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Deutsches Forschungszentrum für Gesundheit und Umwelt

Environmental Modelling for RAdiation Safety II – Working group 9

Comparison between test field data and Gaussian plume model

Laura Urso

Helmholtz Zentrum München Institut für Strahlenschutz

AG Radioecological Modelling and Retrospective Dosimetry(REM)



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Simulation program for determination of population exposure to high doses after the explosion of an RDD device

1) Gaussian model with known metereological parameters

- 2) With at least 3 TLD measurements the free parameters can be inversely determined
- 3) Mathematical approach for inverse modelling: Levenberg-Marquardt Algorithm

Two calculated examples: A) Synthetic data produced with HOTSPOT 2.07

National project: Retrospective dosimetry for the population in emergency situations Contract No 3607S04560

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Equations from SSK report No. 37 pp. 29-30-31

Gaussian dispersion model

Dispersion coefficients a,b,c depend on stability class (from HOTSPOT guide 2.07)

Depletion factor (from HOTSPOT guide 2.07))

Wet deposition

Ground deposition

$$\chi(x, y, z; H) = \underbrace{\frac{1}{2\pi\sigma_y(x)\sigma_z(x)u(x)}}_{1} \underbrace{\exp^{-\frac{y^2}{2\sigma_y(x)^2}}}_{2} \underbrace{\left(e^{-\frac{(z-H)^2}{2\sigma_z(x)^2}} + e^{-\frac{(z+H)^2}{2\sigma_z(x)^2}}\right)}_{3}$$

$$\sigma_{y,z}(x) = \frac{ax}{(1+bx)^c}$$

$$DF(x) = \left[exp(\int_0^x \frac{1}{exp(-\frac{H^2}{2\sigma_z^2(x')}\sigma_z(x'))} dx'\right]^{-\frac{v_d}{u}\sqrt{\frac{2}{\pi}}}$$

$$W(x) = \frac{\Lambda}{\sqrt{2\pi}\sigma_y(x)u(x)} e^{-\frac{y^2}{2\sigma_y^2(x)}}$$

$$B_r(x,y) = Q_r(v_d \ DF(x) \ \chi(x,y,0) + W(x))e^{-\lambda_r t}$$

Dose conversion factors: submersion $g_{w,r}$, inhalation $g_{h,r}$, deposition $g_{b,r}$

submersion dose $H_{wr}(x, y, z) = Q_r \chi(x, y, z) g_{wr}$ inhalation dose $H_{hr}(x, y, 0) = Q_r \chi(x, y, z) g_{hr} 3.34 \cdot 10^{-4}$ deposition dose $H_{br}(x, y, 0) = Q_r(\chi(x, y, 0) v_d DF(x) + W(x)) b g_{br} K_{br}$ External dose $H_{tot}(x, y, z) = H_{wr}(x, y, z) + H_{br}(x, y, 0)$

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submersion $g_{w,r}$ (Gy s / Bq m³) TABLE A.3, deposition $g_{b,r}$ (Gy s / Bq m²) TABLE A.2



Source homogeneously distributed in the air

Source exponentially distributed in the soil with relaxation mass per unit area β

DRY = 0.1 g/cm^2 WET = 1 g/cm^2



MAIN PROGRAM SUBROUTINE FCN.f90 calculates objective function as log10(Dosedata) - log10(Dose) SUBROUTINE LMDIF from MINPACK runs optimisation SUBROUTINE COVAR calculates covariance matrix for error estimation cartesian axis: wind direction is x-axis **INPUT data** namelist:

```
&global_para rnuclide='Tc-99m' wind_ref=3.3d0 theta= 0.0d0
stability_class = 'A' H= 2.5d0 vd= 0.1d0 h_ref=2.0d0
dep_model="DRY"
I_rain = 0.0d0 eq_model='EXPONENTIALX' xdata0=1.0d0 Dt_plot=60.0d0
Qr = 5.8D8/
filename_read: x (km), y(km), Dose(Sv), Surface activity (kBq/m<sup>2</sup>), Dt(s)
```

```
Radionuclide implemented are: Cs-137, I-131, Xe-133, Te-132, Tc-99m
```

OUTPUT data

filename_save:

```
info 1 M 23 N 1 opt_value 436806916.322 NORM 0.216464 unbiased sigmaX 9533334.244
```

+ other output files to produce plots



CODE: LEVENBERG-MARQUARDT ALGORITHM in MINPACK

$F = log_{10}(Dosedata)-log_{10}(Dose)$

If x_{sol} is a solution of a non-linear least square problem then x solves:

and orthogonality condition is $F'(x_{sol})^T F(x_{sol}) = 0$ valid

$$\sum_{i=1}^{m} f_i(x) \nabla f_i(x) = 0$$

The algorithm looks for a correction p such that $F(x+p) \leq F(x)$ To find appropriate p, the algorithm solves the problem: $min\{ ||f=J \cdot p|| \leq D \cdot p|| \leq \Delta\}$ where D is diagonal scaling matrix and Δ is a step bound

LMDIF runs various convergency tests between approximation x and the solution x_{sol}

INFO 1: if the final norm of the residual has K significant decimal digits compared to initial one (the assumed tolerance 10^{-K} is set to square root of machine precision)

INFO 2: the larger components of $(D \cdot x)$ have K significant digits compared to initial ones

INFO 3: if both 1 and 2 are fulfilled

INFO 4: if the norm of the residuals is orthogonal to the Jacobian matrix. This should be examined further: could be F(x)=0, some local minimum and accuracy is not implicit



Test data from HOTSPOT







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Test data from HOTSPOT

- In principle with identical input values and initial guess, initial value for surface activity and dose should be the same as test data. BUT there is a difference of about 4-5% between the two



- HOTSPOT CODE and OP_LM_BfS almost identical: the only difference is integration for Depletion factor!

- In OPT_LM_BfS GAUSS integration is used to increase the number of steps during integration. HOSPOT uses trapezoidal rule but no possibility to check it

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Test data from HOTSPOT: result

info 1 M 23 N 1 opt_value 436806916.322 NORM 0.216464 unbiased sigmaX 20804118.71 (sigmaX divided by M-N) convergence achieved after 9 iterations





Test data from HOTSPOT: cloudshine and groundshine





Test data from HOTSPOT: results

During optimisation, the residuals decrease and mean value goes to zero (1.7 10⁻¹¹)

The norm of the residual decreases from 0.62 to 0.26

There is a clear trend in the residual plot - residual is not random!

Uncertainty on source term decreases with increasing the number of points

Small uncertainty in the result of the fit has to be expected as by fixing the meteorological data the 'shape' of the curve is fixed





TEST 2: 221 measurements of surface activity

&global_para rnuclide='Tc-99m' wind_ref=1.10d0 theta= 0.00d0 stability_class ='B' H= 5.0d0 vd= 0.01 h_ref=2.0d0 I_rain = 0.0d0 Dt=45.0d0 Qr = 9.10D4/

- large uncertainty on deposition velocity v_{d}
- Initial source term (measured) is 910 MBq
- Along x-direction, experimental profile of the plume is NOT an exponential
- --> slow wind and clear Gaussian profile suggest diffusive process also in X direction: possibility for users to choose!
- No source partitioning is included
- objective function which is minimised is log₁₀(Bdata+1) log₁₀(Br+1)



$$diffusivex(x) = e^{-(x-x_0)^2/(2\dot{o}_x^2)}$$

Fitted Gaussian profile $x_0=15$ m, $\sigma_x=5.13$



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info 1 M 221 N 1 opt_value 941237240.30 unbiased sigmaX 20418567.41

Result strongly depends on deposition velocity for $v_d = 0.8$ m/s result is not physical anymore ?



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Experimental data from Prouza et al. TEST 2





The norm of the residual decreases from 40 to 23

The residual clearly follows a trend and is not random but around zero

The standard deviation is very smallagain by fixing meteorological data the form of the curve underlying the fit is fixed!

