

**18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy**

**VALIDATION OF THE LAGRANGIAN PARTICLE MODEL LAPMOD AGAINST THE FULL
SET OF SHORT TERM AND LONG TERM KINCAID TRACER RELEASES**

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Abstract: LAPMOD is a tridimensional non-stationary Lagrangian particle model that can be used to simulate the atmospheric dispersion over complex terrain of gases and aerosols, inert or radioactive. Also, it can simulate the dispersion of odors.

LAPMOD is fully coupled with the meteorological diagnostic model CALMET (Scire et al., 1999a), part of the US-EPA recommended CALPUFF modeling system (Scire et al., 1999b), and it can also use the meteorological input files of the preferred US-EPA model AERMOD (US-EPA, 2004).

LAPMOD is capable of simulating emissions with high time resolution and incorporates numerical schemes to treat plume rise and algorithms for estimating peak concentrations that may be also useful for odor studies and accidental releases. Concentrations can be calculated with different kernel methods, independently of any grid mesh. Use of such kernels greatly reduces the computational times, since very few particles are required to reconstruct the concentration field. This allows to apply the model also on typical regulatory scenarios where the annual average of concentration is often a required parameter to be evaluated.

LAPMOD can compute dry and wet deposition and can describe sources of various shape (buoyant and non-buoyant point, line, rectangle, box, sphere, irregular polygon).

LAPMOD has been applied to simulate the full set of quality 3 Kincaid tracer releases of SF₆ (short term) and SO₂ (long term). The capability of LAPMOD in simulating such datasets has been successfully assessed using the Model Validation Kit (Olesen, 2005) and compared with that of other widely known air quality models.

This poster provides an overview of the LAPMOD modeling system and it shows in detail the results of the validation.

LAPMOD is distributed free of charge in open-source format (<https://www.enviroware.com/lapmod/>).

Key words: *Lagrangian particle model, kernel smoother, model evaluation, Kincaid*

INTRODUCTION

Lagrangian particle dispersion models (LPDMs) simulate pollutant releases by following a number of independent computational particles – each one representing a fraction of the released mass - in a sequence of finite time intervals. The motion of each particle is driven by a time-varying velocity field, which can be divided into an average component, the average wind, plus a fluctuation velocity describing the effects of atmospheric turbulence and those wind variations not included in the mean component. The fluctuation velocity can be described by a non linear form of the Langevin stochastic differential equation.

The development of the Lagrangian particle model LAPMOD started many years ago; its formulation and main features have been recently described in Bellasio et al. (2017). LAPMOD is fully coupled to the diagnostic meteorological model CALMET (Scire et al., 1999a), preprocessor of the dispersion model CALPUFF (Scire et al., 1999b). LAPMOD, through its preprocessor LAPMET, can also use the meteorological input files of the US-EPA preferred dispersion model AERMOD (US-EPA, 2004). LAPMOD describes several types of sources: point, linear, volume, and area, that can arbitrarily vary with time. Point sources may also be buoyant, and the stack-tip downwash and partial plume penetration effects are included. LAPMOD adopts a kernel smoother for the calculation of the concentration field. The model and its pre- and post-processors are available at <https://www.enviroware.com/lapmod>.

STRUCTURE OF THE LAPMOD MODELING SYSTEM

The LAPMOD modeling system structure is schematically represented in Figure 1. The meteorological input of LAPMOD consists of three dimensional fields of wind and temperature, and two dimensional fields of atmospheric turbulence parameters. All these input variables are read directly from the CALMET output file. The geophysical variables needed from LAPMOD (e.g., the roughness length) are also read from the CALMET output file.

The LAPMOD meteorological input file can also be prepared with the LAPMET processor which reads the surface and profile meteorological files of AERMOD, and creates an output file formatted as the CALMET output file. The wind and temperature fields prepared by LAPMET are horizontally homogeneous but vary along the vertical direction. The use of the LAPMET processor is useful for simple applications, when the meteorological fields and stations needed by CALMET are not available, and for validation purposes since the meteorological input files of AERMOD are often provided.

The LAPEMI processor produces the LAPMOD emission file with 1 hour time resolution starting from the annual average emission of each single source and using three temporal modulation profiles: annual, weekly and daily. LAPEMI is useful for processing emissions for permit applications; however, LAPMOD is capable of managing the emission variations up to the time resolution of 1 second. Time resolutions of minutes or less are typical in accidental releases and in odor modeling.

When simulating odor emissions LAPMOD can calculate the 1-hour average concentrations and then estimate the averages over shorter time periods (e.g. 1 or 5 min) by applying a peak to mean ratio (PMR). The PMR for calculating peak odor concentrations from the 1-hour averages is often a constant determined with the Smith (1973) relation (e.g., a value of 2.3). The adoption of this constant is a simplification because the peak concentration varies with atmospheric stability and is not always proportional to the 1-hour average concentration with the same constant factor. LAPMOD contains a routine for calculating peak concentrations as described by Mylne (1992).

LAPOST is the post processor which reads the LAPMOD binary output file, containing for example the hourly concentration results for one year, and calculates the statistics required by the user (e.g., annual average, 1-hour maximum, percentile, etc.).

EVALUATION AGAINST THE SF6 AND SO2 KINCAID FIELD DATA

LAPMOD (version 2017-05-04) has been evaluated using the results of the Kincaid field experiments (e.g. Olesen, 2005), both considering the short-term releases of SF6 and the long-term releases of SO2. For both the experiments, the CALMET like meteorological input files have been built with the LAPMET preprocessor starting from the AERMOD meteorological input files distributed by the US-EPA in the model evaluation databases. Meteorology is therefore horizontally homogeneous, but varies along the vertical direction. The Kincaid power plant is situated in Illinois, USA in an almost flat area with a roughness length of approximately 0.1 m. The power plant has a 187 m stack with an exit diameter of 9 m. The plume rise has been simulated with the algorithm of Webster and Thomson (2002) with $\alpha_1=0.110$, $\alpha_2=0.500$, $\alpha_3=0.655$ and $c_D=0.210$. For all the evaluations, discrete receptors have been placed at the points where the ambient monitoring stations were located. The concentration has been calculated with the Uliasz parabolic kernel.

It is important to observe that the AERMOD plots and statistics reported in the following sections have been obtained with the predictions distributed with the model evaluation databases, which refer to a previous version of the model. The performance of the latest AERMOD version may be different.

Kincaid SF6

The SF6 monitors were placed at ground level at distances ranging from 500 m to 50 km. A quality indicator with values from 0 (worst quality) to 3 (best quality) has been assigned to the observations of Kincaid SF6. Only observations of quality 3 have been used for comparison with the model predictions.

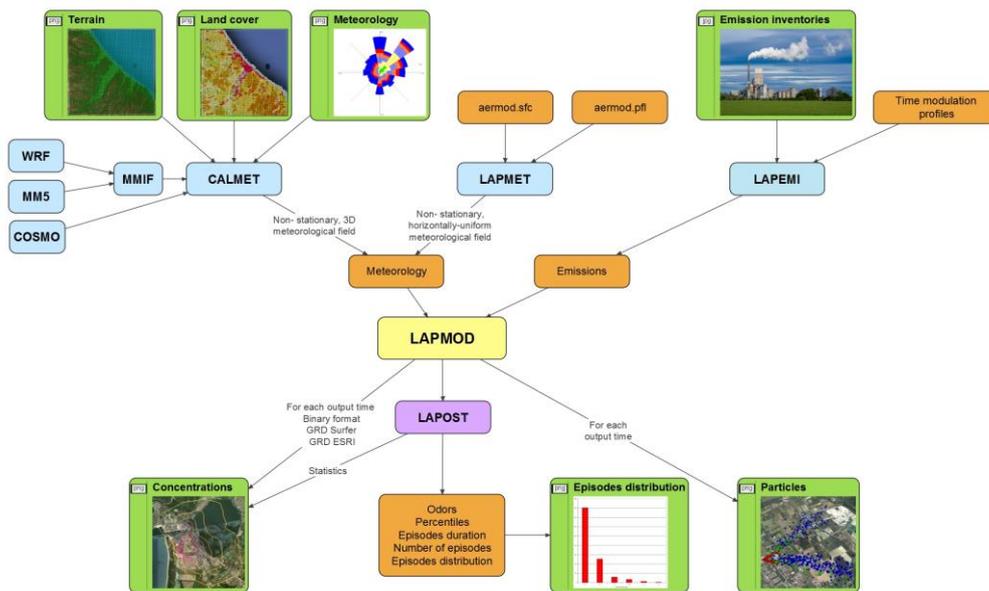


Figure 1. Structure of the LAPMOD model system.

The scatter plot of predictions against observations (Bellasio et al., 2017) shows that the FA2 is 59.5%, while the FA5 is 85.5%. $FA\alpha$ indicates the percent of data which satisfies $1/\alpha \leq C_p/C_o \leq \alpha$, where C_p is the prediction and C_o the observation. The residual box plots for Kincaid quality 3 data are reported in Figure 2. The residuals are shown as a function of the mixing height (Z_i) and of the friction velocity (U^*). Other residuals are shown in Bellasio et al. (2017). The lower and upper whiskers represent the 5th and the 95th percentiles respectively, the lower and the upper part of the gray boxes represent the 25th and the 75th percentile respectively, and the thick black horizontal segment represent the median of the distribution. The horizontal lines represent the FA2 area. The ratio between predictions and observations for a perfect model should always be 1. The LAPMOD results show that the medians of the ratios are almost always close to 1, and a significant proportion of the residuals falls between a factor of 2.

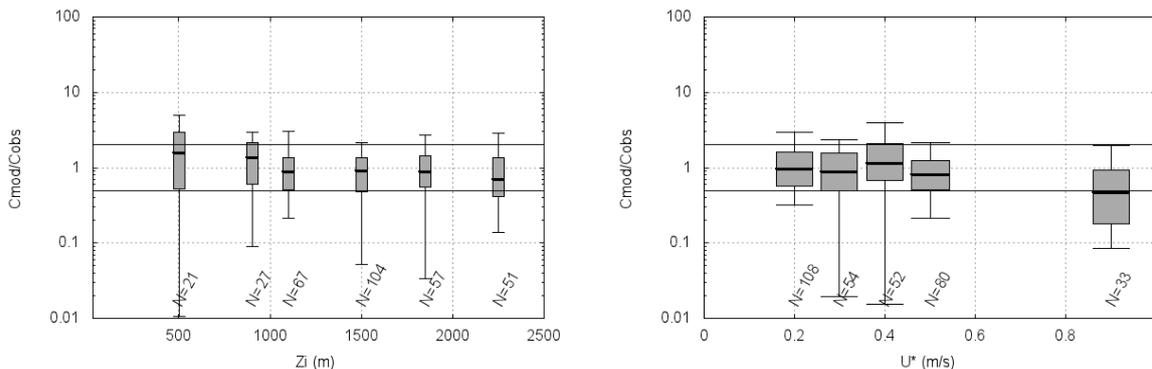


Figure 2. Residual box plot for Kincaid quality 3 data.

The LAPMOD results have been compared against those of other dispersion models using the Model Validation Kit (Olesen, 2005). Table 1 shows the performances of LAPMOD and those of other dispersion models against the SF6 measurements carried out at Kincaid. The other models considered are HPDM (Earth Tech, USA), OML (NERI, Denmark), ADMS 3 (CERC, UK), AERMOD (EPA, USA), ISCST3 (EPA, USA) and NAME (Met Office, UK). Excluding LAPMOD, the data in Table 1 have been obtained from Webster and Thomson (2002). Only the Kincaid observations characterized by a quality indicator equal to 3 have been considered, for a total of 338 data. Both observations and model predictions have been normalized by dividing the concentrations for the emission rate and multiplying by

one thousand. The FS parameter is calculated as $FS = 2 * (\sigma_{Obs} - \sigma_{Mod}) / (\sigma_{Obs} + \sigma_{Mod})$. LAPMOD satisfies the three rules proposed by Chang and Hanna (2004) to evaluate the performance of a model: 1) the fraction of predictions within a factor of two of observations is about 50% or greater (i.e., $FA2 > 50\%$); 2) the mean bias is within $\pm 30\%$ of the mean (i.e., roughly $|FB| < 0.3$ or $0.7 < MG < 1.3$); 3) the random scatter is about a factor of two to three of the mean (i.e., roughly $NMSE < 1.5$ or $VG < 4$).

Table 1. Performance statistics of some dispersion models for the Kincaid observations of quality 3.

Model	Mean	σ	Bias	NMSE	r	FB	FS	FA2
Observations	54.34	40.25	0.00	0.00	1.000	0.000	0.000	1.000
LAPMOD	53.11	48.02	1.23	0.76	0.448	0.023	-0.176	0.595
HPDM	44.84	38.55	9.50	0.75	0.441	0.192	0.043	0.565
OML	47.45	45.48	6.89	1.24	0.146	0.135	-0.122	0.547
ADMS 3	51.7	34.7	2.7	0.6	0.45	0.05	0.15	0.67
AERMOD	21.8	21.8	32.6	2.1	0.40	0.86	0.59	0.29
ISCST3	30.0	60.0	24.3	2.8	0.26	0.58	-0.39	0.28
NAME	40.6	40.4	13.8	1.15	0.279	0.290	-0.005	0.615

In order to evaluate the ability of LAPMOD to represent the extreme concentration values, the robust higher concentration, RHC_R (Cox and Tikvart, 1990), has been calculated. The value of RHC_{11} calculated for the observations is $3.606 \mu\text{g m}^{-3}$, while the one calculated for LAPMOD is $3.707 \mu\text{g m}^{-3}$ and, for comparison, the value calculated by Webster and Thomson (2002) for the NAME model is $4.328 \mu\text{g m}^{-3}$.

Kincaid SO₂

The Kincaid SO₂ study was conducted at the same location as the Kincaid SF₆ study; it involved a buoyant, continuous release of SO₂. The study included about six months of data between April 1980 and June 1981. There were 30 SO₂ monitoring stations providing 1-hour averaged samples from about 2 km to 20 km downwind of the stack. For this long term experiment the comparison has been performed for concentrations paired in time, therefore it is more demanding than the previous comparison for SF₆, that was based on the maximum concentrations observed or predicted over an arc.

The QQ plots for the 1-hour average SO₂ concentration (Bellasio et al., 2017) show that both models underestimate; the LAPMOD concentration distribution is close to the observations up to about $400 \mu\text{g m}^{-3}$, while the underestimation is more pronounced for higher values. On the contrary, for higher concentrations the AERMOD predictions are closer to the observations. The FA2 and FA5 values of both models are lower than those predicted for the SF₆ release because, as anticipated, the SO₂ release predictions and observations at each receptor have been paired in time. The values of these two statistics are similar for the two models (FA2 about 5% and FA5 about 11%). The QQ plots obtained for the 24-hour average SO₂ concentration (Bellasio et al., 2017) show that AERMOD still underestimates the observations, while LAPMOD shows a distribution in good agreement with the measurements.

The period-averaged concentrations at each receptor are shown in **Figure 3**. The LAPMOD average concentrations are in good agreement with the observations, with a FA2 values of 64.3% and 10.7% for LAPMOD and AERMOD, respectively. The RHC_{26} values at each receptor have also been calculated. These values show that, when considering the single receptors instead of the whole 1-hour concentration distribution independently from the position, the ability of LAPMOD to reproduce the peak concentrations improves. Considering the ratio between predicted and observed RHC_{26} , the receptors with such a ratio within the interval [0.85, 1.15] are 28.6% and 39.3% for AERMOD and LAPMOD, respectively.

CONCLUSIONS

This paper describes the LAPMOD modeling system and the evaluation of the atmospheric dispersion model against the SF₆ and SO₂ Kincaid field experiments. LAPMOD is fully linked to the CALMET

diagnostic meteorological model and, through its preprocessor LAPMET, to the meteorological files created by AERMET for AERMOD. The LAPMOD execution times are comparable to those of CALPUFF, therefore LAPMOD is a cost-effective choice for air quality studies. Moreover, the structure of Lagrangian particle models is such that they can highly benefit from parallelization, for example distributing the particles' movements to different processors. LAPMOD is capable of simulating emissions with high time resolution and incorporates numerical schemes to treat plume rise and algorithms for estimating peak concentrations that may be also useful for odor studies and accidental releases. Concentrations can be calculated with different kernel methods independently of any grid mesh. Particle files extracted with the LAPOST processor can be imported in Google Earth and in many GIS systems; it is then possible to track the particles emitted by a specific source and its relative impact.

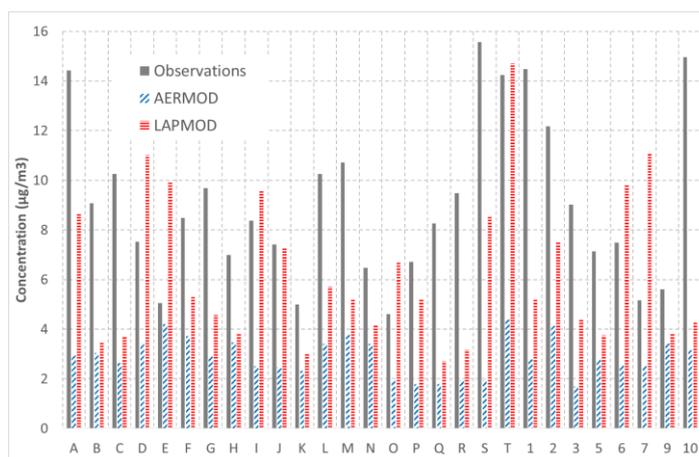


Figure 3. Period averaged concentrations for observations, AERMOD, and LAPMOD predictions.

The validation of LAPMOD against the Kincaid data for short term (SF6) and long term (SO2) averages has given good results, also when compared with the performances of other well known models widely used for regulatory studies. The LAPMOD system is still under development and testing. The Fortran source code of the LAPMOD system is distributed through the Enviroware's web site (<https://www.enviroware.com/lapmod>).

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