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Regulatory Air Pollution Modelling in Poland: Is It Time for an Update?

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Abstract

Over the last two decades, significant changes have taken place in the Polish atmospheric air-quality protection system. With Poland's accession to the European Union, air quality management was introduced, with the aim of improving air quality in areas where limits were exceeded into compliance with the established norms. This management system was based on two components: a system of periodic assessments, which resulted in the classification of administrative zones based on air quality status, and air quality improvement plans, which were developed for zones where limits had been exceeded. Within this system, modern models of pollutant dispersion and transformation in the atmosphere were applied to serve as a complementary tool for assessment of the present state, and as a basic tool for program development. Despite these changes, emission permitting procedures still rely on a methodology developed more than half a century ago, when there were radical differences in the state of air pollution; emission sources; standards; knowledge; data availability; and computational resources. This resulted in substantial discrepancies between the methods used to improve air quality and the tools employed in administrative procedures regarding emissions from sources requiring permits.

This article aims to highlight the possibility of a radical modernization of the procedures used in permitting processes that would align them with contemporary requirements. Here, we focus our attention on stochastic Lagrangian particle dispersion models, which are considered the most accurate and precise in describing the phenomena of pollutant movement in the atmosphere.

1. INTRODUCTION

The establishment of the air quality management system in Poland during the first decade of the current century brought into practice mathematical air quality models that were more suitable for this purpose than the Gaussian plume model that had previously been used in the emission permitting system [Regulation... 2010]. In the Ministry of Environment guidelines issued in 2003 [Łobocki 2003], basic types of mathematical models were discussed, indicating the possibility of using ready-made computer programs developed abroad. Twenty years later, air quality improvement plans developed in recent years (e.g., by Holnicki et al. [2022]) have employed the CALPUFF model [Scire et al. 2000], which represents a significant technological leap compared to the method still used in the permitting procedure. For air quality assessments, such as those of the Chief Inspectorate of Environment Protection (GIOS) [2023, 2024]), and for national-scale air quality prediction, the Eulerian GEM-AQ model [Kaminski et al. 2008] has been utilized. This model integrates the multi-scale GEM meteorological model [Cote et al. 1998]

with its online-coupled air quality modules, which cover transport, chemical and photochemical transformations; secondary pollutant formation (particularly ozone), and aerosol processes. At present, this model is also used as part of the predictive ensemble of the pan-European Copernicus Atmospheric Monitoring Service¹ (CAMS). As a result, both at the national and regional levels, models reflecting the contemporary state of knowledge and technical information capabilities, appropriate for these scales, have been implemented.

Unfortunately, the computational methods used for regulatory purposes (issuing permits for atmospheric emissions) according to the Environment Protection Act [Environment... 2001, Regulation... 2010] have not undergone similar improvements. In the following sections, we will review both the advantages and shortcomings that lead to applicability limitations which should be, though not always are, observed.

¹ <https://atmosphere.copernicus.eu/>

2. THE CHANGING OBJECTIVES

In Poland, the introduction of the Gaussian plume model methodology into the practice of emission permitting took place during the final period of rapid industrialization, which had brought with it a drastic deterioration in air quality. The causes of this decline were primarily attributed to the industrial and energy sectors, although the municipal sector also played a significant role; in urban areas, the growing road-transport sector contributed as well.

The economic problems of the last two decades of the 20th century led to a significant reduction in heavy industry, along with a general decrease in coal consumption, accompanied by shifts in the proportions of various air pollution sources.² The following decades saw stricter air quality standards and the implementation of mechanisms to enforce compliance, which, combined with the economic transformation processes, resulted in a noticeable improvement in air quality. To some extent, air quality has also been affected by climate change; the decrease in the frequency of frosty days has been associated with episodes of high pollutant concentrations due to increased emissions from household heating systems and stagnation tendencies in the atmosphere, while the increase in the occurrence of hot days is often linked to elevated ozone concentrations. Comparing the current situation to that of half a century ago, there is a noticeable relative increase in the contribution of the municipal-residential sector to air pollution, in relation to the energy and industrial sectors, as well as a shift in air-quality standard violations from annual average values to the frequency of exceeding threshold values.

In addition to the aforementioned changes, new issues are emerging that have not yet received adequate attention. These include odour nuisances caused by improperly managed landfills and large livestock farms, as well as the impacts of road transport, population exposure linked to landfill and warehouse fires; transboundary impacts of large facilities (e.g., the Turów dispute); and the development of emergency-response procedures for safeguarding the operation of nuclear power plants. One may also note that the marginal cost of the ongoing air-quality improvement programs will grow in time, as the most cost-effective measures are usually taken first, leaving more expensive or technically-challenging solutions for later stages of implementation. This means that achieving further improvements will require increasingly significant investments and resources.

In view of the evolving air protection challenges, it is essential to update the computational tools supporting

administrative bodies. As noted earlier, the systems used for air quality assessment, zone classification, and the development of corrective programs largely meet contemporary requirements and will primarily require either incremental improvements or the expansion of functionality by introducing new elements. Modernising the third element of the discussed triad — the mathematical model used in permitting procedures — requires greater attention. We will now proceed to discuss this model, highlighting its most significant limitations with regard to the objectives outlined in the current section.

3. THE POLISH REGULATORY MODEL: GAUSSIAN PLUME

Gaussian plume models represent the oldest and simplest group of regulatory air pollution models.

It is assumed that pollutants emitted from a point source located on flat, horizontal, and homogeneous terrain are carried horizontally by the wind and gradually mix with the surrounding air, forming a steady-state pattern of a plume in the shape of a flattened cone. The formula describing the spatial distribution of the passive gaseous pollutant concentration is

$$S(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z u} e^{\frac{-y^2}{2\sigma_y^2}} \left[e^{\frac{-(z-h)^2}{2\sigma_z^2}} + e^{\frac{-(z+h)^2}{2\sigma_z^2}} \right] \quad (1)$$

and can be derived from the averaged mass-conservation equation, assuming that the meteorological conditions appearing in the equation — wind speed and the turbulent mass-exchange coefficient — remain constant along the entire plume. In this formula, Q represents the emission rate of the point source (stack), h is its height above ground level (usually given as an effective height, calculated by considering both the actual height and the thermal and dynamic plume rise), u is the wind speed at height h , y is the distance of the receptor point where the concentration is being calculated, from the plume's centre line, z is the height of this point above the ground, and σ_y and σ_z are the so-called the dispersion coefficients, calculated as a function of the source-receptor distance along the plume's centre line, x [Ministry of Environment 2010]:

$$\sigma_y = Ax^a, \sigma_z = Bx^b \quad (2)$$

Where A , B , a , and b represent constants whose values are determined based on the ratio of the effective height of the emission source to the aerodynamic roughness parameter of the terrain, as well as a parameter m , which is supposed to describe the atmospheric equilibrium state. The above equations constitute the core of the algorithm, which is mandatorily used in Poland for issuing emission permits and also specified in law as the reference methodology.

² For example, according to statistical data, between 1980 and 2010, SO₂ emissions decreased more than fourfold, while emissions from non-industrial sources (the municipal-residential sector, transportation, and communication) increased [Degórska 2016]. The daily, weekly, and annual variability of pollutant concentrations in urban areas clearly indicates the dominant role of these sectors.

As the above model is presumed to describe steady-state conditions (note the absence of time in the above equations), and the wind speed does not appear in the definitions of the coefficients σ_y and σ_z , it is evident that equation (1) will predict infinitely large concentration values when the wind speed approaches zero. This obvious deficiency is circumvented by a recommendation that “if the wind speed is lower than 0.5 m/s, the value of 0.5 m/s should be applied,” which lacks any scientific support.

Considering (i) the need to focus attention on cases of air quality standard violations, which most often occur under calm conditions with low wind speeds, and (ii) the fact that calm conditions occur with a frequency exceeding 20% over large areas of southern Poland [Lorenc 2005], one may raise doubts about the fitness of the discussed model for present-day challenges. At least, investigation of air pollution episodes taking place in low-wind conditions (the majority of wintertime PM exceedances) falls beyond the capabilities of this national reference model.

Unfortunately, this is not the only deficiency of the Gaussian plume models. In general, they should not be used:

- when there is spatial or temporal variability in meteorological conditions within the calculation area;
- in complex topographical or climatic conditions (e.g., mountain valleys, mine dumps and landfills, open pit mines, road tunnels, city centres, sea shores affected by sea breeze), due to their homogeneity and flat-terrain assumptions (unless equipped with special corrections suited to specific terrain conditions);
- computation at distances larger than 10-20 kilometres, depending on spatial variability of meteorological and terrain conditions; or
- in cases of time-varying emissions (at least when the temporal variability of emissions is faster than the plume's passage through the modelling area)

Further, these models:

- do not fully describe the photochemical, chemical, and physical transformations occurring in the atmosphere involving gaseous and particulate pollutants; and
- ignore the complexity of real atmospheric conditions, such as the turning of wind with height due to baroclinicity; or the interplay of Coriolis and drag forces, inertial oscillations; or the multilayer structure of the nocturnal atmospheric boundary layer.

One commonly-mentioned advantage is the model's low demand for computational resources and the simplicity of its structure, which allows for a complete and detailed description of the method in a document of only a few pages — especially for the simplest variants of the model, such as the regulatory model used in Poland. The downside of this simplicity — combined with a well-developed user interface in commercial software — is that it enables analyses to be performed by individuals lacking basic meteorological knowledge who are unable to assess the applicability of the model in specific cases or critically evaluate the results.

4. INPUT DATA

4.1. Meteorological conditions

Essentially, we have three options when selecting meteorological data necessary for modelling pollutant dispersion on a local scale:

a) Using long-term records of measurements and observations taken at surface meteorological stations, schematically classified into a set of scenarios (“meteorological situations”) with their corresponding frequencies of occurrence. This option reduces the computational cost by an order or two orders of magnitude compared to the direct use of hourly data.

b) Direct use of meteorological observations. Here, we deal with two datasets: hourly measurements and observations from surface synoptic stations (“SYNOP” messages) and upper-air data from aerological observatories (“TEMP”) — typically twice per day. The public datasets available from the Polish weather service include SYNOP data from roughly 60 stations and TEMP data from four observatories. Although radar measurements of wind speed are currently available, these data — to the best knowledge of the authors have not yet been used for computing pollutant dispersion in Poland.

The direct use of meteorological observations entered regulatory air pollution modelling at the turn of the 20th and 21st centuries, still in the context of “updated” Gaussian plume models (e.g. Weil and Brower [1984]), significantly improving the quality of the results. However, most of the limitations discussed in the previous section remain in effect. Moreover, the representativeness of data from distant stations is questionable, especially in the case of atmospheric soundings.

c) Using data from meteorological models. Here, climatological reanalysis products, which span extended time periods, play the most crucial role. By utilising historical data, they provide a continuous picture of the variability of meteorological conditions over time and space — unlike the point measurements discussed previously. However, the resolution of computational grids used in reanalyses is still insufficient in spatially diverse areas, such as mountains, coastlines, and cities. For this reason, nested high-resolution models are additionally employed in air quality studies, focusing on much smaller areas. This approach, however, requires significant computational resources and a high level of expertise. In Poland, it has been used in the development of air protection programs. Ideally, these calculations should also include data assimilation of surface observations to reduce divergences between the model-based climatology and the observational data. Unfortunately, in many studies conducted so far in the country, this step has been neglected, leading in many cases to substantial discrepancies.

The most accurate results should be obtained by choosing the last option. However, due to high computational and labour costs, and the vast volume of intermediate results generated, it is reasonable to limit high-resolution

calculations to areas and periods where air quality standard exceedances have been recorded by monitoring stations. One may also note that with the progress of climate change, the consultation of long-term historical climatology becomes more and more questionable.

4.2. Emission data

Emission data are often considered the primary source of uncertainty in air pollution modelling. In fact, most of this information is based on estimates rather than measurements, and different estimation methods lead to considerable discrepancies in the results. Moreover, these data are not available in real-time, and therefore calculations for current periods rely on data from previous years. In regulatory applications, declared values are used. The lack of sufficiently accurate emission data is often cited as a justification for using oversimplified models or methods. On the other hand, using a reliable model can provide feedback to emission estimation when the model results are compared to measurements.

4.3 Terrain data

Terrain features play important role in the transport, dispersion and deposition of air pollutants. Topography modifies air flow, and contributes to the occurrence of spatially varying thermal stratifications in the boundary layer due to non-homogeneous exposure of air to solar radiation. The type of land cover determines its roughness, which directly affects the vertical wind profile, as well as the efficiency of turbulent mixing processes in the lowest layer of the atmosphere. Thus, the efficiency of removing air pollutants by dry subsidence depends, among other things, on the land-use type. The extent and the way in which the above-mentioned processes are taken into account in air pollution modelling depends on the class of the model.

The Polish regulatory model — i.e., the Gaussian plume model — makes simplifying assumptions (flat, homogeneous terrain, steady-state conditions), and so information about the terrain type is taken into account only during the calculation of wind profile and atmospheric diffusion (dispersion) coefficients σ_y and σ_z . The constants A and B appearing in (2) are calculated from the following formulas, developed by Nowicki [1976]:

$$A = 0,088 * \left(6 * m^{-0,3} + 1 - \ln \frac{H}{z_0} \right) \quad (3)$$

$$B = 0,38 * m^{1,3} * \left(8,7 - \ln \frac{H}{z_0} \right) \quad (4)$$

where m is a parameter describing the atmospheric equilibrium state, H is the effective height of the emitter, and z_0 is the aerodynamic surface roughness length.

In advanced air quality models, meteorological and terrain data are entered into specialized modules known as preprocessors, whose function is to prepare in an appropriate format the full input information needed for the air quality model. For example, in the AERMOD system [Cimorelli et al. 2005], a separate terrain preprocessor (AERMAP) provides a physical relationship between terrain features and the behaviour of pollutant plumes. It generates location and height data for each receptor location while providing information that allows the dispersion model to account for the effects of stability-dependent flow patterns around or over hills.

In order to take into account the influence of surface conditions on boundary layer parameter estimates, the surface characteristics (surface albedo, Bowen ratio and effective surface roughness length) are entered into the meteorological pre-processor (AERMET). This calculates the atmospheric parameters needed by the dispersion model, such as atmospheric turbulence characteristics, mixing height, friction velocity, Monin-Obukov length, and surface heat flux.

Another example is the GRAL [Oettl 2015b], a Lagrangian particle dispersion model that is discussed later in this article. This model can be coupled with GRAMM [Oettl 2015a], an Eulerian prognostic non-hydrostatic mesoscale wind field model. It features a terrain-following grid, allowing the effects of terrain on dispersion (e.g., cold-air drainage flows) to be taken into account at all scales. GRAMM solves the conservation equations for mass, enthalpy, momentum, and humidity. A radiation model to take long- and short-wave radiation into account also exists. The surface-energy balance is calculated in a surface module, where several different land-use categories are used to define surface roughness; albedo; emissivity; soil moisture content; specific heat capacity of the soil; and the heat transfer coefficient.

5. LAGRANGIAN PUFF MODELS

This is a newer group of models in which the process of pollutant dispersion is modeled as the movement of certain air volumes containing pollutants — “puffs” — along trajectories determined by wind direction, or through a separate flow model. Examples of this group include RIMPUFF [Thyker-Nielsen et al. 1999], SCIPUFF [Sykes et al. 1998], and CALPUFF [Scire et al. 2000]. Typically, the concentration of pollutants within the clouds is described using Gaussian distribution, whose parameters are usually determined by empirical formulas. However, in the case of the SCIPUFF model, relationships derived from a statistical turbulence model with second-order closure are used, allowing for greater accuracy.

Among this group, the CALPUFF model has gained the most popularity in Poland and is recommended in the Polish guidelines for the modeling of pollutant dispersion in air quality management systems [Łobocki 2003]. It was developed to simulate the transport, dispersion, chemical transformation, and deposition

of air pollutants over various spatial and temporal scales. It consists of three main components: CALMET meteorological module, CALPUFF dispersion module and CALPOST post-processing utilities. The dispersion module incorporates physical processes such as wet and dry deposition, plume rise, and chemical transformations of pollutants, including secondary particulate matter and ozone formation.

In Poland, CALPUFF has been used for research purposes [Holnicki, Kałuszek 2014; Holnicki et al. 2015], developing air protection programs (e.g., Trapp et al. [2007]), regional air quality assessment systems [Fijolek et al. 2003; Fijolek, Trapp 2003], and assessment of large emitters influence on air quality [Szczygłowski, Mazur 2005; Mazur, Michałowski 2001].

While CALPUFF represents a more advanced technology and has fewer limitations than the Gaussian plume models, it also has some notorious weaknesses, such as poor performance under low wind speed conditions, where it tends to overestimate pollutant concentrations due to an artificial stagnation of puffs in a limited area, as shown in Holmes and Morawska [2006], Abdul-Wahab et al. [2011], and Brode [2012]. This deficiency is particularly relevant for the southern regions of Poland, where stable atmospheric conditions and low wind speeds frequently occur, potentially leading to inaccuracies in modelled pollutant dispersion patterns.

6. LAGRANGIAN PARTICLE DISPERSION MODELS

Lagrangian Particle Dispersion (LPD) models simulate the dispersion of pollutants as the movement of a large number (on the order of 10^5) of material points (also known as pseudoparticles), each carrying a certain mass of the substances they transport. The movement of the pseudoparticles is a combination of average flow (wind) and turbulent motions, described as a random field. After calculating the trajectories of individual pseudoparticles, the spatial distribution of pollutant concentrations can be determined, similarly to a plume model. The use of specially-selected kernel functions in the integral operator that converts the set of particle positions into concentrations allows for a reduction in the number of pseudoparticles and the associated computational costs, while still maintaining the required accuracy.

The distinction between Lagrangian particle models and plume models is somewhat blurred, as there are models that allow for both random components in plume motion and concentration distributions within moving particles [De Haan, Rotach 1998]. When computational parameters are properly chosen and meteorological conditions are accurately represented, LPD models yield more accurate results than Gaussian Plume Models (GPMs), although this comes at the cost of higher computational demands.

Models of this class offer several advantages, including:

- the ability to solve inverse problems, i.e., determining emission rates of individual sources based on known concentration fields and meteorological conditions
- demonstrated effectiveness in modelling the dispersion of odorous pollutants
- validation and wide application in modelling the dispersion of traffic-related pollutants
- extensive use, along with plume models, in the meteorological protection of nuclear power plants
- applicability to any source geometry (point, line, area, volume), with any number of sources and any temporal characteristics
- proven effectiveness under low wind speeds and calm conditions
- the ability to simulate dispersion across a wide range of spatial scales, from micro-scale problems (e.g., street canyons) to transcontinental scales, within the limits set by available computational power
- suitability for application in complex terrain, urban areas, and other challenging environments when coupled with an appropriate flow model (meteorological or hydrodynamic)

6.1 Structure

As previously mentioned, in Lagrangian Particle Dispersion (LPD) models, the movement of pseudoparticles is a combination of average flow (wind) and turbulent motions, i.e.,

$$\frac{d\vec{r}}{dt} = \vec{v}(\vec{r}, \vec{v}) + \vec{v}'(\vec{r}, \vec{v}) = \vec{v}(\vec{r}, \vec{v}) \quad (5)$$

where the first term on the right-hand side represents the velocity of the mean flow, and the second term represents the turbulent fluctuation, i.e., the random deviation from the mean value. Integrating this equation allows for the determination of a pseudoparticle's trajectory. The term describing fluctuations is typically modelled as a random process through a stochastic differential equation of the form:

$$d\vec{v} = \vec{a}(\vec{r}, \vec{v})dt + \vec{b}(\vec{r}, \vec{v})dW \quad (6)$$

where the second term on the right-hand side describes random changes in velocity through the increments of the Wiener process dW , with a mean value of zero and variance dt . In homogeneous turbulence, this is the Langevin equation with

$$\vec{a} = -\vec{v}/\tau \quad \text{and} \quad \vec{b} = \sqrt{2\vec{v}^2/\tau} \quad (7)$$

where τ is the Lagrangian timescale of turbulence. With the random component set to zero, the first of the described equations describes the changes in the position of plume centres in the models discussed earlier.

The most important differences in the construction of various models of this class concern the method of modelling fluctuations (see, e.g., Oettl et al. [2001]), and the form of the kernel of the integral operator used to determine concentrations.

6.2. Example Models

Among LPD models, some have been applied for regulatory purposes, and we will focus on those here. The strongest legal backing for this model is found in Germany, where a model of this class (AUSTAL2000) has served as the reference model designated for permitting processes and environmental impact assessments since 2002.³ Procedures related to air protection are described in the TA Luft technical instructions published by the Ministry of the Environment, while the algorithm implemented in the model is detailed in the VDI 3945 standard [VDI Guideline... 2000]. The latest version of the model (AUSTAL v.3, the successor to the program AUSTAL2000) refers to the Annex 2 and 7 of the new version of TA Luft, which entered into force in December 2021 [TA Luft 2021].

Both the source code and executables for Windows and Linux are made available free of charge by the German Federal Environment Agency (Umweltbundesamt).⁴ According to the documentation [Janicke 2024], the program supports both calculations using measurement series and the classification of meteorological situations. It allows for calculations under time-varying emission conditions, in complex terrain (through the use of the kinematic wind field model TALDIA), and around buildings; it also can assess exposure to odorous substances. In the latest version, the modelling of the wet deposition of pollutants is also available.

Unfortunately, the scientific documentation for the model is rather limited, and aside from the aforementioned VDI standard, it is difficult to find scientific publications on the model's structure and its validation. Furthermore, the latter has faced sharp criticism [Schenk 2020]. Additionally, as noted by Langner and Klemm [2011], a comparison of modelling results with measurement data shows significantly better performance for the updated Gaussian model AERMOD than for AUSTAL2000. They found that AERMOD was more efficient for modelling pollutant dispersion in complex terrain, likely due to its enhanced algorithms for handling topographic influences on pollutant flow. On the other hand, AUSTAL2000 was particularly effective when comprehensive meteorological

input data were unavailable, thanks to its capability to simulate dispersion under various data-limited conditions. The study highlighted the fact that AERMOD was significantly faster in terms of computation time, making it more suitable for applications requiring quick assessments. It is also worth noting that the adopted flow model (TALDIA), based on the variational method of minimising deviations at measurement points, produces results that are highly dependent on the initial approximation. It should, therefore, be used more as an assimilation method in combination with a mesoscale meteorological model or hydrodynamic model, rather than as a standalone module. A particularly interesting example is the Austrian GRAL/GRAMM system, developed by the Graz University of Technology (Technische Universität Graz). The work on this system, motivated by the need to create modelling methods suitable for use under low wind conditions or in complex terrain, began in 1999. In 2006, a collaboration was established between Technische Universität Graz and the authorities of the state of Styria,⁵ resulting in a system composed of two models: the mesoscale prognostic model, GRAMM (Graz Mesoscale Model [Oettl 2015a]) and the Lagrangian particle dispersion model, GRAL (Graz Lagrangian Model [Oettl 2015b]).

The GRAMM model is a non-hydrostatic mesoscale prognostic model based on averaged conservation equations of mass, momentum, and energy in the anelastic or Boussinesq approximation formulated in a Cartesian coordinate system. It features alternative parameterisations for turbulent transport: (i) a simple Pandolfo parameterisation based on deformation velocity, Richardson number, and mixing length; (ii) a turbulent kinetic energy (TKE) budget-based closure; and (iii) the standard k- ϵ model, which includes equations for the balance of turbulent kinetic energy and dissipation rate. Surface exchange processes are described using the Monin-Obukhov similarity theory and a parameterised surface heat balance. The current version of the model (23.11) does not include condensation, radiation, or atmospheric chemistry modules. The model's validation covers 22 test scenarios described in the German standard VDI 3783-9 [VDI Guideline... 2017], which involve comparisons with wind tunnel experiment results. Although GRAMM appears fairly basic when compared to other modern mesoscale models, it provides automated integration with the GRAL model, allowing it to be used by properly-trained individuals who are not necessarily specialists in numerical atmospheric dynamics modelling.

The Lagrangian particle dispersion model GRAL possesses all the advantages of the AUSTAL2000 model and is scientifically supported by numerous publications, such as those demonstrating its effective application in complex urban environments and high-resolution simulations [Berchet et al. 2017; Petrov et al. 2024; Patiño et al. 2024]. It

³ Notably, in countries neighbouring Germany, such as Austria and Switzerland, AUSTAL2000 is also used when addressing issues of transboundary pollution transport.

⁴ <https://www.umweltbundesamt.de/en/topics/air/air-quality-control-in-europe/download>

⁵ GRAL is also recommended by the National Health and Medical Research Council of Australia as a regulatory model for calculating the impact of atmospheric emissions from road tunnels.

also features comprehensive and detailed documentation covering both the physical principles and their validation (Oettl 2024).

Validation of this model included four experiments as required by the Austrian guideline RVS 04.02.12, which establishes quality criteria for dispersion models, requiring a Normalized Mean Square Error (NMSE) of 3.0 or less and a Fraction Bias (FB) of 0.3 or less. The GRAL model was evaluated on these four datasets to assess its performance and compliance with these criteria. The first dataset, CALTRANS99, focused on the dispersion of a tracer gas (SF₆) along Highway 99 in California, which is characterized by open terrain and low wind speeds. Emissions were monitored from vehicles travelling in a loop along the highway. GRAL produced an NMSE of 0.5 and an FB of 0.0, meeting the guideline criteria. Although it overestimated peak concentrations, it performed comparably to other models such as ADMS-ROADS and AERMOD.

The second dataset, A2 Biedermannsdorf, monitored NO_x concentrations near the A2 highway in Austria, taking into account high traffic volumes and background concentrations. This site included obstacles, such as a six-meter noise barrier wall. GRAL showed good agreement at most observation points, though slight underestimation was noted 400 metres east of the highway. NMSE values ranged between 0.0 and 0.2, while mean deviations ranged from -0.2 to 0.2, demonstrating compliance with the guideline.

The third dataset, Ehrentalerberg Tunnel, focused on SF₆ dispersion from a tunnel portal under low wind speed conditions. It simulated complex jet stream behaviour caused by meandering wind patterns. GRAL achieved an NMSE of 0.9 and a FB of 0.1 when using the observed turbulence data, which met the guideline criteria. A second simulation using stability classes produced a higher NMSE of 2.2, but remained compliant. GRAL effectively modelled mean concentrations and concentration statistics.

The fourth dataset, Kaisermuehlen Tunnel, examined NO_x dispersion from a 2,150-m tunnel in Vienna that was characterized by complex topography and traffic patterns. The evaluation covered two distinct wind direction scenarios over a 10-month period. GRAL demonstrated variable performance across sites, with NMSE values ranging from 0.4 to 2.4 and FB values between -0.3 and 0.3. While average concentrations were captured well, peak values were sometimes underestimated. Results complied with guidelines, although higher uncertainty was observed due to rough emission estimates.

Overall, GRAL satisfied the Austrian quality criteria across all datasets, confirming its suitability for pollutant dispersion modelling in Austria. Although localized deviations and uncertainties were noted, especially in complex terrain, the model demonstrated reliable performance under varied conditions.

Validation of the GRAL model also includes 15 test cases, according to the German VDI 3783-9, and 26 diffusion experiments. This latter set encompasses all experiments included in the Model Validation Kit (MVK) package

[Olesen 1995]; diffusion experiments under low wind conditions with low emission sources (such as the Idaho and Raaba experiments, where GRAL performed well, while AUSTAL2000 and ADMS completely failed); the Gratkorn experiment, in a mountain valley; the Idaho Falls experiment with a linear emission source; concentration measurements around highways (Elimäki); in a street canyon (Göttinger Strasse, Hanover; Frankfurter Allee, Berlin; Hornsgatan, Stockholm); in a parking lot (Vienna); near a pig farm (Uttenweiler, Germany; Roager, Denmark); near an experimental reactor (EOCR, Idaho); around gas compressors (Texas, Kansas); and at the exits of road tunnels (Ninomiya, Hitachi, Enrei, Japan). In all but one case, the GRAL model provided the best results among the compared models, or results that were very close to the best. Additionally, the model was tested for odour nuisance forecasting around in four experiments in livestock farms, and yielded positive results.

As an example of GRAL's applications, it is worth mentioning the recent study by Petrov et al. [2024], who conducted high-resolution (2-m and 30-m) sensitivity analysis of modelled NO_x emission distribution in Sofia under various meteorological conditions, represented by predefined wind and atmospheric stability. This research highlighted GRAL's ability to account for wind flow dynamics and produce spatially-detailed pollutant concentration maps. Although challenges were encountered in replicating dispersion effects in complex environments, the study underscored GRAL's computational efficiency for long-term simulations and its suitability for analysing emission scenarios to improve air quality or assess population exposure.

Similarly, Berchet et al. [2017] evaluated high-resolution (10 m) GRAL simulations of NO_x concentrations over Zürich, Switzerland. Their study demonstrated the compliance of GRAL's overall performance with the objective criteria of the European Commission expert panel FAIRMODE (Forum for Air-quality Modelling in Europe) [Thunis et al. 2012, Pernigotti et al. 2013]. Despite a persistent tendency to overestimate concentrations, the model was able to successfully capture averaged spatial distributions in different temporal scales, with an emphasis on representing properly diurnal cycles.

Another example is provided by Patiño et al. [2024], who examined the suitability of dispersion models with different levels of complexity for use in urban planning. They found that GRAL/GRAMM, along with a more advanced large eddy simulation (LES) model, PALM, could effectively reflect wind-flow patterns and concentration distributions. Despite limitations related to emission representation and sensitivity to meteorological inaccuracies (present in both simulations), GRAL/GRAMM was recognized as a valuable component of the urban air quality assessment framework. Although it has a simplified structure compared to the LES model PALM, it demonstrated satisfactory performance while requiring much fewer computational resources.

Still another important comparison is presented by Oettl et al. [2001], who evaluate the performance of a Gaussian

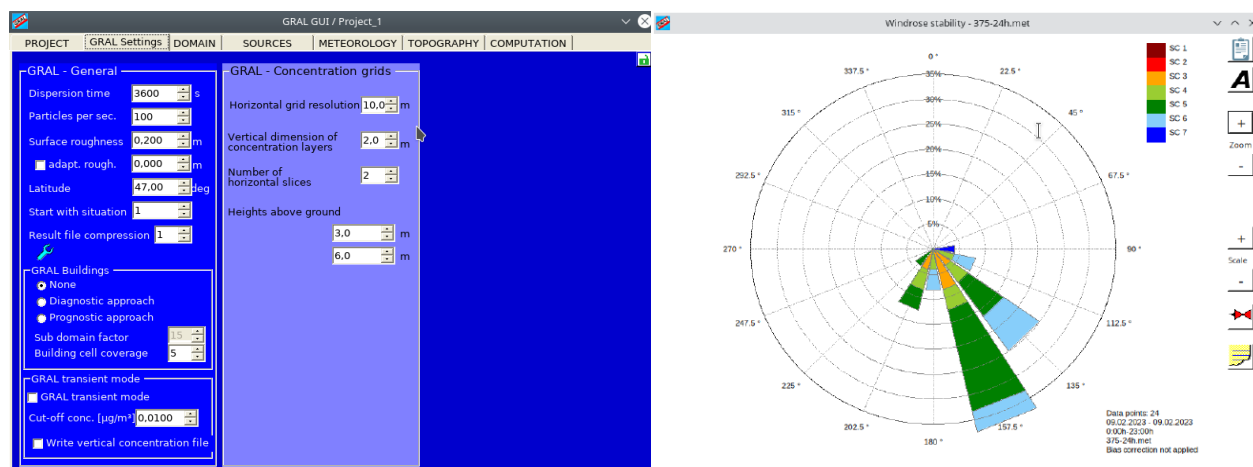


Figure 1. (a) The graphical interface of the GRAL model. (b) A wind rose automatically generated in the GRAL model interface window

plume model, CAR-FMI, and GRAL in predicting NO_x concentrations under low wind speed conditions. Model results were compared with the field measurements from a major road in Elimäki, Finland. The performance of the CAR-FMI model declined when the wind direction became nearly parallel to the road, as well as under the lowest wind speed conditions. In contrast, the GRAL model exhibited greater stability across different wind speeds and directions, providing more accurate results.

GRAL/GRAMM was also compared to CALPUFF in a complex urban environment [Ward, Rollings 2021; Rollings 2022] and showed superior results due to its ability to account for terrain obstacles such as trees, buildings and fences. On the other hand, modeling the impact of microscale terrain features poses problems, primarily with flow modeling. The practical application of full hydrodynamic models at this scale is limited by the immense computational power required.

From the perspective of using the model as a regulatory or reference tool, the terms of its availability under the GNU Public License ver. 3 are of fundamental importance. This also applies to its graphical interface, which, in the case of other models, is most often developed and provided as closed binary code for a fee by third-party companies. The graphical interface, as seen in Fig. 1(a), enables for convenient entry and modification of parameters related to the model settings, such as resolution; number and placement of modelling levels; emission source characteristics; meteorological data; and topography. Within the meteorological data section, users can produce diagnostic graphics, such as wind roses and wind speed histograms, as seen in Fig. 1(b). The results of pollution dispersion simulations can be displayed as concentration isolines superimposed on a topographic map or satellite image. Contaminant concentration maps can also be represented at different predefined heights [Fig. 2].

Another model worth noting is LAPMOD [Bellasio et al. 2017; Bellasio et al. 2018], developed by the Italian

company Environware.⁶ LAPMOD is a complete modelling system, since it is fully coupled with the diagnostic meteorological model CALMET; it works in conjunction with the LAPEMI emission modelling subsystem and the LAPOST result processing and analysis subsystem. It also has another meteorological preprocessor, LAPMET, that can use US-EPA AERMOD meteorological input files (surface and profile). The model has been validated using the standard data set included in the MVK package. The company provides the source code and documentation for these programs free of charge; however, the licence terms restrict their redistribution.

The model offers several alternative parameterizations for buoyancy effects in plumes of hot gases, as well as multiple alternative kernels for the integral operators that can be used to calculate concentrations based on the set of pseudoparticle coordinates; the latter can be highly useful in development work. Another useful feature of the LAPMOD model is the availability of a module designed for solving inverse problems, i.e., source attribution. Analysis demonstrated by ul Haq et al. [2019] highlights the ability of the LAPMOD model to properly simulate the trajectory of released particles within a complex terrain. This feature can be useful for simulating significant extreme events, as shown in Yang et al. [2024], where authors analysed local-scale dispersion of atmospheric Caesium-137 following the Fukushima Daiichi nuclear accident using the CALMET-LAPMOD coupled modelling system.

The final model worth mentioning here is FLEXPART⁷ [Stohl et al. 1998; Stohl et al. 2005; Pissio et al. 2019; Bakels et al. 2024]. This model has primarily been used for simulating the dispersion of pollutants on a large spatial scale — i.e., continental. Two noteworthy aspects are the extensive list of over 200 scientific publications related to the model that are included in the Web of Science database, and the

⁶ <https://www.enviroware.com/>

⁷ <https://www.flexpart.eu/>

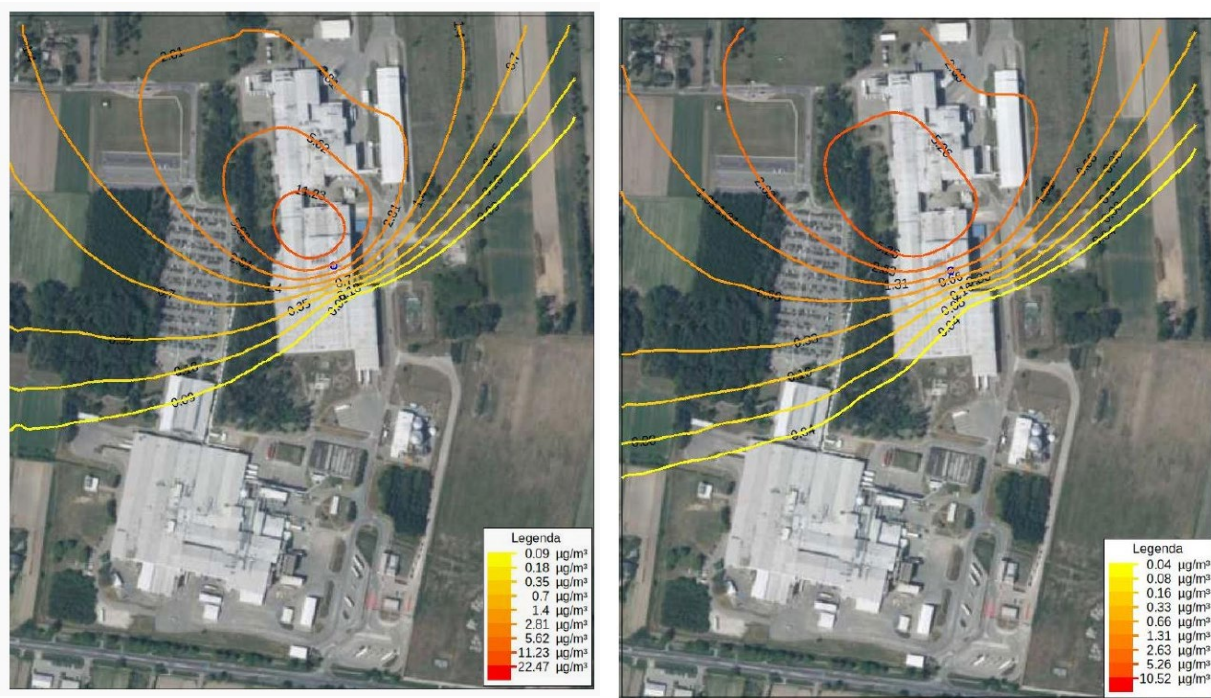


Figure 2. Example of modelled concentration maps from the GRAL model of a pollutant emitted from a point source, superimposed on a satellite map: (a) at a height of 3 m and (b) at a height of 6 m.

availability of the program's source code under the GNU Public License. Another valuable feature is its ability to calculate source-receptor matrices, which are essential for source apportionment. Since it was developed primarily for research rather than regulatory applications, it lacks a graphical user interface, which is often expected by beginners or occasional users. Nevertheless, it is a robust, state-of-the-art model with significant potential for adaptation to practical applications, such as validation of national-scale emission inventories, as presented in Henne et al. [2016].

FLEXPART was also used to investigate the transport pathways and source contributions to black carbon particles in the Arctic region [Zhu et al. 2020], where it proved to be a good emission source detector, attributing near-surface concentrations of black carbon over the Arctic to local anthropogenic emissions in the northern regions of Russia, as well as source regions in nearby Nordic countries. The model has been also successfully used in an integrated forecasting system in the recent study by Foreback et al. [2024], where it simulated back trajectories during heavy pollution events (under stagnant, low-wind conditions and abrupt synoptic weather changes) in Beijing.

Before concluding, it is worth adding a historical note. An LPD model was also developed in Poland during the late 1980s to provide meteorological support for the Żarnowiec Nuclear Power Plant [Uliasz 1990a; Uliasz 1990b]. That work was carried out using an IBM-PC/AT class personal computer, equipped with a 16-bit Intel 286 processor and 1 MB of RAM—four to five orders of magnitude below

the capabilities of today's laptops. Later on, it was also used to analyse air pollution levels in the Iżera Mountains region (the so-called "Black Triangle") [Uliasz et al. 1994], and continued to be developed for several more years [Uliasz 1993; Uliasz et al. 1996; Uliasz, Olendrzyński 1997]. Unfortunately, work on the model was discontinued before the end of the 20th century.

6. SUMMARY AND RECOMMENDATIONS

Calculating the dispersion of pollutants in the atmosphere requires the use of diverse models, appropriately selected based on spatial scale, terrain and climatic conditions, pollutant properties and emission characteristics. On the other hand, legal systems require the clear and unambiguous definition of methods that form the basis for administrative decisions.

Despite over 30 years of efforts to standardise regulatory models for pollutant dispersion in the atmosphere (starting from the first workshop on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes" in Risø, Denmark in May 1992), a consensus on a specific calculation methodology has not yet been achieved among European countries. On the other hand, EU-wide model uncertainty criteria exist, as required by the 2008/50/EC Directive on Ambient Air Quality and Cleaner Air for Europe, Annex I, to fulfil the data quality objectives for ambient air quality assessment. Unfortunately, these do not apply to environmental impact assessment procedures.

The Polish Environment Protection Act of 2001 [Environment Protection Act... 2001] defines the reference method as the one described by the regulation issued pursuant to the act, without any specification of the quality criteria. Entities interacting with the environment and administrative bodies are obligated to apply the reference methodologies. However, the law allows for the use of methods with proven equivalent quality of results or more accurate methods. In the latter case, however, there is a lack of motivation to use more accurate methods, as they are more costly.

Given the current state of knowledge, the Gaussian plume model used in Poland as a reference method is grossly outdated and deserves replacement. Under the current legal framework, a logical approach appears to be the revision of the reference methodology. This would allow for the continued use of simplified models in most straightforward cases, albeit with certain limitations — for example, in situations involving low wind conditions and calms. This would also stimulate the modernization of such models by improving the representation of meteorological conditions, pollutant properties, as well as the refinement of applied parametrizations. Given the present state of knowledge, data availability and computational power, there is plenty of room for improvement.

From this perspective, the reference model should be as universal as possible and thoroughly validated against empirical data in a wide range of physical situations. The best candidates for use in local scales seem to be found within the LPD group, although more advanced puff models, such as SCIPUFF, can be considered for selected applications based on their performance metrics. Drawing on the experiences of Germany and Austria, we propose transitioning to an LPD-class model for these applications. This class model should be defined as the reference method, while the use of simpler models (such as the current one) should be allowed only in cases where consistency with the reference model can be demonstrated.

Needless to say, the transition process is not immediate and would require a series of efforts to develop a methodology that defines how the model should be used in specific situations, taking into account physical scenarios, required input data, and how they are utilized. This publication is intended to serve as a starting point for a substantive discussion, which should precede the decision to undertake such work.

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