

Risk Assessment Perspectives on Air Dispersion Modeling

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ABSTRACT

Risk assessors frequently use air dispersion models to estimate exposure point concentrations in assessing potential risks to human health and the environment. Most typically, models are used to predict ambient concentrations of contaminants emitted from a variety of different sources of concern, and the assessments overlap with air quality assessments required for Clean Air Act (CAA) permitting. For reasons of consistency and facilitating acceptance (both by the public and the regulatory community), risk assessments are often based on the same models used to demonstrate CAA compliance (*i.e.*, the Appendix W models supported by the Office of Air Quality Planning and Standards). The needs of risk assessors, however, sometimes extend beyond CAA compliance requirements for Title V permitting. As examples, risk assessments of combustion source emissions frequently require multi-pathway models to assess contaminant deposition from the atmosphere and subsequent incorporation into terrestrial and aquatic food chain models; near-field deposition of nitrogen and mercury can be of specific concern to ecological and human health issues. Many existing air dispersion models are capable of addressing these problems, but uncertainties in many areas are great, and capabilities of models could be advanced to better serve risk assessment needs. Because the primary target of air dispersion modeling development is the demonstration of CAA compliance, at this point risk assessment applications are supplemental goals. However, risk assessors' use of air dispersion modeling is likely to increase and place greater demands on the air dispersion modeling community. As such, future model development should explicitly account for risk assessment needs to the greatest extent possible. Some observations concerning the air dispersion modeling needs of risk assessment and are explored to promote the dialogue on this topic.

INTRODUCTION

The use of air dispersion modeling in risk assessment is a well-established practice that will likely expand in scope. Residual risk determinations required under CAA Section 112 for Hazardous Air Pollutants are an obvious application in which models used largely for compliance demonstration for criteria pollutants under CAA Section 109 are (and will be) extended to explicitly address human health risk assessment concerns. In cases for which the inhalation exposure pathway is the primary means by which people

contact HAPs, the extension of air dispersion models from criteria pollutants to HAPs is relatively simple, as the focus of air dispersion modeling is predict concentrations of contaminants in air as they disperse from their point of emission into the atmosphere at locations where they are accessible to people. The focus of existing models is in fact coincidental with the goal of estimating the highest risk to any individual, as dispersion modeling applications are generally oriented toward identifying the worst-case maximum impacts. One potential complexity arises in such air only modeling when it is desired to estimate population-based risks over wide geographic areas. In this case, dispersion models must be appropriately selected to account for varying complex terrain and different geographic scales of interest (*e.g.*, local *v.* regional or national).

Demands on risk assessment modeling increase further when the problems of interest extend beyond predicting transport and dispersion in air alone. For contaminants that bioaccumulate, multi-media multi-pathway risk assessment is frequently undertaken to estimate the degree to which pollutants are deposited from the atmosphere, accumulated and transported in soils and waters, and then passed upwards through the food-chain, where they can contribute to indirect exposure. Here, the term indirect is used to indicate that the contaminants are emitted to the atmosphere, but exposure occurs through other media that have assimilated the initially airborne contaminants, sometimes through circuitous steps and processes. Multi-pathway risk assessments evolved to a large extent from the nuclear power industry, which since the late 1970s has required facilities to assess indirect exposures and risks from radionuclides released to the atmosphere^{1,2}.

In the late 1980s, the widespread expansion of the municipal waste-to-energy industry necessitated the development of multi-pathway risk assessment techniques to address public concerns over emissions of various heavy metals and persistent bioaccumulative chemicals such as polychlorinated dibenzo(*p*)dioxins and furans (PCDD/PCDFs). At that time, official, regulatory versions of U.S. EPA air dispersion models lacked reliable models to calculate contaminant deposition, a variable needed as input to subsequent terrestrial and aquatic food-chain models. Consequently, air dispersion models were either modified to include deposition algorithms (through the addition of source code) or the results of the models were used as input to subsequent (usually simple) deposition models. For example, dry deposition rates were typically estimated as the product of ground-level, ambient air concentrations and representative deposition velocities (weighted, by professional judgment, over both spatial and temporal conditions). Wet deposition, which properly must consider scavenging throughout the height of the plume, was often not explicitly calculated, but rather estimated qualitatively using analogies to information from the acid rain literature, and the empirical finding that that, for sulfur and nitrogen deposition, dry and wet deposition processes were of similar order-of-magnitude importance.

The U.S. EPA's development of the COMPDEP model, which around 1990 attempted to codify dry and wet deposition algorithms as well as merge simple and complex terrain modeling procedures, was perhaps the first attempt at an air model that would be useful for multi-pathway risk assessments. The COMPDEP model³ was used in the U.S. EPA's 1997 evaluation of potential health risks associated with the WTI Hazardous Waste

Incinerator⁴ (located in East Liverpool, Ohio), and laid the groundwork for the deposition algorithms that became part of the U.S. EPA's ISCST3 model in 1995. In combination with the U.S. EPA's dioxin reassessment efforts, methods for multi-pathway risk assessment advanced significantly during the mid- to late-1990s. The *Human Health Risk Assessment Protocol*^{5,6} and *Screening-Level Ecological Risk Assessment Protocol*⁷ multi-pathway risk assessment guidance documents developed from this work. Both the HHRAP and the SLERAP recommend ISCST3 as the baseline air dispersion model, but with recent changes to guideline model selection⁸, AERMOD and CALPUFF will likely see widespread application in multi-pathway risk assessments of airborne HAP emission sources.

The capabilities of air dispersion models in predicting contaminant deposition have advanced significantly over time, paralleling the evolution of multi-pathway risk assessment methods. However, as Section 109 compliance requirements remain the principal driver of air dispersion model development, current models do not meet all needs of risk assessors, and new demands on models continue to emerge outside traditional air modeling applications. As such, this paper discusses some perceived needs of risk assessments with respect to air dispersion models in the hopes of (1) expanding the dialogue between risk assessors and the modeling community at large and (2) influencing model development to better anticipate and incorporate the needs of risk assessors within model capabilities.

DEPOSITION MODELING ISSUES

The model AERMOD has recently incorporated relatively advanced deposition algorithms based on the multi-resistance models that consider the various processes that influence wet and dry deposition of both particle-bound and gaseous pollutants⁹. A number of issues are discussed herein regarding AERMOD's deposition algorithms and their implications for model applications and expanded capabilities. Some of these observations are generally applicable to deposition modeling.

AERMOD may overestimate dry deposition

One notable difference in AERRMOD's implementation of dry deposition algorithms as compared with methods previously implemented in the ISCST3 model, merits discussion, because it could result in significantly over-predicted deposition rates. Dry deposition is calculated as the product of an airborne concentration estimated at some reference height and a correspond deposition velocity which itself is modeled as a complex function depending upon contaminant properties, meteorological variables, and characteristics of the receiving surface as in Equation 1:

$$D_{dry} = C_{ref} \cdot v_d$$

where:

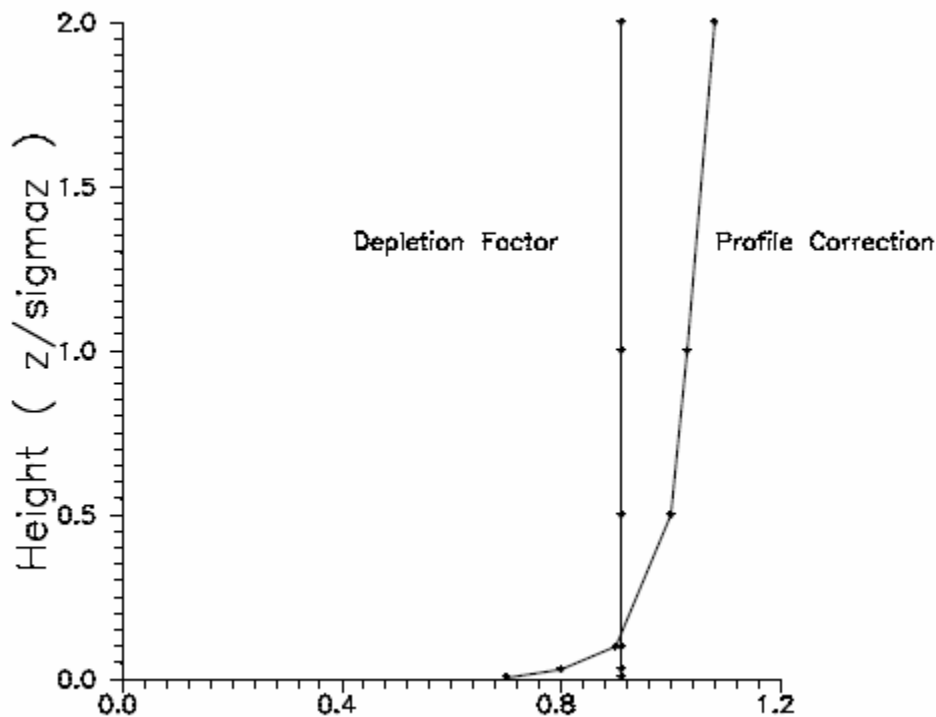
D_{dry} = dry deposition flux

C_{ref} = airborne concentration at some reference height

v_d , = deposition velocity

Importantly, when dry deposition occurs, it depletes pollutant mass from the portion of the plume adjacent to the ground. In contrast, wet deposition reduces contaminant concentrations proportionally throughout the entire vertical structure of the plume in which precipitation washout and scavenging occurs (assuming a first-order removal process). The ISCST3 model accounts for the preferential surface removal of dry deposition by adjusting the vertical concentration profile (Figure 1). The documentation and source code for AERMOD indicate that plume depletion of dry and wet deposition is both implemented using a simple, uniform concentration reduction through the vertical extent of the plume referred to as ‘source depletion.’ The vertical profile adjustment used by ISCST3 to account for surface depletion by dry deposition has not been incorporated into AERMOD. Since depletion of the profile near the surface would more greatly decrease C_{ref} , (compared with the effect of spreading depletion vertically throughout the plume), AERMOD predicts higher dry deposition rates than the ISCST3 model (all other factors being equal). Given the physical reality of the surface depletion effect, AERMOD may in fact be unnecessarily overestimating dry deposition rates, by using a value for C_{ref} that is too high for the reference height at which v_d is calculated.

Figure 1 Difference in vertical concentration profile adjustments between a uniform depletion factor and a surface profile correction (used for dry deposition at a surface). Reproduced from Figure 1-6 of the ISCST3 User’s Manual¹⁰.



AERMOD's deposition algorithms may require prohibitively large modeling studies

AERMOD offers the capability of modeling the deposition of individual gaseous contaminants through the specification of contaminant-specific physicochemical properties. However, air toxics risk assessments can conceivably include dozens, perhaps hundreds, of different contaminants. The U.S. EPA's 1997 WTI risk assessment⁴ considered 139 chemicals of potential concern; the HHRAP guidance⁶ include 203 chemicals of potential concern in its companion database. Running AERMOD over the standard five-year modeling period at hundreds to thousands of receptors can by itself be a time-consuming task for complex source configurations. If it were required that this task be done individually for tens to hundreds of different pollutants, it would easily become prohibitive, both from the standpoints of the potential time required and the complexity of data management.

One potential resolution of this problem is modeling prudence. Risk assessors should apply analyses and prioritization techniques to limit the number of air modeling runs needed to confidently assess risks. Compounds can be excluded from the full, multi-pathway risk assessment model through the use of screening modeling. Alternatively, compounds having similar atmospheric deposition properties can be grouped together for the AERMOD runs. However, a better solution to the problem of the need to assess multiple contaminants may be to develop expanded air dispersion modeling capabilities that will accommodate multiple pollutants within single modeling runs (each with their own physicochemical properties). This procedure is already implemented to a degree in the consideration of particle-bound pollutants, for which a distribution of particle sizes is considered. Incorporation of an array of contaminants would allow simultaneous modeling of a wide variety of multiple species and would result in computational savings by eliminating the need for repeating shared calculations.

The AERMOD system can be expanded to account for local deposition characteristics

AERMOD (through AERMET) characterizes sector-specific surface deposition parameters. AERMET allows the user to specify seasonal surface characteristics (*i.e.*, albedo, roughness length, and Bowen ratio) based on different wind sectors proceeding from the source location. These parameters are made part of the meteorological data files, and subsequently used by AERMOD in predicting dry deposition velocities.

Once specified by wind sector, however, AERMOD treats all receptors within each wind sector as having the same surface characteristics. Dry deposition, however, is a localized phenomenon that depends on the specific conditions of the receiving surface. Treating all locations as having the same surface characteristics averaged over an entire wind sector, may result in reasonable area-averaged deposition estimates. However, local-scale differences in deposition rates can be important to risk assessment because surface characteristics at a critical receptor may differ from those of the sector at large. For example, a farm might be located just outside a highly urbanized area. In this case, the sector may on average be treated as urban land, but the deposition predictions at the farm, which may be of critical importance to the multi-pathway risk assessment, may be

inaccurately modeled due to the unrepresentative reliance on sector-averaged surface characteristics.

This problem could be addressed by expanding AERMOD to allow surface characteristics to be specified at individual receptor locations. For example, seasonal surface types could be specified in AERMOD appropriate for specific land uses (*e.g.*, farms or water surfaces), and land use types optionally specified in conjunction with discrete receptor parameters (allowing for the default assumption of wind sector-averaged values).

ADVANCED MODELING NEEDS

There are many modeling capabilities that risk assessors could use to their advantage as models continue to be developed. Some of these capabilities are described below in the context of limitations currently faced by risk assessors. To some extent, these issues represent areas for which the required research is beyond what is practical as part of pending or planned model development, but they also share characteristics that could be handled through modifications to existing models.

Near-field modeling needs

At some locations dispersion and deposition of pollutants is a potential concern at receptors very close to emission sources. In part, high near-field rates of predicted wet deposition are a consequence of modeled scavenging in the concentrated plume near the emission source. Examples of near-field deposition concerns include mercury potentially deposited to proximate water bodies, and nitrogen deposition (from NO_x and NH₃ emissions) that could affect vegetation as a supplemental nutrient source delivered to soils¹¹. The models and assumptions used for near-field deposition can be of critical importance, even though the algorithms are not necessarily designed for near-field applications. For example, the CALPUFF algorithms that predict nitrogen and sulfur deposition rates are typically focused on estimating acid rain impacts at distant locations (Class I areas). Prudence must therefore be exercised by risk assessors in applying models to near-field locations, but ideally, by model development should address the frequent need to assess near-source impacts.

Near-field modeling concerns are not limited to deposition problems. Some sources, such as ground level fugitive dust, need to be evaluated for very close-by receptors at distances much smaller than those used to develop a Gaussian-type concentration profile (*e.g.*, on the order of tens of meters from the source). Uncertainties in near-field model applications must always be recognized, but model development must also reconcile the unusual demands placed on models by risk assessors. Model validation and testing should be expanded to evaluate the near-field predictive capabilities of models. Most models are verified for ambient concentrations of passive tracers at distances of a few kilometers and beyond, with some models (*e.g.*, those for acid deposition) verified much farther downwind (*e.g.*, > 50 km).

Aerosol-vapor interactions and the influence of background air quality

Some contaminants (*e.g.*, PCDD/PCDFs and other persistent, bioaccumulative chemicals) are present both as vapors and bound to particles. These contaminants are likely to change partitioning in the atmosphere, both over time in response to changing background particle concentrations, and perhaps more dramatically as stack emissions mix into the atmosphere upon their release. The deposition characteristics of aerosols and vapors can differ markedly. For example, dry deposition of fine particulates typically occurs at velocities on the order of 0.1 cm/s, whereas gases that are soluble, lipophilic, and/or reactive can deposit at velocities greater than 1 cm/s to appropriate surfaces. To some extent, the CALPUFF model accounts for the dynamics of particle-vapor behavior in the chemical modules that it uses to model acid rain precursors. Aerosol-vapor interactions may have important implications in the fate and transport of many contaminants, and although this is a topic of active research, future model development should consider methods to model and track these interactions.

An additional consideration when performing source-specific modeling, is the joint consideration of both in-plume and background air quality. For example, the CALPUFF model generally uses a background ammonia (NH₃) concentration as an input to its MESOPUFF chemical mechanism¹². However, because many sources emit significant concentrations of NH₃ in their stack-gas, near-field plume chemistry might be dominated by the source NH₃ concentration. The elevated NH₃ levels are likely to dissipate rapidly below background as stack-gases are diluted by the atmosphere, but source-emitted NH₃ may have relevance in estimating deposition rates close to the point of release¹¹.

Contaminant partitioning, reactive plume chemistry (including aerosols) and removal processes are key factors in understanding contaminant fate and transport, especially with respect to deposition processes. The degree to which these processes can be incorporated into existing models, or whether they demand the development of specialized models, is an important consideration in allocating resources to model development, especially as the issues of interest increase in complexity and challenge state-of-the-art knowledge.

The development of nested regional and local models offer a potential opportunity to better incorporate variability in background concentrations (such as NH₃ levels) required by source-based models. Models such as CALPUFF and AERMOD could utilize the results of regional model simulations developed for similar modeling periods to provide spatial and temporal resolution of background concentrations.

Beyond the first terrain feature

Modeling to identify the location of highest impact from a source has traditionally focused on the first complex terrain feature encountered, with the knowledge that impacts at greater distances will be smaller. Risk assessments, however, often need to focus on receptors such as water bodies, farms, and receptors of special interest, irrespective of their location relative to the first terrain feature. CALPUFF can examine truly complex terrain through 3-D wind fields, but AERMOD is not designed for this purpose. In designing models for widespread application, the modeling community should recognize that risk assessors apply models over wide geographic areas, usually with minimal consideration of the effects of multiple complex terrain features. Aside from the obvious

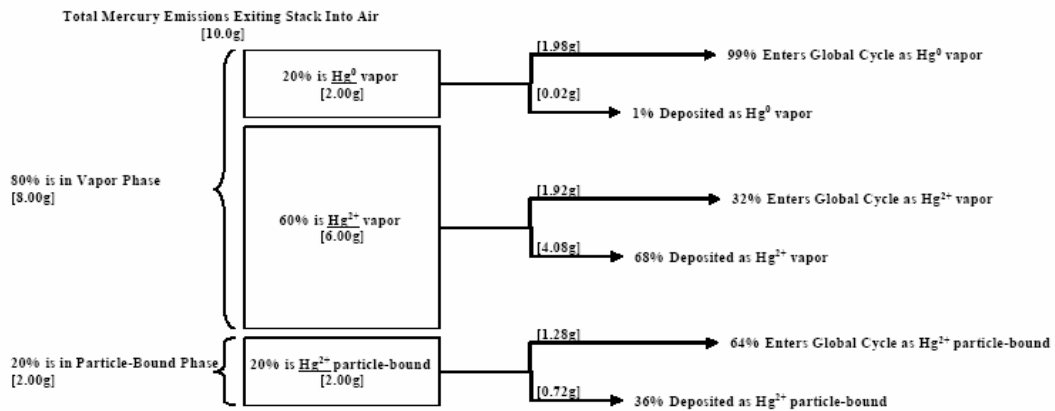
need to recognize uncertainties associated with this practice, specific guidance to risk assessors would be helpful in identifying situations in which models are extended too far beyond their recommended limits.

MERCURY: A POLLUTANT WITH CRITICAL MODELING NEEDS

Mercury has long been a pollutant of special concern to risk assessors, and will continue as such indefinitely because the typical human exposures to mercury are near or at levels of toxicological concern. Mercury is also a difficult environmental contaminant to understand, as natural and anthropogenic sources cycle and intermingle. Local, regional, and global concerns are influenced by different mixes of emissions and relevant atmospheric processes.

Despite the overarching concern over mercury, methods to assess its fate and transport remain highly uncertain. The U.S. EPA’s HHRAP⁶, for example, contains detailed algorithms for predicting mercury fate and transport that begin with an assumed mercury speciation in source emissions among elemental, particle-bound, and divalent forms. Notwithstanding the potentially significant uncertainties associated with either measuring or assuming mercury speciation at the source, the HHRAP proceeds to model mercury by first removing a fraction of each mercury species from consideration in the deposition modeling. This is based on the assumption that fractions of each type of mercury are lost to a “global mercury pool” and are not to be available to be deposited locally (Figure 2). This removal of mercury from the local model is based on findings in the U.S. EPA’s *Mercury Report to Congress*¹³ of a regional-scale model. There is, however, no reason to assume that mercury species will deposit at different rates than would be predicted by the local model itself, because all the mercury is subject to the same atmospheric processes (unless implicit assumptions concerning species inter-conversions are made).

Figure 2 Assumed fate of speciated mercury emissions in the atmosphere, as recommended in the U.S. EPA’s Human Health Risk Assessment Protocol (HHRAP) guidance⁶.



Critical assumptions then follow concerning deposition velocities appropriate for each mercury species. The HHRAP assumes that a negligible amount of elemental mercury deposits locally. Deposition of particle-bound mercury is assumed to occur at the same rate as deposition of other particulate compounds (aside from the assumed “global pool” reduction above). The most critical assumption regarding deposition velocities, however, is typically that made for oxidized mercury vapor (Hg^{2+}) species. Because dry deposition of an atmospheric trace species such as Hg^{2+} is remarkably difficult to measure, the uncertainty in its value may be very large. The HHRAP⁶ recommends a dry deposition velocity of 2.9 cm/s for oxidized mercury vapor species. This value was first used in the U.S. EPA’s *Mercury Report to Congress*¹³, and is based (in part) on a solubility-based analogy with nitric acid as a species that readily deposits to surfaces once the aerodynamic resistance factor is overcome. The assumption has been repeated in many risk assessments, but its validity is difficult to judge. Many other compounds with similar solubility properties are not assumed to deposit at this rate. Nitric acid deposition velocities are among the highest for all contaminants. Empirical nitric acid deposition velocities vary from 0.06 to 4.5 cm/s¹⁴, and encompass the range of 1 to 2 cm/s typically estimated at CASTNET dry deposition sites¹⁵.

The use of a conservative, possibly over-estimated deposition velocity for a critical pollutant such as mercury may seem prudent, but applying the recommended Hg^{2+} deposition velocity of 2.9 cm/s, in combination with myriad other conservative assumptions recommended in the HHRAP, can result in unacceptably high, yet plausible, levels of mercury in fish. Given the inability to distinguish mercury from specific sources, the question of culpability cannot be resolved. On the one hand, the modeled mercury levels may be consistent with mercury levels measured in fish. On the other hand, modeling may over-predict mercury levels in fish that are in fact simply the result of background processes. In this case, the fundamental risk assessment tenet of compensating uncertainty by biasing deposition velocities and other parameters on the high side may serve to confuse the issue of differentiating mercury contributions from individual facilities with respect to background.

In summary, mercury modeling is difficult, and given the need to judge facility impacts against background, modeling cannot be overly conservative if realistic determinations are required. With respect to multi-pathway modeling, research on atmospheric mercury fate and transport modeling is needed on many fronts, especially regarding the critical first step of deposition that places the mercury within terrestrial and aquatic realms. Efforts to improve mercury assessment through future model development, especially validation studies, would also be extremely useful in helping to resolve the significant uncertainties involved in mercury modeling.

CONCLUSIONS

Risk assessors use air dispersion models – sometimes in interesting ways – and their needs may differ significantly from modelers interested in Clean Air Act (CAA) permitting analyses. Predicting contaminant deposition is often a key risk assessment analyses, especially in multi-pathway risk assessments. Unfortunately, relevant and reliable tools for deposition analyses are not always available. The capabilities of

existing models could be developed better meet the needs of multi-pathway risk assessment. More specific and detailed guidance regarding the application of dispersion modeling in settings outside traditional CAA permitting applications is needed, and specific attention to mercury modeling would be welcome. Because the dependence of risk assessors on air dispersion models is likely to increase, it is important that model developers recognize the expanding application of models outside their traditional applications.

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KEYWORDS

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