APPRAISE 3.0: Technical Overview

Technical Report
P266

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R&D Technical Report P266

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Statement of use
This report reviews atmospheric dispersion models and summarises some code intercomparisons. The information within this document is meant for the use by EA staff and others involved in IPC regulatory operations.

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CONTENTS

SYMBOLS and UNITS

The first two columns in the table below identify the symbolic notation used in this report and the dimensions of each quantity. The values of all quantities input to APPRAISE must be expressed in a common units system of mass, length and time, and are output in that same system, for example milligrams (mg), metres (m) and seconds (s).

symbol	meaning	dimensions
A	thickness of the atmospheric mixing layer	length
c	ground level mass concentration	mass per unit volume
q	mass rate of release of pollutant	mass per unit time
d	mass deposition rate	mass per unit area per unit time
T	measurement time	time
E	decay factor	$time^{-1}$
F	vertical dispersion shape factor at ground level	none
h	stack height	distance
G	horizontal dispersion shape factor	none
λ	the decay rate	inverse time
Λ	washout coefficient	$time^{-1}$
r	distance from the source point	length
σ_y	horizontal dispersion coefficient	length
σ_z	vertical dispersion coefficient	length
$S = \Lambda$	Wet deposition rate	$time^{-1}$
T_a	ambient temperature	temperature
T_s	temperature of release	temperature
u	wind speed	length per time
v_{dry}	deposition velocity	length per time
W	wet depletion factor (≤ 1)	none
z	vertical height	length
N	exponent of wind speed dependence on height	none
v_s	vertical velocity of effluent at source point	length per time
D_s	diameter of effluent at source point	length
B	buoyancy parameter	$length^4 \, time^{-3}$
R	horizontal distance to final plume rise	length

EXECUTIVE SUMMARY

This report gives a technical overview of the APPRAISE software written by QuantiSci Ltd for the Environment Agency. APPRAISE is a prototype tool for Integrated Pollution Control (IPC). It calculates various scores and indices of the total and distributed pollution resulting from prescribed processes, taking account of the releases to air, discharges to water and sewer, and other waste arisings for different operating options. The scores and indices of each option may assist Agency inspectors to assess process applications, and to assess the Best Practicable Environmental Option (BPEO). Currently APPRAISE covers a 100km x 100km study area in SE England. Whilst the software is intended primarily as a tool for IPC regulation, it can calculate the combined effects of up to six processes. Its atmospheric dispersion calculation covers an area which includes all locations up to 25km from the furthest in any cardinal direction. Ground level concentrations and soil depositions are made on a mosaic which provides more detail around each source. APPRAISE includes the following features:

- A graphical interface for input of the waste disposal data required for IPC assessments.

- Calculation of pollution measures defined by different regulations for each pollutant (eg a 98%tile of one hour averages).

- Displays of the spatial distribution of predicted, ambient or total measures for regulated pollutants.

- Summaries of the spatial maximum of each pollutant concentration, and comparison to its environmental assessment level.

- A database of pollutant regulations and score factors.

- A database of ambient pollution concentrations in air and water.

- Average and high infills of ambient pollution patterns.

- GIS facilities for pollution display, interrogation, and grid referencing.

1. INTRODUCTION

On April 1st 1996, Her Majesty's Inspectorate of Pollution (HMIP) became part of the new UK Environment Agency (from here on referred to as the Agency), which was established for England and Wales under the Environment Act 1995. The Agency assumes HMIP's previous duties under the Environmental Protection Act 1990 for Integrated Pollution Control of the most technically complex and/or polluting processes in England and Wales. Under the Act, operators of prescribed processes' must apply to the Agency for authorisation before operating the process concerned.

In determining an application for authorisation the Agency needs to ensure that the Best Available Techniques Not Entailing Excessive Cost (BATNEEC) have been used to prevent, or where that is not possible, to minimise and render harmless releases of prescribed and other substances from the process. In addition, where substances are released to more than one medium, operators are required to use BATNEEC to minimise pollution to the environment as a whole, having regard to the Best Practicable Environmental Option (BPEO) available.

As part of the authorisation procedure operators are required to demonstrate that unavoidable releases have been minimised and rendered harmless and the preferred operation can be considered the BPEO. The Agency is in the process of developing guidance on the manner in which environmental and BPEO assessments for integrated pollution control (IPC) can be undertaken, and two consultation documents have been produced. The Orange Book' [HMIP, 1994] set out a number of stages in the investigation of alternative process and abatement options for BPEO assessment. Further refinements were published originally in three volumes [HMIP, 1996], and subsequently as a single volume [Environment Agency, 1997], hereafter referred to as the "Blue Book".

The methodology has three stages as follows:

Stage I involves a preliminary assessment of a base-case option, and alternative options. It includes:

- *Preliminary assessment procedure;*

- *Identification of pollutants released;*

- *Results comparison with Chief Inspectors Guidance Notes;*

- *Chimney height determination;*

- *Determination of compliance with Environmental Quality Standards (EQS's) and Environmental Assessment Levels (EAL's);*

- *Identification of significant releases; and*

- *Selection of practical process techniques.*

Stage II involves an environmental assessment of generated process control and abatement options. It includes:

- *Environmental assessment procedure;*

- *Assessment of long term environmental effects*

- *Assessment of short term effects of releases;*

- *Assessment of other environmental indices;*

- *Other environmental factors; and*

- *Identification of BPEO.*

Stage III involves the determination of the site specific BPEO option.

As the Agency make more use of IPC tools, those tools will be of great use to applicants, i.e. to the operators of prescribed processes. Operators need access to environmental quality standards and assessment levels to explore process options and select the BPEO for their business. The critical use of a common set of tools should promote constructive debate on regulation and improve the quality of applications, to the benefit of all.

This document gives a technical overview of Version 3.0 of a prototype tool, named APPRAISE (Assessment of Prescribed Process Releases And Integrated System Evaluation). It is one of four documents produced by QuantiSci Ltd under contract P4-029.

- P.R.Maul, N.S.Cooper, B.E.A.Fisher and A.Venter, Atmospheric Dispersion Models for Integrated Pollution Control: The Use of Second Generation Models and the Importance of Plume Rise, Environment Agency R&D Technical Report P264, 1997;

- R.C.Brown, APPRAISE : Technical Overview of Version 3.0, Environment Agency R&D Technical Report P266, 1998;

- R.C.Brown, APPRAISE : User Guide for Version 3.0, Environment Agency R&D Project Record P4/i029/02 , 1998;

- D.J.Waters, P.R.Maul, K.J.Clarke, R.C.Brown and A.Venter, APPRAISE II : Review of Aquatic Dispersion Models, QuantiSci Report ENV2-6032A-REVB Version 1.0, February 1998;

For completeness, the current document retains material unchanged from the technical overview of Version 2.0 of APPRAISE, which was described in a previous document [Brown and Waters, 1997], and which was one of a series of reports [Brown, 1997, Brown and Waters, 1997, Brown et al, 1997, Maul et al, 1997] produced under a previous contract for HMIP (CPR2/41/1/125).

APPRAISE is a software tool designed to assist IPC in England and Wales. It is conceived as a tool primarily for routine releases, and the current prototype runs on a Unix workstation. Version 3.0 automates many of the procedures advocated in the E1 Guidance Notes for processes within a 100 km by 100 km study area in the South East of England, centred at grid reference TL 5000 0000. Questions of timescales and objectives are closely linked with the activities of planning and regulation. Whilst the two are closely interlinked, planning seems more closely allied to issues covering wider spatial and temporal scales. Planners and regulators may require somewhat different types of software to support their decisions. Planning over long timescales is likely to involve quite different models than those used in APPRAISE, which was developed largely, but not wholly as a tool for regulating applications. APPRAISE provides evaluations of regulatory indices for processes involving a wide range of pollutants. Its planning use is limited to a small number (6) of processes.

APPRAISE Version 1.0 was developed on a PC under Microsoft Windows, and had grown to the point where it was constrained by 16 bit addressing limitations. Under a previous contract for HMIP (HMIP/CPR2/41/1/125), the software was ported to a 32 bit system selected by the client, a Sun Sparc20 workstation with a Unix based operating system, Solaris, where it runs in the Motif window environment. After further enhancements, this software became APPRAISE Version 2.0. Substantial changes were required to port the geographical data used, which necessitated "padding" the database from about 30Mb to 80Mb. This database has remained unchanged under the current contract (P4-029).

2. AQUEOUS DISPERSION MODEL

The aqueous dispersion model in APPRAISE is one of simple dilution in a river flow model which is calibrated to different watersheds that intersect the study area.

2.1 River Flow Model Calibration

Five hydrometric regions intersect the study area. They are:

- Thames - 39

- Lee - 38

- Stour - 36

- Rhoding - 37

- Cam/Ouse - 33

The numbers are the codes used by the Institute of Hydrology. The river flow model interpolates water flow F as proportional to the sum L of upstream river lengths, $F = KL$. This model is used to derive pollutant concentrations in the study area, and is calibrated using flow data from the Institute of Hydrology for the monthly flows at gauging stations in those regions during the years 1973 through 1993. A detailed discussion was given in a previous report [Waters et al, 1994]. In brief the procedure was as follows. Some filtering was applied to reject gauging stations which had very few records, or were within 10km from a river source where the flow model might be poor, and for the same reason, all flows less than or equal to 0.1 ms^{-1} were ignored. All data for the exceptional drought year of 1976 were ignored. The sum of upstream lengths was calculated at river confluences throughout the river network, and geographically associated with the gauging stations in the river network. The model flow was then fitted to the measured flows and lengths in each recorded month. This procedure was adopted for each hydrometric region in turn. The root mean square deviation of such fits is typically about 30% of the gauging station mean flows. The calibration data is stored in ASCII file 'flowfact.dat'.

2.2 River Network and Pollutant 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. These 'posts' are river confluences, and occasionally isolated points on long river sections without confluences. 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 $Q_{s,j} = V_j c_{s,j}$, 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 w has its discharge. These discharges are taken as $Q_{s,j} = V_j c_{s,j} \prod_{k=1}^{M_w} (1 - R_{s,k})$, where $R_{s,k}$ is a retention factor for pollutant s at sewage treatment stage k, and M_w is the number of treatment stages at sewage works w. The retention factors are stored in an ASCII list of pollutant assessment levels for water (see Section 4.6). Once all discharges have been injected, they are traced downstream and summed where necessary at river confluences.

2.3 Derivation of Different Concentration Measures

The accuracy of the upstream length model is adequate for predicting flows and 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 is adopted. The monthly flow records in each region are summarised by the average and the minimum of flow per length factors, K_{av} and K_{min}. These factors are 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 are estimated by assuming the cumulative probability distribution formula below, assuming that $C > C_{av}$,

$$P(C) = \frac{1}{2} + \frac{1}{2} \left[\frac{(C - C_{av})}{(C_{max} - C_{av})} \right]^B , \tag{2.1}$$

with a power $B = \frac{1}{2}$, so that as $C \to C_{max}$, $P(C)$ approaches one like $\frac{1}{2} + \frac{1}{2}[1 - x]^{1/2}$ as $x \to 0$. This implies a plausible long tailed probability density function $p(C) = dP(C)/dC$, 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

$$C(P) = C_{av} + (C - C_{av})[2P - 1]^{1/B} . \tag{2.2}$$

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

3. THE ATMOSPHERIC DISPERSION MODEL

3.1 Introduction

The model of atmospheric dispersion in the demonstrator Version of APPRAISE is an implementation [Brown, 1993] of the Gaussian plume model known as R91 [Clarke, 1979]. The code was developed to meet the client's requirements from the first demonstrator model (APPRAISE 1.0). An outline of the R91 model is first given, followed by the Agency requirements, before describing the current implementation.

3.2 The R91 Model

APPRAISE calculates ground level concentrations and depositions from up to six chosen processes, each having one stack. The salient features of the model are described below.

3.2.1 Pollutant Concentrations at Ground Level

The ground level concentration of a pollutant released from a continuous process acting as a single point source are evaluated using

$$c = qEFGH, \tag{3.1}$$

where q is the rate of release of the pollutant, $E = \exp(-\lambda t)$, is the decay of the pollutant during a travel time t, λ its decay rate, F and G are vertical and horizontal shape factors at ground level (with dimensions of inverse length), and $H = 1/u$ is the dilution due to mixing with air at wind speed u.

The above expression for c may represent either a non sector averaged or sector averaged form of the R91 model as given by equations (4) and (6), or equations (7) and (8) of [Clarke, 1979]. This is facilitated by using F and G factors here that absorb the $1/(\sigma_z\sqrt{2\pi})$ and $1/(\sigma_y\sqrt{2\pi})$, or $1/(\sigma_z\sqrt{2\pi})$ and $1/(r\alpha)$ factors which appear explicitly in those equations, where α is the sector width in equation (8). Thus the vertical dispersion factor at ground level is given by

$$F = 2g(h,\sigma_z) + 2g(2A + h,\sigma_z) + 2g(2A - h,\sigma_z), \tag{3.2}$$

where h is the effective source height above ground allowing for plume rise, σ_z is the vertical dispersion length and $g(s,\sigma) = \exp -[\frac{1}{2}(s/\sigma)^2]/(\sigma\sqrt{2\pi})$ is a gaussian probability density.

The above expression for F is simply $1/(\sigma_z\sqrt{2\pi})$ times equation (5) of the R91 report at ground level ($z = 0$).

The horizontal dispersion factor is given by $G = g(y,\sigma_y)$ for the non sector averaged, or $G = 1/(r\alpha)$ for a sector averaged forms, where r is the distance from the source. The vertical

dispersion length σ_z was calculated from the formulae of Hosker given in [Clarke, 1979]. It depends on the atmospheric stability, the distance from the source, and the roughness of the terrain. In APPRAISE Version 1.0, predictions were made for sector averaged concentrations, using $\alpha = \pi/6$.

APPRAISE models plume rise, and included stack tip downwash using formulae taken from [Wilson, 1993]. We note a typographical error in that reference below.

The downwash (in m) is taken to be

$$max[0, 1.5 - \frac{v_s}{u}],\qquad (3.3)$$

where v_s is the exit gas velocity at the source point (the stack top).

This downwash is subtracted from plume rise, which is taken to be the larger of buoyancy and momentum rises, and is calculated as follows.

In unstable and neutral conditions buoyancy rise is calculated as

$$\frac{1.6B^{\frac{1}{3}}(3.5R)^{\frac{2}{3}}}{u},\qquad (3.4)$$

where B is a buoyancy parameter described below, and R is the distance to final plume height, given by $R = 14B^{\frac{2}{5}}$ when $B < 55$, and otherwise by $R = 34B^{2/5}$. The buoyancy parameter is given by $B = gv_s(\frac{1}{2}D_s)^2 f$, where g is the acceleration due to gravity at the Earth's surface (9.81 m s-2), D_s is the diameter (in m) of the effluent at that point, and f is a volumetric contraction factor given by

$$f = [1 - \frac{T_a}{T_s}],\qquad (3.5)$$

where T_a is the ambient air temperature and T_s is the temperature of the effluent at the release point, both in degrees Kelvin. (We note a typographical error in Wilson's paper, which uses a contraction factor of $[T_s - T_a/T_s]$.) APPRAISE takes T_a to be 283 degrees Kelvin, equivalent to 10 degrees C. Under the same conditions momentum rise is calculated as

$$3D_s\frac{v_s}{u}.\qquad (3.6)$$

In stable conditions the buoyancy rise is calculated from

$$2.6\left[\frac{B}{u\psi}\right]^{\frac{1}{3}},\qquad (3.7)$$

where

$$\psi = g\frac{1}{T_a}\frac{dT_a}{dz},\qquad (3.8)$$

and dT_a/dz is the ambient vertical temperature gradient, taken to be 0.02 degrees per metre in slightly stable conditions, or otherwise to be 0.035. Under the same conditions the momentum

rise is calculated as the smaller of $3D_s v_s/u$ and

$$\frac{1.5}{u^{\frac{1}{6}}} \left[\frac{v_s^2}{u} \frac{T_a}{T_s} (\frac{1}{2}D_s)^2 \right]^{\frac{1}{3}}. \tag{3.9}$$

The calculated net plume rise is added to the physical height of a stack to give its effective source height.

3.2.2 Pollutant Depositions to Ground

Deposition rates are evaluated for wet and dry deposition mechanisms, including the effect of wet depletion, using the formula

$$d = qEGH(WS + Fv_{dry}), \tag{3.10}$$

where WS is an average factor for wet depletion and wet deposition, given by expressions in [Jones, 1981], and used a washout coefficient $\Lambda = 10^{-3}\text{s}^{-1}$, and v_{dry} is a dry deposition velocity which could differ for each pollutant. Dry depletion is not included in concentration or deposition predictions, as it requires a numerical integration which would have a substantial effect on the calculation speed.

3.2.3 Spatial Distributions and Spectral Measures

In the R91 report, the effects of different weather categories, wind speeds and directions are summed in equation (9) of [Clarke, 1979], which predicts the average concentration in a given sector. Whilst this formula might have been used, it applies to specific choices of other parameters which are inconvenient. In particular, it applies to a single source, a specific distance r, and a single terrain roughness. To cater for more than one source, allow for a range of distances within a mosaic grid, and a variety of terrain roughness scales, the sum must be generalised to integrate over such extra dimensions. The most efficient way of doing so is to use a sampling scheme, generally referred to as the Monte Carlo method [James, 1980].

In APPRAISE 1.0 terrain roughness lengths of 0.01, 0.04, 0.1, 0.4, 1.0 or 4.0m were sampled with equal probability in the calculation, and independently of distance or angle. Spectra of concentrations and depositions due to weather variations were elicited by sampling statistics for the joint probabilities $p_{kjn} = p(k, u_j, \theta_n)\Delta u_j \Delta \theta_n$ of each stability category k, wind speed slot j and wind sector n recorded at Stansted airport. These spectra represented the distribution of measurements made over a 24 hour averaged period, as discussed in 3.3.1. The wind speed (at ten meters height) is recorded as being within one of six slots $[u_j, u_j + \Delta u_j]$, and the wind direction within one of twelve equal angular sectors of width $\Delta \theta_n$.

Meteorological statistics used in APPRAISE include six contigous wind speed ranges. The first of these is calms. These are unfortunately incompatible with this or any other Gaussian plume

model. To avoid this difficulty, the joint probability table is adjusted to redistribute the small calm probability into the next speed slot, sharing it equally amongst all wind angular sectors, so as to yield an adjusted set of weights w_{kjn}.

The wind speed at ten meters height is used to calculate H. At other heights the wind speed is found from a category and roughness dependent power law, $u(z)/u(10) = (z/10)^N$, where N is given in Table 1 of the R91 report [Clarke, 1979]. The wind at the real source height is used to calculate plume buoyancy, whilst the speed at the effective source height is used to calculate the travel time used to estimate any decay.

Predictions are made within a spatial mosaic of square tiles, whose sizes decreased as the distance to any source decreased.

3.3   Implementation

The R91 implementation in APPRAISE 2.0 and 3.0 was developed to produce different statistical measures of pollutation required by the Agency as described below.

3.3.1   Spectral Measures of Pollution

Results were required for different regulatory reference periods of 10 min, 15 min, 30 min, 1 hr, 4 hrs, 8 hrs and 24 hrs. Each pollutant might have several regulations, each having one of those reference periods, and a spectral measure, a mean, a median or a quoted percentile. These periods correspond to the time ΔT over which a measurement is made, and over which fluctuations in wind direction are averaged. This influences the amount of horizontal dispersion to be modelled as follows.

Horizontal dispersion may be modelled as Gaussian in the angle around the nominal wind direction divided by the distance from the source, viz $G = g(\theta - \theta_n, \sigma_\theta)/r$. In angular terms, the dispersion parameter σ_θ is taken as the vertical dispersion parameter divided by the distance from the stack, and augmented by wind direction fluctuations, viz:

$$\sigma_\theta^2 = \left[\frac{\sigma_z}{r}\right]^2 + 0.065^2 \frac{7}{u}\Delta T \tag{3.11}$$

which is equation (B5) on page 69 of R91 divided by r, where ΔT is the measurement time in hours, and u is in m s^{-1}.

A sector averaged value for concentration may be considered as a prediction with wind direction fluctuations averaged over a 24 hour measurement duration. However, to use the non sector averaged form with Pasquill categories, ΔT is strictly limited by the lifetimes of those categories. With this in mind an upper limit of six hours [Jones, 1985] is imposed in APPRAISE. This limitation is a consequence of using long term meteorological statistics for joint probability. It

is possible to avoid this limitation by adopting a different approach using hourly meteorological statistics. However, to achieve *the same reliability* for long term predictions, it would have been necessary to use a sample of such hourly data over *many years*. Such an approach would require a huge increase in computational time without clear benefits.

3.4   Architecture

The key to the design was the need to cope with increased calculation loads implied by the requirements, and hinged on the observation that many R91 model factors are independent of the particular pollutant, or only dependent via its regulation period or deposition parameters.
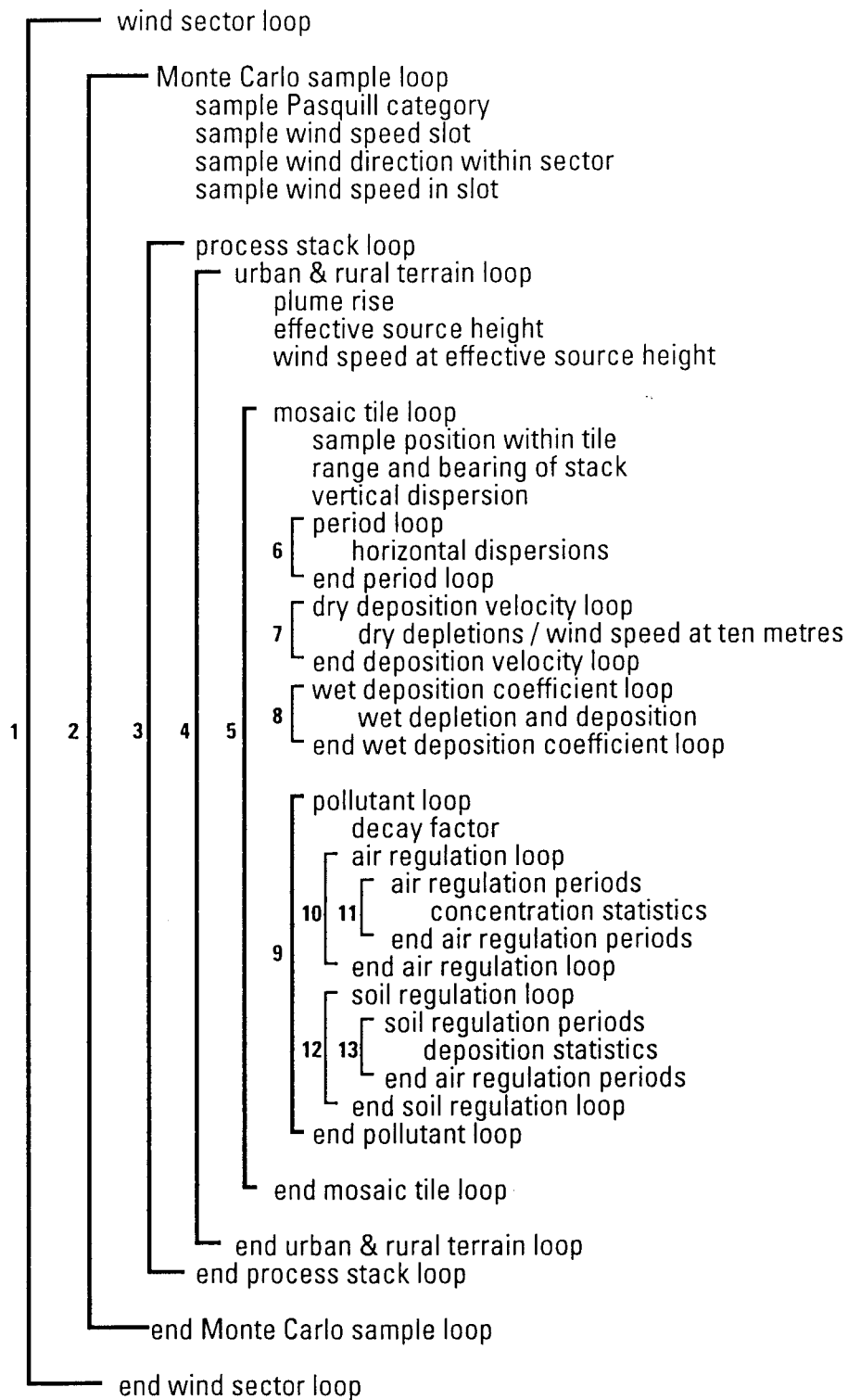
Deposition is pollutant dependent in the R91 model and could have posed a large calculation load. Its prediction is less certain than that of concentration. Wet and dry processes are not wholly distinct, but are parameterised by a pollutant washout coefficient and a dry deposition velocity. In practice these values are not well determined [Jones, 1983], partly because they are determined by natural conditions and features that exhibit wide variations. Washout is influenced by rainfall rate, rain droplet size, rainfall distribution and updrafts, the affinity of a pollutant for water, its vapour pressure. Dry deposition velocity depends on particle size, density, wind speed and ground cover, and pollutant chemistry. The uncertainties cover an order of magnitude [Smith, 1991]. Given the uncertainties and load penalties, predictions were chosen for a fixed number of washout coefficients and dry deposition velocities which spanned the likely range of values.

By calculating generic factors for a small fixed number of periods and deposition parameters, and devising a method for calculating spectral measures without storing spectra, it was possible to restrict the major computational effort to generic factors, and minimise the overhead of individual pollutants. Dry depletion then became affordable in the calculations for concentration and deposition.

APPRAISE 3.0 provides predictions for only two roughness lengths, representative of rural and urban scenarios. Although the roughness length must carry some uncertainty, the concept that rural and urban scenarios are distinguishable is probable, and separate calculations are therefore preferable.

The heart of the code structure is depicted in a simplified manner by the schematic of Figure 3.1. In that figure the outermost loop over wind sectors (1) improves the angular quality of the spatial distributions by giving each sector its own Monte Carlo calculation.

All sampling occurs within the Monte Carlo loop (2), so that all processes and mosaic tiles experience the same climate.

wind sector loop
  Monte Carlo sample loop
      sample Pasquill category
      sample wind speed slot
      sample wind direction within sector
      sample wind speed in slot

    process stack loop
      urban & rural terrain loop
        plume rise
        effective source height
        wind speed at effective source height

      mosaic tile loop
        sample position within tile
        range and bearing of stack
        vertical dispersion
        period loop
6   horizontal dispersions
        end period loop
        dry deposition velocity loop
7   dry depletions / wind speed at ten metres
        end deposition velocity loop
        wet deposition coefficient loop
8   wet depletion and deposition
        end wet deposition coefficient loop

        pollutant loop
          decay factor
          air regulation loop
10 11   air regulation periods
              concentration statistics
              end air regulation periods
9   end air regulation loop
          soil regulation loop
12 13   soil regulation periods
              deposition statistics
              end air regulation periods
          end soil regulation loop
        end pollutant loop

      end mosaic tile loop

    end urban & rural terrain loop
    end process stack loop

  end Monte Carlo sample loop

end wind sector loop

1 2 3 4 5

Figure 3.1: Schematic of Air Dispersion Calculation

The climate is sampled by firstly choosing at random one of the Pasquill categories A to G, and one of the wind speed slots. The relative frequency of weather with the chosen sector, category and slot is then held as a weight for the sample.

A precise wind direction and speed is then established as follows:- The wind direction is chosen uniformly at random within a sector, but the wind speed is chosen not uniformly within its speed slot; lower values in each slot are chosen more frequently, consistent with typical speed spectra.

Within the Monte Carlo loop, the calculations proceed to the process option loop (3), where the polluting stack is selected, and then to a loop (4) over two roughness lengths typical of urban and rural terrains. Within these loops the plume rise is calculated to find the effective source height. The wind speed at the effective source height is then calculated to allow a conservative regulatory estimate of travel time.

The next loop (5) ranges over a mosaic of spatial tiles. This mosaic is constructed to cover an area which encompasses all selected stacks (one per process), has a border of 25km around the edge, and decreasing tile size with decreasing distance from each stack. Tiles can be at most 10km on a side, and shrink by a factor of two as a stack is approached. The minimum tile size is $10/2^6 = 0.15625$km. For a single stack the mosaic area is simply a 50km sided square centred to within 5km on the stack. The centering is not exact, because the mosaic must register with a fixed 5km sided grid in which ambient levels are available. The effect is a grid with a quasipolar behaviour around each stack which is suitable for resolving the expected spatial peaks.

Within the mosaic tile loop (5), the position within each tile is sampled uniformly, so that the spectrum of results represents the position over each tile as a whole. The range and bearing of the current stack are then found, and the vertical dispersion factor is calculated at ground level. At this point there are three small loops. The first of these (6) is one to calculate a horizontal dispersion factor for every regulatory reference period. After this is complete, there follows a loop (7) to calculate a dry depletion factor [Jones, 1981] divided by the ten metre wind speed, for a fixed number of fixed dry deposition velocities, 0, 10^{-4}, 10^{-3} and 10^{-2} m s^{-1}.

After that there is a loop (8) to calculate the product of wet depletion and wet deposition factors for two values of wet deposition coefficient, 10^{-4}s^{-1} and 10^{-3}s^{-1}. Some extra variability in wet deposition is allowed by making predictions on a sample by sample basis. Rain is assumed to fall 20% of the time only when the Pasquill category is D (neutral stability), corresponding to an absolute probability of about 10%. If it does not rain, both values of wet depletion times deposition are zero.

Inside the loop over pollutants (9) there are only a few multiplications and additions to perform once the decay factor has been evaluated. The calculations for concentration and deposition are organised in loops (10) and (11) over the regulatory reference periods that apply to each. Inside these loops the concentration and deposition samples c and d are calculated from the formulae overleaf.

$$c = qEHFG, \tag{3.12}$$

$$d = qEH[F v_{dry} + WS], \tag{3.13}$$

where q is the rate of release of the pollutant, $E = \exp(-\lambda t)$ is the decay of the pollutant during a travel time t, F and G are vertical and horizontal shape factors at ground level with dimensions of inverse length, and $H = 1/u$ is the dilution due to mixing with the air at wind speed u.

Plume rise is modelled in the same manner as described in Section 3.2. From these sample values the program updates three statistics for concentration or deposition rate, $y = c$ or $y = d$,

- the number of times that y exceeds a very low threshold, $y_0 = 10^{-24}$, in mg m^{-3} for concentrations, or mg m^{-2} s^{-1} for deposition rates,

- the sum of weighted y values,

- the maximum y.

The first pair of each set are later divided by the sum of weights to yield $p(y > y_0)$, y_{av} and y_{max}. These are stored for every regulatory reference period and pollutant, and for urban and rural terrains. The storage is not a simple array, since every pollutant may have a different number of regulations, involving a number of reference periods. However a storage index is calculated to ensure efficient packing. The speed of this code allows increased sampling; currently this is set at 100 per angular sector.

3.5   Spectral Measures

The above statistics provide the average or maximum concentration or deposition for any pollutant and reference period directly, and also allow estimates of different spectral measures of concentration or deposition values by assuming that either spectrum may be described by the following shape.

$$p(y) = p_0 \delta_{y,0} + p_1 \exp(-sx), \tag{3.14}$$

where $x = y/y_{max}$, i.e. c/c_{max} or d/d_{max}, and $\delta_{x,0}$ is the Kronecker delta function,

$$\delta_{0,0} = 1, \tag{3.15}$$

$$\delta_{x \neq 0,0} = 0, \tag{3.16}$$

and s is a slope describing the spectral shape. The first term accounts for the numerous occasions when the wind is not blowing any appreciable pollution towards the position of interest. The chance of that happening with a uniform wind rose may be estimated as about (11/12), or over 90%. If the wind rose is uniform this is the chance of the wind being outside a ($2\pi/12$) angular sector, a value commensurate with wind fluctuations over 24 hours. With smaller averaging

times, it may be argued that the expected value for p_0 would be even higher. The second term models the spectral decay which is qualitatively expected on statistical grounds. We have observed that this type of shape is indeed representative of spectra from calculated samples at a wide range of distances from a single source. An example of a sample spectrum using the same R91 model in QuantiSci's QUEST shell is shown in Figure 3.2 below.
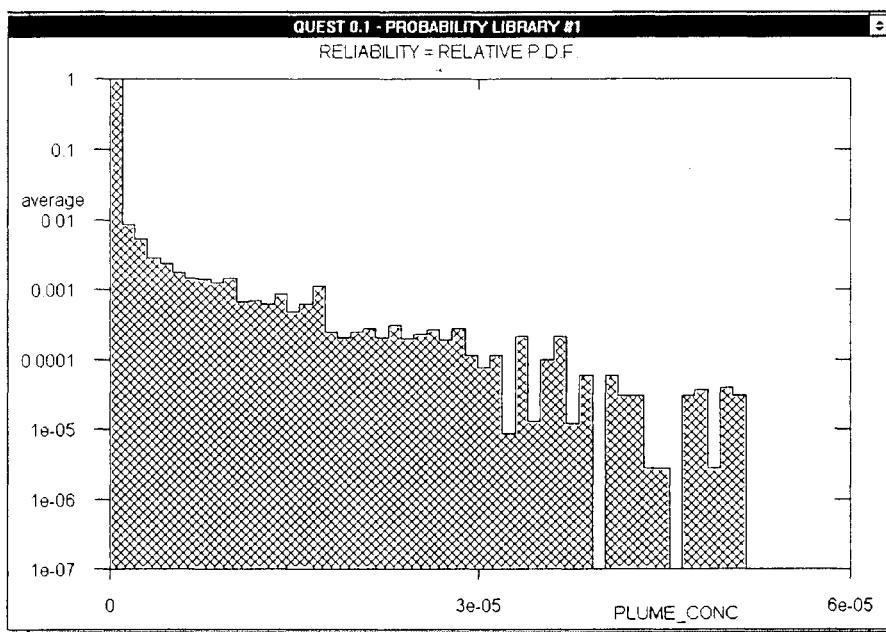
Figure 3.2: A typical R91concentration spectrum

We equate $p_0 = 1 - p(c > y)$ or $p_0 = 1 - p(d > y)$, and find

$$p_1 = \frac{s(1 - p_0)}{1 - \exp(-s)}.$$ (3.17)

The spectral slopes are then readily found by iteratively solving

$$x_{average} = (1 - p_0)\left[\frac{1}{s} - \frac{\exp(-s)}{1 - \exp(-s)}\right].$$ (3.18)

Spectral estimates are then made from

$$x(P) = \frac{1}{s}\ln\left[\left(1 - \frac{P - p_0}{1 - p_0}(1 - \exp(-s))\right)^{-1}\right],$$ (3.19)

where P is the required percentile expressed as a probability. (Note that regulations with $P < p_0$ are satisfied by $x = 0$.) This method of estimating percentiles is much faster than the direct approach of storing sample values for every tile, and searching them later. Although it is clearly an approximation, it is justified by observation and is accurate enough given the expected accuracy of the R91 model [Jones, 1985]. Coupled with the increased sample rate, the use of this estimator is simple and practical way of avoiding enormous overheads associated with storing concentration and deposition spectra for each pollutant in each tile.

4. POLLUTANTS

4.1 Requirements

The pollutant database structure in APPRAISE Version 3.0 is organised around the lists in the Agency's 'Blue Book' [HMIP, 1996, Environment Agency, 1997]. APPRAISE uses its database for several purposes, namely:

- to control the lists of pollutants that appear in each disposal pathway interface,

- to control which predictions were made for which pollutant,

- to control what spectral measures are possible for each pollutant, and

- to determine which pollutants may require ambient pollution data.

There are separate lists for pollutants with

- concentration assessment levels in air

- concentration assessment levels in water

- assessment levels for releases to land via deposition

- hazard scores

- global warming potentials

- photochemical ozone creation potentials

These lists are implemented as simple ASCII files described below.

4.2 Global Warming Potentials

Tables 7.1 and 7.2 of the 'Blue Book' are implemented by file 'chem_gwp.dat' in the following format:

- *Name*

- *Agency global warming potential*

The entry for methane is:-

- METHANE

- 21

4.3 Photochemical Ozone Creation Potentials

Table 8.1 of the 'Blue Book' is implemented by file 'chem_pocp.dat' in the following format:

- *Name*

- *Agency photochemical ozone creation potential*

The entry for methane is:-

- METHANE

- 3.4

4.4 Concentration Assessment Levels in Air

Tables A1 and A2 of the 'Blue Book' are implemented by file 'chem_air.dat' in the following format:

- *Name*

- *Number of assessment levels*

- *The assessment levels (see below)*

- *Half life in air (s)*

- *Dry deposition velocity (ms^{-1}) and washout coefficient (s^{-1}) followed by the molar weight of the pollutant*

Note that the dry deposition velocity and washout coefficient are in practice restricted by the selection built in to the code, viz one of 0, 10^{-4}, 10^{-3} and 10^{-2} m s^{-1} for dry deposition, and 10^{-4}s^{-1} and 10^{-3}s^{-1} for washout (see Section 3.4).

Each assessment level has the following format; an *identification* string, followed by the measurement period, (1 MONTH, 8 HR, 4 HR, 1 HR, 30 MIN, 15 MIN or 10 MIN), followed by a measure string (MEAN, MEDIAN, MAX, or *percentile*, and followed by the value of the assessment level in mg m^{-3}. The *identification* string may be used to indicate whether the level value is for long or short term assessment, or is an environmental quality standard. Note that the first assessment level with the identifier LONG is taken as the *EAL* for deriving environmental quotients as described in sections 6.2 through 6.5. The *percentile* string is of the form *xx*PERCENTILE, where *xx* is desired percentage of the spectrum of pollution concentration.

The entry for nitrogen dioxide provides a good example of all these features:-

- *NITROGEN DIOXIDE*
- *3*
- *LONG 8 HR MEAN 0.04*
- *SHORT 30 MIN MEAN 0.286*
- *EQS 1 HR 98PERCENTILE 0.2*
- *1e9*
- *1e-3 1e-4 46*

Note that the molar weight of the pollutant is only required as an ambient conversion factor for gases at NTP where ambient concentrations are given as parts per billion. Cases where this is not required have a value of zero.

4.5   Assessment Levels for Releases to Land via Deposition

Table C1 of the 'Blue Book' is implemented by file 'chem_soil.dat' in the following format:

- *Name*
- *Maximum rate of deposition (mg $m^{-2} s^{-1}$)*

The entry for copper is:-

- COPPER
- 0.25

4.6 Concentration Assessment Levels in Water

Tables B1 and B2 of the 'Blue Book' are implemented by file 'chem_water.dat' in the following format:

- *Name*

- *Number of assessment levels*

- *The assessment levels (see below)*

- *Half life in water (s)*

- *Average removal factors at primary, secondary and tertiary sewage treatments (dimensionless)*

The assessment levels have the same format as those for air. Again note that the first assessment level with the identifier LONG is taken as the EAL for deriving environmental quotients as described in sections 6.2 through 6.5.

The entry for chromium and compounds in dissolved form is :-

- CHROMIUM & COMPOUNDS,dissolved

- 4

- LONG 1 MONTH MEAN 250

- CYPRINIDSOFT 1 MONTH MEAN 150

- SALMONIDHARD 1 MONTH MEAN 50

- SALMONIDSOFT 1 MONTH MEAN 5

- 1e9

- 0.4 0.61 0.1

4.7 Hazard Scores

Tables E1 and E2 of the 'Blue Book' are implemented by file chem_haz.dat in the following format:

- *Name*

- *Agency unit hazard score total*

The entry for methanol is:-

- METHANOL

- 200

In all cases each data item must be separated from its neighbour(s) by at least one blank.

4.8   Use of Pollutant Lists

4.8.1   Releases to Air

The user interface for entering releases to air is made up of pollutants gleaned from four of the above lists:-

- concentration assessment levels in air (chem_air.dat)

- assessment levels for releases to land via deposition (chem_soil.dat)

- global warming potentials (chem_pocp.dat)

- photochemical ozone creation potentials (chem_gwp.dat)

The user interface does not repeat pollutants which occur in different lists with the same name, although of necessity there are overlapping chemical groups.

4.8.2   Discharges to Water

The user interface for entering discharges to air is made up of pollutants from the list of concentration assessment levels in water (chem_water.dat).

4.8.3   Discharges to Sewers

The user interface for entering discharges to sewers is also made up of pollutants from the list of concentration assessment levels in water (chem_water.dat).

4.8.4   Waste Arisings

The user interface for entering waste arisings is made up of pollutants from the list of hazard scores (chem_haz.dat).

4.8.5 Assessment Levels for Environmental Quotients and Integrated Indices

The environmental assessment level used to calculate the indices described in Sections 6.2, 6.3, 6.4 and 6.5 is taken as the first regulation that is identified as long term in each medium. If no such level is available, APPRAISE uses the first short term one.

4.8.6 Assessment Levels for Displaying Tolerability of Pollution

Any assessment level for a pollutant may be selected to gauge the tolerability of spatial distributions in displays for predicted process contribution, ambient, or sums of process and ambient measures. Measures of predicted process contributions are described in Sections 5.1 and 7.1. For interface details see the User Guide [Brown, 1998].

5. THE ROLE OF AMBIENT DATA

The selection and interpolation of ambient data for infilling patterns of ambient pollution has been described in detail in a previous report [Brown and Waters, 1997]. The link between ambient data and background is described below.

5.1 Ambient and Background

Whilst ambient concentrations are in themselves of interest to the Agency, their role in AP-PRAISE is primarily for use in estimating background pollution which may be added to process contributions. Unfortunately the use of ambient to estimate background has serious pitfalls. A process that has been operating during the period over which ambient measurements have been taken will already have contributed to existing ambient levels, i.e. In general, the existing ambient will be measured as

$$AEC_{exist} = AEC_{pre} + \beta PC_{exist} \tag{5.1}$$

where AEC_{pre} is the pre-existing ambient concentration. In general $0 \leq \beta \leq 1$ because measured values of ambient pollution levels may be made in spatial positions or over durations which preclude the full contribution from an existing process option. For example, they may occasionally be made upstream of a water discharge, or upwind of an air release. It is incorrect to assume that $\beta = 1$ in general. A further danger is that if we assumed that $\beta = 1$, it would be tempting to derive that pre-existing ambient for use as a background estimate, viz. $AEC_{pre} = AEC_{exist} - PC_{exist}$. This would allow us to estimate total concentrations for existing and alternative options as

$$Total_{exist} = AEC_{pre} + PC_{exist} = AEC_{exist} \tag{5.2}$$

$$Total_{alt} = AEC_{pre} + PC_{alt} = AEC_{exist} - PC_{exist} + PC_{alt}. \tag{5.3}$$

Unfortunately these estimates are an unfair comparison of existing and alternative options because the existing and alternative totals are subject to different uncertainties. In terms of the independent measured ambient and predictions, the existing total involves just the measured ambient, but the total for alternative options involves the measured ambient and two predictions. This scheme is therefore an unsound basis for comparing existing and alternative options. To 'keep the playing field level', it is essential that any totals should be made on an equal basis of measurement and prediction. This is possible if the 'ambient' measurements may be used directly as an estimate of background, so that totals are estimated for existing and alternative options in the same way, viz.

$$Total_{exist} \approx AEC_{exist} + PC_{exist} \tag{5.4}$$

$$Total_{alt} \approx AEC_{exist} + PC_{alt}. \tag{5.5}$$

For these estimates to be accurate, the 'ambient' values must not include any significant contribution from the process of interest. To ensure this, APPRAISE allows the user to edit its

ambient data to use measurements which do not include such contributions. Such edits are thought practical because process contributions are peaked around the release site. In the case of air concentrations, edits might be necessary within 10 km of the release point, whilst for water concentrations, values might be required for a longer distance downstream of the discharge point, this depending on the flow dilution encountered. In many cases it is likely that the changes required will be within the uncertainty scoped by the range of ambient values at any point. APPRAISE reinterpolates ('infills') its ambient patterns after any edits.

6. QUOTIENTS AND INDICES

6.1 Procedures for BPEO Assessment

The 'Blue Book' provides three scores and an integrated environmental index (IEI) which gauge environmental hazards. APPRAISE calculates these together with the Agency IEI and three alternative IEI's.

The generalised hazard score (HS) ?? covers disposals not made via releases to air, water or sewer, termed waste arisings. The two other scores cover the potentially deleterious effects of air releases indirectly on human health and the environment due to the creation of ozone near ground level $(POCP)$, and via changes in the earth's atmosphere which may produce global warming (GWP).

The IEI's are described in the following sections.

6.2 The Agency IEI

The Agency IEI is built from environmental quotients defined for each pollutant s and medium m (air, soil or water) as the spatial maxima of

$$EQ_{s,m} = PC_{s,m}/EAL_{s,m} \qquad (6.1)$$

where $PC_{s,m}$ is the process contribution to the concentration or deposition rate, and $EAL_{s,m}$ is an assessment level or quality standard defined by the Agency. The quotients $EQ_{s,m}$ are summed over pollutants s for each medium m to yield medium quotients EQ_m; these are added to yield the IEI. The EQ_m and the IEI are reported in a summary window as described in Section 7.1.

6.3 A Population Weighted IEI

A population weighted IEI was calculated using population density data supplied by the Agency. The data consisted of population census data interpolated to 1km sided squares in the study area. The population N in each square, was used as a density to define new $EQ_{s,m}$ by the value of the PC/EAL quotient where $NPC_{s,m}/EAL_{s,m}$ was maximum. This excludes all $EQ_{s,m}$ outside the study area. Corresponding 'weighted' medium EQ_m and a 'weighted' IEI are reported in the summary window.

6.4 A Spatial Average IEI

A spatial average of $PC_{s,m}/EAL_{s,m}$ quotients is also calculated for each pollutant and medium. The averaging takes place over a 50 km sided square centred on a single source, or more if several sources are selected. The predicted area is always a rectangle which covers selected sources,

and extends 25km further in each cardinal direction. The average quotients are summed over pollutants to obtain an average EQ_m for each medium, and their sum provides the average IEI. The 'average' medium EQ_m and 'average' IEI are reported in the summary window.

6.5 A Modified IEI

The Agency's IEI uses environmental quotients defined by the process contribution to pollution, rather than the total of process and background. It is possible to define tolerability quotients by

$$TQ_{s,m} = (PC_{s,m} + BK_{s,m})/EAL_{s,m} \tag{6.2}$$

where $BK_{s,m}$ is a non-process contribution, or background. Background concentrations are usually estimated from ambient environmental concentrations $(AEC_{s,m})$, as discussed in section 7.1. At first sight, these $TQ_{s,m}$ could be used to define an alternative IEI, but there is a serious problem; the sum of such quotients is not well conditioned to the choice of pollutants. It is not clear whether an IEI derived from these quotients should include all pollutants measured from a process, those measured as significant, all those measured, all those that could conceivably be emitted, or even all pollutants of interest to the Agency. The associated changes to the sum of tolerability quotients need not be negligible; hence the problem. A better alternative is to modify the Agency index with weights which reflect the current state of the environment. Here we have used weights $w_{s,m}$ proportional to $AEC_{s,m}/EAL_{s,m}$ although many other possibilities could be considered. Such weights could be used as was done with population data. For this purpose APPRAISE takes a slightly different approach. The weights for pollutants in each medium are scaled so that their sum over pollutants equals the number of pollutants in the sum. Modified quotients EQ_m are then defined for each medium by a weighted sum of the normal $EQ_{s,m}$ quotients,

$$EQ_m = \sum_s w_{s,m} EQ_{s,m} \tag{6.3}$$

Addition of these new medium EQ_m gave a weighted IEI in terms of the weights and the normal environmental quotients. The weight scaling facilitates comparison of the modified IEI with the Agency IEI. The modified EQ_m and IEI are reported in the summary window. The use of weights may be attractive from several administrative viewpoints. A weighting scheme could be held fixed for a number of years. They could then be made available to industry to assist in forward planning. Planned changes in the weighting scheme could be published ahead of their introduction to give industry time to plan ahead. A weighting scheme could be used to exert regulatory pressure for particular types or in particular areas of pollution, by raising weights, and could be publicly justified by observed trends in ambient levels.

6.6 Comments

It is not clear which of the above indices offers the best prospects for gauging BPEO. A published simulation of uncertainties in the Agency IEI [Brown and Waters, 1997] suggests that

in practice the differences may be less significant then their uncertainties.

A common feature of the different indices is that they attempt to gauge environmental effects which operate over different timescales. Unfortunately they do not offer an integrated approach to disposals which produce prompt effects with those whose effects which occur after a delay of months or years. As an example, they do not account for leachate pollution from landfills. A similar related omission is that of the effects of distributed soil additives which leach to rivers. However a consideration of the effects of landfill disposals is given in the separate waste arisings hazard score.

7. SUMMARY OUTPUT FROM CALCULATIONS

A summary window is produced following a calculation of process pollution. The user may add his or her comments to the window, and the information may be saved to file for later printing.

7.1 The Information

The information that is presented falls into six categories:

- Date and User Name,

- Details of User Selections,

- Pollution Scores: HS, $POCP$, GWP,

- Regulatory View of the Spatial Distribution of Pollution,

- Regulatory Indices summarising Pollutant Distribution, and

- User Comments.

Examples are shown in a previous case study report [Brown and Wilson 1996b]. The following sections briefly describe the five classes of information presented in the summary.

7.2 Date and User

The date is taken from the operating system. The logon name of the user is recorded to nominally identify the person who ran the calculation. Both of these data are often useful at a later date in discussing results.

7.3 Details of User Selection

Following the date and user name are the following details of selections which influence the calculation and its status:

- Selected meteorological station name, (either Bedford, Stansted, London or Heathrow),

- File reference from process application file,

- Site address,

- Contact name,

- Contact address,

- Grid reference.

7.4 Hazard Scores

Following the selection details come lists of individual scores for pollutants and their total under three categories: a general hazard score for waste arisings; and two scores for pollutants released to air (their photochemical ozone creation potential (POCP), and the global warming potential (GWP)).

7.5 Regulatory View of the Spatial Distribution of Pollution

The calculations of the spatial distributions of pollutants in air, deposited to soil, and in surface waters are summarised in corresponding sections. The following tableau is presented for each pollutant.

	Predicted	Ambient	Total
Max Value :	$max(PC_{EAL})$	$max(AEC_{gm})$	$max(PC_{EAL} + AEC_{gm})$
Divided by EAL :	$max(PC_{EAL})/EAL$	$max(AEC_{gm})/EAL$	$max(PC_{EAL} + AEC_{gm})/EAL$
	$Grid.Ref.$	$Grid.Ref.$	$Grid.Ref.$

$$EAL : \ regulation\ definition\ and\ limit$$

where PC_{EAL} is the spectral measure of the predicted process contribution that is required by the regulation definition of the EAL, whose definition is given with its limiting value below each tableau. The AEC_{gm} is the *geometric mean* of the infilled low and high ambient values described in Section 5.1. The quoted maxima are spatial peaks. As a result, the figures in the **Predicted** and **Ambient** columns do not necessarily sum to make the figure under **Total** ; they are generally found at different positions, as an examination of their grid references will confirm. The first of the three figures divided by the EAL is the Agency environmental quotient for the pollutant.

7.6 Regulatory Indices summarising Pollutant Distribution

Here a breakdown is given for the indices described in Sections 6.2 tthrough 6.5, that is the Agency index, the (population) weighted index, the averaged index and the modified index suggested by QuantiSci. The breakdown is by the EQ for air, soil and water, and their index total.

7.7　User Comments

The above information in the summary window cannot be changed by the user without rerunning the calculation (though of course its printed form could be altered). However an extra window is provided in which any comments may be typed or edited. These are added to the end of the summary window when changes are completed.

8.　OUTLOOK

The APPRAISE project has clarified many of the thorny conceptual and technical issues which underpin a software implementation of the Agency's IPC methodology. It should be remembered that APPRAISE was conceived as an initial ('level 1') screening tool. It should not be compared with research models, or with advanced studies for 'difficult' applications. A period of in-house use of APPRAISE by practically experienced inspectors would now be appropriate. This could 'iron out' operational matters, and establish a firm foundation for the future construction of a valuable IPC tool to asist the Agency.

In future development for more advanced IPC tools, it will be necessary to cope with topographic and coastal effects in modeling air dispersion and soil deposition, with much larger amounts of data for the whole of England and Wales.

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