VALIDATION OF THE EULERIAN POLLUTION TRANSPORT MODEL POLTRAN ON THE KINCAID DATA SET

Dimiter Atanassov
National Institute of Meteorology and Hydrology (NIMH),
66, Tsarigradsko chaussee, 1784 Sofia, BULGARIA

INTRODUCTION

PolTran is an Eulerian dispersion model combined with a numerical Atmospheric Boundary Layer (ABL) model (*Atanassov*, 2000). It has been first presented at the Fifth International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. The attention has been then focused on the model's general construction. After finding some encouraging results concerning the chosen approach, some improvements of the model have been made in order to prepare it for simulation of processes in the real nature (*Atanassov et al.*, 2000). The present study is the first validation of the model on a data set from the Model Validation Kit.

Two specific things of the study are worth mentioning. The model is designed to use the output products of a numerical weather centre, that reflects in the corresponding way on the construction of the meteorological pre-processor. Second, PolTran is a typical representative of Eulerian models that are supposed to be not good enough in local scale problems. The application of the model to the typical local Kincaid experiment is the real challenge here.

MODEL'S DESCRIPTION

Meteorological pre-processor

The meteorological pre-processor is described in (*Atanassov*, 2000) and no significant changes have been made in it later. For the present it is a non-stationary 1D numerical Atmospheric Boundary Layer (ABL) model. All the basic processes in the ABL (momentum, turbulence, heat, short and infrared radiation, humidity, soil heat transfer) are handled by the corresponding differential equations. The model is able to work using only the products of a numerical weather centre, mostly as upper boundary conditions and to simulate the energy balance at the soil-atmosphere interface, particularly in prognostic mode. It can optionally use surface measurement in a diagnostic mode.

Dispersion model

The pollutants' advection, assuming as a horizontal, is described by the numerical Eulerian scheme TRAP *(Syrakov,* 1996, 2000). The improvements after the version PolTran-1-2 have been made, mainly in the diffusion modelling (*Atanassov et al.,* 2000). The vertical transport is assumed to be caused only by the turbulent diffusion and is calculated according to the equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z} K_z(z,t) \frac{\partial C}{\partial z} \tag{1}$$

where t is time, z is the vertical coordinate, C is the pollutant's concentration in the air, $K_z(z,t)$ is the profile of the turbulent coefficient calculated by the ABL model. In addition to the horizontal advection, the horizontal turbulent diffusion is also taken into account. By analogy to the vertical one, it is calculated according to the equations:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} K_h(z,t) \frac{\partial C}{\partial x}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial y} K_h(z,t) \frac{\partial C}{\partial y} \qquad (2)$$

where x, y are the horizontal coordinates, $K_h(z,t)$ is the horizontal turbulent coefficient which for the present is calculated by

$$K_h(z,t) = d_1 + d_2\, K_z(z,t) \qquad (3)$$

where d_1, d_2 are coefficients varied in the present simulations. Equations (1,2) are solved numerically. The top of the domain is assumed to be impervious for the pollutants, but a thick enough upper layer is acting as a reservoir, absorbing the pollutants when their concentration below is bigger, and releasing them when their concentration below is smaller. The deposition velocity concept

$$V_d C = K_z \frac{\partial C}{\partial z} \qquad (4)$$

is used to set the lower boundary condition for the equation (1), where the deposition velocity V_d is varied in the following model tests. The pollutants are assumed to pass free through the horizontal bounds of the domain, due to both advection and diffusion.

The present model version is announced as PolTran-1-2.5. The “1” stands for the 1 dimensional meteorological pre-processor. As the pollutant’s movement is considered 2 dimensional concerning the advection and 3 dimensional concerning the diffusion, the second index referred to dispersion is “2.5”.

KINCAID SIMULATIONS

Model configuration

For simulation of the Kincaid field measurements, the space structure of the PolTran model is specified in the following way. Despite the ABL model is designed to work using input data only at the top of the boundary layer, the wind and the temperature measurements at 10m, 50m and 100m are used in the present simulations. In this way, the model validation is focussed on the turbulence and dispersion modelling. The ABL model has 28 vertical grid layers. The grid is established in such way, that some of its levels exactly coincide with the mentioned above measurement heights. The differential equations for wind and temperature (see *Atanassov*, 2000) are solved numerically in layers between the measurements heights, and the measurements themselves are used as boundary conditions. The radiosonde data at 850hPa from the file RAWIN.DAT, interpolated in time, are used as upper boundary conditions for the layer above 100m. The dispersion calculations are performed in 10 vertical layers. The Kincaid source is in the 6th layer. Depending on the buoyancy effect, calculated by a modified Briggs formula, the emission penetrates sometimes in the 7th layer. The upper reservoir layer is between 1000 and 3000m. The data from RAWIN.DAT at 700hPa are used for calculation of the pollutants’ movement in the reservoir layer. The wind and turbulence profiles calculated by the ABL model are rearranged (averaged) in a corresponding way for the 10 layers of the dispersion model, and used as inputs for the dispersion calculations.

The runs are performed in 200x200 horizontal grid with grid step of 500x500m., covering an area of 100x100km. The source is in the central 100x100 grid cell.

The time step of the ABL model is 60s and the time step in dispersion calculation is 30s. The ABL calculations start before the tracer release always at 00 o'clock local time. The dispersion calculations are carried out for the hours given in the file SF6_KIN.DAT of the Model Validation Kit. The release hours in the file SF6_ALL.DAT that are not included in SF6_KIN.DAT, are not considered.

MODEL VALIDATION RESULTS

At the present study, the validation of the PolTran model is made in terms of arcwise maximum concentrations (*Olesen*, 1995). First, the position of the arcwise maximum established in the Model Validation Kit for the concrete hour and arc is located with respect to the numerical grid of the model. Then, the value of the arcwise maximum is juxtaposed to the concentration value predicted by the model in the corresponding grid cell.

All the 1284 arc-hours collected during the Kincaid campaign are included in the model validation. For the hours when some meteorological data are missing, several ways to avoid the problem have been tried. The results discussed hereafter are obtained by interpolation of the missing data in time and when necessary in space.

Hana's BOOT package (*Hanna et al.*, 1991) is used for statistical assessments. The results for the datasets with quality indicator Q3 and those for Q23 are presented in Table 1 and Table 2 correspondingly. Some trial changes in the turbulence sub-model have been made and different model runs have been performed with them. The matter of the trials will not be discussed here. Nevertheless, the statistical assessments corresponding to them are presented in the first 4 rows of the two tables (marked with extension t1, t2, t3 and t4) in order to demonstrate the sensitivity of the statistical assessments to the turbulence simulations. For these cases: d_1=1.0, d_2=1.5, V_d= 0.1; in the 5th row are presented the results for d_2=2.5. In the last rows of the tables, below the bolt line, the results of the models validated at the Mol workshop (*Olesen*, 1995) are presented for comparison with the present PolTran validation.

Table 1. Validation of the model PolTran-1-2.5 on the Kincaid dataset, subset Q3 (338 observations): statistics for maximum arcwise concentration.

Model	Mean	Sigma	Bias	NMSE	COR	FA2	FB	FS
C_OBS	54.34	40.25	0.0	0.0	1.0	1.0	0.0	0.0
PolTran_t1	86.55	90.10	-32.21	2.08	.134	.393	-.457	-.765
PolTran_t2	62.16	62.84	-7.82	1.38	.192	.524	-.134	-.438
PolTran_t3	68.58	79.18	-14.24	1.82	.203	.476	-.232	-.652
PolTran_t4	67.01	78.38	-12.68	1.84	.195	.476	-.209	-.643
PolTran_t4*	56.69	55.76	-2.35	1.29	.170	.521	-.042	-.323
HPDM	44.84	38.55	9.50	.75	.441	.565	.192	.043
IFDM	29.42	26.03	24.92	2.00	-.132	.423	.595	.429
INPUFF	34.61	26.76	19.72	1.29	.140	.497	.443	.403
OML	47.45	45.48	6.89	1.24	.146	.547	.135	-.122
ADMS	86.32	103.78	-31.99	2.45	.228	.518	-0455	-.882

Table 2. Validation of the model PolTran-1-2.5 on the Kincaid dataset, subset Q23 (586 observations): statistics for maximum arcwise concentration.

Model	Mean	Sigma	Bias	NMSE	COR	FA2	FB	FS
C_OBS	40.96	39.27	0.0	0.0	1.0	1.0	0.0	0.0
PolTran_t1	81.32	88.63	-40.36	3.04	.128	.361	-.660	-.772
PolTran_t2	53.75	58.05	-12.79	1.80	.242	.473	-.270	-.386
PolTran_t3	57.62	70.12	-16.66	2.29	.241	.437	-.338	-.564
PolTran_t4	56.14	69.16	-15.18	2.29	.239	.439	-.313	-.551
PolTran_t4*	49.10	51.80	-8.14	1.66	.233	.468	-.181	-.275
HPDM	42.37	38.61	-1.40	1.16	.337	.514	-.034	.017
IFDM	29.79	28.81	11.17	2.06	-.007	.395	.316	.307
INPUFF	30.41	26.82	10.55	1.49	.244	.437	.296	.377
OML	38.42	43.84	2.54	1.63	.264	.437	.064	-.110
ADMS	89.59	121.28	-48.63	4.73	.131	.435	-.745	-1.022

CONCLUSION

The performance of the PolTran-1-2.5 model is comparable to the performance of the other models that have been validated to the Kincaid experiment of the Model Validation Kit. This could be considered as a success of Eulerian model in local scale applications. The model possesses the advantages of Eulerian models and enables many opportunities for further improvements that will be subject of some next studies.

REFERENCES

Atanassov, D., 2000: Local Scale PC-oriented Eulerian Pollutant Transport Model PolTran-1-2, *Int. J. Environment and Pollution*, vol.14, Nos. 1-6, pp.217-224.

Atanassov, D, D. Ivanova, D. Terziyski, 2000: Eulerian Air Pollution Transport Model PolTran-1-2.5 and some trial runs for the region of Sofia, *Journal of Environmental Protection and Ecology,* special issue, pp.48-55.

Hanna, S, D. Strimaitis, J. Chang, 1991: Hazard response modeling uncertainty (A quantitative method), Volume 1: User's guide for software for evaluating hazardous gas dispersion models, Sigma Research Corporation, 234 Littleton Road, Suite 2E, Westford, MA, 01886.

Olesen, H., 1995: The model validation exercise at Mol: overview of results, *Int. J. Environment and Pollution*, vol.5, Nos. 4-6, pp.761-784.

Syrakov, D., 1996: On the TRAP advection scheme-Description, tests and application, *Proc. of the first REMAPE Workshop "Regional Modelling of Air Pollution in Europe*", Copenhagen, Denmark, September 1996,

Syrakov D., 2000: On the use of a flux-type advection scheme on non-homogeneous grid, *Proceedings of the EUROTRAC-2 Symposium 2000, 27-31 May, 2000, Garmish-*Partenkirhen, Germany, Springer-Verlag, Berlin, Heidelberg 2001, p. 255.