1.14 A NEW MODEL VALIDATION DATABASE FOR EVALUATING AERMOD, NRPB R91 AND ADMS USING KRYPTON-85 DATA FROM BNFL SELLAFIELD

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INTRODUCTION

The emission of krypton-85 (^{85}Kr) from nuclear fuel reprocessing operations provide a classical passive tracer for the study of atmospheric dispersion. This is because of the persistence of this radioisotope in the atmosphere, due to its long radioactive halflife and inert chemistry; and the low background levels that result due to the limited number of anthropogenic sources globally.

The BNFL Sellafield site in Cumbria (UK) is one of the most significant point sources of ^{85}Kr in the northern hemisphere, with ^{85}Kr being discharged from two stacks on the site, MAGNOX and THORP. Field experiments have been conducted since October 1996 using a cryogenic distillation technique (Janssens et al., 1986) to quantify the ground level concentration of ^{85}Kr. This paper reports on the construction of a model validation database to allow evaluation of regulatory atmospheric dispersion models using the measured ^{85}Kr concentrations as a tracer. The results of the database for local and regional scale dispersion are presented.

THE KRYPTON-85 DATABASE

The database is specifically tailored to provide data for modelling and statistically analysing air concentrations of ^{85}Kr and requires several underlying archives to perform this task. These underlying archives contain: meteorological data, emissions data, receptor locations and summary information from each monitoring period. To ensure that modelling assessments are only made using checked and validated data, the archives can not be modified using the database’s graphic user interface.

Meteorological archive

Hourly meteorological data, for the period 01-01-96 to 31-03-00, are contained in the meteorological archive. These data were obtained from temperature, wind speed and wind direction profiles that were measured on the 48 m high mast at the Sellafield meteorological station, adjacent to the site. Boundary layer parameters for running ADMS were determined from these data using flux-profile relationships as detailed in Hill et al. (2001). The Pasquill-Gifford stability class, required by the older generation NRPB R91 model (Clarke, 1979), was estimated from the Monin-Obukhov length using the relationship derived by Golder (1972) for a roughness length of 0.3 m. This roughness length is typical of agricultural areas and consistent with the roughness length used when modelling the atmospheric dispersion of material released from the Sellafield site. Meteorological data, formatted for AERMOD, were produced using the AERMET pre-processor.

Emissions archive

The emissions archive in the ^{85}Kr database contains the measurements from the THORP and MAGNOX stack monitors between August 1996 and May 2000. Data between August 1996 and August 1997 were entered into the database as daily averages, however hourly data were typically available from August 1997. The algorithms in the ^{85}Kr database are written such that hourly emission data is used when available.

Receptor archive
The receptor archive contains details of the geographical location of the monitoring sites, related to the locations of the THORP and MAGNOX stacks. The receptor location data that were used with the NRPB R91 dispersion model were in the form of distances and wind bearings between each stack and monitoring site. Whilst, data formatted for inclusion with the ADMS and AERMOD models were in the form of Cartesian co-ordinates.

Summary information
The field experiments to monitor ^{85}Kr air concentrations are detailed in the summary information archive. This archive includes the start and end times of the sampling runs, the name of the measurement site (corresponding to the location in the receptor archive), the measured air concentration of ^{85}Kr (in Bq m^{-3}) and a summary of the cryogenic distillation analysis. A summary of the monitoring data is shown in Table 1.

Table 1. Details of the field measurements of ^{85}Kr air concentrations used in the model validation study

Duration	**Number of measurements**	**Air concentration (Bq m^{-3})**		
		Maximum	**Minimum**	**Average**
2 hours	55	5510	3.2	513
15 - 48 hours	120	1543	1.2	136
164 – 168 hours	13	364	1.9	55
All	188	5510	1.2	240

INTEGRATION OF DISPERSION MODELS IN THE DATABASE
A Microsoft Excel database was developed to store the results of the ^{85}Kr field experiments and to allow the configuration and execution of regulatory atmospheric dispersion models. As the database is modular in construction it is possible to add additional models as they become available or sensitivity test multiple configurations of the same model. The three models that are currently interfaced with the database are AERMOD (versions 99351 and 02222) (see Cimorelli et al., 2002), ADMS (version 3.1) (CERC, 2001) and NRPB R91 (Clarke, 1979).

AERMOD Interface
An interface to the AERMOD model was created to automate the reformatting of emissions databases, running the model and importing the time-averaged air concentrations predicted for each monitoring period. Template AERMOD input (".inp") files were used to allow the evaluation of AERMOD configurations based on effective stack heights (determined from wind tunnel studies on the Sellafield site) and using the integrated buildings and terrain preprocessors (PRIME and BPIP).

The AERMET meteorological preprocessor was used to determine the boundary layer structure for input into AERMOD. AERMET input was supplied from ADMS formatted files using the ADMS to SAMSON converter integrated in the LAKES AERMET VIEW software and through a separate "site data" file containing the full timeseries of measured temperature and wind profiles from the Sellafield meteorological tower. AERMET surface and profile files were created for each year of data and stored external to the database.

ADMS Interface

The interface to the ADMS model used a similar method of modifying template files to that used for running AERMOD. ADMS met files were created for each of the field experiments. Model predictions of dispersion factors (DF, in s m^{-3}) for each stack were imported into the database. Average concentrations for each of the monitoring periods were calculated using equation (1), where n is the number of hours of monitoring data and Q is the emission rate in Bq s^{-1}.

$$\chi_{MODELLED} = \frac{\sum (Df_{THORP}\ Q_{THORP} + Df_{MAGNOX}\ Q_{MAGNOX})}{n} \qquad (1)$$

The use of template ADMS input files allowed the consideration of different model configurations. Three generic modelling scenarios were run:

- Effective stack heights (termed ESH).
- Coastal effects using effective stack heights (termed COAST).
- Building effects, with a main building defined for each stack in conjunction with a roughness length map for the site (termed BUILD).
- Terrain effects, through running the FLOWSTAR module (termed TERRAIN)

NRPB R91 Interface

An embedded Visual Basic version of the NRPB R91 model was included in the ^{85}Kr database. This embedded version of NRPB R91 was tailored to produce predictions of dispersion dispersion factors for use in equation (1). A modified version of the model was also tested. These modifications included the use of wind speeds at release height (rather than at 10 m) and the use of measured rather than calculated values of the standard deviation of the wind direction (σ_θ). Effective stack heights, specific to the NRPB R91 model, of 92.5 m and 80 m were used for THORP and MAGNOX stacks respectively.

STATISTICAL ANALYSIS OF MODEL PERFORMANCE

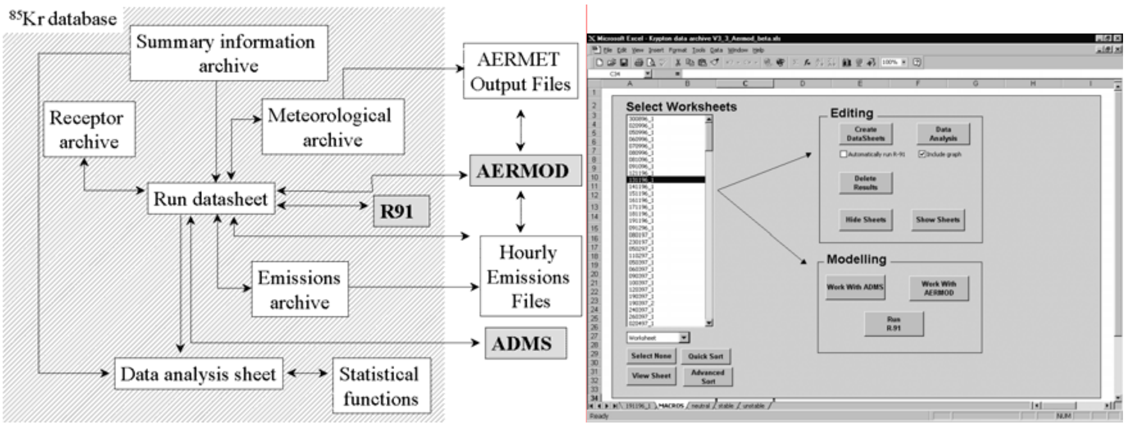
Statistical analyses could be applied to the entire dataset or to smaller subsets of data corresponding to specific conditions, including receptor locations and meteorological conditions. For example, later in this paper we compare the performance of the three atmospheric dispersion models for dispersion close to the site and for dispersion to receptors at distances of greater then 10 km from the site.

The following statistical functions are included in the database:

- Mean Bias (MB)
- Fraction of predictions within factors of 2, 5 and 10 (F2, F5, F10)
- Correlation statistic squared (R^2)
- Normalised mean squared error (NMSE)

DATABASE STRUCTURE

The structure of the database is shown in Figure 1 (a). This illustrates the transfer of data from the four data archives, leading to the creation of "Run datasheets" containing model input data and simulation results for each of the monitoring periods. The database was implemented using Visual Basic in Microsoft Excel, a screenshot from the "front end" of the database is shown in *Figure 1 (b).*



(a) *(b)*

Figure 1. (a) Structure of the krypton database (shown in light grey hatching) showing the four data archives, three dispersion models (in grey), the datasheets created for each run and the data analysis sheets. (b) screenshot of the model validation database

RESULTS

The atmospheric dispersion models were compared for two scenarios: local dispersion to receptors within 3 km of the site and dispersion on a regional scale to receptors greater than 10 km from the site. The sensitivity of the model predictions to the methods used to include the effects of the site buildings on dispersion was evaluated by running ADMS and AERMOD using Effective Stack Heights (ESH), the BUILD module of ADMS and the BPIP and PRIME modules of AERMOD. The 90 % confidence limits of each of the model evaluation statistics was determined using bootstrap resampling (with replacement) with 5000 realisations per statistical test. The results of the model evaluation are shown in Table 2.

DISCUSSION

The model evaluation results, presented in Table 2, demonstrate that for local dispersion all three models overpredict air concentrations when configured using Effective Stack Heights. A significant reduction in the bias of the AERMOD and ADMS models was achieved through the application of their integral buildings modules, with mean bias values not significantly different from unity. The remainder of the statistical tests showed a general trend of improvement in model performance when buildings and terrain modules were applied. For situations where effective stack heights were used, the modified configuration of the NRPB R91 was found to provide results that were comparable with the predictions of the second generation models.

The results of the evaluation of the models for regional scale dispersion are also shown in Table 2. Overall the NRPB R91 model performed well when compared with the regional dataset, though no statistically significant differences were found between the models. This may be partially due to the relatively small sample size considered in this analysis.

CONCLUSIONS

A model validation database has been developed containing data from dispersion model validation experiments conducted using the ^{85}Kr release from the BNFL Sellafield site as a tracer. This database has been used to provide a validation of the regulatory models: ADMS, AERMOD and NRPB R91. For dispersion within a few kilometres of the site configurations of ADMS and AERMOD using their buildings and terrain modules were found to outperform the effective stack height configurations.

When effective stack heights were used, the modified configuration of the NRPB R91 model was found to provide similar results to the AERMOD or ADMS models. For dispersion over longer distances no statistically significant differences were found between the model configurations. Further model validation experiments at a regional scale would be required to confirm this result.

Table 2. Results of the statistical analysis of model performance

Model	**Config.**	**MB**	**F2**	**F5**	**F10**	**R2**	**NMSE**
			LOCAL DISPERSION (N =188)				
NRPB R91	**Standard**	4.14*	0.20*	0.53*	0.67*	0.32	22.38*
	Modified	2.29*	0.35	0.58	0.76	0.36	9.03
ADMS 3.1	**BUILD**	1.63	0.36B	0.66B	0.77	0.47	6.74
	ESH	2.75*	0.32	0.59	0.77	0.52	17.11*
	COAST	2.68*	0.33	0.59	0.77	0.51	17.42*
AERMOD 99351	**BPIP**	1.33	0.31	0.6	0.74	0.4	3.94B
	ESH	2.71*	0.21*	0.48*	0.70	0.61	12.89
AERMOD 02222	**PRIME**	1.03B	0.32	0.65	0.78B	0.41	4.07
	ESH	2.49*	0.26	0.54*	0.75	0.61B	9.84
			REGIONAL DISPERSION (N=12)				
NRPB R91	**Standard**	0.60	0.27	0.64	0.82	0.17	2.64
	Modified	0.32	0.27	0.45	0.82	0.13	5.93
ADMS 3.1	**FLAT**	0.17	0.18	0.45	0.64	0.11	13.26
	TERRAIN	0.22	0.27	0.45	0.82	0.39	9.20
AERMOD 02222	**FLAT**	0.37	0.27	0.64	0.82	0.60	3.55
	PRIME	0.30	0.27	0.55	0.82	0.53	5.18

*Notes: B Highest performing model configuration, * model configuration found to be significantly different from the highest performing configuration at the 90 % confidence limit.*

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