# NAME III Documentation

# Implementation of cloud gamma modelling within NAME III

**Author**

**P. Bedwell**[1]

[1] HPA-RPD, Chilton, Didcot, Oxfordshire, OX11 0RQ

# 1. Introduction

This note expands upon and furthers the note developed by Wellings and Mortimer, 2008, with the aim of providing a more detailed approach to implementing cloud gamma modelling in NAME III.

There are two distinct aspects to implementing cloud gamma modelling in NAME, the modelling of atmospheric dispersion using particles and using puffs. Approaches which lend themselves to particles are considered in detail here. The use of puffs for cloud gamma modelling in NAME will be considered separately, but a short section at the end of the note touches on the use of puffs for cloud gamma modelling.

# 2. Particle Approach

## 2.1 Lagrangian particle approach

### 2.1.1 Method

Wellings and Mortimer, 2008, recommended an approach detailed in a paper by S. Raza and R. Avila entitled "A 3D Lagrangian particle model for direct plume gamma dose rate calculations" (Raza and Avila, 2001).

$$\dot{D}_\gamma(x_0, y_0, z_0) = \frac{kK\mu_a E_\gamma}{\rho} \sum_{p=1}^{N} \frac{B(E_\gamma, \mu r)\exp(-\mu r) q(x', y', z')}{4\pi r^2} \qquad \text{Eq1}$$

where:

- $q$, the radioactivity of the $p$th particle at $(x', y', z')$ (Bq or $s^{-1}$);
- $k$, the factor for converting the absorbed dose in air to absorbed dose in tissue (dimensionless);
- $K$,dose conversion factor (rad kg $MeV^{-1}$);
- $\rho$, local air density (kg $m^{-3}$);
- $\mu_a$, energy absorption coefficient ($m^{-1}$);
- $\mu$, linear attenuation coefficient in air ($m^{-1}$);
- $\dot{D}_\gamma(x_0, y_0, z_0)$, dose rate (Gy $s^{-1}$);
- $x_0, y_0, z_0$, co-ordinates of the receptor point (x,y - lat-long or horizontal Cartesian co-ordinates; z – m agl);
- $E_\gamma$, photon energy (MeV);
- $B$, buildup factor;
- $r$, distance between the particle and the receptor (m).

Raza and Avila, 2001 derived Eq1 from the formula for dose-rate from a plume detailed in Eq2, but rather than integrating over the volume of the plume, the recommended approach sums over the total number of particles released.

$$\dot{D}_{\gamma}(x_0,y_0,z_0) = \frac{kK_{a}B(E_{\gamma},\mu r)\exp(-\mu r)q(x',y',z')dx'dy'dz'}{4\pi r^2} \qquad \text{Eq2}$$

Eq1, above, is not in the appropriate form to apply HPA's recommended parameter values for calculating cloud gamma dose. Thus Eq1 has been revised such that the endpoint is exactly the same but the parameters used to derive that endpoint have been slightly modified. The result is Eq3, below.

$$\dot{D}_{\gamma}(x_0,y_0,z_0) = E_{perunitair\,kerma}K_{air,perunitfluence}\sum_{p=1}^{N}\frac{B(E_{\gamma},\mu r)\exp(-\mu r)q(x',y',z')}{4\pi r^2}$$

Eq3

where:

- $K_{air,per\ unit\ fluence}$ = air kerma per unit fluence (Gy $m^2$)
- $E_{per\ unit\ air\ kerma}$ = effective or organ dose per unit air kerma for isotropic (uniform in all directions) irradiation (Sv $Gy^{-1}$ for effective dose conversion and Gy $Gy^{-1}$ for organ dose conversion).

Note that it can be shown that scaling by the air kerma per unit fluence values are equivalent to scaling by:

$$\frac{kK_{a}B}{\Xi}$$

The units of which are: (rad kg $MeV^{-1}$ x $m^{-1}$ x MeV) / kg $m^{-3}$. Note that 1 Gy is approx equal to 100 rad.

k is also equivalent to $E_{per\ unit\ air\ kerma}$.

Eq3 (which is of the form of Eq1, recommended by Raza and Avila, 2001) does not account for the photon intensity, as in the equation for photon flux in HPA models PLUME and ESCLOUD (see the equation at the bottom of page 2 of the report by Wellings and Mortimer, 2008 or equation 4 in Section 3.3.1 of the External Irradiation Chapter of the HPA's Models and Data Handbook).

It was agreed between J Smith and P Bedwell that the photon intensity should be included and therefore Eq4, below, is the full cloud gamma dose equation which is implemented into NAME III for dispersion modelling using particles (and not puffs).

$$\dot{D}_{\gamma}(x_0,y_0,z_0) = E_{perunitair\,kerma}K_{air,perunitfluence}\sum_{p=1}^{N}\frac{fB(E_{\gamma},\mu r)\exp(-\mu r)q(x',y',z')}{4\pi r^2} \qquad \text{Eq4}$$

where "f" is the photon intensity.

Eq4 estimates cloud gamma dose rate, which is averaged over time (but not space) or is an instantaneous value in NAME III. Cloud gamma dose rates are in units of Sv $s^{-1}$ for effective dose rate and units of Gy $s^{-1}$ for organ dose rate. NAME also includes the

capability to integrate the dose rates over time, thus estimating cloud gamma effective dose in units of Sv and cloud gamma organ dose in units of Gy.

It is important that Eq4 above is coded properly into NAME III. The exponential term, describing the fraction of the direct gamma ray 'beam' which reaches the receptor and the a build-up factor, which accounts for the scattered radiation reaching the receptor, written out explicitly, would be of the form of Eq5. The difficulty with the equation in this form lies with the positive exponent in the exponential term used to describe the Berger build-up factor. b(E) is positive for photon emissions of energies ranging from 4 MeV to 0.04 MeV. The linear attenuation coefficient, μ, is positive for all photon energies. Therefore, for the majority of photon emissions, as the distance between the particle and the receptor, r, increases, the term exp(b(E)μr) tends to infinity. Thus as r gets very large 'B(Eγ,μr)exp(-μr)' cannot be calculated in NAME III (and the dose estimated is represented as NAN, not a number). This is important because when averaging or integrating the contributions to dose at a single receptor, if any one of the contributions is NAN, then no dose estimate can be made at that receptor. Eq6 can be fashioned by re-arranging Eq5. Eq6 includes exponential terms with only negative exponents (as b(E) < 1). Thus as r increases, the terms exp(-μr) and exp(μr(b(E)-1) tend to zero. Implementing Eq6 as opposed to Eq5 into NAME III prevents the numerator in Eq4 from 'blowing up' as r becomes increasingly large.

$$B(E_\gamma, \mu r)\exp(-\mu r) = (1 + a(E)\mu r \exp(b(E)\mu r))\exp(-\mu r) \qquad \text{Eq5}$$

$$B(E_\gamma, \mu r)\exp(-\mu r) = \exp(-\mu r) + a(E)\mu r \exp(b(E)\mu r - \mu r)$$

$$B(E_\gamma, \mu r)\exp(-\mu r) = \exp(-\mu r) + a(E)\mu r \exp(\mu r(b(E) - 1)) \qquad \text{Eq6}$$

Note that NAME III will give a warning if the photon energies entered in the NAME input file is outside of the range 0.01-10 MeV. The bounds on this warning can easily be extended, but this does not prevent NAME from running.

### 2.1.2 Photon Flux

The photon flux, also termed, fluence, is defined as the number of photons passing through a unit area per second ($m^{-2}$ $s^{-1}$) and is described by Eq7a, below. This equation considers the radioactive concentration on the particle (Bq), an exponential term describing the fraction of the direct gamma ray 'beam' which reaches the receptor, a build-up factor, which accounts for the scattered radiation which reaches the receptor, the photon intensity (also termed, photon frequency) and the surface area of a sphere of radius, r, where r is the distance between a particle and the receptor.

$$PF(x_0, y_0, z_0) = \sum_{p=1}^{N} \frac{fB(E_\gamma, \mu r)\exp(-\mu r)q(x', y', z')}{4\pi r^2} \qquad \text{Eq7a}$$

The radioactive concentration, q, is evaluated on each particle for each timestep.

### 2.1.3 Distance between particle and receptor

The distance between a particle and the receptor, r, is estimated by Eq8, below.

$$r = \left[ (x_0 - x)^2 + (y_0 - y)^2 + (z_0 - z)^2 \right]^{\frac{1}{2}} \qquad \text{Eq8}$$

where:

- x, y, and z, the co-ordinates of the particle;
- $x_0$, $y_0$ and $z_0$, the co-ordinates of the receptor.

NAME III calculates the distance between two points for lat-long and Cartesian horizontal coordinate systems. NAME assumes that the vertical coordinate is in metres above ground level (m agl). r is evaluated for each particle at each timestep.

It is important to set boundary conditions on the upper and lower limits of r.

For r very large the particles may be such a large distance from the receptor that the photons emitted make no contribution to dose. Under such circumstances an upper bound on r will place a lid on the amount of computation required and therefore limit runtime.

There exist three terms in Eq4 and Eq6 which are dependent on the distance between the particles and the receptor and therefore, for large r, have the potential to dominate Eq4, resulting in the calculation of trivial doses. These terms are:

i) $1/r^2$,
ii) $a(E)\ \mu r \exp(\mu r\ (b(E)-1))$,
iii) $\exp(-\mu r)$.

Firstly consider the term $1/r^2$. If r = 1000 m, $1/r^2$ = 1.0E-06 $m^{-2}$. If r = 10000 m, $1/r^2$ = 1.0E-08 $m^{-2}$. If r = 100000 m, $1/r^2$ = 1.0E-10 $m^{-2}$. At 100 km, $1/r^2$ is 1.0E-10 $m^{-2}$ which is not particularly small.

Consider the second term. a(E) varies from 0.025-4.366 across the range of photon energies considered here. Relatively speaking, this term is not small and therefore would not determine very small doses. b(E) < 1 and therefore 'b(E) – 1' is always negative. b(E) varies between 0.174 and -0.0464 and therefore 'b(E) – 1' varies between -0.826 and -1.0464. Consider μr exp(kμr) in term ii, where k = b(E) – 1. μ varies between 6.21E-01 and 2.64E-03. Thus for r ranging from 1000 to 100000 m (as considered above), μr ranges from 2.64E+00 to 6.21E+04. Using the most conservative value of k (-0.826), then if μr = 2.64E+00, then μr exp(kμr) = 0.30; if μr = 2.64E+01, then μr exp(kμr) = 8.9E-09; if μr = 2.64E+02, then μr exp(kμr) = 5.2E-93 etc. There are two points worth noting here. Firstly as r and therefore μr increases (μ remains constant for an individual photon), the increase in μr is not comparable to the decrease in exp(kμr). The term exp(kμr) dominates here and therefore as μr increases μr exp(kμr) rapidly decreases. Secondly, for the same range of r, as r increases, the term ii, a(E) μr exp(μr (b(E)-1)), is observed to tend towards significantly smaller values than term i, $1/r^2$, and therefore term ii is deemed to be dominant in determining very small doses.

On analysis, terms ii and iii are comparative in their impact upon dose. Either term could be considered when deriving the upper limit of r for calculations of cloud gamma dose. Term ii, exp(μr(b(E)-1)), is considered here.

A suitable value for 'μr (b(E)-1)' must be determined, whereby at the upper bound, $r = r_{max}$.

$$\Phi = \mu r_{max} (b(E)-1) \qquad \text{Eq9a}$$

Therefore,

$$r_{max} = \Phi / (\mu (b(E)-1)) \qquad \text{Eq9b}$$

In an effort to determine a suitable value for, Φ, a number of model runs were performed, estimating dose for three fabricated radionuclides, emitting a photon with an energy of 0.01, 0.5 and 10 MeV, respectively (describing the full range of likely photon energy's, depicting, very small, moderate and very large photon energies, respectively). These model runs indicate that for Φ = 30, only doses greater than $10^{-20}$ Sv are routinely estimated for all photon energies. There should not be a requirement to estimate doses smaller than $10^{-20}$ Sv but to border on the side of caution, Φ is set to 50. For Φ = 50, only doses greater than $10^{-30}$ Sv are routinely estimated for all photon energies. exp(-50) is very small i.e. 1.9E-22 Sv. The full details of the NAME III runs can be found in: Testing\r_boundarycondition\for_large_r.

$$r_{max} = 50 / (\mu (b(E)-1)) \qquad \text{Eq9c}$$

It is evident that terms ii and iii dominate over term i when it comes to minimising dose for large r and it also evident that the two terms have a similar impact. It should be noted that there do exist distances whereby the $1/r^2$ term is smaller than the two exponential terms (for example for small r and large photon energies) but under such conditions the contribution to dose is deemed to be significant.

Thus Eq9c is applied in the NAME III code as an upper bound on r. If $r > r_{max}$ then the photon flux, PF(j) = 0; else the photon flux is calculated using the Lagrangian particle approach, as described above.

For r very small there is the potential for the $1/r^2$ term to blow up and therefore cause the calculation of dose to fail. Therefore the NAME III code has been edited to consider a lower bound on r, $r_{min}$. A value of $r_{min}$ = 1 mm was deemed appropriate as a lower bound. If $r < r_{min}$, then the NAME III code assumes a value of 1 mm for r.

### 2.1.4 Linear Attenuation Coefficient

The fraction of direct radiation which reaches the receptor is dependent on the distance between the particle and the receptor, r, and the linear attenuation coefficient, μ, (LAC). The LAC is dependent upon the material through which the beam passes and the energy of the photons (note that the terms photon and gamma ray are often used interchangeably). The LAC increases as the atomic number of the absorber increases. The LAC decreases as the energy of the gamma rays increases (and the energy of the gamma rays varies with radionuclide). NAME assumes that the material

through which the gamma rays travel is air. No account is made of gamma rays travelling through materials such a water vapour, water droplets or ice crystals.

Table 3.1 in the External Irradiation Chapter of the HPA's Models and Data Handbook (MDH) includes values of LAC for a fixed number of photon energies in the range 0.01-10 MeV (taken from Hubbell, 1982). These values are applied in the NAME III code (see Section 2.3 for further details).

### 2.1.5 Gamma dose build-up factor

Build-up factors, $B(E_\gamma,\mu r)$, account for the component of the scattered radiation which emerges at the receptor point. HPA currently recommends the use of the Berger build up factor (Jaeger et al, 1968). However Raza and Avila, 2005 in a paper: 'Calculation of immersion doses from external exposure to a plume of radioactive material', recommend the use of Geometric Progression (GP) build-up factors (Faw and Shultis, 1999, which subsequently references Harima et al, 1986). It is apparent that build-up factor approximations, such as GP and Berger, have been compared to build up factors derived from 1$^{st}$ principles as defined by equation 6.58 in Faw and Shultis, 1999. The result of such comparisons is that the Berger and GP approximations provide very similar estimates for distances up to 4 km between receptor and particle. Beyond a distance of about 4 km the Berger form over predicts the build-up when compared with the GP form.

Currently Berger build-up factors have been implemented in NAME III, on the basis of HPA-RPD's current recommendation (within their Models and Data Handbook). The GP approximation was not applied, despite the recommendation by Raza and Avila, 2005, as it is thought that in the majority of dispersion scenarios, the use of the GP approximation is not likely to significantly enhance the 'accuracy' of the estimates of cloud gamma dose (i.e. the contributions to dose from distances greater than 4 km are generally assumed to be negligible). However this reasoning is not based in anyway on scientific fact and it may be of use to perform a review of the two approaches and their benefits for HPA applications, in particular, determining the scenarios whereby estimates of cloud gamma dose are dependent upon the gamma dose build-up factor approach applied. The GP approximation is certain to be more computationally expensive but it is uncertain whether this would be to such an extent that it may significantly increase run time. If required, replacing the Berger approach with the GP approach in NAME III is likely to take 2-3 hours.

Note that a review of the Berger build-up factor coefficients to be used may be pertinent. There exist significant differences between the coefficients recommended by the HPA (Jaeger et al, 1968) and those coefficients detailed in Table E.6, Faw and Shultis, 1999 (to the extent that some of the Faw and Shultis coefficients are outside of the error bounds of the HPA recommended values). The values in Faw and Shultis, 1999 reference Chilton, Eisenhauer and Simmons, 1980.

Some scoping calculations have been undertaken in an effort to quantify the impact of using Berger build-up factor coefficients derived by the two different approaches identified above; Jaeger et al (currently adopted by the HPA) and Faw & Shultis. It is assumed that r = 10 m and values of LAC are taken from the Hubbell, 1982 (as applied by HPA). Berger build-up factors have been calculated for three different

coefficients scoping the range of photon energy's and are displayed in Table 1, below. It is evident from Table 1 that the difference between the estimated Berger build-up factors is small, most notably for large photon energies. Therefore, for this comparison at least, the values of the Berger build-up factors are independent of the source of the data.

Table 1. Berger build-up factors

| | Faw & Shultis | Jaeger et al |
|---|---|---|
| 0.015 MeV | 1.1467 | 1.1695 |
| 0.5 MeV | 1.2607 | 1.1999 |
| 10 MeV | 1.0082 | 1.0083 |

Interestingly, Raza and Avila, 2005, reference Faw and Shultis, 1999 in relation to the GP approach, but do not reference Faw and Shultis, 1999 in relation to the Berger approach. Instead Raza and Avila, 2005, reference Lamarsh, 1983 when deriving Berger build-up factors for use.

Berger build-up factors are estimated using Eq10a, where a and b are the Berger build-up factor coefficients and are currently referenced from Jaeger et al, 1968 (via the HPA's MDH). These coefficients are dependent on the gamma-ray energy, the attenuation medium, and the nature of the response (i.e. the medium of the material in which we want to estimate the kerma value). NAME III assumes that air is both the attenuation medium and the response medium.

$$B(E_\gamma, \mu r) = 1 + a\mu r \exp^{b\mu r} \qquad \text{Eq10a}$$

### 2.1.6 Air kerma

Air kerma is effectively the dose (or dose rate) in air (at the position of the receptor) in units of Gy (or Gy $s^{-1}$). The air kerma is estimated by scaling the photon flux, PF ($m^{-2}$ $s^{-1}$), by the air kerma per unit fluence, $K_{air,per\ unit\ fluence}$ (Gy $m^2$). Values of $K_{air,per\ unit\ fluence}$ are taken from Table A.21 in ICRP 74 (ICRP, 1996). Note that values of air kerma per unit fluence were not taken from the External Irradiation Chapter of the MDH, which details the values from Table A.1 of ICRP 74. Following consultation with Joe Wellings, Kelly Jones, Rick Tanner and Jon Eakins (all employees at the HPA), Jon advised that re-normalisation had been carried out on those values in Table A.1, introducing further uncertainty/errors on these values. However there only exists a 2% difference in the values given in the Tables A.1 and A.21.

### 2.1.7 Effective and Organ Dose

Effective (or whole body) dose (Sv) and organ dose (Gy) are estimated by scaling the air kerma by $E_{per\ unit\ air\ kerma}$, the effective or organ dose per unit air kerma for isotropic (uniform in all directions) irradiation (in units of Sv $Gy^{-1}$ when converting to effective dose and Gy $Gy^{-1}$ when converting to organ dose).

Values of $E_{per\ unit\ air\ kerma}$ are taken from the External Irradiation Chapter of the HPA's MDH (Table 3.2) which are derived in ICRP 74 (ICRP, 1996). The factors for

isotropic irradiation are assumed to be appropriate for calculating gamma doses from material in the air (and are assumed to be applicable irrespective of whether the receptor is in or below the plume). Factors for other irradiation geometries are given in ICRP 74, and can be used in NAME III if deemed appropriate (these values are not hard wired into the code). Organ absorbed doses per unit air kerma have also been ascertained from ICRP 74, for lung, thyroid and bone surface. These organs are considered in NAME III as agreed by Stephanie Haywood (see email titled: Cloud gamma doses and dated 16th Sept 08, for details).

All values of $E_{\text{per unit air kerma}}$ collated to date are applicable to adults only. It was agreed with Stephanie Haywood that the cloud gamma calculations would consider a range of additional age groups, notably 10 year old child and 1 year old infant, and foetus if possible. ICRP 74 does not include child nor infant effective or organ doses per unit air kerma, however it does detail some references which may be of use, notably Yamaguchi, 1994 which details age dependent effective gamma dose applicable to 0, 1, 5, 10 and 15 year olds. ICRP 74 also references Zankl et al, nd[a] which details organ doses to an eight week old infant and a seven year old child. A review of the most suitable data for use may be appropriate here.

Currently NAME III is coded to only account for adult effective and organ doses as a result of external exposure from the plume. No coding has been implemented to explicitly account for child, infant or foetus effective and organ doses, however the nature of the approach implemented in NAME III allows a 'fix' to calculate cloud gamma doses to additional age groups. This fix requires the user to enter child or infant doses per unit air kerma under the headings for adult doses per unit air kerma.

A decision needs to be made regarding whether NAME III should be coded to be able to explicitly calculate cloud gamma dose for different age groups and if so, how best to implement this. Multiple "Set of Cloud Gamma Parameters" headers could be used in the Species block along with multiple "Cloud Gamma Parameters:" blocks, with each block referring to a different age group and the headers being non-age specific e.g. 'Bone surface dose pu air kerma' (as opposed to 'Adult bone surface dose pu air kerma', 'Child bone surface dose pu air kerma', etc). Alternatively the number of parameters which can be entered within the "Cloud Gamma Parameters:" block could be extended to include dose per unit air kerma coefficients for additional age groups. This approach is probably preferable but could make the "Cloud Gamma Parameters:" block rather long. This addition to the code is likely to take approximately two hours to implement, plus time for testing.

### 2.1.8 Shielding

Currently no account for shielding has been made in NAME III. Stephanie Haywood noted (see email titled: Cloud gamma doses and dated 16th Sept 08, for details) that ideally NAME III would incorporate the ability to consider shielding by way of a user input location factor. Including location factors in NAME III is feasible but not straightforward. Incorporating location factors into the cloud gamma parameters block of a NAME III input file is not very satisfactory as location factors are not photon energy dependent. Incorporating location factors into the species block of a NAME III input file is again not very satisfactory as location factors are not species dependent. Location factors could be added to the Output Requirements – Fields: block but Dave

wished to limit the additions to this block where possible. Perhaps shielding could even be added as a new block, however this requires more effort, for the inclusion of only one additional parameter. Dave raised concerns over including shielding in NAME without updating headers describing the cloud gamma dose output in NAME III output files such that the location factor(s) or at least the use of location factors was indicated in some way. Pete advised that location factor was only ever likely to be location dependent i.e. dependent on the receptors. Pete thought that it may be easier for HPA to apply a location factor to cloud gamma dose as part of the HPA's post processing of dose output from NAME III. HPA should consider how to account for shielding when estimating cloud gamma dose.

### 2.2 How cloud gamma parameter values are implemented in NAME III

All cloud gamma parameters are read into NAME III through the NAME III input file. None of the parameters are hard wired into the code. An example of the key blocks in the NAME III input file are highlighted in Figure 1, below.

```
Species:
Name,           Category, Half Life, Daughter, Branching Ratio,
KRYPTON-85, RADIONUCLIDE,  3.37E+08,         ,                ,

Set of Cloud Gamma Parameters, UV Loss Rate, Surface Resistance, Deposition Velocity,
                        KR-85,     0.00E+00,                   ,            0.00E+00,

Wet Type, Molecular Weight, Material Unit
       0,                0,            Bq


Cloud Gamma Parameters:KR-85
Photon Energy, Photon Intensity, Linear Attenuation Coefficient, B Build-up Factor a,
5.14E-01,              4.30E-03,                       1.12E-02,            1.73E+00,

B Build-up Factor b, Air kerma pu fluence, Adult effective dose pu air kerma,
           9.91E-02,             2.45E-16,                           6.76E-01,

Adult thyroid dose pu air kerma, Adult lung dose pu air kerma,
                        7.49E-01,                     7.21E-01,

Adult bone surface dose pu air kerma
                            7.06E-01
```

Figure 1. Section of a NAME III input file used to estimate cloud gamma dose

A key aspect of a NAME III input file used to estimate cloud gamma dose is that the text defined under the "Set of Cloud Gamma Parameters" column heading within the "Species" block must be the same as the respective "Cloud Gamma Parameters" block heading, e.g. "KR-85", in Figure 1.

If including a Cloud Gamma Parameters block all (four) of the dose per unit air kerma values (in the aforementioned block) must be detailed in the NAME III input file irrespective of whether or not output requests (in the Output Requirements – Fields: block) for all (or even any) types of cloud gamma dose (effective, lung, bone surface and thyroid) are selected.

Also note that if "Set of Cloud Gamma Parameters" is inadvertently left blank NAME III will attempt to calculate cloud gamma dose but all output in the output file will be zero (or blank if zero's are ignored).

### 2.3 Deriving all cloud gamma parameters

Stephanie Haywood and Jane Simmonds recommended the following radionuclides for primary use in NAME III when calculating cloud gamma dose:

$^{135}I$, $^{132}I$, $^{134}I$, $^{88}Kr$, $^{133}I$, $^{131}I$, $^{132}Te$, $^{87}Kr$, $^{133}Xe$, $^{135}Xe$, $^{134}Cs$, $^{103}Ru$, $^{105}Ru$, $^{140}Ba$, $^{41}Ar$ and $^{85}Kr$.

Currently in NAME the maximum number of radionuclides which may be considered for a run outputting cloud gamma dose is 16, defined by the global parameter, 'MaxCGSpecies'. Note that MaxCGSpecies will not constrain NAME to the 16 radionuclides highlighted above if there is a wish to consider additional radionuclides. MaxCGSpecies can very easily be increased to consider a greater number of radionuclides. However, as presented in the Section 2.7, due to the computationally expensive nature of the cloud gamma calculations, there exist only a limited number of runs which can be performed with 16 or more radionuclides.

A spreadsheet was used to collate the photon energies and photon intensities for all the radionuclides highlighted above. Both binned and non-binned photon energies were collated from Oak Ridge, USA and ICRP 38 datasets, respectively. This spreadsheet can be found at: Photon_Energy_&_Intensity.xls.

The non-binned photon energies posed a problem in that a single radionuclide may emit photons of many different energies. For example, $^{132}I$, emits 120 different photons (as detailed in ICRP38.RAD). It is assumed here that the radioactive significance of each photon is measured by the product of the photon energy and photon intensity. The cumulative percentage contribution to the total cloud gamma dose from the radioactively significant photons for each radionuclide was estimated. For example for $^{132}I$, the 19 most radioactively significant photons result in an estimated contribution of 90% of the total cloud gamma dose; 28 photons result in a contribution of 95% of the total cloud gamma dose; 41 photons result in a contribution of 98% of the total cloud gamma dose; 50 photons result in a contribution of 99% of the total cloud gamma dose; and 75 photons result in a contribution of 100% of the total cloud gamma dose (accurate to 0 decimal places i.e. >99.5%). Currently the maximum number of photon energies permissible for a single radionuclide in the code has been set to 20. This can be modified simply but the larger the number of energies per radionuclide considered the more computationally expensive each run will become and the longer the runs will take to complete. A review may be required to identify the minimum number of the most radioactively significant photons which can be considered without compromising unduly on the 'accuracy' of the cloud gamma dose estimations. This should be performed for all 16 radionuclides considered here. If a large number of photons must be considered in an effort to 'accurately' calculate the cloud gamma dose estimations, the use of binned photon energies may be recommended. In fact if the number of binned energies is less than the true number of photon energies for a single radionuclide I would recommend that binned energies are utilised in NAME III. It is recognised that cloud gamma dose is not linearly proportional to the product of photon energy and photon intensity but this is likely to be reasonable gauge.

Table 3.1 in the External Irradiation Chapter of the HPA's MDH includes the linear attenuation coefficients for a fixed number of photon energies in the range 0.01-10

MeV (Hubbell, 1982). However these do not necessarily apply to the energies of photons emitted from radionuclides e.g. for $^{85}$Kr, a photon of energy 514 keV is emitted. Similarly, Berger build-up factors, air kerma values per unit fluence and effective and organ doses per unit air kerma are all a function of energy and are all given for a fixed number of discrete photon energies in the range 0.01-10 MeV. ICRP 74 (ICRP, 1996) recommends an approach for interpolating air kerma values per unit fluence and effective and organ doses per unit air kerma (paragraph 191):

"When precise interpolation is required, it is recommended that interpolation between values of the conversion coefficients given in Table A.21 be carried out using a 4-point (cubic) Lagrangian interpolation formula on a linear-log scale".

There exists a lack of clarity in the ICRP advice as to which variable should be linear and which should be logged. In consultation with Rick Tanner (of the HPA) it was agreed that the photon energies should be considered on a linear scale and the air kerma values per unit fluence and effective and organ doses per unit air kerma on a log scale.

ICRP do not appear to give advice on how to interpolate linear attenuation coefficients and Berger build-up factors. Rick Tanner advised that it is immaterial whether a linear-linear or linear-log scale interpolation method is applied. A scoping calculation re-enforced Rick's advice (detailed in CG_Params.xls). Therefore an interpolation between values of linear attenuation coefficients and values of Berger build-up factors using a 4-point (cubic) Lagrangian interpolation formula on a linear-linear scale is assumed.

The interpolation of the linear attenuation coefficients, Berger build-up factors, air kerma per unit fluence values and dose per unit air kerma values are all performed in: CG_Params.xls. The air kerma per unit fluence values are also converted from units of pGy cm$^2$ to units of Gy m$^2$ for use in NAME (by dividing by $10^{16}$).

NAME III has been coded such that it has the ability to calculate cloud gamma dose from any radionuclide and any photon energy. However NAME III does not include a database or any form of data storage and therefore the associated cloud gamma parameters for each radionuclide currently have to be added to the NAME III input file. To minimise the effort required to incorporate the cloud gamma parameters in NAME III input files a Cloud Gamma Parameters text file has been created (..\Version5_2c\Resources\Defns\Cloud_Gamma_Params.txt or Cloud_Gamma_Params.txt), analogous to the Species text file, which includes all 16 recommended radionuclides, their photon energy emissions and their associated cloud gamma parameters. The file contains two sets of cloud gamma parameters. The first set considers non-binned photon energies and their associated cloud gamma parameters. This dataset is not comprehensive in that for some radionuclides, such as $^{135}$I, only the top 20 'radioactively significant' photons are included. The number of photons considered per radionuclide can be extended but consideration of the impact on run time must be accounted for before increasing the global parameter 'MaxEnergies' which is currently set to 20. The second set of cloud gamma parameters considers binned photon energies and their associated cloud gamma parameters. For each radionuclide considered, values of linear attenuation coefficients, Berger build-up coefficients, air kerma per unit fluence and adult doses

per unit air kerma have been included for all 12 photon energies, irrespective of whether there is a respective value for photon intensity. It is envisaged that if the user wishes to use cloud gamma parameters from the binned photon energies section, only the rows of data including values of photon intensity should be copied to the NAME III input file. The user can use non-binned and binned energy related cloud gamma parameter data in a single NAME III input file, but not in combination for a single radionuclide. For example binned data could be used for I-135 and non-binned data for Kr-85 but a combination of binned and non-binned data should not be used for either I-135 or Kr-85.

Note that it is also deemed of value to create 'default' NAME input files for 'standard' model runs whereby estimates of cloud gamma dose are requested.

### 2.4 Output from NAME III

NAME III includes output of instantaneous and average effective and organ dose rates in units of Sv $s^{-1}$ and Gy $s^{-1}$, respectively and integrated effective and organ dose in units of Sv and Gy, respectively. Photon flux ($m^{-2}$ $s^{-1}$) can also be output which is of use for testing purposes and adds flexibility to the code but is not an endpoint typically used by HPA. Note that dose and dose rate is summed over photon energy for a single radionuclide but is not summed over radionuclide for a source including multiple radionuclides. However if HPA require total dose or total dose rate summed over radionuclide this may be an area for future development of NAME.
Note that there is no constraint to consider air concentrations (or any other output quantity) as an output requirement when estimating cloud gamma dose.

### 2.5 Code changes to NAME III to incorporate cloud gamma modelling – the Lagrangian particle approach

Below is a summary of how the NAME III code has been modified to account for cloud gamma modelling. The summary of the code added considers the Lagrangian particle approach only (and not the semi-infinite approach, which is considered subsequently). The development version of the files can be found in: file:/home/h05/appb/Version5_2c/Code_NameIII. Old files are named …..01.F90. Newly updated files are named ……F90. Note that the files include the previous update of the decay chain modelling for atmospheric dispersion (but not for deposition).

#### 2.5.1 Input

In the ReadInputFiles subroutine on the fifth pass through the main input file the CloudGammaParamses are read into NAME III. The CloudGammaParamsInputNames Subroutine is called (from the same module) to initialise the Cloud Gamma block and if there exists a 'Cloud Gamma Parameters:' block in the input file, the Tokens2CloudGammaParams Subroutine is called (from the same module).

In the SpeciesInputNames Subroutine, the column key (i.e. column header) "Set of Cloud Gamma Parameters" was added, such that the Species block could be

associated with the respective Cloud Gamma Parameters block (via the naming of the block).

The Subroutine, "CloudGammaParamsInputNames" was added to initialise the Cloud Gamma Parameters block i.e. to define the content and format of such a block.

The Subroutine, "Tokens2CloudGammaParams" was added to initialise the Cloud Gamma Parameters and, where appropriate, to perform checks on the values being read into NAME. From this routine the "AddCloudGammaParams" Subroutine is called (in Species.F90 module).

### 2.5.2 MainNAMEIII

In the Program NameIII CloudGammaParamses is called from the Subroutine, "ReadInputFiles" in Input.F90.

The subroutine, "SetUpSpecieses_iCloudGammaParams" is called (from the Species.F90 module), which sets up the indices in Species for referring to sets of cloud gamma parameters.

The subroutine RunToRestartDumpOrSuspendOrEndOfCase is called to pass the argument, "CloudGammaParamses".

### 2.5.3 Case

The output fields in the output module have been updated accordingly (line 22).

In the Subroutine, "RunToRestartDumpOrSuspendOrEndOfCase, CloudGammaParamses has been added as an argument. This routine carries out the loop over successive updates of the met and flow module instances, calling LoopOverSyncTimes once between each update time.

In the Subroutine, "RunToSyncTimeOrMetFlowUpdateOrEndOfCase, CloudGammaParamses has been added as an argument. This routine carries out the loop over successive times when the particle/puffs are synchronised, calling LoopParticlePuffsAndTimeSteps once between each synchronisation time and also calling CalcParticleResults.

In the Subroutine, "LoopParticlePuffsAndTimeSteps", CloudGammaParamses has been added as an argument. This routine evolves the particles and puffs, carrying out the looping over particles/puffs and timesteps, calling CalcParticleResults twice. In the first instance CalcParticleResults is called for: output of sets of particle/puff information for particles/puffs that have just been released, which calculates contributions for output times which the particle/puff can contribute to. In the second and third instances CalcParticleResults is called for: calculating contributions for output times which the particle/puff can contribute to (T and T1 (or T+1)). In the fourth instance CalcParticleResults is called for: calculating contributions for output travel times which the particle/puff can contribute to.

In the Subroutine, "CalcParticleResults", ParticleCloudGamma Subroutine is called from Particle.F90 module if one the output field requests is Cloud Gamma Dose.

### 2.5.4 Species

Data is not passed to or from the Species.F90 module. Within this module the CloudGammaParamses and CloudGammaParams arguments are defined.

The following Types have been defined in Species.F90:

CloudGammaParams, defines the cloud gamma parameters for a single set of cloud gamma parameters i.e. for a range of energies but only one species. The arguments defined by this type include: name, number of energies, photon energy and intensity, linear attenuation coefficient, Berger Build Up Factor Coefficients, Air Kerma per unit Fluence, Effective or Organ Dose per unit Air Kerma.

CloudGammaParamses, defines the collection of sets of cloud gamma parameters.

There exists a function to initialise a collection of cloud gamma parameters: InitCloudGammaParamses. CloudGammaParameters (linking cloud gamma parameters to a species) is initialised in the function, InitSpecies. All of the cloud gamma parameters are initialised via the function: InitCloudGammaParams. The Subroutine, AddCloudGammaParams, adds a set of cloud gamma parameters to a collection of sets of cloud gamma parameters. The function: FindCloudGammaParamsIndex, finds the index of a set of cloud gamma parameters in the collection of all such sets of parameters. The function, CloudGammaParamsEq, tests for equality of cloud gamma parameters. Finally the Subroutine, SetUpSpecieses_iCloudGammaParams sets up indices in Species for referring to sets of cloud gamma parameters.

### 2.5.4 Co-ordinateSystem

A subroutine, "CalcDistanceBetweenTwoPoints" has been developed to calculate the distance between two points for lat-long and Cartesian horizontal coordinate systems, so that the distance between each particle and receptor can be ascertained (assuming the vertical coordinate is in 'm agl'). This subroutine calls the Subroutine MetricCoeffs, which passes the metric coefficients for lat-long and Cartesian horizontal coordinate systems such that irrespective of the co-ordinate system considered the distance between points can still be evaluated. These distances are passed to the Particle.F90 module.

### 2.5.6 Particle

The Subroutines, ParticleCloudGamma and ParticleFluence have been added. ParticleCloudGamma identifies and reads in the appropriate values for the grids (including identifying the position of the particle and receptor), species and cloud gamma parameters. The subroutine, "CalcDistanceBetweenTwoPoints" is called (from the Co-ordinateSystem.F90 module) to calculate the distance between each particle and receptor. This is called twice, depending on whether the grid is structured or unstructured. Either way, the ParticleFluence Subroutine is called (it was deemed unnecessary to code this twice). The ParticleFluence Subroutine performs the

calculation of photon flux, for all photon energies at a each timestep but for only a single species and a single particle at a time. In addition, boundary conditions are placed on r, the distance between the particle and the receptor in this subroutine. The photon fluxes are then passed back to the ParticleCloudGamma Subroutine, which then sums the photon fluxes for each energy and each species over all particles. The Results%Fields%(iField)%Std array has been setup to pass photon energies to the Ouput.F90 module (in the $7^{th}$ element of this array) along with the photon flux values, and temporal and spatial details.

### 2.5.7 Output

The Photon Flux field request and the adult effective and organ cloud gamma dose requests have all been added. This includes codes for the cloud gamma quantity in the field requirements and information on the cloud gamma quantity in field requirements. There are 5 requests in total including lung, thyroid and bone surface organ dose. This coding can be found in lines 409-791.

In defining FieldReq_ type, an index for Photon Flux, 'iPhotonFlux' has been added. This will enable the calculation of output requests which use photon flux as an intermediary step. See line 1315 for details.

In the Function InitFieldReq, iPhotonFlux is set to 0. This ensures iPhotonFlux is 0 if Photon Flux is not a required output. If Photon Flux is required, iPhotonFlux will be set to a non-zero integer subsequently in the code. See line 3391 for details.

In the Subroutine SetUpReqs, lines 6018-6060, code has been added to set up an extra field request i.e. if adult effective or organ doses are requested an extra field request for photon flux is setup as this must be calculated first. In addition a coding 'short cut' has been added (lines 6422-6428) which avoids chains of reference between field requirements.

In the Subroutine ProcessFields, lines 8889-8892, 8904 and 8971-8978, code has been added to locate other fields required e.g. Photon Flux field via iPhotonFlux. Lines 9016-9027 were added to call the subroutine, DeriveCloudGammaDose.

The subroutine DeriveCloudGammaDose (lines 9469-9622) calculates the cloud gamma dose (and dose rate) field at each timestep (including summing over all photon energies for a single radionuclide) from the photon flux calculated in the Particle.F90 module.

The subroutine OutputFields was edited (lines 11292-11335), such that the headers for the adult effective and organ cloud gamma dose fit within the 26 character limit in the NAME III output files. Lines 11407-11422 were added such that when integrating over the cloud gamma dose rate to calculate the cloud gamma dose, the units in the output file are given in Sv or Gy as appropriate (rather than Sv $s^{-1}$ or Gy $s^{-1}$, respectively).

## 2.6 Passing Cloud Gamma related data

Below details how the cloud gamma parameter data (defined as CloudGammaParamses) is passed through the NAME III:

Read Input Files in Input.F90
-> Program NameIII in MainNameIII.F90;
-> RunToRestartDumpOrSuspendOrEndOfCase Subroutine in Case.F90;
-> RunToSyncTimeOrMetFlowUpdateOrEndOfCase in Case.F90;
-> LoopParticlePuffsAndTimeSteps in Case.F90;
-> CalcParticleResults in Case.F90 (also called direct from RunToSyncTimeOrMetFlowUpdateOrEndOfCase);
-> ParticleCloudGamma in Particle.F90.

## 2.7 Testing

It is important to test the cloud gamma modelling approach implemented in NAME III. There are two aspects to this testing. Firstly NAME III should be tested to ensure that the approach has been correctly implemented, there are no bugs apparent and that NAME III cloud gamma dose output is verified against other approaches and/or models. This could be done by comparing output from NAME III with other models for analogous scenarios, such as PC COSYMA and HOTSPOT for instantaneous/accidental releases and PC CREAM and ADMS for continuous/routine release scenarios. However, when comparing against other models, some account must be made of the differences in the air concentrations estimated. The danger with comparing such models is that all the differences may lie in the dispersion of the release and not the approach used to calculate cloud gamma doses. However it is anticipated that the differences in the dispersion between models should not be so variable that no agreement in cloud gamma dose between models can be observed. It should be noted that a full review of the overall differences between cloud gamma dose estimates (inclusive of the differences resulting from the dispersion) from a range of models would be beneficial at a later date. In addition, there exist two scenarios whereby relatively simple hand calculations can be performed and the output compared against the code; the semi-infinite cloud approximation and a point source approximation. Both of these methods of testing NAME III also avoid the issues (alluded to above) with dispersion modelling.

The second aspect of testing NAME III, investigates the conditions under which the calculation of cloud gamma dose via the approach implemented in NAME are applicable. This part of the testing focuses on a range of model runs and whether the respective output is informative or noisy.

***Note that the NAME III output included in the tables below was derived from versions of NAME in my own directory. Because of changes added to NAME by other members of the dispersion team whilst I have been developing and implementing cloud gamma modelling in NAME, output from version5_2a in apdg may differ slightly to that detailed here.***

### 2.7.1 Testing against hand calculations

a) Semi-infinite cloud approximation

A model run was setup in NAME III to replicate uniform air concentrations over relatively large horizontal and vertical spatial scales. Values of air concentration output from NAME can be used in the semi-infinite approach as described in Wellings and Mortimer, 2008 and detailed below (Eq11a), to estimate the absorbed dose rate in air, $D_A$. The absorbed dose rate in air is subsequently scaled by the adult dose per unit air kerma to estimate the adult effective cloud gamma dose for comparison with output from NAME III.

$$\dot{D}_A = kC\sum_{j=1}^{n} I_j E_j \qquad \text{Eq11a}$$

where
- k = conversion factor
  = $2.0\ 10^{-6}$ Gy $y^{-1}$ per MeV $m^{-3}$ $s^{-1}$,
- C = air concentration (Bq $m^{-3}$)
  = 1.84E-01 Bq $m^{-3}$,
- n = no. of photons specified for nuclide
  = 1,
- I = photon intensity
  = 4.30E-03,
- E = photon energy (MeV)
  = 5.14E-01 MeV.

The conditions of the release are described below:

i) Source Term. 1.0E+10 Bq instantaneous release of $^{85}$Kr. Modelled using a release of 100000 particles. Source centred on the grid mid-point and at 500 m above ground level, with dimensions 10 x 10 x 1 km.

ii) Met Conditions. Wind speed = 5 m $s^{-1}$. Heat Flux = 200 W $m^{-2}$. Boundary Layer Depth = 1000 m. A moderate wind speed and a large heat flux resulting in the release mixing relatively quickly throughout the boundary layer without the plume being advected too rapidly downwind.

iii) Output Grid. The number of grid points consider are 3 x 3 x 2 (in the x, y, z planes, respectively). The total dimensions covering all grid points are: 1 x 1 x 1 km. The grid points are therefore 500 m apart in the horizontal and at 250 m and 750 m above ground level in the vertical plane. Air concentrations (Bq $m^{-3}$) output at each of these grid points and are averaged over the 5 minutes post release (at 30 second intervals). One receptor point considered for output of the adult effective cloud gamma dose rate (Sv $s^{-1}$), at the horizontal mid point of the source term and air concentration grids, at 1 m above ground level and, as air concentrations, averaged over the 5 minutes post release (at 30 second intervals).

The full details of the NAME III run can be found in: Testing\Semi_Inf_Cloud.

Estimating the cloud gamma dose rate via the semi-infinite approach (hand calculation):

The mid point air concentration is applied in the calculation of absorbed dose rate in air i.e. at the same location as the receptor point from which adult effective cloud gamma dose rate is output. The 18 average air concentrations output over the 1 x 1 x 1 km grid, range from 1.71E-01 to 1.91E-01 Bq $m^{-3}$. The small variability in air concentrations observed implies the relative uniformity in the concentrations over such spatial scales.

$D_A$ = 8.13E-10 Gy $y^{-1}$

For $^{85}$Kr the adult effective dose per unit air kerma is 6.76E-01 Sv $Gy^{-1}$.

Adult effective dose rate = 5.50E-10 Sv $y^{-1}$
or
Adult effective dose rate = 1.74E-17 Sv $s^{-1}$

NAME III estimates an adult effective dose rate of 1.77E-17 Sv $s^{-1}$ using the Lagrangian particle approach. This compares very well with the value derived using the semi-infinite cloud approach, 1.74E-17 Sv $s^{-1}$. This gives confidence in the Lagrangian particle approach implemented within NAME III and NAME's ability to estimate cloud gamma dose under conditions of uniform air concentrations. Potentially this is a challenging modelling scenario for the particle approach in NAME because of the models method of representing uniform air concentrations with discrete particles, whereby there exists the prospect for individual particles to distort doses as a result of their proximity to the receptor. $^{85}$Kr was used in this testing because it emits only one photon and therefore simplifies modelling and hand calculations, however $^{85}$Kr is not deemed to be the most restrictive radionuclide (of those considered here) for this scenario. $^{133}$Xe would be the most suitable radionuclide (of those considered here) for testing in such a scenario because the photons it emits have relatively large linear attenuation coefficients (i.e. a significant portion of the gamma rays from the photons emitted are attenuated over relatively short distances, therefore placing a greater emphasis on the distance between the particles and receptor when estimating the contribution to dose). As a result of a similar test to that for $^{85}$Kr (see Testing\Semi_Inf_Cloud\Xe133 for details), it is evident that there exists an equally good agreement the between the Lagrangian particle approach (estimated adult effective dose rate of 2.59E-16 Sv $s^{-1}$) and the semi-infinite cloud approach (estimated adult effective dose rate of 2.66E-16 Sv $s^{-1}$) for a release of $^{133}$Xe. If photon emitting radionuclides with even larger linear attenuation coefficients are to be modelled in NAME then further testing may be required, however the testing carried out to date gives confidence in the Lagrangian particle approach implemented in NAME III for any magnitude of linear attenuation coefficients.

b) Point source approximation

A model run has been setup in NAME III which replicates a point source. Thus using an approach recommended in the External Irradiation Chapter of the HPA's Models and Data Handbook, a hand calculation can be performed to estimate the photon flux, PF, from a point source, as detailed below (Eq7b). Note that the photon intensity, f, is included in Eq7b, such that the calculation of the photon flux is in agreement with the method applied in NAME III.

$$PF(x_0, y_0, z_0) = \sum_{p=1}^{N} \frac{fB(E_\gamma, \mu r)\exp(-\mu r)q(x', y', z')}{4\pi r^2} \qquad \text{Eq7b}$$

where: q = source strength (Bq)
= 1.0E+10 Bq,
$\mu$ = linear attenuation coefficient ($m^{-1}$)
= 1.12E-02 $m^{-1}$,
r = distance between point source and receptor (m)
= 500 m,
B = energy deposition build-up factor,
$E_\gamma$ = initial gamma ray energy (MeV)
= 0.514 MeV,
f = photon intensity/frequency
= 4.3E-03.

$$B(E_\gamma, \mu r) = 1 + a\mu r \exp^{b\mu r} \qquad \text{Eq10b}$$

where: a, b = photon energy dependent parameters,
a = 1.73,
b = 9.91E-02.

The conditions of the release are described below:

i) Source Term. 1.0E+10 Bq instantaneous release of $^{85}Kr$. Modelled using a release of 1 particle (as a point source). Source centred on the grid mid-point and at ground level, with no dimensions (dx, dy, dz = 0, 0, 0).

ii) Met Conditions. Wind speed = 0 m $s^{-1}$. Heat Flux = -5 W $m^{-2}$. Boundary Layer Depth = 100 m. Calm conditions and a negative heat flux modelling a stable atmosphere, in an effort to repress the dispersion of the particle from the point of release.

iii) Output Grid. Four receptor points are considered. At each receptor point the photon flux is calculated. All receptors are 500 metres from the horizontal mid point and the source of the release, 1 m above ground level and averaged over a 15 second period post release.

The full details of the NAME III run can be found in: Testing\Point_Source.

Estimating the photon flux the point source approximation (hand calculation):

B = 1.79E+01

PF = 9.07E-01 $m^{-2}$ $s^{-1}$

NAME III estimates photon fluxes of 9.01E-01 $m^{-2}$ $s^{-1}$, 8.16E-01 $m^{-2}$ $s^{-1}$, 1.00E+00 $m^{-2}$ $s^{-1}$ and 9.07E-01 $m^{-2}$ $s^{-1}$, relating to positions (x-500, y), (x, y-500), (x, y+500) or (x+500, y), respectively (where x, y is the release point). There exists a very good agreement in the photon flux approximated by NAME III, 9.06E-01 $m^{-2}$ $s^{-1}$ (averaged over the four receptors) and that estimated using the hand calculation applying the point source approximation, 9.07E-01 $m^{-2}$ $s^{-1}$. The negligible difference

between approaches is to be expected as the methods of calculation are very similar. The agreement between approaches presented here further enhances the confidence in the Lagrangian particle approach implemented within NAME III. Note that in the 15 second period post release it is evident that the particle does 'disperse' (although the movement of the particle is somewhat limited) and does not remain at the point of release, as assumed in the hand calculation. A superior approach for testing here would have been to modify the code in NAME III such that no dispersion of the particle released could take place. However this would have required unnecessary additional effort and the approach applied was deemed to be sufficient for the purposes of the testing undertaken here.

### 2.7.2 Testing against other model output

a) Instantaneous/accidental release scenario

For an instantaneous/accidental release scenario a comparison of NAME III with HOTSPOT and PC COSYMA is performed. Below is a summary of the assumptions made and a comparison of the estimated output.

The conditions of the NAME III release are described below:

i) Source Term. An instantaneous release of 1.0E+10 Bq of $^{85}$Kr. Modelled using a release of 10000 particles. Source height = 10 m above ground level, with no dimensions (dx, dy, dz = 0, 0, 0).

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m. Note that no deposition is considered (because $^{85}$Kr is a noble gas).

iii) Output Grid. Three receptor points are considered, at 1, 2 and 5 km along the plume centre line (PCL). Time integrated air concentrations (TIAC) and adult effective cloud gamma doses are estimated at these points. Both are integrated over 1 hour post release (at one minute intervals). The air concentrations are estimated within grid boxes 20 x 20 x 20 m. All adult effective doses are estimated at a height of 1 m above ground level.

The full details of the NAME III run can be found in: Testing\COSYMA_Comp\NAME_Output or Testing\HOTSPOT_Comp\NAME_Output. The model input in PC COSYMA and HOTSPOT are defined such that they replicate the NAME III model input as closely as possible. Neither PC COSYMA nor HOTSPOT specifically defines a 1 hour integration period. In PC COSYMA a 1 hour phase release is assumed. In HOTSPOT I think it is assumed that the contribution at each receptor is integrated over the time taken for the plume to pass that point, which for the distances considered here, is in affect analogous to NAME and PC COSYMA. The full details of the HOTSPOT run can be found in: Testing\HOTSPOT_Comp. The full details of the PC COSYMA run can be found in: Testing\COSYMA_Comp.

Model Output

Table 2. Adult Effective Cloud Gamma Dose (Sv)

| | NAME III | PC COSYMA | HOTSPOT |
|---|---|---|---|
| **1 km downwind** | **2.5E-12** | **4.7E-12** | **2.5E-11** |
| **2 km downwind** | **1.3E-12** | **2.3E-12** | **8.5E-12** |
| **5 km downwind** | **5.2E-13** | **7.7E-13** | **2.2E-12** |

Table 3. Time Integrated Air Concentration (Bq s $m^{-3}$)

| | NAME III | PC COSYMA | HOTSPOT |
|---|---|---|---|
| **1 km downwind** | **4.5E+04** | **8.7E+04** | **2.1E+05** |
| **2 km downwind** | **3.0E+04** | **3.1E+04** | **7.2E+04** |
| **5 km downwind** | **1.5E+04** | **7.8E+03** | **1.9E+04** |

In summary the adult effective cloud gamma doses estimated by NAME III are in good agreement with PC COSYMA estimates (within a factor of 2 at all downwind distances considered here). The agreement with HOTSPOT estimates are less robust. NAME III estimates of adult effective cloud gamma dose are within a factor of 10 of the HOTSPOT doses. The NAME III estimates of dose are smaller than those of the other two models but this is to be expected as typically NAME's estimates of TIAC are less than those in PC COSYMA and HOTSPOT. The relatively good agreement between models presented here further enhances the confidence in the Lagrangian particle approach implemented within NAME III. However, it is recommended that further time and effort be spent on such a model comparison. Extensions to this model comparison should ensure that all the input parameters considered in the model runs are analogous and if not, how this will impact upon model output. Further consideration of the model output should be made, especially with regard to the differences in the approaches applied. Additional scenarios may also be considered when extending any model comparison, for example, consideration of how the models compare at greater distances downwind.

b) Continuous/routine release scenario

For a continuous/routine release scenario a comparison of NAME III with ADMS and PC CREAM is performed. Below is a summary of the assumptions made and a comparison of the estimated output.

The conditions of the NAME III release are described below:

ix) Source Term. A continuous release of 1.0 Bq $s^{-1}$ of $^{85}Kr$ over a 24 hour period. Modelled using a release of 200000 particles over the 24 hour period. Source height = 10 m above ground level, with no dimensions (dx, dy, dz = 0, 0, 0).

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m. Note that no deposition is considered (because $^{85}Kr$ is a noble gas).

iii) Output Grid. Three receptor points are considered, at 1, 2 and 5 km along the PCL. Average air concentrations and adult effective cloud gamma dose rates are estimated at these points. Both are averaged over 24 hours post release (at one hour intervals for dose calculations and 5 minute intervals for air concentration calculations). The air concentrations are estimated

within grid boxes 20 x 20 x 20 m. All adult effective doses are estimated at a height of 1 m above ground level.

The full details of the NAME III run can be found in: Testing\ADMS_Comp\NAME or Testing\PCCREAM_Comp\NAME. The model input in ADMS and PC CREAM are defined such that they replicate the NAME III model input as closely as possible.

The full details of the ADMS run can be found in: Testing\ADMS_Comp. The full details of the PC CREAM run can be found in: Testing\PCCREAM_Comp.

Model Output

Table 4. Adult Effective Cloud Gamma Dose Rate (Sv $s^{-1}$)

| | NAME III | ADMS | PC CREAM |
|---|---|---|---|
| **1 km downwind** | **2.3E-22** | **2.1E-22** | **3.2E-22** |
| **2 km downwind** | **1.1E-22** | **8.2E-23** | **1.3E-22** |
| **5 km downwind** | **5.1E-23** | **2.2E-23** | **3.5E-23** |

Table 5. Average Air Concentration (Bq $m^{-3}$)

| | NAME III | ADMS | PC CREAM |
|---|---|---|---|
| **1 km downwind** | **5.6E-06** | **3.8E-06** | **6.5E-06** |
| **2 km downwind** | **7.5E-07** | **1.1E-06** | **2.0E-06** |
| **5 km downwind** | **3.7E-07** | **2.5E-07** | **4.2E-07** |

In summary the adult effective cloud gamma dose rates estimated by NAME III are in good agreement with PC CREAM and ADMS estimates (within a factor of 2 and a factor of 3, respectively, at all downwind distances considered here). The NAME III estimates of dose are greater than those of ADMS and yet at 2 of the 3 distances downwind the average air concentrations estimated by NAME III are less than ADMS. This anomaly may require further investigation. The relatively good agreement between models presented here further enhances the confidence in the Lagrangian particle approach implemented within NAME III. However, it is recommended that further time and effort be spent on such a model comparison. Extensions to this model comparison should ensure that all the input parameters considered in the model runs are analogous and if not, how this will impact upon model output. Further consideration of the model output should be made, especially with regard to the differences in the approaches applied. Additional scenarios may also be considered when extending any model comparison, for example, consideration of how the models compare at greater distances downwind.

### 2.7.3 Further testing – Ensuring the 3D Lagrangian particle model approach has been correctly implemented in NAME III

There exist a number other parts of the NAME III code which must be tested to ensure that the 3D Lagrangian particle model approach has been correctly implemented. These include:

i) Multiple photon energy's.
ii) Multiple radionuclides.
iii) Organ doses.
iv) Instantaneous dose rates.

v) In combination with decay chain modelling.
vi) Photon Flux.
vii) Integrated dose.
viii) Domain.

i) Multiple photon energy's

All the runs detailed so far have been performed using $^{85}$Kr which emits a single photon. A run (analogous to the instantaneous/accidental release scenario performed for $^{85}$Kr, above) including $^{41}$Ar was performed to test that NAME III could successfully calculate cloud gamma doses for multiple photon emissions. The run completed successfully and the output appears to be in the right ball park but these values should be compared with output from PC COSYMA. The full details of the NAME III run can be found in: Testing\OtherRadionuclides\Ar41.

ii) Multiple radionuclides

All the runs detailed so far have been performed using a single radionuclide. A run (analogous to the instantaneous/accidental release scenario performed for $^{85}$Kr and $^{41}$Ar in separate runs, above) including $^{85}$Kr and $^{41}$Ar was performed to test that NAME III could successfully calculate cloud gamma doses for a single run including multiple radionuclides. The run completed successfully and the output appears to be in the right ball park. The output are in agreement with the output for $^{85}$Kr and $^{41}$Ar modelled individually – need to ensure that the Ar41 run above is ok. The full details of the NAME III run can be found in: Testing\OtherRadionuclides\Kr85&Ar41.

iii) Organ doses

All the runs detailed so far have output adult effective cloud gamma dose. NAME III has been coded such that it can also calculate adult lung, adult thyroid and adult bone surface cloud gamma doses. A run (analogous to the instantaneous/accidental release scenario performed for $^{85}$Kr, above) to calculate adult lung, adult thyroid and adult bone surface cloud gamma doses was performed to test that NAME III could successfully calculate all forms of cloud gamma dose output as coded into the model. The run completed successfully. A hand calculation was performed to test the organ doses calculated by NAME. The ratio of the adult effective dose per unit air kerma and the three adult organ doses per unit air kerma were calculated. The ratios were then applied to the adult effective dose estimates output from NAME in an effort to estimate the adult organ doses. The NAME III output and the hand calculations were all in agreement. The full details of the NAME III run can be found in: Testing\OrganDoses.

iv) Instantaneous dose rates

All the runs detailed so far have output integrated cloud gamma dose (Sv) or averaged cloud gamma dose rate (Sv $s^{-1}$). NAME III has been coded such that it can also calculate instantaneous cloud gamma dose rates (Sv $s^{-1}$). A run (similar to the instantaneous/accidental release scenario performed for $^{85}$Kr, above) to

calculate adult effective cloud gamma dose rates at discrete times (60 times, at 1 minute time steps for an hour post release) was performed to test that NAME III could successfully calculate instantaneous cloud gamma dose rates. The run completed successfully. Output was compared against integrated cloud gamma doses for the same run (Testing\Noise\InstantRelRuns\Noise7). The output compared very well but further testing against other models may be of use at a later date. The full details of the NAME III run can be found in: Testing\InstantCldGDR.

v) In combination with decay chain modelling

A run was performed to test that NAME III could successfully model the radioactive decay of a parent to a daughter radionuclide and calculate adult effective cloud gamma dose from both the parent and the daughter product. The run completed successfully and the output appears to be in the right ball park but these values should be compared with output from PC COSYMA (PC COSYMA does account for decay chain modelling). The full details of the NAME III run can be found in: Testing\with_decay_chain_mod.

vi) Photon Flux

A run (similar to the instantaneous/accidental release scenario performed for $^{85}$Kr, above) to calculate average photon flux and instantaneous photon flux was performed to test that NAME III could successfully output all forms of photon flux. The run completed successfully. A hand calculation was performed to test the photon flux values output by NAME. The NAME III output and the hand calculations were all in agreement. The full details of the NAME III run can be found in: Testing\PFTestingRuns.

vii) Integrated dose

For some cloud gamma dose calculations the time integrated dose may be required at all receptor points and whereby the entire plume has passed all such receptor points. To ensure the cloud gamma output file is generated, “E”, must be added under the ‘Output Format’ header within the “Output Requirements - Fields:” block, for at least one of the output requirements (not necessarily, the cloud gamma output requirement). Without this addition, if all of the particles have left the domain then NAME III will stop performing the calculations and despite the request, no values of integrated dose will be output.

viii) Domain

When calculating cloud gamma dose (or any output requirement for that matter) ensure the domain used is minimised, thus particles dispersing away from the receptors (and therefore not contributing significantly to dose) will exit the domain and no longer be included in the model calculations, therefore minimising run time. However, care must be taken to ensure that particles are not lost from the domain which would have otherwise made a significant contribution at one or more of the receptors considered.

### 2.7.4 Testing of the applicability of the 3D Lagrangian particle model approach for calculating cloud gamma dose as implemented in NAME III

It is evident that the 3D Lagrangian particle model approach for calculating cloud gamma dose is the most suitable approach for implementation into NAME III. However there still exist some conditions under which this approach will not be applicable. The aim of this section is to highlight such conditions as a result of performing numerous NAME model runs.

One of the primary issues is to identify the conditions whereby the output is depicted by clearly defined contours of cloud gamma dose and is not noisy. The factors affecting the 'clarity' of the output include: the size and extent of grid boxes; the number of particles released and also the linear attenuation coefficient of the photons emitted. At the edges of the plume (i.e. off axis/off the 'plume centre line') and at the furthest downwind extent of the plume the output will always be noisy to some degree. This is unavoidable as there will always be a relatively small number of particles which are spread over a relatively large volume of the atmosphere but this is also representative of the extremities of the plume. Assuming no external forcing, the plume is never going to have a distinct edge or boundary. To a large degree, the more particles released in a NAME III run, the more 'clutter-free' the output. However the cloud gamma model calculations are relatively computationally expensive and the domains of interest may be large e.g. Europe wide for a continuous release estimating collective doses. For such a run, significantly increasing the numbers of particles released will significantly increase run time, to the extent that the run times are so large that the run time does not justify the run itself.

#### 2.7.4.1 Instantaneous/accidental release scenarios

A number of runs have been performed in NAME III, whereby the numbers of particles, and the grid size and extent have been modified to gauge the distance the model run remains clutter-free (or if it is clutter-free at all) and the run time. Note that the PC used to perform the runs had a CPU (processor speed) of 3 GHz (model name: Intel(R) Core(TM)2 Duo CPU E6850 @ 3.00GHz).

The conditions of the NAME III model run are described below:

i) Source Term. An instantaneous release of 1.0E+10 Bq of $^{85}$Kr. Source height = ground level (0 m), with dimensions of dx = 0.01, dy = 0.01, dz = 0 m.

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m. Note that no deposition is considered (because $^{85}$Kr is a noble gas). Wind direction = 270 degrees.

iii) Output. Adult effective cloud gamma dose are estimated, averaged over 24 hours post release (at one hour intervals) All adult effective doses are estimated at a height of 1 m above ground level.

Table 6. Distance NAME III model runs, for an accidental/instantaneous release, remain 'clutter-free' (or if it is clutter-free at all) and run time

| | | Number of Particles | | | |
|---|---|---|---|---|---|
| Maximum observed downwind extent / integration time | Size of grid boxes | 100 | 1000 | 10000 | 100000 |
| 35 km / 1 hr | 100 x 100 m | Output very noisy; no contour detail. Run time = ~30 seconds. (12) | Output noisy; contour detail evident to ~6 km. Run time = ~5 minutes. (13) | Output clear; contours smooth; contour extent = ~35 km. Run time = ~50 minutes. (14) | No run performed. |
| | 1 x 1 km | Output very noisy; no contour detail. Run time = few seconds. (7) | Output noisy; vague contour detail. Run time = few seconds. (8) | Output a little noisy; contour detail evident. Run time = ~1 minute. (9) | Output not noisy; contour detail evident but 'blocky'. Run time = ~10 minute. (10) |
| 240 km / 6 hrs | 1 x 1 km | Output very noisy; no contour detail. Run time = ~1 minute. (17) | Output noisy; vague contour detail. Run time = ~10 minutes. (18) | Output a little noisy; contour detail evident to 240 km. Run time = ~1.5 hours. (19) | Output a tiny bit noisy; contours smooth; contour extent to 240 km. Run time = ~16 hours. (20) |
| | 10 x 10 km | Output very noisy; no contour detail. Run time = few seconds. (22) | Output very noisy; no contour detail. Run time = few seconds. (23) | Output a little noisy; vague contour detail and blocky. Run time = ~3 minutes. (24) | Output a little noisy; vague contour detail and blocky. Run time = ~30 minutes. (25) |
| 950 km / 24 hrs | 1 x 1 km | No run performed. | Output very noisy; no contour detail. Run time = ~14 hours. (27) | Output very noisy; contour detail to 110 km; no subsequent contour detail. Run time = ~5 days & 21 hours. (28) | No run performed. |
| | 10 x 10 km | No run performed. | No run performed. | Output very noisy; no contour detail. Run time = ~1 hour. (31) | Output noisy; vague contour detail. Run time = ~14 hours. (32) |

Note that the number in brackets in each cell of Table 6, refers to the run number. The full details of all the NAME III runs can be found in: Testing\Noise\InstantRelRuns.

In summary, Table 6 suggests that for an instantaneous/accidental release scenario, a scoping run, providing a guide of the magnitude and extent of cloud gamma dose, can be performed using a minimum of 1000 particles and relatively few receptor points, at a runtime of the order of a few seconds or a few minutes. An example is Figure 2, below (Run 10, Table 6). However, if the user requires a clear and detailed plot of the magnitude and extent of cloud gamma dose, which is not 'blocky' (due to the large grid size and limited number of receptors) and is not noisy, then a minimum of 10000

particles and a relatively large number of receptor points are required, resulting in a runtime of at least one hour. An example is Figure 3, below (Run 14, Table 6).

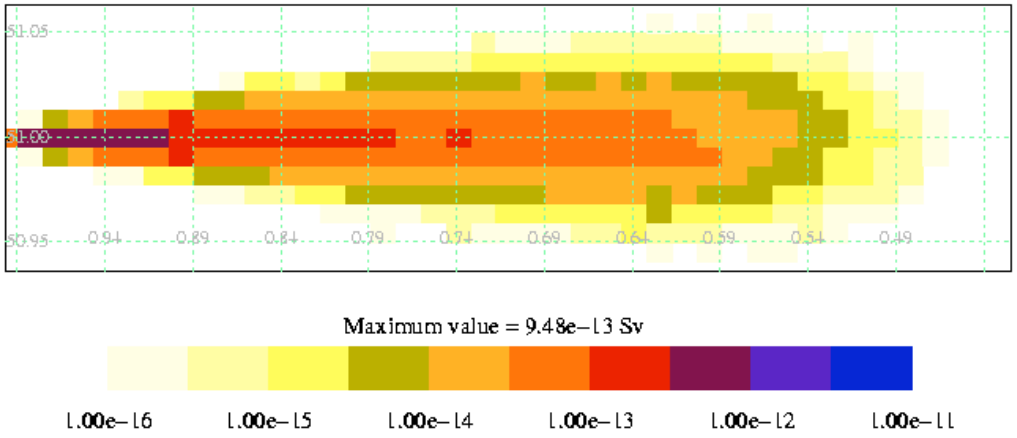


Figure 2. Adult effective cloud gamma dose (Sv), integrated over 1 hour, resulting from a 1.0E+10 Bq instantaneous release of $^{85}Kr$ using single site met data, on a 1 x 1 km grid.

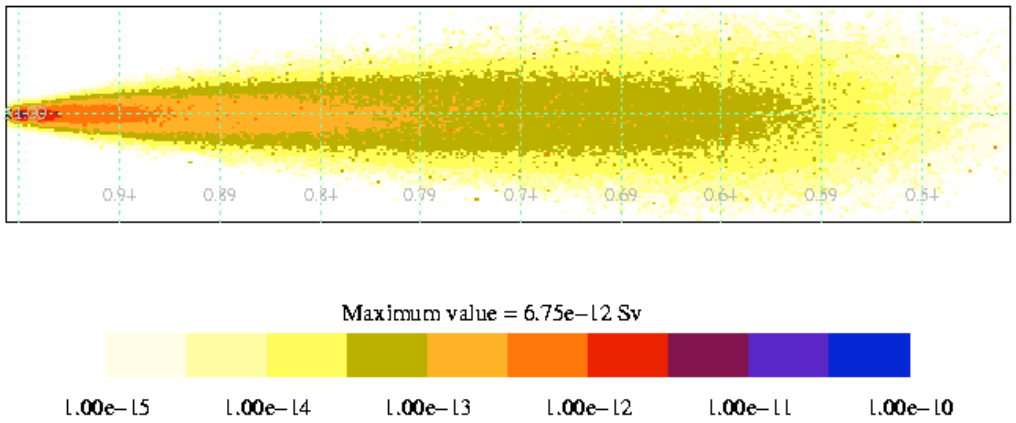


Figure 3. Adult effective cloud gamma dose (Sv), integrated over 1 hour, resulting from a 1.0E+10 Bq instantaneous release of $^{85}Kr$ using single site met data, on a 100 x 100 m grid.

From the NAME III model runs performed to date, for an instantaneous/accidental release of the type likely to be performed by HPA-RPD, most, if not all of the release should be able to be modelled using the Lagrangian particle approach. This assumes that cloud gamma dose calculations are required up to and including 10's of km's from the release. If the release is significantly large, such that cloud gamma dose estimates in the range of 100's of km's from the release are required, the semi-infinite approach is likely to be used in conjunction with the Lagrangian particle approach.

Below, I have suggested how cloud gamma doses may be calculated (if required) in the event of an accidental release:

i) An initial run(s) would be performed for a handful of receptors at key locations for a wide range of radionuclides. Two examples, one utilising

single site met data and the other utilising NWP met data are considered. These can be run on a timescale suitable for an emergency i.e. of the order of seconds. Examples can be found in: Testing\Acc_Rel_Scen\Unstructured_Grid and Testing\Acc_Rel_Scen\Unstructured_Grid2, relating to single site and met and NWP met, respectively.

ii) Plotting plumes would clearly also be beneficial, however to plot plumes may take of the order of minutes or hours depending on the clarity and detail required from the plot. Minimising the number of radionuclides to just include those deemed key, minimising the number of receptors, the size of the domain, the domain extent of the NWP met data and the number of particles will all minimise run time. In a single run, 1 hour increments in the release duration can be considered to avoid repeating the same run for progressively longer release durations (for example: Testing\Noise\InstantRelRuns\Noise17\Inc_Hrs_RD). Also in a single run, one hour increments in the estimated integrated dose can be considered, thus avoiding repeating the same run for progressively longer output times (for example: Testing\Noise\InstantRelRuns\Noise17\Inc_Hrs_Output).

Figures 4 and 5 below depict the adult effective cloud gamma dose at relatively short distances (up to 10 km) and relatively large distances (of order of 100's km) from the release, respectively.

The conditions of the NAME III model run in Figures 4 and 5 are described below:

i) Source Term. An instantaneous release of 1.0E+10 Bq of $^{85}$Kr. Modelled using a release of 10000 particles. Source height = ground level (0 m), with dimensions of dx = 0.01, dy = 0.01, dz = 0 m.

ii) Met Conditions. NWP met (for the period: 29/06/2008 11:00:00 to 29/06/2008 15:00:00). Regional met data used (Spatial grids = 40 x 40 km; temporal grid = 3 hourly). Met data domain = Europe and all of the Northern Atlantic Ocean. Note that no deposition is considered (because $^{85}$Kr is a noble gas).

iii) Output. Adult effective cloud gamma dose is estimated (Sv). Doses integrated over the 4 hour period post release (at one minute intervals). Output in Figure 4 is estimated at a height of 1 m above ground level, using the Lagrangian Particle approach. Output in Figure 5 is estimated for grid boxes of 1 km x 1km x 0.1 km (x, y, z) using the Semi Infinite approach.

The full details of all the NAME III runs can be found in: Testing\Acc_Rel_Scen\Run15.

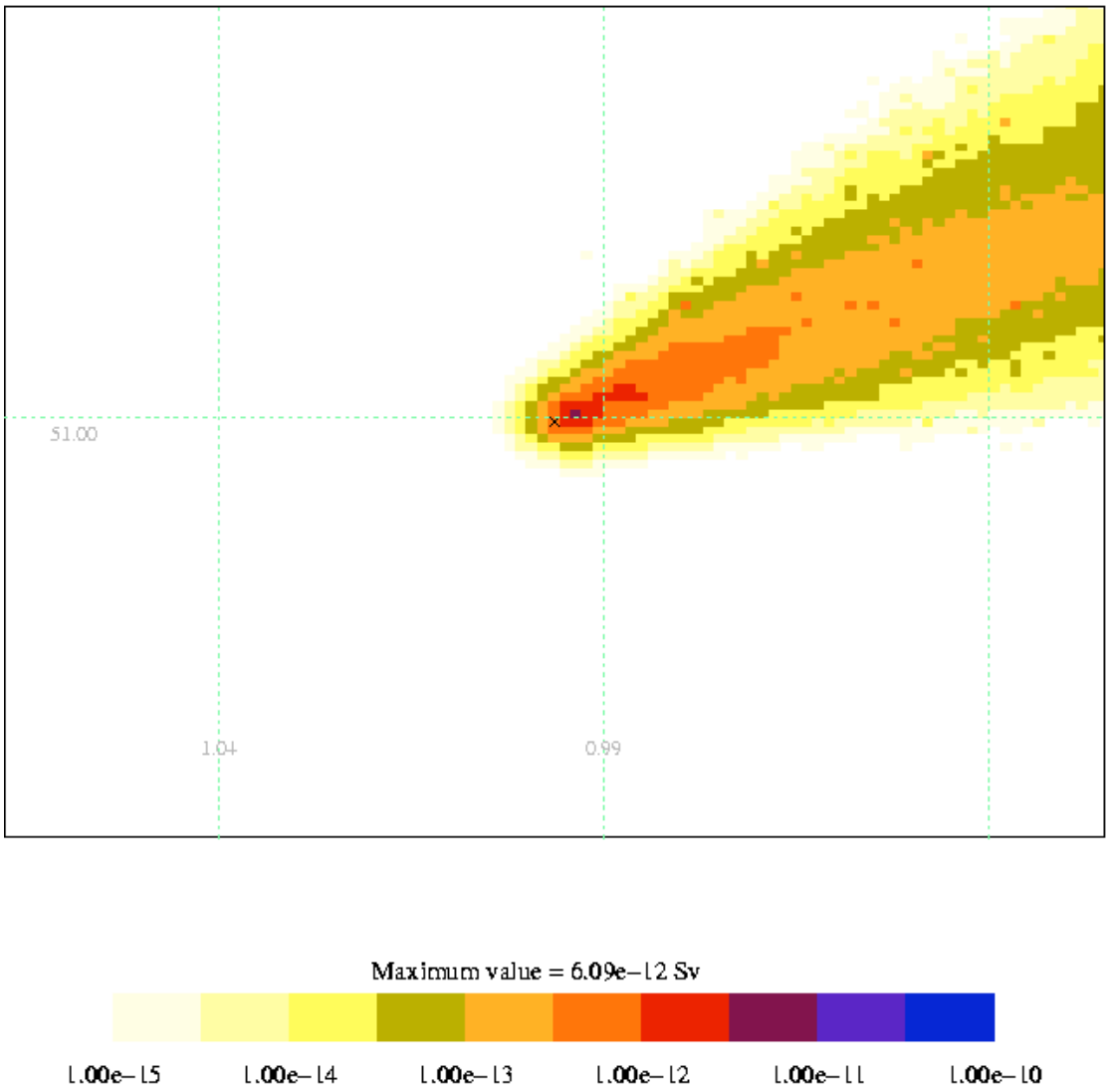


Figure 4. Adult effective cloud gamma dose (Sv), integrated over 4 hours, resulting from a 1.0E+10 Bq instantaneous release of $^{85}$Kr using NWP met data, for a release of 10,000 particles on a 100 x 100 m grid (using the Lagrangian Particle approach).

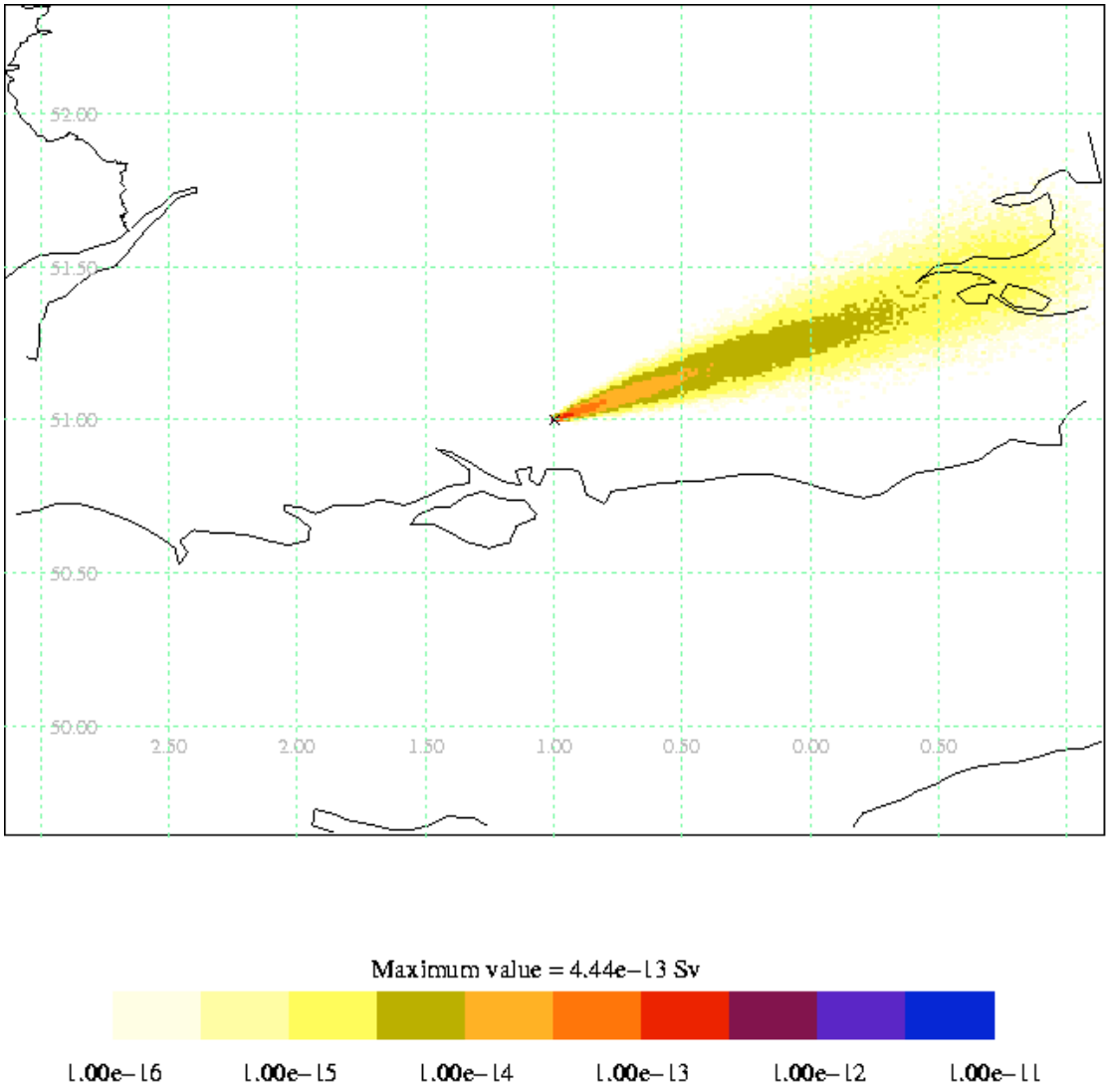


Figure 5. Adult effective cloud gamma dose (Sv), integrated over 4 hours, resulting from a 1.0E+10 Bq instantaneous release of $^{85}Kr$ using NWP met data, for a release of 10,000 particles on a 1 x 1 km grid (using the Semi-infinite approach).

#### 2.7.4.2 PRA release scenarios

From the NAME III model runs performed to date, for a PRA type run, typical of those performed by HPA-RPD, the run is likely to require the combined use of the semi-infinite and the Lagrangian particle approach. This assumes that cloud gamma dose calculations are required up to and including 100's of km's from the release. Below, I have suggested how cloud gamma doses may be calculated (if required) in probabilistic risk assessments.

A PRA type run requiring (individual) hourly runs for a whole year (365 x 24 runs), using NWP met data is likely to be costly (in terms of runtime). One potential option to reduce runtime would be for each 24 hour period, to consider 24 different sources in a single run (one for each hour) despite the species and quantity of each species released in each source being the same. Using this approach saves CPU because the

same NWP met data does not have to be repeatedly read in to NAME (reading in NWP met data can be a significant expense when performing NAME runs). An alternative approach would be to produce cut outs of the met data. For example, for each proposed nuclear site the NWP met data around that site e.g. on a 200 $km^2$ domain centred on the site, could be cut out, from the hourly 12 km x 12 km Mesoscale met data, for example. For a years data set (for example) the cut out data could be read in to NAME at a significantly smaller cost than the full domain (which for the Mesoscale met includes all of the UK and Ireland, most of France, the Low Countries and parts of Scandanavia). If either approach or a combination of the two approaches were to be applied a script or an extension to the HPA's NIFTY front end could be developed which would increment and update the appropriate parameters in the NAME III input file to perform a run over timescales of a year or more (thus automating the run).

Output of the form of Figures 4 and 5 could be produced, however these would be replicated for every hour over one or more years worth of NWP met data.

#### 2.7.4.3 Continuous/routine release scenarios

For routine release calculations HPA-RPD are likely to need to calculate collective doses out to significant distances (e.g. 3000 km – over much of Europe). In addition HPA-RPD are likely to need to calculate critical group doses out to much shorter distances (e.g. approximately 10 km from the release). Both types of release will require a continuous release over a year or mores NWP met data.

From the NAME III model runs performed to date, for a continuous/routine release of the type likely to be performed by HPA-RPD, it is envisaged that all releases modelled over a European domain will use the Semi Infinite approach. However, it is envisaged that all releases modelled over 20 $km^2$ domains (for example) will use the Lagrangian Particle approach. Below, I have suggested how cloud gamma doses may be calculated (if required) in the event of a continuous/routine release assessment for a) long range collective dose calculations and b) short range critical group dose calculations:

a) Long range collective dose calculations

The conditions of the NAME III model run in Figure 6 (and Table 7) are described below:

i) Source Term. A continuous release of 1.0E+03 Bq $s^{-1}$ of $^{135}I$. Modelled using a release of 100 particles per hour for an entire year (01/01/2008 00:00:00 to 01/01/2009 00:00:00). Source height = ground level (0 m), with dimensions of dx = 0.01, dy = 0.01, dz = 0 m.

ii) Met Conditions. NWP met (for the period: 01/01/2008 00:00:00 to 01/01/2009 00:00:00). Regional met data used (Spatial grids = 40 x 40 km; temporal grid = 3 hourly). Met data domain = Europe and all of the Northern Atlantic Ocean.

iii) Output. Adult effective cloud gamma dose rate is estimated (Sv $s^{-1}$). Dose rates averaged over a 1 year period post release (at six hour

intervals). Output is estimated for grid boxes of 100 km x 100 km x 0.1 km (x, y, z) using the Semi Infinite approach.

Table 7. Clarity and detail of output and run time, for a range of NAME III model runs (continuous/routine releases for long range collective dose calculations).

| | | Number of particles per hour | | |
|---|---|---|---|---|
| Radionuclides considered | Size of grid boxes and domain | 20 | 100 | 500 |
| $^{135}$I only | European domain (17°W to 32°E & 34°N to 66°N) 100 x 100 km grid (33 x 35 grid points) | - | Output 'blocky' but not noisy; contour detail evident. Run time = ~22 hours. (1) | - |
| | Smaller European domain (10°W to 20°E & 40°N to 60°N) 100 x 100 km grid (21 x 23 grid points) | Output 'blocky' but not noisy; contour detail evident. Run time = ~4.5 hours. (3) | Output 'blocky' but not noisy; contour detail evident. Run time = ~9 hours. (4) | Output 'blocky' but not noisy; contour detail evident. Run time = ~48 hours. (2) |
| | Smaller European domain (10°W to 20°E & 40°N to 60°N) 10 x 10 km grid (211 x 231 grid points) | Contour detail smooth and clear (not noisy). Run time = ~4.5 hours. (6) | - | - |
| All 16 radionuclides | Smaller European domain (10°W to 20°E & 40°N to 60°N) 100 x 100 km grid (21 x 23 grid points) | Output 'blocky' but not noisy; contour detail evident. Run time = ~5 hours. (5) | - | - |

Note that the number in brackets in each cell of Table 7, refers to the run number. The full details of all the NAME III runs can be found in: Testing\Version5_2e under folders named, "Cont1", Cont2", etc.

From Table 7 it is evident that the number of particles released per hour is a key parameter impacting upon runtime (compare Cont3 and Cont2 in Table 7). The size of the dispersion domain is also clearly significant in determining runtime (compare Cont1 and Cont4 in Table 7). It is also likely that reducing the size of the domain of the NWP met data used would also significantly reduce runtime, however this has not been tested here. If it is satisfactory for output to be 'blocky' (due to the large grid size and limited number of receptors), a run with a release of 20 particles per hour on a grid of 100 x 100 km appears to be sufficient (see Figure 5, below – derived from Cont1 in Table 7), however further investigation is recommended. There appeared to be little difference in the output observed across the range of numbers of particles released per hour (20-500). If the output is required to be clearer and contours smoother then the grid size must be reduced and the number of receptors increased. This does not directly increase runtime (compare Cont3 and Cont6 in Table 7) but a result of decreasing grid size is the requirement to increase the number of particles per hour which could in turn significantly increase runtime (further investigation is recommended). It also appears that increasing the number of radionunclides considered has little impact on runtime (compare Cont3 and Cont5 in Table 7). 100 x 100 km grids (as in Figure 6, below) may be more appropriate for estimating cloud

gamma doses on a European domain and 10 x 10 km grids may be more appropriate for estimating cloud gamma doses on a UK domain.

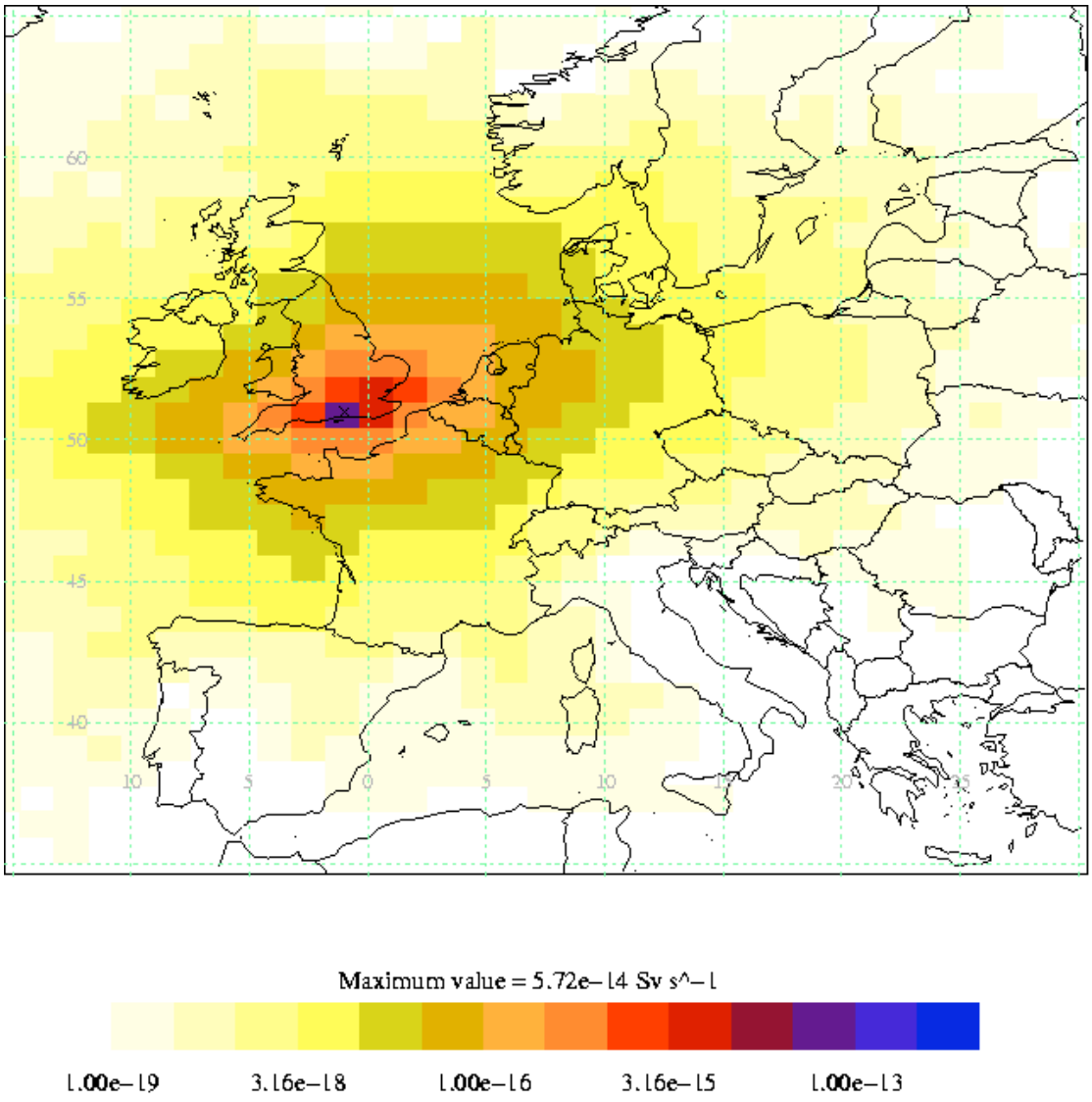


Figure 6. Adult effective cloud gamma dose rate (Sv $s^{-1}$), averaged over 1 year, resulting from a 1.0E+03 Bq $s^{-1}$ continuous release of $^{135}I$ using NWP met data, for a release of 100 particles per hour on a 100 x 100 km grid (using the Semi Infinite approach).

b) Short range critical group dose calculations

The conditions of the NAME III model run in Figure 7 are described below:

i) Source Term. A continuous release of 1.0E+03 Bq $s^{-1}$ of $^{135}I$. Modelled using a release of 500 particles per hour for an entire year (01/01/2008 00:00:00 to 01/01/2009 00:00:00). Source height = ground level (0 m), with dimensions of dx = 0.01, dy = 0.01, dz = 0 m.

ii) Met Conditions. NWP met (for the period: 01/01/2008 00:00:00 to 01/01/2009 00:00:00). Regional met data used (Spatial grids = 40 x 40 km; temporal grid = 3 hourly). Met data domain = Europe and all of the Northern Atlantic Ocean.

iii) Output. Adult effective cloud gamma dose rate is estimated (Sv $s^{-1}$). Dose rates averaged over a 1 year period post release (at six hour intervals). Output is estimated at 1 m above ground level on 100 x 100 m grids using the Lagrangian Particle approach.

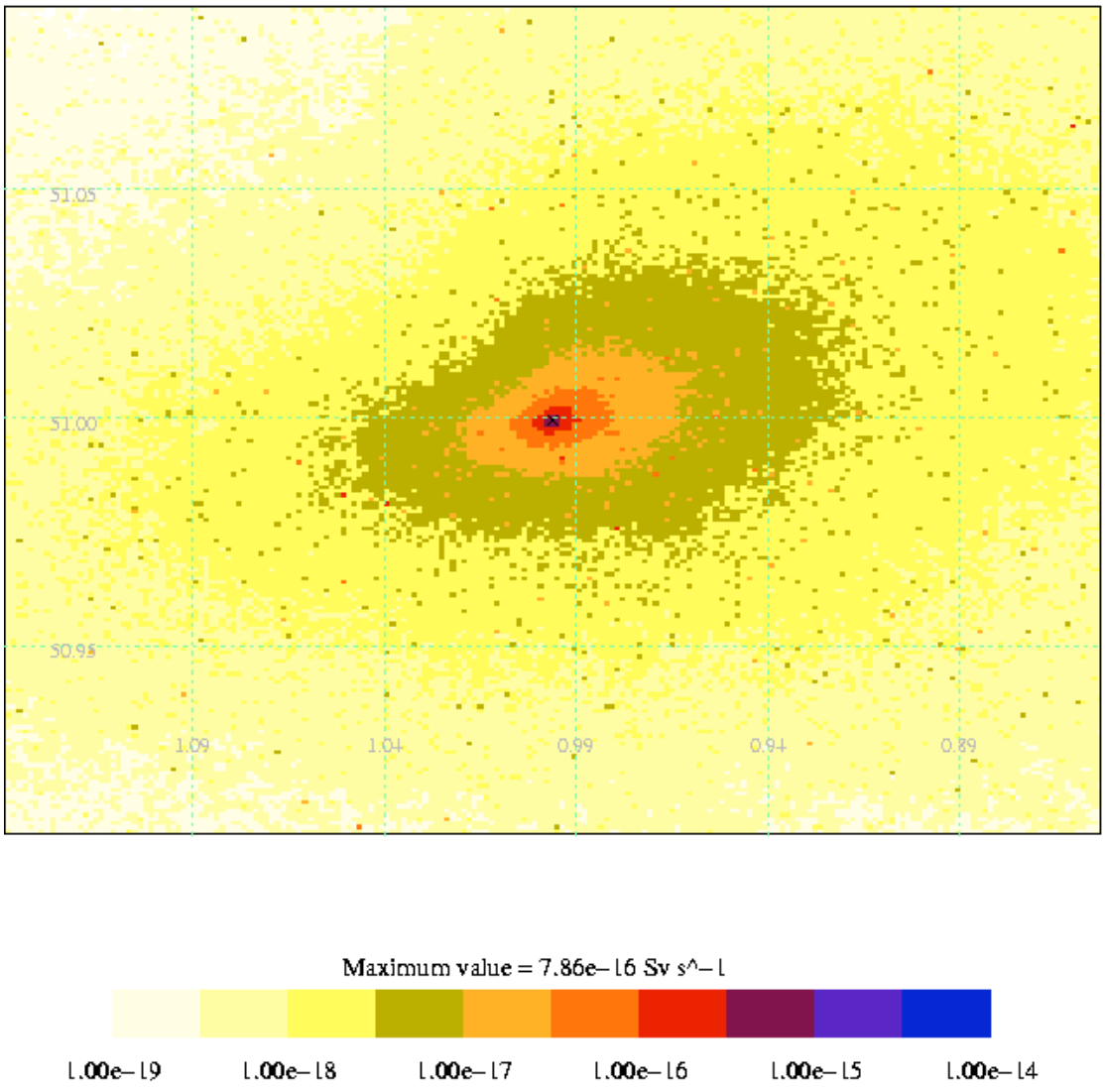


Figure 7. Adult effective cloud gamma dose rate (Sv $s^{-1}$), averaged over 1 year, resulting from a 1.0E+03 Bq $s^{-1}$ continuous release of $^{135}I$ using NWP met data, for a release of 500 particles per hour on a 100 x 100 m grid (using the Lagrangian Particle approach).

From the NAME III model runs performed to date, it is suggested that a minimum of 500 particles per hour are released for short range critical group dose calculations. Any fewer particles and there is deemed to be a lack of clarity in the model output

when plotted. The model run considering a release of 500 particles per hour took approximately 6.5 hours (compared to 3.5 hours for an analogous model run considering a release of 100 particles per hour). As well as particle release rate, the domain size of the NWP met data and the number of radionuclides considered are also likely to impact significantly on model runtime. It certainly seems unnecessary to use the full Mesoscale domain (for example) (covering all of the UK and Ireland, most of France, the Low Countries and parts of Scandanavia) when only an area 20 $km^2$ may be required. Further consideration is recommended. It is thought that detail greater than that provided by a 100 x 100 m is unlikely to be required and in any event is likely to be very computationally expensive.

The full details of all the NAME III runs used to derive Figure 7 can be found in: Testing\Cont_Rel_Scen\Run3.

#### 2.7.4.4 Other considerations

**How many photon energies can NAME III handle?**

For a run with only a handful of receptor points, a moderate number of particles and a relatively short averaging and/or integrating period, akin to those in Testing\OtherRadionuclides\I132, any number of photon energies can be considered for a single radionuclide. In such runs, 6 receptors and an instantaneous release of 10,000 particles are considered, resulting in a runtime of order of seconds. The difficulty the user is faced with here is adding the potentially large number of photon energies to the NAME III input file. The process of adding photon energies to NAME III input files can be simplified by using: ..\Version5_2c\Resources\Defns\Cloud_Gamma_Params.txt and/or by setting up default NAME III input files. For a NAME III run with a large number of receptor points and/or a large number of particles released over a relatively large domain, the number of photon energies should be limited. However there is never any need to run with more than 12 photon energies per radionuclide, because HPA currently utilises an approach which considers photon energies across 12 separate bins. Currently the maximum number of photon energies allowed for any one radionuclide in NAME III is limited to 20. This upper bound can easily be increased if deemed necessary.

**How many radionuclides can NAME III handle?**

An unstructured grid with a handful of receptor points can comfortably model cloud gamma dose for all 16 radionuclides identified as key. For example in runs 1-3 in Testing\OtherRadionuclides\ManyRadionuclides for 6 receptors and an instantaneous release of 10000 particles, a release of 16 radionuclides will run over the order of seconds. For a run considering 16 radionuclides and 61 x 31 (~2000) receptors, a run time of 1.5 and 15 minutes applies to instantaneous releases of 100 and 1000 particles, respectively (see runs 4-5 in Testing\OtherRadionuclides\ManyRadionuclides for details). By limiting the number of particles released and the number of receptor points considered in a structured grid it is possible to run NAME, even for up to 16 radionuclides, for relatively short runtimes. Clearly the run time is also dependent on the number of photon energies considered for each radionuclide (see above for details). Note that currently the maximum number of radionuclides applicable in any

NAME run is limited to 16. This upper bound can easily be increased if deemed necessary.

**Integration (or averaging) times and sync time**

A number of runs were performed investigating the impact of integration timesteps on model output and runtime. It is observed that where the doses are large, varying the integration timesteps made relatively little difference to the estimated dose (variation of a factor of 2). At the edges of the plume where the doses are much smaller varying the integration timesteps made a relatively large difference to the estimated dose (many orders of magnitude difference in some instances). However it is apparent that large changes in the integration timesteps make only a small difference to runtime. Therefore integration and average timesteps of 1 minute and sync times of 30 seconds are suggested for the majority of cloud gamma model runs. However further input and/or investigation may be necessary. The full details of all the NAME III runs can be found in: Testing\IntTimes.

**NWP met data**

It is likely that NWP met data will be used in the estimation of cloud gamma doses for a range of assessments performed by the HPA. Outlined below are the types of NWP met data which are likely to be required if HPA were to use NAME III to estimate cloud gamma dose in the range of assessments they undertake.

For an accidental/instantaneous release of the type likely to be modelled by HPA-RPD, it is envisaged that if NWP met data were to be used for a model run when estimating cloud gamma dose Mesoscale met or NWP met on smaller grids are deemed to be most suitable.

For a PRA assessment of the type likely to be modelled by HPA-RPD, it is envisaged that if NWP met data were to be used for a model run when estimating cloud gamma dose Mesoscale met or NWP met on smaller grids are deemed to be most suitable. A cut out of the NWP met applicable to each site of interest is likely to be of use.

For an continuous/routine releases (long range collective dose calculations) of the type likely to be modelled by HPA-RPD, it is envisaged that if NWP met data were to be used for a model run when estimating cloud gamma dose, Reg NAE (or perhaps NAE or Regional) met are deemed to be most suitable.

For an continuous/routine releases (short range critical group dose calculations) of the type likely to be modelled by HPA-RPD, it is envisaged that if NWP met data were to be used for a model run when estimating cloud gamma dose, 4 x 4 km met or NWP met on smaller grids are deemed to be most suitable. A cut out of the NWP met applicable to each site of interest is likely to be of use.

Table 8. Range of NWP met data available for use in NAME III

| NWP Met Description | Domain | Temporal Grid | Spatial Grid | History |
|---|---|---|---|---|
| Global | Global | 3 hourly | 40 x 40 km | Historically coarser grid. Long term dataset. |
| Regional (subset of Global dataset) | Europe & North Atlantic Ocean | 3 hourly | 40 x 40 km | Historically coarser grid |
| NAE | Europe and most of the North Atlantic Ocean | Hourly | 12 x 12 km | Always 12 x 12 km grid. No archive. |
| Reg NAE (cutout of NAE dataset) | Europe | Hourly | 12 x 12 km | Always 12 x 12 km grid. |
| Mesoscale | UK & Ireland, most of France, the Low Countries & parts of Scandanavia | Hourly | 12 x 12 km | Historically coarser grid. Long term dataset. |
| 4 x 4 km | UK, Ireland, & NE France | Hourly | 4 x 4 km | Always 4 x 4 km grid. |
| 1.5 x 1.5 km | Likely to be smaller than 4 x 4 km. | Hourly | 1.5 x 1.5 km | To be released at the end of 2009. |

Note that the spatial grids are defined here in terms of km's, however in truth the grids are denied in lat/long co-ordinates and the values in km's are only approximate.

## 2.8 Semi-infinite Cloud Approach

It is evident from Section 2.7.4 that there will exist instances whereby HPA will wish to calculate cloud gamma dose or dose rate (for a combination of: number of receptor points, spatial and temporal dispersion domain, number of particles released, met data and a numbers of radionuclides and associated photon energies) but the Lagrangian particle approach will not be a suitable approach.

The estimation of absorbed dose in air from a plume emitting photons is most simply achieved by use of a Semi-infinite cloud model (Simmonds et al, 1995). Implicit in this approach are the assumptions that the air concentration is uniform over the volume of the plume from which photons can reach the point at which the dose is delivered and that the cloud is in radiative equilibrium: the amount of energy absorbed by a given element of cloud is then equal to that released by the same element.

Thus at relatively long distances from the source of a release where there exists a relatively low density of particles the Lagrangian particle approach to cloud gamma modelling will typically result in noisy output and dose estimates associated with a large degree of uncertainty. In contrast, at similarly large distances from the release, air concentrations are likely to be relatively uniform and the Semi-infinite cloud

approach will typically result in a good approximation of dose. Thus the Semi-infinite approach has been coded into NAME III.

### 2.8.1 Method

Using the Semi-infinite cloud approach, the cloud gamma dose rate (effective and organ dose rates in units of Sv $s^{-1}$ and Gy $s^{-1}$, respectively) is expressed as:

$$\dot{D}_\gamma = kC\sum_{j=1}^{n} I_j E_j A_j \qquad \text{Eq11b}$$

where k = conversion factor
= 2.0 $10^{-6}$ Gy $y^{-1}$ per MeV $m^{-3}$ $s^{-1}$,
C = air concentration (Bq $m^{-3}$)
n = no. of photons specified for nuclide
I = photon intensity
E = photon energy (MeV)
A = dose per unit air kerma (Sv $Gy^{-1}$ or Gy $Gy^{-1}$ depending on whether the dose is an effective dose or an organ dose per unit air kerma, respectively).

### 2.8.2 Output from NAME III

Analogous to the Lagrangian particle approach for calculating cloud gamma dose, the Semi-infinite approach implemented in NAME III can be used to derive output of instantaneous and average effective and organ dose rates in units of Sv $s^{-1}$ and Gy $s^{-1}$, respectively, and integrated effective and organ dose in units of Sv and Gy, respectively. However, photon flux ($m^{-2}$ $s^{-1}$) cannot be output. Note that dose and dose rate is not summed over radionuclide for a source including multiple radionuclides. However if HPA require total dose or total dose rate summed over radionuclide this may be an area for future development of NAME.

Note that there is no constraint to consider air concentrations (or any other output quantity) as an output requirement when estimating cloud gamma dose.

### 2.8.3 Code changes to NAME III to incorporate cloud gamma modelling – the Semi-infinite cloud approach

Below is a summary of how the NAME III code has been modified to account for cloud gamma modelling. The summary of the code added considers the Semi-infinite cloud approach only (and not the Lagrangian particle approach, which is considered previously). The development version of the files can be found in: H:\Version5_2h. Old files are named …..01.F90. Newly updated files are named ……F90. Note that the files include the previous update of the decay chain modelling for atmospheric dispersion (but not for deposition).

#### 2.8.3.1 Input

The column key, "Semi-infinite approx?" has been added to the FieldReqsInputNames subroutine, applicable to the "Output Requirements – Fields:" block. The default value is "No" i.e. to use the Lagrangian particle approach when calculating cloud gamma dose. The subroutine, "Tokens2FieldReqs" is updated accordingly.

#### 2.8.3.2 Output

It is worth noting that the Semi-infinite approach uses the same output requests as the Lagrangian particle approach. The alternative approach would have been to apply different output requests for different approaches but this would potentially result in many different output requests and could prove confusing if the same quantity, "Cloud Gamma Dose" could be calculated using different output requests. Care however needs to be taken in the output file as the approach used to calculate the cloud gamma dose will not be detailed (however Dave thought that this could be added to a row in the output file which could also be used to state if decay is switched on or off for deposition). Pete and Dave agreed that if further approaches were to be implemented into NAME III (e.g. the line source approach) the current method used to calculate Cloud Gamma Dose would need to be reviewed (i.e. the use of the column key "Semi-infinite approx?" in the "Output Requirements – Fields:" block). Pete believes that HPA are unlikely to require any further approaches for calculating cloud gamma dose in NAME III (e.g. the two approaches implemented to date should be more than adequate when modelling line sources) but that this issue should be considered further by HPA.

The argument, "SemiInfApproach" was added to the Type, "FieldReq_". A check was added in the Function, "InitFieldReq", which raised an error if the Semi-infinite approximation is selected in a NAME III input file without selecting one of the four cloud gamma output requests. A check to ensure that field requirements are equal is performed in the Function, "FieldReqEq" and the Function, "FieldReqEquiv". SemiInfApproach is included in all the extra field requests (ExtraFieldReq) in the "SetUpReqs" Subroutine, which includes an extra field request for calculating the cloud gamma dose by way of the Semi-infinite cloud approach, whereby Quantity = 'Air Concentration'. In the Subroutine, "ProcessFields" the Subroutine, "Derive_CldGammaDose_via_SemiInfApproach" is called. The Subroutine, "Derive_CldGammaDose_via_SemiInfApproach" is added and used to calculate the cloud gamma dose using air concentrations estimated by NAME.

### 2.8.4 Semi-infinite model runs and NAME III input files

The NAME III input file is set up very similarly if using the Lagrangian particle approach or Semi-infinite approach (see Section 2.2 for further details). The primary difference is the inclusion of the column key (column heading), "Semi-infinite approx?" in the Output Requirements - Fields: block (see Figure 8 for details).

```
Output Requirements - Fields:
Name,                          Quantity,        Species,   Source,      H-Grid,
Req 4, Adult Effective Cloud Gamma Dose,     KRYPTON-85,         ,    CG_Grid1,

  Z-Grid,  T-Grid, Z-Coord, BL Average, T Av or Int, Av Time, # Av Times, Sync?,
AC_Grid1,  TGrid1,        ,          ,         Int,   06:00,        180,    No,

   Graph?,  Screen?, Disk?,  Across, Separate File,  Output Format,  Output Group,
```

```
      No,       No,    Yes,      TZ,             T,            IAE,  Fields_grid4,

Semi-infinite approx?
                  Yes
```

Figure 8. Section of a NAME III input file used to estimate cloud gamma dose via the Semi-infinite approach

A key difference in the NAME III input files when applying the Lagrangian particle approach and the Semi-infinite cloud approach to calculate cloud gamma dose lies in the spatial grids used in the "Output Requirements – Fields:" block. When using the Lagrangian approach the size and position of the grids is only of importance in terms of defining the locations of the receptors, for example, Z-Grid should be set to $z_o$ = 1 m (or there abouts) as this approximates the height of the centre of a 'typical' person. There is no requirement to define grids on the basis of the contribution to dose from particles as this is independent of the grids. All particles contribute to dose irrespective of whether they are in the same grid box as the receptor (or regardless of them residing in a grid box at all). However the Semi-infinite cloud approach is derived from air concentrations averaged over each grid box and applied to the receptor residing within that same grid box. Therefore the dimensions of H-Grid and Z-Grid for the Semi-infinite approach must be specified with more care. For the Semi-infinite approach to be applicable, air concentrations should be uniform and relatively large grid boxes should be applied e.g. 500 x 500 x 500 m. Using relatively small grid boxes for the Semi-infinite approach may well give erroneous answers because small grids boxes will contain relatively few particles which is likely to result in estimates of 'noisy' air concentrations.

### 2.8.5 Testing

It is important to test the cloud gamma modelling approach implemented in NAME III. NAME should be tested to ensure that the approach has been correctly implemented, there are no bugs apparent and that cloud gamma dose output is verified against other approaches and/or models. It should be noted that a full review of the overall differences between cloud gamma dose estimates from a range of models would be beneficial at a later date. The testing of the Semi-infinite approach will incorporate hand calculations, intercomparison of NAME III model runs and comparison of NAME output against output from HPA's PC CREAM model.

A second aspect of testing NAME III, investigating the conditions under which the calculation of cloud gamma dose via the Semi-infinite approach implemented in NAME are applicable, has been performed and is detailed in Section 2.7.4.

#### 2.8.5.1 Testing against hand calculations

Hand calculations were performed to estimate cloud gamma dose using the Semi-infinite cloud approach. Three air concentrations were randomly selected from: H:\Cloud_Gamma_Mod\Testing\Version5_2h\Run1\Fields_grid1_C1_T1_200606291105.txt and applied to the approach detailed in Section 2.8.1. The cloud gamma dose rates calculated by hand were in agreement with those calculated by NAME in: Testing\Version5_2h\Run1\Fields_grid3_C1_T1_200606291105.txt. This gives

confidence that the method for calculating cloud gamma dose via the Semi-infinite approach, as detailed in this note, has been correctly implemented into NAME III.

#### 2.8.5.2 Testing NAME III by way of comparison of different NAME model runs

**Comparison of NAME III runs for receptors relatively close to the source**

i) In Section 2.7.1 a NAME III model run was setup to replicate uniform air concentrations over horizontal and vertical spatial scales of the order of km's. The same model run was used here to estimate cloud gamma dose via the Semi-infinite cloud approach implemented in NAME.

The source term and met conditions of the model run are as detailed in Section 2.7.1 but there exist some differences in the output grid. The number of grid points consider are 3 x 3 x 2 (in the x, y, z planes, respectively). The dimensions covering all grid points are: 1 x 1 x 1 km. The grid points are therefore 500 m apart in the horizontal and at 250 m and 750 m above ground level in the vertical plane. Air concentrations (Bq $m^{-3}$) AND cloud gamma dose rate (Sv $s^{-1}$) output at each of these grid points are averaged over the 5 minutes post release (at 30 second intervals).

On the basis of this single model run, cloud gamma dose rate was estimated via three different methods, detailed below.

a) Estimating cloud gamma dose rate by hand via the Semi-infinite approach (assuming an air concentration of 1.84E-01 Bq $m^{-3}$, taken from Testing\Semi_Inf_Cloud or Testing\Version5_2h\Run1:

Adult effective dose rate = 1.74E-17 Sv $s^{-1}$

b) Estimating cloud gamma dose rate directly from NAME III using the Lagrangian particle approach (taken from Testing\Semi_Inf_Cloud):

Adult effective dose rate = 1.77E-17 Sv $s^{-1}$

c) Estimating cloud gamma dose rate directly from NAME III using the Semi-infinite cloud approach (taken from Testing\Version5_2h\Run1):

Adult effective dose rate = 1.75E-17 Sv $s^{-1}$

The spreadsheet in: Testing\Version5_2h\Run2\Cld_Gamma_Dose_Rate.xls details how NAME III comes to estimate the adult effective dose rate in this instance.

All three estimates of cloud gamma dose rate compare very well. This gives confidence in the Semi-infinite cloud approach implemented within NAME III and NAME's ability to estimate cloud gamma dose under conditions of uniform air concentrations.

.

ii) In Simmonds et al, 1995 it is stated that for photons of less than 20 keV energy, a semi-infinite cloud model will always be adequate. Therefore a comparison of the Lagrangian particle approach (for a relatively large number of particles) and the Semi-infinite approach has been undertaken.

The conditions of the NAME III model run considered here are described below:

i) Source Term. An instantaneous release of 1.0E+10 Bq of X-2 (a fabricated radionuclide with a photon energy of 10 KeV and photon intensity of 1). Source height = ground level (0 m), with dimensions of dx = 0.01, dy = 0.01, dz = 0 m.

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m.

iii) Output. Adult effective cloud gamma dose rate is estimated (Sv $s^{-1}$). Dose rates averaged over a 1 hour period post release (at one minute intervals). 12 receptors along the plume centre line at the source, 500 m downwind, 1km downwind, 1.5 km downwind, etc up to 5.5 km downwind. Horizontal grids 500 x 500 m. For cloud gamma dose estimated via the Lagrangian Particle approach, z = 1 m agl. For cloud gamma dose estimated via the Semi-infinite cloud approach, the vertical dimensions of the grid box were set to 500 m.

Table 9. Adult effective cloud gamma dose rate (Sv $s^{-1}$)

| | Particles released | | | | | |
|---|---|---|---|---|---|---|
| | 10000 | | 100000 | | 1000000 | |
| Distance downwind (km) | Lagrangian Particle Approach | Semi Infinite Approach | Lagrangian Particle Approach | Semi Infinite Approach | Lagrangian Particle Approach | Semi Infinite Approach |
| 0 | **1.4E-18** | **2.0E-18** | 1.2E-17 | 2.0E-18 | **7.6E-18** | **2.0E-18** |
| 0.5 | **6.9E-18** | **2.6E-18** | **5.0E-18** | **2.6E-18** | 1.1E-16 | 2.6E-18 |
| 1 | **3.2E-18** | **2.3E-18** | **7.8E-19** | **2.3E-18** | 1.1E-17 | 2.3E-18 |
| 2 | 4.9E-22 | 1.7E-18 | **1.9E-18** | **1.7E-18** | 1.5E-17 | 1.7E-18 |
| 3 | 6.9E-22 | 1.3E-18 | 1.1E-20 | 1.3E-18 | **5.1E-19** | **1.3E-18** |
| 4 | 1.4E-20 | 1.1E-18 | 7.4E-20 | 1.1E-18 | **5.8E-18** | **1.1E-18** |
| 5 | 3.5E-22 | 9.2E-19 | 1.2E-19 | 9.1E-19 | **1.7E-18** | **9.1E-19** |

Note that values within a factor of 5 of each other are highlighted in bold.

Full details of the model runs in Table 9 can be found in:
Testing\Version5_2h\Run4 for a release of 10000 particles;
Testing\Version5_2h\Run3 for a release of 100000 particles;
And in Testing\Version5_2h\Run5 for a release of 1000000 particles.

I do not believe that this test adds much in the way of confidence in the Semi-infinite approach implemented in NAME III but I do believe it adds value when comparing model approaches for calculating cloud gamma dose. It is evident that there exists reasonable agreement between the two approaches but not across the board for all downwind distances considered and for all numbers of particles released. Further consideration may be of use.

iii) ESCLOUD is the only (Check?) model used by HPA which gives the user the choice to use the Semi-infinite model, however HPA can no longer run this model. PC CREAM does not give the user the choice to use the Semi-infinite model. However, PC CREAM does include the Semi-infinite model, which is applied to the first

gamma energy level considered i.e. 10 keV and thereafter uses the finite model. Thus the Semi-infinite approach in NAME III is tested here against output from PC CREAM for $^{55}$Fe which has very low energy photon emissions.

The conditions of the NAME III model run considered here are described below:

i) Source Term. A continuous release of 1.0 Bq $s^{-1}$ of $^{55}$Fe. Modelled using a release of 200000 particles over the entire 24 hour period (29/06/2006 00:00:00 to 30/06/2006 00:00:00). Source height = 10 m above ground level, with dimensions of dx, dy, dz = (0,0,0). Only the four photons deemed to contribute most to dose were considered.

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m. Wind direction = 270 degrees.

iii) Output. Adult effective cloud gamma dose rate is estimated (Sv $s^{-1}$). Dose rates averaged over a 24 hour period post release (at one hour intervals). Output is estimated for 6 receptor points over grid boxes of 1000 m x 1000 m x 500 m (x, y, z) using the Semi-infinite approach.

The full details of all the NAME III runs can be found in: Testing\Version5_2h\Run6.

Further investigation is required to ascertain why there exists a significant difference in dose rate between the two models despite all air concentrations being within a factor of 2.

**Air Conc (Bq m-3)**

| | PC CREAM | NAME III |
|---|---|---|
| Dist downwind (km) | | |
| 1 | 6.5E-06 | 3.8E-06 |
| 2 | 2.0E-06 | 1.5E-06 |
| 5 | 4.2E-07 | 4.6E-07 |

Note that the air concs above should be the same as those in Table 5, however the version used there was an earlier version of v5_2a of NAME III with fewer code changes in.

**Dose Rate (Sv s-1)**

| | PC CREAM | NAME III |
|---|---|---|
| Dist downwind (km) | | |
| 1 | 1.8E-24 (5.8E-17 Sv y-1) | 2.2E-25 |
| 2 | 5.7E-25 (1.8E-17 Sv y-1) | 8.5E-26 |
| 5 | 1.2E-25 (3.7E-18 Sv y-1) | 2.5E-26 |

**Comparison of NAME III runs for receptors at relatively large distances from the source**

Cloud gamma dose output from the two approaches (Lagrangian particle and Semi-infinite cloud approach) have been compared at relatively large distances from the source. At distances of order of 10's-100's km (and greater), the air concentration will typically be well mixed within the boundary layer, for any type of release within the boundary layer and any met condition. Thus, the Semi-infinite approach should compare well with the cloud gamma dose calculated using the Lagrangian particle approach at such distances (as long as the distances aren't so great that output derived via the Lagrangian particle approach is very noisy). Note that further investigation is required to identify the distances the Semi-infinite approach should be used (across the full range of atmospheric conditions e.g. in turbulent, unstable conditions I would expect the semi-infinite approach to be applicable at much shorter distances from the source than in stable conditions).

The conditions of the NAME III model run considered here are described below:

i) Source Term. An instantaneous release of 1.0E+10 Bq of $^{85}$Kr. Modelled using a release of 100000 particles. Source height = 0 m i.e. ground level, with dimensions (in m) of dx, dy, dz = (0.01, 0.01, 0).

ii) Met Conditions. Wind speed 5 m $s^{-1}$. Boundary layer depth = 800 m and heat flux = 0 W $m^{-2}$ i.e. representative of Pasquill Stability Category D. No precipitation. Surface roughness = 0.3 m. Wind direction = 270 degrees.

iii) Output. Adult effective cloud gamma dose is estimated (Sv). Dose rates averaged over a 6 hour period post release (at two minute intervals). Output is estimated for 241 x 51 receptor points. The Lagrangian particle approach estimates dose at 1 m agl. The Semi-infinite approach estimates dose over grid boxes of 1000 m x 1000 m x 100 m (x, y, z).

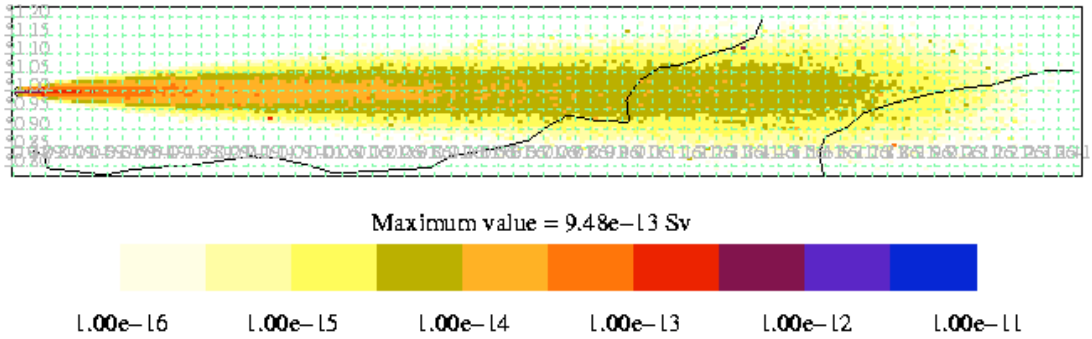


Figure 9. Adult effective cloud gamma dose (Sv), integrated over 6 hours, resulting from a 1.0E+10 Bq instantaneous release of $^{85}$Kr, using single site met data, for a release of 100000 particles at 1 m agl (using the Lagrangian particle approach).

Full details of the model run in Figure 9 can be found at: Testing\Noise\InstantRelRuns\Noise20.

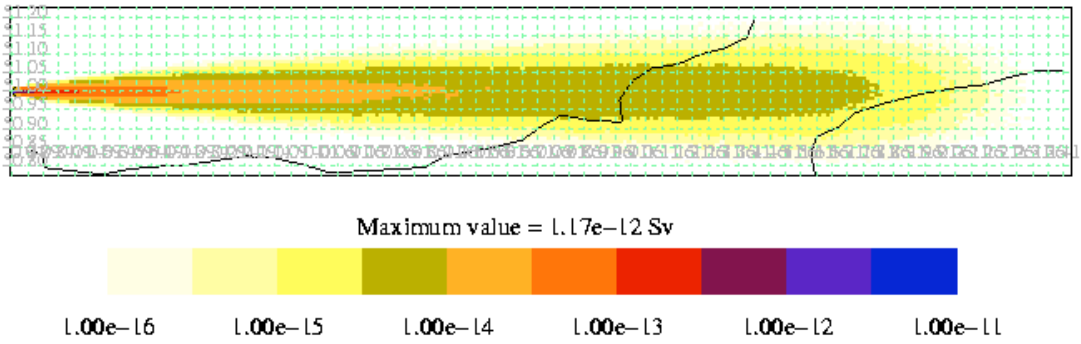


Figure 10. Adult effective cloud gamma dose (Sv), integrated over 6 hours, resulting from a 1.0E+10 Bq instantaneous release of $^{85}Kr$, using single site met data, for a release of 100000 particles on a 1 x 1 x 0.1 km grid (using the Semi-infinite approach).

Full details of the model run in Figure 10 can be found at: Testing\Version5_2h\Run7.

It is evident that Figures 9 and 10 are in very good agreement and therefore give confidence in the Semi-infinite approach implemented in NAME III. It is worth noting that the model run used to derive the output in Figure 9 took 16 hours to complete; in contrast the model run in Figure 10 took 6 minutes to complete. The output derived in Figure 10 is also less noisy than that in Figure 9.

### 2.8.6 Application of the Semi-infinite approach

To date NAME III includes the Lagrangian particle approach and the Semi-infinite cloud approach for calculating cloud gamma dose but there is no option to switch between the two approaches (see Section 2.8.7 for further details). Therefore I have outlined where I think the use of the Semi-infinite approach is most suited.

The Semi-infinite approach unlikely to be required for accidental releases or PRA assessments in the range of 10's of km's but for releases of 100's km it may be required. For continuous/routine release assessments the Semi-infinite approach is likely to always be required for collective dose calculations but unlikely to ever be required for critical group dose calculations. See Section 2.7.4 for further details.

For photons of less than 20 keV energy, a Semi-infinite cloud model will always be adequate.

### 2.8.7 Merging the Lagrangian particle approach and Semi-infinite cloud approach

To date NAME III includes the Lagrangian particle approach and the Semi-infinite cloud approach for calculating cloud gamma dose but there is no option to switch between the two approaches. At some point in the future it would be of use to consider merging the two approaches. CERC have attempted to merge finite and semi-infinite approaches in their model, ADMS and any related documentation should be reviewed if a merger of approaches were to be implemented in NAME III. Below I have outlined a number of issues which should be considered if HPA and/or the Met Office were to add the ability to switch between approaches in NAME III.

At relatively large distances downwind from the release it is likely that the plume will be uniformly mixed within the boundary layer and hence the semi-infinite approach could be applied (and as the particles released become widely spread the Semi-infinite approach should be applied). There are two issues to consider here. Firstly, determining one or more "triggers" which will initiate a timely change in approach. Secondly, ensuring that there is not a significant "step" in dose at the point where the approaches are switched.

We may wish to consider the distance between the nearest particle and the receptor point as a trigger, but this may be large as a result of a plume on the ground having particles spread far apart (in which case we would want to switch approaches) or could be large as a result of the plume being high in the boundary layer (i.e. as a result of a large release height or a large amount of buoyancy in the plume released), in which case there may be many particles in close proximity but they are all along way from the receptor (in which case we would not want to switch approaches).

A trigger may be defined by the distance between particles i.e. the distances between the particle nearest to the receptor and the particle nearest to the particle nearest to the receptor or perhaps the distances between the three particles nearest the receptor. However the structure of NAME III does not really lend itself to this approach as it handles one particle at a time (and does all the calculations and manipulations on this particle before moving onto the next, looping over all particles).

Perhaps triggers could be based on the positions on the particles from the previous timestep? Clearly this may be problematical if the timesteps are large or the particles are moving significantly over relatively small timesteps. Potentially the last distance moved by each particle and the change in distance moved by the particles over all the previous timesteps could be determined (Check?) or something to this end, which could then be used if the trigger was based on the positions of the particles from the previous timestep. If particle positions were used to trigger the switch between approaches this would require storing all particles positions, which, if there are a lot of particles, as you would expect there would be for a run calculating cloud gamma dose, could be computationally expensive. As I understand, NAME III already stores the particle position at each timestep and the old particle position at the previous timestep.

Perhaps the trigger to switch between approaches could be based on air concentration i.e. if the air concentration is uniform over x distance in the horizontal and vertical? The trigger would apply for sigma y and sigma z large, perhaps in accordance with boundary later depth. NAME III does output sigma z but it does not output sigma y and therefore an approach to determine if the concentration is uniform, most notably in the horizontal, would be required. Consideration of whether to switch approaches when the Lagrangian particle approach is no longer applicable or when the Semi-infinite cloud approach is applicable may also need to be considered. I think the latter is the better approach, based on the much shorter runtime when calculating cloud gamma dose via the Semi-infinite approach, however this may require further thought.

Note that at energies of a few tens of keV, photon attenuation is very large and a plume with a uniform concentration over a radius of a few tens of metres can be

considered Semi-infinite (as detailed in Jones, 1980, page 11). Therefore the attenuation coefficient or the energy of the photons should be accounted for when considering a trigger(s) for switching between approaches.

## 3. Puffs

Cloud gamma modelling utilising puffs has not been considered here, however this may be of use and worth considering for future work. Puffs may be particularly of use in the near range, where running with large numbers of particles can be very expensive and running with small numbers of particles can lead to output being noisy. A potential application is for accidental releases which necessitate that where runtime is short but without compromising on output detail and clarity?

Sources of information describing the puff approach in NAME can be found in: Proceedings of the 11th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes – A new puff modelling technique for short range dispersion applications, Thomson and Jones.

Any review of how puffs may be used with cloud gamma modelling should consider the approaches implemented in the HPA's Gaussian models: PC CREAM, ESCLOUD and PC COSYMA. Consideration of a RISO report (Thykier-Nielsen et al, 1995) to see how they handle puffs (and any other relevant reports) should also taken into account.

## 4. Summary (including future work & useful files)

A Lagrangian particle approach (as recommended by Raza and Avila, 2001) for estimating cloud gamma dose and a Semi-infinite approach (as detailed in Wellings and Mortimer, 2008) for estimating cloud gamma dose were implemented in NAME III.

### 4.1 Future work

Areas for consideration of future work in the field of cloud gamma modelling in NAME III include:

i) Cloud gamma dose summed over radionuclide. Currently output of cloud gamma dose is only a function of radionuclide.
ii) A method to enable the ability to merge the Lagrangian particle approach and Semi-infinite cloud approach for calculating cloud gamma dose in NAME III.
iii) Full review and in depth model comparison.
iv) How HPA wishes to include shielding in cloud gamma dose calculations. Currently no shielding is considered.
v) If and how HPA wishes to include child and infant cloud gamma dose calculations. Currently all doses calculated are applicable to adults only.
vi) HPA should consider if further approaches for calculating cloud gamma dose in NAME III are required.

vii) HPA and Met Office should consider if it would be of use to use puffs to estimate cloud gamma dose. Currently only the particle scheme is used to estimate cloud gamma dose.

### 4.2 Useful files and their respective filepaths

Detailed below are the filenames and paths of the relevant files for running NAME III to estimate cloud gamma dose.

All modifications to NAME III to incorporate the ability to perform cloud gamma modelling have been added to the version 5_2a in:
file:/net/home/h03/apdg/NameIII/NameIIIDevVersions/Version5_2a/Code_NameIII
This version of NAME III has been compiled and run using some of the model runs I have described previously in this document. The model output produced by the version of NAME III in 'apdg' and the development versions in my own space, for a handful of model runs, are in very good agreement.

A text file, 'Cloud_Gamma_Params.txt', detailing the cloud gamma parameters required in the Cloud Gamma Parameters block of a NAME III input file when estimating cloud gamma dose in a NAME III model run can be found in:
file:/net/home/h03/apdg/NameIII/NameIIIDevVersions/Version5_2a/Resources/Defns
Note that this has not yet been tested by HPA and therefore, until tested, all parameters used from this file should be used with caution.

An example NAME III input file, 'Example_Cloud_Gamma_Dose.txt', for estimating cloud gamma dose using NAME III can be found in:
file:/net/home/h03/apdg/NameIII/NameIIIDevVersions/Version5_2a/Runs

## 5. References

Chilton A B, C M Eisenhauer and G L Simmons (1980). Photon Point Source Buildup Factors for Air, Water, and Iron. Nucl. Sci Eng. 73, 97-107.

Faw RE, Shultis JK. Radiological assessment: sources and doses. La Grange Park, IL: American Nuclear Society; 1999.

Harima Y, Sakamoto Y, Tanaka S and Kawai M (1986). Validity of the Geometric Progression Gamma-Ray Buildup Factors. Nucl. Sci. Eng. 94, 24-35.

Hubbell J H (1982). Photon mass attenuation and energy-absorption coefficients from 1 keV to 20 MeV. Int J Appl Radiat Isot 33 1269-1290.

ICRP (1996). Conversion Coefficients for use in Radiological Protection against External Radiation. ICRP Publication 74. Ann. ICRP, Vol 26, No 3/4

Jaeger R G et al (eds). (1968) Engineering compendium on radiation shielding. Vol 1, Shielding fundamentals and methods. Springer-Verlag

Lamarsh J R (1983). Introduction to nuclear engineering. Boston, MA: Addison-Wesley.

Raza S and Avila R (2005). Calculation of immersion doses from external exposure to a plume of radioactive material. Health Physics Vol 89, No 3, 247-254.

Raza S and Avila R (2001). A 3D Lagrangian particle model for direct plume gamma dose rate calculations; JRP, 21 (2), 145-154.

Simmonds, J R, Lawson G and Mayall A (1995). Methodology for assessing the radiological consequences of routine releases of radionuclides to the environment. RP 72. EUR 15760 EN.

Thykier-Nielsen S, Deme S and Lang, E (1995). Calculation Method for Gamma Dose Rates From Gaussian Puffs. Riso-R-775(EN).

Yamaguchi, Y (1994). Age-dependent effective doses for external photons. Radiat. Prot. Dosim., 55 123-129.

Wellings J and Mortimer K (2008). Proposal for integration of cloud-gamma dose calculations into NAME III. RPD-EA-13-2008.

Zankl, M., Petoussi, N., Drexler, G. (nd[a]). Tomographic Anthropomorphic Models, Part III: Organ Doses to an Eight Week Old Baby and a Seven Year Old Child due to Parallel and Environmental Exposure Geometries, GSF-Bericht. GSF-Forschungszentrum fur Umwelt und Gesendheit, Neuherberg (in preparation), for age dependent organ gamma doses.