or has a licence to use, other aquatic flow and dispersion models which would have to be taken into further consideration.

Key words:

Water Quality; BPEO; Dispersion Modelling.

1. INTRODUCTION

APPRAISE has been developed over the last five years and a number of 'back-to-back' projects have incrementally enhanced this regulatory 'multi-media modelling decision support system'. Primarily, the original HMIP 'EAS' contract (Waters et al., 1994) identified the need for those models that currently reside in this prototype system. Subsequent projects have however improved the functionality of the models and in certain circumstances radically improved the performance e.g. reduced uncertainty of model predictions, improved the complexity of calculations, increased the number of pollutants modelled. Enhancements were often achieved by testing new model additions/components using standalone software (e.g. QUEST).

Identifying a conceptual system representation and appropriate individual model performance is important for robust decision making, but necessarily is limited to processes that can be practically explored and incorporated. This naturally varies between media and ultimately this leads to disparate levels of understanding and reliability of multi-media model predictions. Primarily an aim of this work is to review the suitability of more complex aquatic models, than those which currently reside in APPRAISE. Secondly, there is an attempt to explore the robustness of the whole system approach by understanding what is practically achievable within media (i.e. cost-effective reduction in uncertainty) and the comparative complexity for modelling dispersion in each medium.

The early APPRAISE demonstrator, and now the existing prototype, have been test bed systems. APPRAISE has developed incrementally and therefore the details of inter-media modelling complexity have not developed in concert. The result is that some media are better understood and represented than others. Before we attempt to understand the limitations and perhaps standardise the level of detail of modelling, we must consider the following questions:

what level of modelling complexity is achievable and practical within media ?

and, perhaps more fundamentally, is there a scientific and regulatory need for inter-media consistency of complexity of modelling ?

When making a determination of processes under IPC, using any model, the uncertainties in the predicted outputs depend on how the uncertainties in the inputs are developed through the model processes and pathways, i.e. the sensitivity of the system to a given release scenario. It is desirable that the system is robust to the range of scenarios it is required to handle, i.e. it should not have radically different output uncertainties for different scenarios. If this were not the case, scenarios that consider release to more than one medium will be inherently more uncertain, and perhaps more difficult to authorise. This places a requirement for robustness either on its sensitivities, and/or its input uncertainties. As control of these two areas is necessarily limited, they are critical to an appropriate IPC determination.

More general issues that need to be considered when assessing the sophistication of aquatic models to be incorporated include:

- the resolution of output from one model (medium) is consistent with inputs to another model (medium);
- where and what are the greatest modelling uncertainties in the system and where should additional effort be expended (e.g. are the current levels of uncertainty acceptable when compared to the relevant regulatory criteria);
- is the modelling naturally more complicated in certain media ?
- is national data availability a major limiting factor ?
- is the modelling complexity for each medium appropriate for the number of releases being assessed and the immediacy of their impact ?

It is important to consider, prior the review of models, the purpose and objectives of the APPRAISE 'regulatory' system. These have implications for the level of modelling detail that has been incorporated and the degree of uncertainty that is deemed acceptable. The initial objectives were to:

- Develop an integrated system to allow the environmental impacts of process options to be analysed and visualised (quickly and efficiently).
- Derive pollutant concentrations in air and water, and depositions to soil which can be compared to the appropriate regulatory limits.
- Provide a national scale system to promote inter-regional standardisation of decisions.
- Select suitable regulatory models (i.e. not detailed research models).
- Provide a consistent and standardised approach that is useable by non-specialists.
- Minimise the time taken to audit in-coming authorisations.

In principle, IPC software should model releases to all media (i.e. air, soil and water). The atmospheric component has been covered in a separate report [Maul et al., 1997] and although the subject of this report is primarily a detailed analysis of the aquatic environment, we believe it is the responsibility of the contractor to briefly consider some of the problems of modelling releases to soils. However, the uncertainty associated with modelling releases to soil is large and resolving the situation is not straight forward. Soil contaminant residence times (i.e. storativity and delays) are extremely variable, from days to many years, and estimating soil-to-water transfer is complicated. Ultimately the robustness of any integrated index (for regulation) is a function of the weakest link. Under certain release scenarios the soil environment is very important and thus a brief overview of improvements in modelling soil is presented in Section 5.

The report is structured as follows.

Section 2 reviews aquatic dispersion models for freshwater and estuarine environments and mainly considers:

- the general modelling constraints including: integration into the existing framework; and modelling freshwater and estuarine processes on a national scale within an interactive regulatory decision support system;

- the ability to incorporate a simple estuarine scoping model;

- the appropriateness of the existing freshwater modelling approach; and

- what from a cost-benefit perspective is the best way forward.

Section 3 attempts to consider the issue of consistency of complexity of inter-media modelling and summarises some of the limitations of incorporating more complex representations (i.e. what is possible versus what is practical). A brief discussion of the soil environment is also included.

Section 4 is a general discussion and **Section 5** summarises the main conclusions and recommendations.

2. AQUATIC DISPERSION MODELLING

2.1 Existing APPRAISE Approach

APPRAISE already has a simple freshwater aquatic model, that also considers discharges from sewage treatment works, and is described in Section 2.1.2. The estuarine component is not yet represented and Section 2.3.5 is the first attempt to scope this environment. Chemical transformations are not modelled in any part of the system.

2.1.1 Network and flows

The rate at which pollutants enter surface waters is first calculated as a mass flow rate Q. River flows F are then used at different points in the river network to predict the pollutant concentrations C = Q/F. This is correct for existing discharges, whose water input is already included in the flows F, and is conservatively pessimistic for new discharges.

The river network plays a central role in this calculation. This network was originally derived in 1991 from AA 1:200,000 digital satellite data of river images. The network consists of a set of 'posts' derived from the end points of digitised tracks. For the most part these posts are river junctions. Occasionally they are just isolated points on rivers. At each post there are 'signs' with distances and flow directions to destination posts. This information allows rapid tracing of water or pollutant movement through the river system.

To calculate the mass flow rates of pollutants, APPRAISE uses the river network to inject, trace, and where necessary sum, the mass flows. The injection points are taken as the nearest upstream post to the closest river point on the network.

The rate at which pollutant mass enters a river is calculated by firstly injecting all discharges from selected processes. From direct disposals to water the discharges are taken as $Q_{sj} = v_j \, c_{sj}$, where V_j is the volumetric flow rate of effluent from process j, and $c_{s\,j}$ is the concentration of pollutant s in that effluent. Indirect discharges to water via sewers are injected at the post where the associated receiving sewage works has its discharge. These discharges are taken as $Q_{sj} = V_j \, c_{sj} \, \prod_{k=1}^{M_w} (1 - R_{sk})$, where R_{sk} is a retention factor for pollutant j at sewage treatment stage k, and M_w is the number of treatment stages at sewage works w_j. Once all discharges have been injected, they are traced downstream and summed where necessary at river confluences.

2.1.2 Aqueous concentration measures

The accuracy of the upstream length model was adequate for predicting flows in order to derive concentrations, but not sufficiently high to warrant using the fitted flow per length factors as a statistical basis to estimate different spectral measures of flow and concentration. Instead the following approach was adopted. The monthly flow records in each region were summarised by the average and the minimum of flow per length factors, K_{av} and $K_{\min}$.

These factors were then used in each region to estimate average and maximum concentrations, $C_{av} = Q/(K_{av}L)$ and $C_{\max} = Q/(K_{\min}L)$.
Other spectral measures were estimated by assuming the cumulative probability P(C) distribution formula below:

$$P(C) = \tfrac{1}{2}+\tfrac{1}{2}\,[(C - C_{av}) \,/\, (C_{\max} - C_{av})]^{B};\ C > C_{av})$$

with a power $B = \frac{1}{2}$ so that as $C -> C\max$, P(C) approaches one like $\frac{1}{2} + \frac{1}{2}\,[1 - x]^{1/2}$ as x -> 0. This implies a plausible long tailed probability density function $\mathrm{P(C)} = \mathrm{dP(C)/dC}$, and at the average concentration, this formula gives $P(C_{av}) = -\frac{1}{2}$. It is not expected to be suitable for concentrations below the average.

Using the above maximum, APPRAISE predicts the concentration for a given percentile (expressed as a probability) by

$$C(P) = C_{av} + (C_{\max} - C_{av})[2P-1]^{1/B}.$$

For example, a 95%tile concentration would be $C_{av} + 0.81*(C_{\max} - C_{av})$.

2.2 General Considerations

Following a summary of the existing position, it is important to mention a number of general issues/constraints in the freshwater and estuarine environment, before specific models and codes can be justly appraised in the following sections. Some of these limitations are imposed by the existing regulatory and software framework and others are dictated by the practicalities of conceptually and parametrically modelling these environments. This section serves to define some of the boundaries of the problem and enable effort to be focused in the model review.

General modelling constraints include:

- identification of a 'fit-for-purpose' conceptual model (ensuring the main features and processes, can be, and are represented);
- the availability of data (practical decision support systems often need to provide information in the absence of detailed data, which can be costly to collate on a national scale) at the selected spatial and temporal scales;
- the speed of response (the system needs to supply model predictions in reasonable timescales); and
- the acceptability of uncertainty in model predictions.

In general the level of model process detail required and the timescales of interest are dictated by the regulatory resolution. Generally the impacts are immediate in the atmosphere, medium term in the aquatic environment and much longer term in the soil environment, where the residence times can be of the order of a hundred years. The level of detail of process modelling reflects the need to incorporate complexity and the technical ability to do so. Hence, it is important to appreciate the original objectives of the APPRAISE system mentioned in the Introduction.

2.3 Modelling Discharges to Estuaries

Estuaries can be defined as semi-enclosed coastal bodies of water that have a free connection with the open sea and within which seawater is measurably diluted with freshwater. IAEA[1991] discusses the different types of estuary. Estuaries are usually classified according to their physical oceanographic characteristics, particularly the magnitude of vertical mixing. Estuaries can be 'stratified or salt wedge', 'partially mixed' or 'well mixed'.

If the turbulent energy of the tidal current is sufficient to break down the stratification caused by density differences between saline and fresh water, the estuary becomes vertically well mixed, although there may remain lateral inhomogeneities. The Severn is an example of a 'well mixed' estuary. Discharges into well mixed estuaries are often modelled in a similar way to discharges to coastal environments. Simmons et al [1995] suggest that 'well mixed' estuaries generally have a tidal range of more than 4 m.

In estuaries where turbulence is insufficient to produce full vertical mixing, the estuary will be stratified, with salinity levels increasing with depth. In such estuaries it is important to incorporate the effects of stratification in models for contaminant dispersion. Simmons et al [1995] suggest that 'stratified' estuaries generally have a tidal range of less than 2 m.

In between 'well mixed' and 'stratified' estuaries lie 'partially mixed' estuaries. This section initially discusses more sophisticated compartmental, semi-analytic and numerical models which can be considered more consistent with 'second generation' approaches. The section concludes with a description of a scoping model which offers a practical approach to initiating an estuarine component within APPRAISE.

2.3.1 Practical limitations

The generic nature of the APPRAISE system restricts the ability to build in site specific estuarine models. Estuaries could be classified in as 'stratified', 'well mixed' or 'partially mixed'. Currently there is no estuarine model in APPRAISE and the first step is likely to incur the implementation of a simple empirical scoping model. In general, estuaries are complex systems and often require detailed models to produce accurate predictions. The ability to model estuaries using a simple empirical approach will depend on the ability to extract and represent the major processes for each estuary class/type.

Practical limitations to modelling estuarine systems on a national scale include:

- lack of site specific data and poor characterisation;
- realistic predictions often require sophisticated models incorporating a large number of processes and parameter ranges (e.g. retention times, freshwater and tidal flows, sediment dynamics etc); and
- problems of incorporating sediment dynamics and contaminant residence times.

Major features and processes to be represented either explicitly or implicitly include:

- freshwater flow;
- water depth;
- tidal variations/excursions;
- degree of mixing;
- physical dimensions; and
- sediment dynamics.

These issues are considered in more detail in Section 2.3.5

This section has attempted to define the modelling constraints and enable attention to focus on potential models and concepts of relevance. Consideration has not been given to the detailed mathematics because that is an extensive exercise. The remit is to recommend whether consistency of complexity is required and what level of detail is appropriate in these different environments (see Sections 3, 4 and 5).

2.3.2 Compartment models

The compartment volume will be based upon the tidal excursion either side of the discharge point, and the loss term due to water removal from the compartment will be the ratio of the freshwater flow to compartment volume, plus a term to account for diffusive losses. The loss rate or transfer rate to sediments (depending on whether a single or multi-compartment model is being used) will need to take into account the tide-averaged salinity of the estuary at the discharge point, since metal-sediment sorption rates are salinity-dependent. However, if the estuary is stratified this may not be a sensible approximation.

Simmons et al [1995] state that it is difficult to construct simple generic models for estuaries, but give examples of compartment models for 3 European Estuaries. In stratified estuaries it will be necessary to employ more than one compartment in the vertical, but for well mixed estuaries compartment models can be set up which represent lateral mixing only. The NRPB model for the Severn Estuary [McColl, 1988] is an example of a compartment model for a well-mixed estuary. This model has been validated against measurements of salinity and Cs-137, and illustrates that multi-compartment models can be applied successfully to contaminant dispersion in well-mixed estuaries.

2.3.3 Semi-analytic models

The semi-analytic approach in which a frame of reference is used which moves with the tide, is well suited to relatively simple estuary models. By removing the tidal component of the water movement, only the uni-directional freshwater flow component remains, which simplifies the mathematics. Such models have a long history of use for modelling water quality [Mollowney, 1973].

2.3.4 Numerical models

There are a large number of numerical computer codes which are used to model the transport of various contaminants in estuaries. The major limitation is that the contaminant-sediment interaction is not adequately represented. For conservative contaminants these interactions are not significant, but for others, the sorption onto the solid phase is critical in determining the ultimate aqueous and deposited sediment concentrations.

Two-dimensional numerical codes such as MIKE21, mainly considered for short term dispersion in the marine environment, could be used for environmental assessments in estuaries. For some estuaries one-dimensional codes such as MIKE11 may be appropriate (with the pollutant being well mixed across the estuary), but the same intensive site-specific input data for model calibration is required. These codes generally consist of a hydraulic module which calculates the tidal flow of water within the estuary, and water quality modules which advect and disperse the pollutants, and simulate the water chemistry. A metal-sediment module would include concentrations of dissolved metal in the water column and bed sediments, concentrations of adsorbed metals on suspended and bed sediments, suspended sediment concentrations and bed sediment depths.

A two-layer version of MIKE11 is available, which would allow some representation of stratified estuaries. However, as for the two-dimensional models discussed previously, these sophisticated codes require much site-specific bathymetric data on the channel geometry's, tidal boundary conditions, and dispersion coefficients. Each model constructed must be calibrated to the site.

The WRc code QUESTS [Clark et al, 1993] (which also operates within a statistical framework) has both 1D and 2D capabilities. WRc have developed QUESTS models for the Environment Agency for the following areas: Humber, Wash, Deben, Stour, Orwell and Harwich, Colne, Blackwater, Crouch and Roach, Thames and Medway. These numerical models can be used to model processes occurring over a few tidal cycles, and to resolve the movement of pollutants up and down the estuary within a tidal cycle. For longer term predictions, it would be possible to use residual freshwater flows down the estuary in these models, so effectively averaging out the intra-tidal water movement, although QUESTS also can be used for longer time frames. This has also been done in the one-dimensional model RALEE [Howorth et al, 1993] discussed below.

AEA Technology employed RALEE for the Esk Estuary using many of the modelling features of the CUMBRIA code for the Irish Sea. Advective water velocities down the estuary were derived from measured freshwater flows (monthly averages were used), and diffusion coefficients were derived from a consideration of salinity profiles along the estuary.

Sorption coefficients were taken to vary with salinity. Seasonal erosion and accretion were modelled in each discretised cell, but with no net gain or loss; the mass accrued in the summer is balanced by the mass lost in the winter. In addition, long term sedimentation was modelled. The estuary bed was represented by three layers, with transport in the vertical being represented by advection/diffusion.

As the model is time dependent, it can be used to investigate, for example, variations in transport through the spring-neap cycle. Although RALEE was applied to radionuclide discharges from Sellafield by specifying radionuclide concentrations at the mouth of the estuary, the model could be applied to situations where there is a direct release of radionuclides/contaminants into the estuary.

Perianez and Abril [1996] describe a numerical model where activity is partitioned between four phases: dissolved, suspended sediment, large bottom sediment and fine bottom sediment. Rate constants are used between the four phases instead of equilibrium sorption coefficients, with laboratory experiments being carried out to provide data to estimate the values for these parameters.

From a computational perspective many of these models could be incorporated into APPRAISE, within a limited impact of calculation time. The big limiting factor is the availability of data on a national scale. This precludes the use of more detailed approaches and tilts the balance towards more simplistic approaches, one of which is presented in the next section. This is a better progressive development step and still allows more detailed models to be used for calibration purposes rather than for regular decision making.

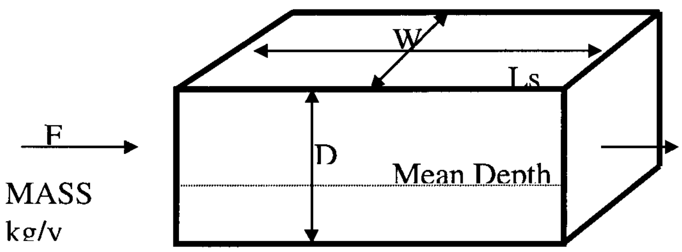
2.3.5 Estuarine scoping model

The most useful first step to incorporate an estuarine component in APPRAISE is to develop a simple scoping model. A simple compartmental approach is likely to be the best way to derive estimates of average and maximum contaminant concentrations. A relatively easy calibration exercise would be to compare the results with more complex codes, for specific estuaries where data is available.

In order to produce scoping calculations, the following variables will be needed:

- estuary width;
- water depth;
- tidal excursion (perhaps utilising estuary shape and bed slope);
- freshwater flow; and
- generic settling velocities and Kd's.

Hence the objective is to estimate the effective volume to which the discharge occurs including the input from the freshwater (see Figure 2.1). The volume will be calculated by assessing the mean depth, mean width and mean tidal excursion (i.e. length estimation). Low summer flow and summer neap tides will be used to estimate maximum contaminant concentrations. The introduction of a loss factor (based on suspended solid concentration, K_d and deposition/settling velocity) seems an added complication at this stage.



where,
Ls = Tidal Excursion
D = Depth
W = Mean Width

Figure 2.1 Single compartment model for a well mixed estuary

The average concentration, C_t could be calculated by:

- estimating the flux of pollutant into the estuary via diffuse (catchment) and direct sources;
- calculating the loss due to sedimentation; and
- estimating the estuary compartment water volume.

Hence, the following equation for C_t could be used:

$$C_t \simeq \left(\frac{R+P}{F_f + F_s}\right) \exp\left[-\lambda \frac{D_d}{D}\right]$$

where R is the background pollutant input to V (kgs^{-1})

P is the point source release(s) input to V (kgs^{-1})

F_s is the saltwater flow ($m^3 S^{-1}$); F_f is the freshwater flow

λ is the partition coefficient (dimensionless)

D_d is the settling depth ($V_d \bullet T$) (m)

D is the estuary depth (m)

where $F_s = V_s / \Delta T, Vs = \frac{1}{2} \Delta D w L_s, \; Vs = \frac{1}{2} \frac{\Delta D}{D} V$

and • D is the tidal height range.

The maximum would be a function of highest input and lowest water

throughput, i.e. likely to be summer low flow into a neap tidal volume. It is proposed that this will be a useful first approach to incorporate an estuarine component in APPRAISE.

2.4 Discharges to Freshwater Environments

Pollutants can enter lakes and rivers from a number of primary sources including: direct discharges via pipes; effluent from sewage treatment works and runoff from land. APPRAISE already has an aquatic flow and concentration model that attempts to scope the impact of the first two sources to rivers (Brown and Waters, 1997; Waters et al; 1995). Estimates of distributed pollution sources are however, subject to great uncertainty and they are currently implicitly incorporated through the use of real measurement data to calibrate the model.

The uncertainties in the current 'proportional upstream length' flow model approach was presented in Brown and Waters (1997) and is summarised in Section 2.1. The root mean square fit was about 30% of the mean station flows. Although the accuracy of the upstream length model was adequate for predicting flows to find concentrations, the fitted flow per length factors were not accurate enough to statistically estimate spectral measures of flow and concentration. In this instance, the monthly flow records in each region were summarised by the average and the minimum of flow per length factors K_{av} and K_{min} and these were used to calculate the average and maximum concentrations.

Prediction of water quality of large fresh water bodies concerned with water movement induced by inflows, outflows and prevailing winds, with the aims of predicting the effective residence times of pollutants in inflows, and water quality changes resulting from design characteristics and stratification. Although there is no dedicated lake model in APPRAISE at present, a simple classification scheme may be appropriate that included factors such as hydraulic residence times (using inflows, outflows and storativity), area and depth. This should be investigated in the next phase of work.

Most discharge points on rivers will require significant dilution to ensure environmental quality standards are not breached. Where the process is located in the 'valley' or 'plain' stage of a river section, there will naturally be depositional environments where sediment dynamics could play an important role for in-stream concentration of contaminants.

As with other aquatic environments, the main endpoint of interest from the dispersion stage of the contaminant assessment will be water concentration, including suspended solids. Given the current set of regulations there is no need to explicitly calculate the sediment concentration, as there are no specific criteria. We must assume that as long as the water concentrations are maintained below some critical value, the long term accumulation of contaminants in deposited sediments will not cause any adverse effects.

The main processes and features which are often modelled in river systems include:

- water flow and dispersion;
- frequency of bank full events/exceedences;
- suspended solid concentrations and contaminant sorption onto the solid phase; and
- in-stream sediment dynamics (re-suspension, deposition and accumulation).

If an annual average and a maximum concentration estimate are required, average flow and a low flow statistic (e.g. 95th percentile) will suffice. Where flow or stage data are absent they can be extrapolated from the nearest flow gauge (often local to large operational sites). Sediment deposition and accumulation could be predicted from channel characteristics, particle size and concentration, flooding frequency and water and deposition velocities. The number of bank full events will be needed especially if there is a likelihood for in-stream sediment removal and particularly from tidal or deep river sections. Substance specific sorption or partition coefficients will also be required. These parameters could be extremely important in depositional environments such as estuaries.

2.4.1 Practical limitations

Specific constraints to modelling freshwater systems on a national scale include:

- geographically locating all pollution sources (discharge points);
- estimating inputs from diffuse sources of pollution;
- calibrating a catchment flow model (at the appropriate temporal resolution);
- validating water quality predictions using measured/sample concentration data; and
- handling missing (flow and quality) data through interpolation and extrapolation.

With the incorporation of the existing freshwater model into APPRAISE many of the above issues have been considered. Conceptually we must identify the processes to be explicitly, implicitly modelled and omitted and this will be partly dictated by the resolution of the regulatory criteria. Major processes that need to be modelled include:

- water flow and dispersion;
- suspended solid concentrations and sorption; and
- in-stream sediment dynamics (re-suspension, deposition and accumulation).

Often there are no simple ways to incorporate or scope complicated phenomena. Either they are ignored, they are implicitly incorporated or a serious attempt must be made to explicitly incorporate the effects from them.

2.4.2 River models

There are numerous models that have been developed to predict contaminant transport in surface waters. Many of the codes are detailed research models that require considerable input data and site calibration before they can be used. A representative list is presented in Table 2.1.

Table 2.1 Some representative river models

Model	Reference	Steady Flow	Variable Flow	Dimension
ADZ	Wallis et al [1989]	*		1S
DYNTOX	Ambose et al [1988]		*	1S
EXAMS	Burns et al [1982]	*	*	1D
HSPF	Johanson et al [1984]		*	1D
HYDRA	Elsevier[1992]		*	1D
MIKEII	Danish Hydraulics Institute	*	*	1D
OTTER	Hancox et al [1996]		*	1D/S
PRAIRIE	Welsh [1992]		*	1D/S
PRISE	Elsevier[1992]	*		1D
QUAL2E	Barnwell [1985]	*		1D
QUASAR	Whitehead [1993]		*	1D/S
SALMON-Q	Reeve and Garland [1992]	*		1D
SIMCAT	Gill and Murrell [1993]			1S
TOMCAT	Bowden and Brown [1983]	*		1S
WASPS	Ambose [1987]		*	3D

Note: S indicates stochastic, D deterministic

For general water quality simulation and assessment the Environment Agency have used codes such as SIMCAT and TOMCAT. These are stochastic models developed to track river quality on a catchment scale and therefore require details of the whole river network. The data requirements are therefore considerable. Hence they may be of limited practical use for national-scale impact assessments using APPRAISE systems although there is evidence of their application to predict down-stream concentrations.

QUASAR is another water quality and flow model that was developed for setting and monitoring river quality objectives for river networks but subsequently superseded by Questor. It would be of limited value for generic impact assessment modelling.

MIKE11/12 has already been referred to as a potentially applicable 1D estuary modelling, and could be used for pollutant discharges to rivers. However, it is another sophisticated engineering software package for the one-dimensional simulation of flow, water quality and sediment transport in rivers (and other water bodies). It is a modular code with a flexibility to model a range of processes. It does require a lot of input data and therefore, is unlikely to be of use for routine impact assessments.

PRAIRIE (Pollution Risk from Accidental Influxes into Rivers and Estuaries) has been developed by AEA Technology for HSE, DoE and the Environment Agency. It uses a one-dimensional time dependent finite difference solution of the advection-diffusion equation which can be used in either deterministic or stochastic mode. It has access to various chemical databases, and has been applied to chemical pollutants such as pesticides. The methods are largely based on those advocated by the US Environmental Protection Agency.

OTTER has a catchment model, a river model and a lake model. The river model is based on that used in PRAIRIE, using semi-empirical methods to derive flow velocities and dispersion coefficients in each river section. It was developed for inputs from atmospheric deposition, but could be applied for direct inputs into rivers or lakes. Calculations from the river model in OTTER have been compared with ADZ, which requires the concentration profile of the pollutant near the source as an input (and so can not be considered to be a complete predictive tool).

Often the major limitation in the models discussed above is the failure to explicitly incorporate pollutant-sediment interactions. For conservative pollutants these interactions are not significant, but for many contaminants they are critical in determining the ultimate concentration in the water column, regardless of the accumulated sediment concentration. Many of these codes are too sophisticated for the impact assessment of routine pollutant discharges i.e. modelling of adsorption, transformation, decay, retardation in dead zones and algal development. Superfluous processes could be modelled by using default parameters, but the need to consider each aspect of the model, and to make decisions regarding the inclusion or otherwise of particular processes, would make most unnecessarily complicated. They are also data hungry, because of the need to consider site specific factors, and therefore of limited application, unless detailed field surveys are practicable.

Perhaps the most appropriate role of these more sophisticated codes is in the quantification of uncertainties in data and parameter inputs. Hence, they can be used when there is a need to explore an issue in greater detail, or various release scenarios require further explanation.

For long term trends and effects much simpler mixing zone models could be employed. The basis of the mixing zone model is that some way downstream from a discharge point of constant concentration to a river, mixing in the water across the whole cross section of flow will be complete. The concentration in the river may then be estimated as the rate of mass input divided by the flow rate. Uncertainty may be estimated by using the average, the minimum or some statistical representation of the flow rate (e.g. 95th percentile) and reflects the current approach taken in APPRAISE.

As already experienced in APPRAISE the water is a complicated system to represent. Considerable effort was expended in the early development stages to derive a topologically acceptable flow network. The enhancements made in APPRAISE II case study area highlighted the considerable effort that would need to be expended to propagate the new, but simplistic flow model, to the whole of England and Wales (Section 2.1 and Brown and Waters, [1998]). This situation in conjunction with the relative good uncertainty performance means from a cost-benefit perspective, the best way forward is to continue with the existing approach.

Secondly as concluded with the estuarine environment, the introduction of more complex models would have considerable data implications and in many locations this data would not be readily available, without a considerable data gathering exercise.

2.4.3 Models for lakes

The simple compartment models developed for coastal discharges can be used for well mixed lakes. If the lake is stratified this may not be a sensible approximation. Some of the models discussed in Section 4.2 above can be applied to lakes. These include OTTER and COASTOX. The model in OTTER is a compartment-type model, representing the lake ecosystem. Another model used in the RODOS programme is LAKECO [Heling, 1995] developed by KEMA, Arhem, The Netherlands. This is also a compartment-type model.

The need to incorporate a lake model must depend on the number of pollutant releases that occur to, or above, such water bodies. A simple scoping model would be more in keeping with the existing APPRAISE aquatic modelling approach. Further work is required in this area before a suitable model could be proposed.

3. CONSISTENCY OF COMPLEXITY

When modelling several media simultaneously there are some obvious constraints and limitations. A compromise is set by what is possible and what is practical. For example, the ability to introduce more complex models in the atmosphere can be realised because the data requirements are similar. Where possible, it is important that we introduce the latest scientific advances which will ultimately improve uncertainties and decision making. However, there are a number of candidates and enhancements in one medium must not continue at the ignorance of the others. The following section considers some of the limitations to improving the whole system performance and clearly sets out where certain developments are just not practical.

3.1 IPC Methodology and APPRAISE Constraints

General constraints imposed by the IPC methodology and existing APPRAISE software framework include:

- the feasibility of integrating codes (as opposed to underlying models, if they are available);
- attention to the need for some consistency of complexity of modelling (i.e. outputs from one model are suitable inputs to another);
- restricted visualisation of the model output (i.e. the greater the resolution of the model predictions the greater the need to visualise the information at a higher resolution, with data cost implications);
- uncertainty in the Agency strategy, including the future of the IEI assessment concept and the wider direction of IPPC regulation;
- the need to predict concentrations on temporal scales relevant to the regulatory limits without extrapolation;
- the spatial resolution of the system predictions (i.e. England and Wales); and
- the ability of the models to perform under typical conditions and ensure the users recognise their limitations.

To some extent these constraints have played an important role in the form of the existing system. We must continually appraise these criteria and ensure their relevance now and in the future.

3.2 Soil Modelling

It is not the responsibility of this report to recommend enhancements to the modelling of soils. However, given the uncertainties associated with modelling the soil environment as presented in Brown and Waters [1997] and the current use of the IEI concept in the authorisation decision some comment is necessary.

The ways in which pollutants reach the soil include the following:- the spreading of sewage sludge on land, washoff from fertilised fields and via dry and wet atmospheric deposition. In the majority of soil contamination problems contaminant transport is dominated by advection and hydrodynamic dispersion. In some cases, such as migration of volatile contaminants in unsaturated rocks, transport may be controlled by diffusion [Arthur and Zhou, 1993]

Contaminant transport from the soil to the aquatic environment will depend on the relative temporal magnitude of retardation mechanisms such as sorption, precipitation/dissolution, acid/base reactions, complexation, hydrolysis, substitution reaction, redox reactions, biological transformation, and partitioning of the contaminant among coexisting phases (e.g. volatilization). Hence, calculating soil to water transfer is a complicated process and subject to great uncertainty. It figures that some pollutants tightly sorbed to the solid phase may never reach the freshwater environment, particularly within the lifecycle of the process.

In Waters et al. [1993] the features and processes to be modelled included:

- allowance for the distinction between major soil types;
- inclusion of the estimate of the effective rainfall;
- an estimate of the soil moisture content;
- a substance specific partition coefficient (Kd);
- a substance specific decay rate/biodegradation; and
- an appropriate spatial averaging of the calculations.

There is an abundance of soil models ranging from fugacity models to compartment models. Fugacity models require spatial information on soil moisture storage, soil organic carbon content, partitioning coefficient and solubility. At present these parameters are not available on an areal weighted national catchment scale and considerable digitising effort would be necessary to derive such values. Therefore this precludes their use within APPRAISE at present.

Modelling of contaminants in soil is often performed as part of groundwater modelling by including a linear compartment model for transfer through soils to the foodchain etc. Examples of such models are those that were tested in the international BIOMOVS II program [BIOMOVS 1995]. The objective of this working group of the BIOMOVS project was to compare models that can be used to assess the long term impact of radioactive releases from uranium mill tailings, involving multiple pathways, multiple contaminants and multiple environmental receptors. A secondary objective was to examine how these models can be used to assess the fate of stable toxic elements. The models that were used in the BIOMOVS project, and the extent to which modelling of contaminants in soil are addresses in these models, are listed in Table 3.1.

Table 3.1 Models tested in the BIOMOVS project.

Model	Retention in soil	Other soil features
ECOSR	yes	n
ETP/AECB	yes	n
GEOLE/ABRICOT	Kd function	n
IMPACT	Leaching and erosion modelled separately	
JAERI	y	n
RESRAD	y	n
SACO	y	n
SONS	y	Surface soil modelled separately from root zone soil
SENES	Kd function	Surface soil modelled separately from root zone soil

The models listed in Table 3.1 are of varying complexity. They are generally based on standard screening level conceptual models. With some models the user manual describes in detail the modelling approach and transfer algorithms (e.g.ETP/AECB). The SONS and SENES models have the most complex representation of the soil compartment, with the latter containing a detailed two layer soil model which incorporates atmospheric deposition, irrigation water application, leaching in soil water and surface runoff.

Apart from the models listed in Table 3.1, many other models have been developed that are capable of simulating simple or complex geologic media, single-phase or multiphase flow, saturated or unsaturated conditions, and transport and fate processes [Arthur and Zhou, 1993]. A review of these models as well as those listed in Table 1 should enable a recommendation to be made as to how to best represent the soil compartment in a decision support system, taking into account level of complexity, etc.

4. DISCUSSION

Several freshwater and estuarine models were considered in Section 2 and assessed in the light of regulatory, APPRAISE and environmental modelling constraints. Considerable effort was spent on all these issues to minimise the review of unsuitable models. These constraints will impact on the form of the models and affect their ultimate practicality of application within a national decision support system. The primary objective was therefore to assess the current approach and consider the potential to practically incorporate a more complex conceptual representation. This decision needs to be made not only in the context of the aqueous medium but also in the light of other representations and uncertainties in the system and a need to ensure that outputs from one model/medium are appropriate inputs to another model/medium.

Currently, the atmospheric component is setting the pace following numerous developments and enhancements over the past few years. One issue that supports this position is the similarity and availability of data required by second generation atmospheric models. Thus it was timely to take a step back and assess whether such a development strategy was appropriate and best spend of resources. The incremental evolution of the methodology has been instrumental in the development of APPRAISE, and the testing of regulatory concepts has been of fundamental importance. When APPRAISE is used in this testing mode inconsistencies of complexity are naturally less important. The primary importance is assessing the scope of the methods and how might the latest scientific concepts be adopted in a widely distributed model. However, when an operational viewpoint is taken, where real decisions need to be made by users, the practicality of the approach is much more important.

One major limitation or control on the form of the system is the assessment methodology and the associated resolution and uncertainty in the regulatory criteria. The quality of the authorisation decision will be a function of the weakest link, and at present this is often the soil environment, i.e. the uncertainty associated with soil concentrations over short and long temporal scales.

Although it is theoretically possible to adopt sophisticated models to represent a complex range of features and processes, practically this is impossible (e.g. inability to calibrate and validate models by the unavailability of data at a national scale). We must recognise the limitations of a regulatory decision support system (i.e. not just those of the current APPRAISE prototype) and support the concept of shadow models. They provide an opportunity to carry out more detailed investigations where uncertainties in predictions are currently unacceptable, or where simple models, which fail to incorporate all processes and features, produce concentrations above the assessment criteria or some other trigger level.

One of the major difficulties following the identification of the major processes and features to be conceptually incorporated, was how are they to be explicitly and implicitly modelled on a national scale (i.e. all catchments in England and Wales). Naturally, the unavailability of data and parameter values, means many important processes must be either implicitly represented or even ignored. Although scientifically this may be disappointing, it is the only practical way forward given the constraints. In such circumstances we must rely on uncertainty and bias audits and understand the implications, and robustness of, the system outputs. Where uncertainties are unacceptable, further more detailed model predictions will be required. For this reason alone the existing freshwater modelling approach is deemed acceptable. Propagating the flow model to England and Wales, without even contemplating higher resolution data, is already a significant exercise. However, this does not prevent more complex models being incorporated in later versions of APPRAISE.

Ultimately the 'fit-for-purpose' aim of the system is to derive predictions that are commensurate with the resolution and robustness of the regulatory levels. Where appropriate we must interpolate and extrapolate results, and this naturally introduces further uncertainties. It seems wasteful to produce predictions at a higher resolution than necessary and introduce uncertainties from upscaling effects. Hence, if regulatory criteria are expressed as annual limits, then providing higher resolution temporal results may not bring any benefits concerning the confidence in the decision. Averaging data over time, smoothes out some of the more detailed processes and may support a less detailed approach.

As a result of the dramatic increase in computing power available in recent years, it is now quite feasible to run complex software packages which include hydrographical models such as the Danish Hydraulics Institute package MIKE21 and the WRc package QUESTS for coastal or estuarine sites, and access results quickly. If short term EQS are derived then these packages are extremely powerful for modelling short term dispersion, however, the major limitation would be data availability, and therefore these models in general would not be appropriate for generic impact assessments. However, there would appear to be no reason why such models should not be used in a calibration / validation mode or to investigate the potential consequences of accidental discharges.

It is interesting to compare the field of aquatic dispersion modelling with that of atmospheric dispersion modelling. In the atmospheric environment better models of dispersion in the atmospheric boundary layer have been produced in the last 10-15 years, and these have been incorporated in a number of `second generation' codes. The improvements in physical understanding (essentially a better conceptual model for the processes involved compared with the empirical Gaussian plume models) can be incorporated into dispersion models, and suitable input data can generally be measured.

In the aquatic environment, detailed models for dispersion, generally based on numerical solutions of the advection-dispersion equations, are available, and the currently available computing power means that these could be applied to pollution discharges. In this case, however, the detailed input data that would be required are generally not available. In addition, the timescales of interest are often very different, i.e. of the order of an hour for dispersion in the atmosphere, but of the order of a year for the aquatic environment. It is our conclusion therefore that the current position of inter-media differences is justified and appropriate given the comments above.

5. CONCLUSIONS AND RECOMMENDATIONS

The main conclusions which have been drawn from the review are as follows:

- The current IPC methodology which adopts the IEI concept (i.e. adding EQ's for all media) requires that all uncertainties in media concentration predictions are investigated and minimised wherever possible to improve the robustness of the authorisation decision.

- The conceptual representation of media features and processes is a function of the methodology, the regulatory decision support system and the chosen environmental model (with particular respect to data availability).

- No individual model can be recommended for all aquatic dispersion calculations; the choice will depend upon the time and distance scales of interest, and the uncertainties present in other stages of the assessment being undertaken.

- Numerous models have been reviewed and their potential application within a national decision support system is limited by the availability of data not potential computing power. For example, commercially available hydrodynamic and water quality models software packages such as MIKE21 (developed by the Danish Hydraulics Institute) are extremely powerful for modelling short term dispersion, but are data-hungry.

- In light of the above findings it is concluded that the existing freshwater modelling approach is fit-for-purpose.

- A simple estuarine scoping model has been presented as a first attempt to introduce this component into APPRAISE. It will calculate average and maximum concentrations by estimating average and minimum compartmental volumes.

- The resultant inconsistency in complexity of modelling features and processes in different media is acceptable as long as outputs from one model/medium are suitable inputs to another.

- The soil system is a complex environment and storativity and retardation effects introduce great uncertainties into temporal concentration predictions. This component is a weak link in the system and restricts the ability to incorporate realistic soil-to-water transfers.

Research requirements in the area of aquatic dispersion modelling need to be evaluated in the light of limitations in data availability, and uncertainties in other components of radiological assessments. The areas where there would appear to be most scope for fruitful development are:

- extrapolation of the flow model to the whole of England and Wales (including best fits for ungauged areas);

- detailed specification, calibration and validation of a simple estuarine scoping model with more detailed hydrodynamic and water quality studies.

- a detailed investigation into all uncertainties and how they affect the regulatory decision process

- further investigation into soil modelling and resolving soil-to-water transfers

The first two areas would be directly applicable to current assessments for annual critical group doses, whilst the second two involve more fundamental research of a longer term nature.

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