

Review

Sub-Grid Scale Plume Modeling

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Abstract: Multi-pollutant chemical transport models (CTMs) are being routinely used to predict the impacts of emission controls on the concentrations and deposition of primary and secondary pollutants. While these models have a fairly comprehensive treatment of the governing atmospheric processes, they are unable to correctly represent processes that occur at very fine scales, such as the near-source transport and chemistry of emissions from elevated point sources, because of their relatively coarse horizontal resolution. Several different approaches have been used to address this limitation, such as using fine grids, adaptive grids, hybrid modeling, or an embedded sub-grid scale plume model, *i.e.*, plumein-grid (PinG) modeling. In this paper, we first discuss the relative merits of these various approaches used to resolve sub-grid scale effects in grid models, and then focus on PinG modeling which has been very effective in addressing the problems listed above. We start with a history and review of PinG modeling from its initial applications for ozone modeling in the Urban Airshed Model (UAM) in the early 1980s using a relatively simple plume model, to more sophisticated and state-of-the-science plume models, that include a full treatment of gas-phase, aerosol, and cloud chemistry, embedded in contemporary models such as CMAQ, CAMx, and WRF-Chem. We present examples of some typical results from PinG modeling for a variety of applications, discuss the implications of PinG on model predictions of source attribution, and discuss possible future developments and applications for PinG modeling.

Keywords: air quality modeling; plume-in-grid; source attribution; plume chemistry; grid resolution

1. Introduction

Multi-pollutant three-dimensional (3-D) grid models are widely used to predict the impacts of emission controls on the atmospheric concentrations and deposition of pollutants such as ozone (O_3) , fine particulate matter $(PM_{2.5})$, and mercury (Hg) and other air toxics. Such a grid-based approach necessarily averages emissions within the volume of the grid cell where they are released and cannot resolve processes that occur at much smaller scales. For example, the averaging process may be appropriate for sources that are more or less uniformly distributed at the spatial resolution of the grid system but may lead to significant errors for sources that have a spatial dimension much smaller than that of the grid system, such as elevated point sources. The stack emissions from these sources lead to plumes that initially have dimensions of tens of meters, whereas the horizontal resolution in grid-based air quality models is typically several kilometers in urban applications and up to about 100 km in regional applications. Thus, the grid model cannot resolve the sharp concentration gradients between the plume and the background atmosphere, and the artificial dilution of stack emissions leads to (1) lower concentrations of plume material; (2) unrealistic concentrations upwind of the stack; (3) incorrect representation of the transport of the emitted chemicals; and (4) incorrect chemical reaction rates due to the misrepresentation of the plume chemical concentrations and turbulent diffusion. The misrepresentation of plume chemistry in a grid model is amplified for cases when the plume chemistry is significantly different from the ambient chemistry, such as power plant plumes rich in NO_x, where both experimental studies, e.g., [1,2], and theoretical studies, e.g., [3,4], have shown that the rates of ozone and acid formation in the plume differ significantly from background rates. The errors introduced by coarse grid resolution impact not only the ambient concentrations, but also the dry and wet deposition of chemical species.

Techniques that have been adopted to address sub-grid scale errors associated with grid models include the use of multiple nested fine grids, including one-way and two-way nesting, adaptive grid modeling, hybrid modeling, and plume-in-grid (PinG) modeling. The last approach, which is the focus of this paper, has been primarily used for simulating elevated point source plumes within a grid model. However, as discussed below, the technique can be readily applied to many other sub-grid scale applications. In the following sections, we first briefly discuss the various approaches that are commonly used in grid models, and then present a detailed discussion on PinG modeling starting from the first applications of this approach nearly three decades ago to the current state-of-the-science.

2. Sub-Grid Scale Plume Modeling Approaches

2.1. Nested Grid Modeling

Because sub-grid scale errors are a direct result of coarse grid resolutions, one approach to resolve such errors is to use grids with very fine resolution. However, this can become computationally of the horizontal grid resolution on model results.

prohibitively expensive for large domains, due to both the large number of grid cells that must be stored and solved as well as the smaller time steps that must be used in the solution due to the Courant number restriction on the model time step. Consequently, domain-wide fine-grid simulations are restricted to small domain and/or short duration simulations, and nested grid modeling is generally used for larger domains. In this approach, one or more fine grids are employed over regions of special interest within the larger domain (e.g., urban regions within a regional domain or regional domains within a continental domain), sometimes with multiple levels of nesting (e.g., global > continental > regional > urban). Typical horizontal grid resolutions used in many air quality modeling applications vary from about 100 km for a global domain to 36 km, 12 km, and 4 km for continental, regional, and

Nested grid modeling is now routinely employed in air quality modeling applications, and almost all current operational models include some kind of nested grid modeling capability. In some models, grid nesting is achieved by sequential applications of the model starting with the outermost coarse grid domain and ending with the innermost coarse grid domain. Thus, the nesting is one-way, *i.e.*, information flows from the coarse grids to the inner grids and there is no feedback from the inner to outer grids. Processors are available that read the coarse grid simulation outputs to extract information (initial and boundary conditions) required for simulating the inner grids. The U.S. EPA Community Multiscale Air Quality (CMAQ) model [9] is an example of a widely used one-way nested model.

urban domains, respectively. Several nested grid modeling studies, e.g., [5–8], highlight the importance

In other models, the nested grid capability is built-in and the multiple grid simulations can be conducted simultaneously with two-way flow of information between the coarse and fine grids. Examples of such models are the Urban and Regional Multiscale (URM) model [10–13], the Comprehensive Air quality Model with extensions (CAMx) [14,15], the Weather Research and Forecasting/Chemistry (WRF/Chem) model [16] and the variable grid Urban Airshed Modeling (UAM-V) system [17]. CAMx offers up to four levels of nesting and 10 nested grids, and also includes a capability, referred to as "flexi-nesting", which allows for reconfiguration of nested grids during a simulation and the in-line interpolation of coarse grid inputs to the fine grid when inputs for the fine grid are not available. WRF/Chem provides the capability of coupled meteorological-air quality simulations allowing for the investigation of feedback among chemistry-aerosol-cloud-radiation-climate, e.g., [18], and a global-through-urban version of the model has recently been developed [19,20].

The URM model evolved from the CIT airshed model [21], and uses a two-dimensional transport scheme based on the streamline upwind Petrov-Galerkin (SUPG) finite element method [22]. This scheme allows the use of different size elements to generate the model grid, making it possible to construct grid meshes that use coarse and fine scales most effectively in the modeling domain. Thus, the multiscale modeling approach in the URM model differs from the approach used in the other nested grid models in that there is a single solution for any finite element in the URM as compared to the multiple solutions for each grid in the traditional approach. Kumar *et al.* [13] applied the model to the northeastern U.S. for an ozone episode in July 1988 for several different grid configurations, including an 18.5 km resolution uniform grid and two multiple-nested grid configurations with three and five levels of nesting and fine scales (4.625 km resolution) over the Northeast Corridor and other

urban areas. They found that the nested grid configurations resulted in broader and higher predicted peak ozone regions in the Northeast Corridor, compared to using coarse scales over the whole domain.

While fine grid and nested grid modeling are commonly used practical tools to address some coarse grid resolution issues, they are not a panacea. Grid resolutions finer than 1 km are typically not used, because of the excessive computational resource requirements, and sometimes because the parameterizations in a particular model may not be adequate for grid cell sizes lower than 1 km. Examples of some CMAQ and CAMx nested grid applications with the finest grid resolution at 1 km are provided in [23–27]. However, even a resolution of 1 km is inadequate to resolve sub-grid scale features, such as plumes from elevated point sources, whose initial dimensions are of the order of a few tens of meters.

Another disadvantage of the nested grid approach discussed above is that the grids are static or fixed, *i.e.*, they do not change during the simulation. Thus, the resolution and the extent of each grid must be determined *a priori* and remain fixed throughout the simulation and the selection of grids must be made carefully. The static nested grid approach does not allow the capability to adjust to dynamic changes in grid resolution requirements, e.g., the transport of point source plumes in different directions and to large downwind distances, where the grid resolution may be insufficient to resolve the plume. A refinement to the nested grid approach, referred to as adaptive grid modeling, addresses this limitation.

2.2. Adaptive Grid Modeling

In the adaptive grid modeling approach, the grid system is modified dynamically during a simulation, based on certain aspects of the calculated fields, to respond to dynamic changes in solution resolution requirements, e.g., to follow the chemical evolution of plumes. Adaptive grid algorithms for meteorological and air quality models were developed more than a decade ago, e.g., [28–36], but their use in functional or operational models is more recent and still evolving. Initial applications of the adaptive grid approach in an air quality model for an ozone episode are described by Odman *et al.* [37] and Odman and Khan [38] who incorporated the Dynamic Solution Adaptive Grid Algorithm-Piecewise Parabolic Method (DSAGA-PPM) algorithm of Srivastava *et al.* [34–36] in the Multiscale Air Quality Simulation Platform (MAQSIP) model [39], the prototype for CMAQ. The model was also used by Unal and Odman [40] to predict the air quality impacts of biomass burning. Belwal *et al.* [41] and Constantinescu *et al.* [42] describe an adaptive grid approach in corporated in the Sulfur Transport Eulerian Model (STEM) [43].

The adaptive grid approach of Odman and coworkers [34–38] is a mesh refinement algorithm where the number of grid cells remains constant and the structure (topology) of the grid is preserved. Thus, finer resolution can be achieved in selected regions by permitting coarser resolution elsewhere. Grid nodes move continuously during the simulation, and grid cells are automatically refined or coarsened for a more accurate solution. The movement of the grid nodes is controlled by a weight function determined by user-defined criteria (e.g., NO_x concentration gradients for tracking power plant plumes). While Odman *et al.* [37] were able to demonstrate success with their initial application of the approach for simulating an ozone episode, the inclusion of the adaptive grid algorithm into a photochemical model with nonlinear chemistry imposed a significant computational burden due to the short time step required by smaller grid scales. Subsequently, a variable time step algorithm that allows each grid cell to have a unique time step was developed [44,45]. This algorithm was incorporated into CMAQ to develop an adaptive grid version of the model, referred to as adaptive grid CMAQ or AG-CMAQ, and the model has been applied to study the air quality impacts of biomass burning plumes [46,47]. In this application, grid resolutions as fine as 100 m × 100 m were used to capture the sub-grid scale nature of these plumes [47].

Adaptive grid modeling is an important advancement over the static nested grid approach and shows promise in addressing many of the limitations of traditional grid modeling. However, the approach has not yet been routinely applied in an operational mode for long-term multi-pollutant air quality simulations over large domains and with hundreds of sub-grid scale plumes. Garcia-Menendez and Odman [48] provide additional information on the state-of-the-science of adaptive grid modeling and what the future holds.

2.3. Hybrid Modeling

In the hybrid modeling approach, concentrations from a grid-based chemical transport model and a local plume dispersion model are combined to provide contributions from photochemical interactions, long-range (regional) transport, and details attributable to local-scale dispersion. Hybrid modeling has been extensively used over the last few years, motivated by the increasing concern about population exposure to hazardous air pollutants (HAPs), especially in the vicinity of the sources of these pollutants. As mentioned previously, a traditional grid model, which provides average concentrations for grid volumes, cannot provide the fine-scale details in the concentration patterns and capture "hot spots", required for calculating population exposure. For example, measurements of ultrafine particles near freeways and other roadways, e.g., [49–52], show that exposures near the roadway are up to 10 times greater than those at background locations and drop to background levels within a few hundred meters of the roadway.

Ching *et al.* [53,54] developed an approach where they accounted for sub-grid spatial variability using the results of grid model simulations conducted with a fine spatial resolution and proposed the use of additional models, such as a Gaussian dispersion model, to superimpose sub-grid scale variability on the grid model results. Touma *et al.* [55] discuss the pros and cons of the hybrid approach *versus* other sub-grid scale approaches, including PinG modeling. Isakov and Venkatram [56] used a hybrid modeling approach for a case study in Wilmington, California, a community that contains a diverse array of emissions sources, including petroleum refineries, heavily traveled freeways, distribution centers, and local businesses, all located in close proximity to or interspersed with residential and mixed-use development. Examples of hybrid modeling for other urban regions, such as Houston, Texas; Philadelphia, Pennsylvania; New Haven, Connecticut; and Detroit, Michigan are provided in [24,57–60]. Cook *et al.* [61] discuss the development of local scale emissions for hybrid modeling to simulate air quality near roadways. Other hybrid modeling approaches are discussed in [62–64]. The application of hybrid modeling to predict the local-scale air quality impacts of airport emissions is discussed in [65,66].

While hybrid modeling is a promising approach to incorporate sub-grid scale variability in a gridded concentration field, it has some limitations and may not be the right approach for some

applications. Most of the examples of hybrid modeling cited above have used a steady-state Gaussian dispersion model, such as the Industrial Source Complex (ISC) Short Term, Version 3 (ISCST3), or its replacement, the American Meteorological Society (AMS)/EPA Regulatory Model (AERMOD), for calculating local scale impacts. These models cannot handle non-linear chemistry and are inappropriate for secondary pollutants. Furthermore, steady-state models cannot be applied in areas with very complex wind fields, because their formulation is based on the assumption that wind fields are uniform over the modeling domain, e.g., [55]. Non-steady-state puff models with a treatment of chemistry comparable to that in a photochemical grid model, such as the Second-order Closure Integrated puff model with Chemistry (SCICHEM) [67], can correct these deficiencies. The puff model can be applied off-line, as in the hybrid modeling discussed above, with the grid model providing the regional or large-scale background but not being affected by the puff model, or in-line, within the grid model, allowing two-way feedback between the grid model and local scale calculations. In the following section, we discuss the latter approach, referred to as PinG modeling.

2.4. Plume-in-Grid Modeling

In the PinG modeling approach, the errors associated with the grid-averaging of stack emissions or other sub-grid scale variations are reduced by imbedding a puff or plume model within the grid model. The embedded model tracks the sub-grid scale process (e.g., elevated point source emissions) until the fine scale variability becomes unimportant (referred to as the "puff dumping" or "hand-over" point), at which point the grid model takes over the calculations for that process while the embedded model continues tracking sub-grid scale processes.

PinG modeling has a long history, particularly for ozone modeling, and is now being used for multi-pollutant modeling as well, as discussed later in this review. The first sub-grid scale treatment of plumes in 3-D air quality models, referred to as the Plume-Airshed Reactive-Interacting System (PARIS), was developed by Seigneur *et al.* [68], who embedded a simple puff model into the Urban Airshed Model (UAM) [69], and used it to calculate ozone concentrations in urban areas such as Los Angeles, California, and St. Louis, Missouri. Morris *et al.* [14,70] describe a plume-in-grid treatment in the variable grid version of UAM (UAM-V). Other early PinG treatments include those of Sillman *et al.* [71]; Myers *et al.* [72], who implemented PinG treatment in the SARMAP Air Quality Model (SAQM) [73]; and Kumar *et al.* [74], who incorporated a sub-grid scale treatment of plumes in URM. Initial versions of CMAQ also included a plume-in-grid treatment [75,76], based on a reactive plume model developed by Gillani [77].

These early PinG models treated plumes at a sub-grid scale, thereby eliminating some of the errors associated with the grid model. However, they could not represent the complex dispersion processes associated with the plume mixing into the background air because the plume dimensions were represented by simple geometric functions (columns, grids, ellipses, or Gaussian distributions). Physical phenomena such as the effect of wind shear on plume dispersion, the effect of plume overlaps (e.g., under conditions of flow reversal or merging of adjacent plumes), and the effect of atmospheric turbulence on chemical kinetics were not represented in these models. In the last decade, new plume models, such as SCICHEM [67], have been developed that address the above deficiencies and also include a detailed treatment of atmospheric chemistry. SCICHEM has been embedded into CMAQ,

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e.g., [78,79], to develop a PinG model, referred to as CMAQ-APT (where APT stands for Advanced Plume Treatment). The PinG treatment in the CAMx grid model also uses a plume model that has some attributes of SCICHEM [80]. SCICHEM has also recently been incorporated in WRF/Chem [81]. Advanced PinG treatments of puff dispersion and chemistry have recently been incorporated in European models, such as the Polyphemus air quality modeling system [82,83]. The PinG approach has also been used to track biomass burning plumes within a grid model, e.g., [84], including the adaptive grid CMAQ discussed in Section 2.2 [85].

In the following section, we discuss two PinG air quality models that have been applied in the recent past.

3. Two Operational Plume-in-Grid Air Quality Models

3.1. Model Descriptions

CAMx and CMAQ-APT are two widely used air quality models that include plume-in-grid modeling capabilities. Both consist of a reactive plume model, based on SCICHEM [67], embedded within the host grid model (CAMx and CMAQ). Plume transport and dispersion are simulated using a second-order closure approach to solve the turbulent diffusion equations [86,87]. The plume is represented by a myriad of three-dimensional puffs that are advected and dispersed according to the local micrometeorological characteristics. Each puff has a Gaussian representation of the concentrations of emitted inert species. The overall plume, however, can have any spatial distribution of these concentrations, since it consists of a multitude of puffs that are independently affected by the transport and dispersion characteristics of the atmosphere. The plume model can simulate the effect of wind shear since individual puffs will evolve according to their respective locations in an inhomogeneous velocity field. As puffs grow larger, they may encompass a volume that cannot be considered homogenous in terms of the meteorological variables. A puff splitting algorithm accounts for such conditions by dividing puffs that have become too large into a number of smaller puffs. Conversely, puffs may overlap significantly, thereby leading to an excessive computational burden. A puff-merging algorithm allows individual puffs that are affected by the same (or very similar) micro-scale meteorology to combine into a single puff. Also, the effects of buoyancy on plume rise and initial dispersion are simulated by solving the conservation equations for mass, heat, and momentum.

Chemical species concentrations in the puffs are treated as perturbations from the background concentrations. The chemical reactions within the puffs are simulated using a general framework that allows any chemical kinetic mechanism to be treated. The puff chemical mechanism is the same as the host grid model mechanism for consistency. SCICHEM allows the option of explicitly simulating the effect of turbulence on chemical kinetics for selected reactions. This effect is more pronounced near the stack and requires additional computational time for its simulation [67].

In CMAQ-APT, the treatment of chemistry in the plume model is identical to that in the host grid model, and includes gas-phase chemistry, aerosol chemistry, and aqueous-phase chemistry. In the CAMx Plume-in-Grid (PinG) model, two approaches are available that provide different levels of chemical complexity [80]. Both approaches share common design features for puff initialization, puff structure, transport, and growth. They deviate in how they treat chemistry and when they transfer mass

from puffs to grid cells. The first PinG approach in CAMx is aimed at treating the early chemical evolution of large NO_x plumes when mostly inorganic gas-phase reactions are operative. The method is called the Greatly Reduced Execution and Simplified Dynamics Plume-in-Grid approach (referred to as "GREASD-PiG"), and can be used in both ozone and particulate matter (PM) simulations. The second approach treats the full suite of gas-phase photochemistry for all types of point sources and thus incorporates much more chemical complexity than the GREASD-PiG approach. This treatment is referred to as the Incremental Reactions for Organics and NO_x (IRON) Plume-in-Grid (referred to as "IRON-PiG"). PM is not treated in IRON-PiG.

In both CAMx and CMAQ-APT, the host grid model concentrations serve as the background (ambient) concentrations for the embedded plume model calculations, and are also updated whenever plume-to-grid transfer occurs. In CMAQ-APT, the transfer of puff material to the 3-D grid system is triggered when the puff size is commensurate with the grid cell size [78,79]. The model also includes an option to use a chemical dumping criterion for situations where the physical criterion may result in premature transfer of the plume material to the grid [78]. The grid cell size approach is also used in the IRON-PiG version of CAMx to determine when puffs are ready to be transferred to the host model. To prevent a sudden shock to the system by dumping the entire puff at once, the CAMx dumping approach uses a technique, referred to as "puff leakage", that allows puff mass to be transferred to the grid in a more continuous manner [80]. In the GREASD-PiG implementation in CAMx, the number of puffs is limited by dumping the puffs when oxidant formation begins, which usually occurs before the puff sizes are comparable to the grid resolution.

With both CAMx and CMAQ-APT, it is possible to sample concentration fields at a finer scale than the grid model resolution. CAMx has an optional sampling grid that allows surface-layer puff sampling of model species on a user-defined grid of arbitrary horizontal resolution, similarly to the way nested grids are defined [80]. Sampling grids are entirely passive, and intended to provide a display of the plume concentrations at scales much smaller than typically used for the finest computational grids (*i.e.*, <1 km), primarily around and downwind of a source complex. In CMAQ-APT, sampling at finer scales than the grid model resolution is achieved by post-processors that sample the puffs at arbitrary locations and combine the puff perturbation concentrations at these locations with the gridded concentration field, e.g., [79].

The computational overhead associated with simulating a large number of point sources explicitly with the plume component of the model can be significant in a PinG model. In the past, this limitation has restricted the application of these models to short duration simulations with less than 50 PinG sources, e.g., [79,88]. This limitation has been overcome in both CMAQ-APT and CAMx by parallelizing the code to take advantage of multi-processor workstations and workstation clusters that are commonly used today for air quality model simulations. In CMAQ-APT, the grid model parallelization is based on domain decomposition using the Message Passing Interface (MPI), and Karamchandani *et al.* [89] recently parallelized the plume component using puff decomposition and MPI. In CAMx, which uses Open-MP (OMP) on shared-memory systems and MPI on distributed-memory systems, the parallelization of the plume model depends on which of these two approaches is selected. If OMP is selected, then the main puff loop is parallelized using OMP (similar to the puff decomposition approach in CMAQ-APT). If MPI is selected, each thread or processor

solves the puffs within its subdomain (*i.e.*, grid decomposition is used for both the grid and embedded puff models).

3.2. Model Applications

The first version of CMAQ-APT only included gas-phase chemistry in the plume component and was used for ozone episode applications in the northeastern U.S with 30 PinG point sources [78], and central California with 10 PinG point sources [88]. Results from the northeastern U.S. simulations showed that the use of the PinG approach had a significant effect on the spatial patterns of ozone and nitric acid surface concentrations downwind of the sources considered for PinG treatment to distances of 100 to 200 km. Results from the central California application were qualitatively similar to those from the northeastern U.S. application, but the effects of the PinG approach were smaller. This was attributed to the relatively smaller magnitude of NO_x emissions from large point sources in California as compared to the eastern United States.

The model was extended for particulate matter by including aerosol and aqueous-phase treatments in the plume model that were consistent with those used in the host grid model [79]. The model was applied to the southeastern United States with a 12 km horizontal grid resolution for the months of January and July 2002. Emissions from fourteen coal-fired power plants (CFPPs) in Alabama, Georgia, Florida and Mississippi were explicitly simulated with the PinG treatment. The model was evaluated with routine measurements as well as with detailed measurements corresponding to plume events from the Southeastern Aerosol Research and Characterization study (SEARCH) network. While model performances with and without the PinG approach were almost identical with the routine measurements, the PinG approach was found to capture the SEARCH plume events better than the non-PinG approach. In addition, the use of the PinG model had a significant effect on the spatial patterns of particulate sulfate and total inorganic nitrate (gas-phase nitric acid + particulate phase nitrate) concentrations. The effects were largest in the four states containing the 14 power plants selected for PinG treatment. However, differences in sulfate and total inorganic nitrate concentrations were also predicted in some of the surrounding states.

The next stage in the development of CMAQ-APT was the inclusion of mercury (Hg) treatment [90,91]. The model was applied for 2001 over a domain covering the U.S. at 36 km horizontal resolution [91]. The top thirty Hg emitting power plants in the U.S. were selected for explicit plume treatment. The PinG treatment resulted in improved performance for Hg wet deposition over a purely Eulerian grid-based model, partial correction of over-predictions of wet deposition downwind of coal-fired power plants in the northeastern U.S., and in decreases of approximately 10% in simulated dry and wet deposition over large parts of the eastern U.S. with larger decreases near the plants selected for PinG treatment.

CMAQ-APT was also used to estimate the decrease in atmospheric nitrogen deposition in Escambia Bay and its watershed in Florida and southern Alabama due to planned emissions controls of NO_x and SO_2 at a nearby coal-fired power plant [92]. Using the PinG treatment resulted in less simulated dry deposition of atmospheric nitrogen than a purely gridded model, approximately half as much in the immediate vicinity of the plant and by 10% over the Escambia Bay watershed. In another APT modeling study, the export of reactive nitrogen (nitrogen oxides and their oxidation products, collectively referred to as NO_y) from 25 coal-fired power plants in the U.S. to the global atmosphere was investigated [93]. The results from the study showed that the APT simulation predicted 31% greater simulated export of NO_y compared to the purely grid-based modeling approach.

CMAQ-APT was recently adapted to develop a prototype model that could be used to simulate near-roadway concentrations due to mobile emissions from roadways [94]. The motivation for the study was the increasing concern about population exposure to hazardous air pollutants (HAPs), especially in the vicinity of the sources of these pollutants. The model was applied to a 51 km stretch of a busy interstate highway in New York City. For this prototypical application, the roadway was treated as a series of adjacent elongated area sources (approximately 1700) where each source represented a road segment, and the emissions of each source were explicitly simulated with the plume component of the model [94]. The model was able to successfully capture the observed spatial variability in exposure levels from near the source to several hundreds of meters from the source.

The parallelized version of CMAQ-APT, as part of a comprehensive modeling system entitled AMSTERDAM (the Advanced Modeling System for Transport, Emissions, Reactions and Deposition of Atmospheric Matter), was applied to the central and eastern United States for summer and winter periods in 2002 [89,95]. Over 150 coal-fired power plants in the domain were selected for PinG treatment in this application. Although similar model performances were obtained with and without PinG treatment, the results showed significant differences in the specific nature of the predicted spatial distribution of ozone and PM_{2.5} concentrations. For example, a comparison of the 8-hour average ozone concentrations predicted from the PinG and grid-only configurations showed that using the PinG approach resulted in decreases of up to 13 ppb and increases of about 8 ppb in predicted ozone concentrations. The effect of using the PinG approach on PM_{2.5} also showed regions of both decreases and increases in PM_{2.5} concentrations. The decreases were generally larger in magnitude than the increases, *i.e.*, the PinG configuration generally resulted in significantly lower PM_{2.5} concentrations (by up to 12 μ g m⁻³) over large portions of the modeling domain and slightly higher (by less than1 μ g m⁻³) PM_{2.5} concentrations.

PinG applications with CAMx also show that overall model performance is little changed with the PinG approach, but the spatial distribution of ozone and $PM_{2.5}$ concentrations can be substantially different, especially near sources. In a northeast Texas ozone modeling study for the summer of 2005, the CAMx GREASD-PiG option was used to treat emissions from selected major NO_x emitters in the modeling domain [96]. The model was able to successfully capture the general observed transport of the plume from the Dolet Hills power plant, located in Louisiana, southwestward into northeast Texas, on 8 September 2005. The Dolet Hill plume observations were conducted by Baylor University's Piper Aztec aircraft. The model correctly simulated the ozone and NO_y plume enhancements and the approximate plume length, but predicted plume ozone maximums closer to the Dolet Hills plant than in the observations. It also displaced the modeled plume slightly to the southeast of the observed plume due to a small bias in the MM5 wind directions used to drive the model [96].

4. Summary and Future Directions

This paper has described and compared various approaches used in air quality models to resolve fine scale processes. Our review focuses on one such approach, PinG modeling, that has been widely used in

previous and current operational air quality models. Early PinG models were primarily developed and applied for ozone modeling and included a simple treatment of plume dispersion and transport. However, today's PinG models are increasingly being used to look at multipollutant issues, consistent with the "one-atmosphere" approach used in current models, and incorporate a state-of-the-science treatment of both plume dispersion and chemistry. Like other fine scale modeling approaches, PinG modeling imposes computational overhead in a grid model simulation. However, the parallelization of the PinG codes and the widespread availability of multi-processing workstations has addressed this limitation to a large extent.

The ability of the PinG approach to resolve a range of scales along with the capability to simulate detailed atmospheric chemistry makes it a practical tool to address sub-grid scale resolution issues. The prototypical roadway application [94] demonstrates that the PinG approach can be applied in non-traditional settings, such as near-source exposure assessments, compliance with 1-hour NO₂ standards (recently revised in the US [97]), or the air quality impacts of airports. Adding the capability to conveniently simulate different source types, such as line sources, would increase the utility of PinG models for such applications. Another improvement to current PinG models would be the ability to operate with meteorological inputs at a finer scale than the host grid model resolution. In all the PinG applications to date, the meteorology and other inputs, such as terrain elevations, that drive the plume model are at the same grid resolution as the host model. Using finer scale meteorology will allow a more accurate treatment of sub-grid scale transport.

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References

- Richards, L.W.; Anderson, J.A.; Blumenthal, D.L.; Brandt, A.A.; McDonald, J.A.; Waters, N.; Macias, E.S.; Bhardwaja, P.S. The chemistry, aerosol physics, and optical properties of a western coal-fired power plant plume. *Atmos. Environ.* **1981**, *15*, 2111–2134.
- 2. Gillani, N.V.; Meagher, J.F.; Valente, R.J.; Imhoff, R.E.; Tanner, R.L.; Luria, M. Relative production of ozone and nitrates in urban and rural power plant plumes 1. Composite results based on data from 10 field measurement days. *J. Geophys. Res.* **1998**, *103*, 22593–22615.
- 3. Karamchandani, P.; Koo, A.; Seigneur, C. Reduced gas-phase kinetic mechanism for atmospheric plume chemistry. *Environ. Sci. Technol.* **1998**, *32*, 1709–1720.
- 4. Karamchandani, P.; Seigneur, C. Simulation of sulfate and nitrate chemistry in power plant plumes. *J. Air Waste Manag. Assoc.* **1999**, *49*, 175–181.
- 5. Taghavi, M.; Cautenet, S.; Foret, G. Simulation of ozone production in a complex circulation region using nested grids. *Atmos. Chem. Phys.* **2004**, *4*, 825–838.
- 6. Arunachalam, S.; Holland, A.; Do, B.; Abraczinskas, M. A quantitative assessment of the influence of grid resolution on predictions of future-year air quality in North Carolina, USA. *Atmos. Environ.* **2006**, *40*, 5010–5026.

- Queen, A.; Zhang, Y. Examining the Sensitivity of MM5-CMAQ predictions to explicit microphysics schemes and horizontal grid resolutions, Part III—The impact of horizontal grid resolution. *Atmos. Environ.* 2008, 42, 3869–3881.
- Mircea, M.; Cappelletti, A.; Briganti, G.; Vitali, L.; Pace, G.; Marri, P.; Silibello, C.; Finardi, S.; Calori, G.; Zanini, G. Impact of Horizontal Grid Resolution on Air Quality Modeling: A Case Study over Italy. In *Proceedings of the 13th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, Paris, France, June 2010.
- Byun, D.; Schere, K.L. Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.* 2006, 59, 51–77.
- 10. Odman, M.T.; Russell, A.G. Multiscale modeling of pollutant transport and chemistry. *J. Geophys. Res.* **1991**, *96*, 7363–7370.
- 11. Odman, M.T.; Russell, A.G. A multiscale finite element pollutant transport scheme for urban and regional modeling. *Atmos. Environ. Part A Gen. Top.* **1991**, *25*, 2385–2394.
- 12. Kumar, N.; Odman, M.T.; Russell, A.G. Multiscale air quality modeling: Application to Southern California. J. Geophys. Res. **1994**, 99, 5385–5397.
- 13. Kumar, N.; Russell, A.G. Multiscale air quality modeling of the Northeastern United States. *Atmos. Environ.* **1996**, *30*, 1099–1116.
- 14. Morris, R.E.; Yarwood, G.; Emery, C.; Wilson, G. Recent Advances in CAMx Air Quality Modeling. In *Proceedings of the AWMA 94th Annual Meeting and Exhibition*, Orlando, FL, USA, June 2001.
- 15. Morris, R.E.; Yarwood, G.; Emery, C.A.; Wilson, G. Recent Advances in Photochemical Air Quality Modeling Using the CAMx Model: Current Update and Ozone Modeling of Point Source Impacts. In *Proceedings of the AWMA 95th Annual Meeting and Exhibition*, Baltimore, MD, USA, June 2002.
- 16. Grell, G.A.; Peckham, S.E.; Schmitz, R.; McKeen, S.A.; Frost, G.; Skamarock, W.C.; Eder, B. Fully coupled "online" chemistry within the WRF model. *Atmos. Environ.* **2005**, *39*, 6957–6975.
- 17. Morris, R.E.; Yocke, M.A.; Myers, T.C.; Mirabella, V. Overview of the Variable Grid Urban Airshed Model (UAM-V). In *Proceedings of the AWMA 85th Annual Meeting*, Pittsburgh, PA, USA, June 1992.
- Zhang, Y.; Wen, X.Y.; Jang, C.J. simulating chemistry-aerosol-cloud-radiation-climate feedbacks over the continental U.S. using the online-coupled Weather Research Forecasting Model with chemistry (WRF/Chem). *Atmos. Environ.* 2010, 44, 3568–3582.
- Zhang, Y.; Pan, Y.; Wen, X.-Y.; Dong, X.-Y.; Karamchandani, P.; Streets, D.G.; Skamaroc, W.C.; Grell, G.A. Simulating Climate-Air Quality Interactions Using Global-through-Urban WRF/Chem. In *Proceedings of the 11th Conference on Atmospheric Chemistry/the 89th AMS Annual Meeting*, Phoenix, AZ, USA, January 2009.
- 20. Zhang, Y.; Pan, Y.; Wen, X.-Y.; Chen, Y.-S.; Hemperly, J.; Karamchandani, P.; Streets, D.G.; Jang, C. Global-through-Urban WRF/Chem: A Unified Model for Simulating Aerosol-Climate Interactions and Evaluating Co-Benefit for Air Quality and Climate Change. In *Proceedings of the Joint Workshop of EMEP's Task Force on Measurements and Modeling (TFMM) and the Task Force on Hemispheric Transport of Air Pollution (TF HTAP)*, Paris, France, June 2009.

- 21. McRae, G.J.; Goodin, W.R.; Seinfeld, J.H. Development of a second-generation mathematical model for Urban air pollution-I. Model formulation. *Atmos. Environ.* **1982**, *16*, 679–696.
- Brooks, A.N.; Hughes, T.J.R. Streamline upwind/Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations. *Comput. Methods Appl. Mech. Eng.* 1982, 32, 199–259.
- Sokhi, R.S.; San José, R.; Kitwiroon, N.; Fragkou, E.; Pérez, J.L.; Middleton, D.R. Prediction of ozone levels in London using the MM5-CMAQ modelling system. *Environ. Model. Softw.* 2006, 21, 566–576.
- 24. Stein, A.F.; Isakov, V.; Godowitch, J.; Draxler, R.R. A hybrid modeling approach to resolve pollutant concentrations in an urban area. *Atmos. Environ.* **2007**, *41*, 9410–9426.
- 25. Shrestha, K.L.; Kondo, A.; Kaga, A.; Inoue, Y. High-resolution modeling and evaluation of ozone air quality of Osaka using MM5-CMAQ system. *J. Environ. Sci.* **2009**, *21*, 782–789.
- 26. Morris, R.E.; Kemball-Cook, S.; Nopmongcol, U.; Parker, L. Fine-Scale Modeling with CMAQ and CAMx for Air Toxics, PM and Ozone in Detroit. In *Proceedings of the AWMA Guideline on Air Quality Models: Next Generation of Models Conference*, Research Triangle Park, NC, USA, October 2009.
- Fann, N.; Roman, H.A.; Fulcher, C.M.; Gentile, M.A.; Hubbell, B.J.; Wesson, K.; Levy, J.I. Maximizing health benefits and minimizing inequality: Incorporating local-scale data in the design and evaluation of air quality policies. *Risk Anal.* 2011, *31*, 908–922.
- Tomlin, A.; Berzins, M.; Ware, J.; Smith, J.; Pilling, M.J. On the use of adaptive gridding methods for modelling chemical transport from multi-scale sources. *Atmos. Environ.* 1997, 31, 2945–2959.
- 29. Hart, G.; Tomlin, A.; Smith, J.; Berzins, M. Multi-scale atmospheric dispersion modelling by use of adaptive gridding techniques. *Environ. Monit. Assess.* **1998**, *52*, 225–238.
- Bacon, D.P.; Ahmad, N.N.; Boybeyi, Z.; Dunn, T.J.; Hall, M.S.; Lee, P.C.S.; Sarma, R.A.; Turner, M.D.; Waight, K.T.; Young, S.H.; *et al.* A dynamically adapting weather and dispersion model: The Operational Multiscale Environment Model with Grid Adaptivity (OMEGA). *Mon. Weather Rev.* 2000, *128*, 2044–2076.
- Khan, M.; Odman, T.; Karimi, H. Reducing Uncertainty of Air Quality Models through Coupling Adaptive Grids with GIS Techniques. In *Proceedings of the 2nd ICGESA International Conference on GIS for Earth Science Applications*, Izmir, Turkey, September 2000.
- 32. Ghorai, S.; Tomlin, A.S.; Berzins, M. Resolution of pollutant concentrations in the boundary layer using a fully 3D adaptive gridding technique. *Atmos. Environ.* **2000**, *34*, 2851–2863.
- Odman, M.T.; Khan, M.N.; McRae, D.S. Adaptive Grids in Air Pollution Modeling: Towards an Operational Model. In *Proceedings of the 24th (Millennium) NATO/CCMS International Technical Meeting on Air Pollution Modeling and its Application*, Boulder, CO, USA, 15–19 May 2000; Gryning, S.E., Schiermeier, F.A., Eds.; Kluwer Academic/Plenum Publishers: New York, NY, USA, 2000; pp. 541–549.
- 34. Srivastava, R.K.; McRae, D.S.; Odman, M.T. An adaptive grid algorithm for air-quality modeling. *J. Comput. Phys.* **2000**, *165*, 437–472.
- 35. Srivastava, R.K.; McRae, D.S.; Odman, M.T. Simulation of dispersion of a power plant plume using an adaptive grid algorithm. *Atmos. Environ.* **2001**, *35*, 4801–4818.

- 36. Srivastava, R.K.; McRae, D.S.; Odman, M.T. Simulation of a reacting pollutant puff using an adaptive grid algorithm. *J. Geophys. Res.* **2001**, *106*, 24245–24257.
- Odman, M.T.; Khan, M.; Srivastava, R.; McRae, D.S. Initial Application of the Adaptive Grid Air Quality Model. In *Air Pollution Modeling and its Application XV*; Borrego, C., Schayes, G., Eds.; Kluwer Academic/Plenum Publishers: New York, NY, USA, 2002; pp. 319–328.
- 38. Odman, M.T.; Khan, M.N. Adaptive Grid Air Quality Model: Application to an Ozone Episode. In *Proceedings of the 12th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association*, Norfolk, VA, USA, May 2002.
- Mathur, R.; Shankar, U.; Hanna, A.F.; Odman, M.T.; McHenry, J.N.; Coats, C.J., Jr.; Alapaty, K.; Xiu, A.; Arunachalam, S.; Olerud, D.T., Jr.; *et al.* Multiscale air quality simulation platform (MAQSIP): Initial applications and performance for tropospheric ozone and particulate matter. *J. Geophys. Res.* 2005, *110*, D13308.
- Unal, A.; Odman, M.T. Adaptive Grid Modeling for Predicting the Air Quality Impacts of Biomass Burning. In *Proceedings of the 2nd International Wildland Fire Ecology and Fire Management Congress*, Orlando, FL, USA, November 2003.
- Belwal, C.; Sandu, A.; Constantinescu, E.M. Adaptive Resolution Modeling of Regional Air Quality. In *Proceedings of the 2004 ACM Symposium on Applied Computing*, Nicosia, Cyprus, 14–17 May 2004; ACM: New York, NY, USA, 2004; pp. 235–239.
- 42. Constantinescu, E.; Sandu, A.; Carmichael, G. Modeling atmospheric chemistry and transport with dynamic adaptive resolution. *Comput. Geosci.* **2008**, *12*, 133–151.
- 43. Carmichael, G.R.; Peters, L.K.; Saylor, R.D. The STEM-II regional scale acid deposition and photochemical oxidant model-I. An overview of model development and applications. *Atmos. Environ. Part A Gen. Top.* **1991**, *25*, 2077–2090.
- Odman, M.T.; Hu, Y. A Variable Time-Step Algorithm for Air Quality Models. In *Air Pollution Modeling and Its Application XVII*; Borrego, C., Norman, A.-L., Eds.; Springer: New York, NY, USA, 2007; pp. 411–420.
- 45. Odman, M.T.; Hu, Y. A variable time-step algorithm for air quality models. *Atmos. Pollut. Res.* **2010**, *1*, 229–238.
- 46. Odman, M.T.; Hu, Y.; Yano, A.; Garcia-Menendez, F.; Achtemeier, G.L.; Goodrick, S.L.; Naeher, L.P. Development of a Modeling System for Prescribed Burn Emissions and Air Quality Impacts. In *Proceedings of the 16th Conference on Air Pollution Meteorology*, Atlanta, GA, USA, January 2010.
- 47. Garcia-Menendez, F.; Yano, A.; Hu, Y.; Odman, M.T. An adaptive grid version of CMAQ for improving the resolution of plumes. *Atmos. Pollut. Res.* **2010**, *1*, 239–249.
- 48. Garcia-Menendez, F.; Odman, M.T. Adaptive grid use in air quality modeling. *Atmos.* 2011, submitted for publication.
- 49. Zhu, Y.; Hinds, W.C.; Kim, S.; Sioutas, C. Concentration and size distribution of ultrafine particles near a major highway. *J. Air Waste Manag. Assoc.* **2002**, *52*, 1032–1042.
- 50. Zhu, Y.; Hinds, W.C.; Kim, S.; Shen, S.; Sioutas, C. Study of ultrafine particles near a major highway with heavy-duty diesel traffic. *Atmos. Environ.* **2002**, *36*, 4323–4335.
- 51. Zhu, Y.; Hinds, W.C.; Shen, S.; Sioutas, C. Seasonal trends of concentration and size distribution of ultrafine particles near major highways in Los Angeles. *Aerosol Sci. Technol.* **2004**, *38*, 5–13.

- 52. Weijers, E.P.; Khlystov, A.Y.; Kos, G.P.A.; Erisman, J.W. Variability of particulate matter concentrations along roads and motorways determined by a moving measurement unit. *Atmos. Environ.* **2004**, *38*, 2993–3002.
- 53. Ching, J.; Pierce, T.; Palma, T.; Hutzell, W.; Tang, R.; Cimorelli, A.; Herwehe, J. Application of Fine Scale Air Toxics Modeling with CMAQ to HAPEM5. In *Proceedings of the 3rd Annual CMAS Models-3 Conference*, Chapel Hill, NC, USA, October 2004.
- 54. Ching, J.; Herwehe, J.; Swall, J. On joint deterministic grid modeling and sub-grid variability conceptual framework for model evaluation. *Atmos. Environ.* **2006**, *40*, 4935–4945.
- 55. Touma, J.S.; Isakov, V.; Ching, J.; Seigneur, C. Air quality modeling of hazardous pollutants: Current status and future directions. *J. Air Waste Manag. Assoc.* **2006**, *56*, 547–558.
- 56. Isakov, V.; Venkatram, A. Resolving neighborhood scale in air toxics modeling: A case study in Wilmington, CA. J. Air Waste Manag. Assoc. 2006, 56, 559–568.
- 57. Isakov, V.; Irwin, J.S.; Ching, J. Using CMAQ for exposure modeling and characterizing the subgrid variability for exposure estimates. *J. Appl. Meteorol. Climatol.* **2007**, *46*, 1354–1371.
- Isakov, V.; Touma, J.S.; Burke, J.; Lobdell, D.T.; Palma, T.; Rosenbaum, A.; Ozkaynak, H. Combining regional- and local-scale air quality models with exposure models for use in environmental health studies. *J. Air Waste Manag. Assoc.* 2009, *59*, 461–472.
- Wesson, K.; Baker, K.; Nopmongcol, U.; Yarwood, G.; Sakulyanontvittaya, T.; Strum, M.; Thurman, J.; Camalier, L.; Ensley, D.; Timin, B.; *et al.* Comparing Models/Methods for Estimating Multipollutant Fine-Scale Air Quality Concentrations. In *Air Pollution Modeling and its Application XX*; Steyn, D.G., Rao, S.T., Eds.; Springer Science: Dordrecht, The Netherlands, 2010; pp. 81–85.
- 60. Wesson, K.; Fann, N.; Morris, M.; Fox, T.; Hubbell, B. A multi-pollutant, risk-based approach to air quality management: Case study for detroit. *Atmos. Pollut. Res.* **2010**, *1*, 296–304.
- Cook, R.; Isakov, V.; Touma, J.S.; Benjey, W.; Thurman, J.; Kinnee, E.; Ensley, D. Resolving local-scale emissions for modeling air quality near roadways. *J. Air Waste Manag. Assoc.* 2008, 58, 451–461.
- 62. Galmarini, S.; Vinuesa, J.F.; Martilli, A. Modeling the impact of sub-grid scale emission variability on upper-air concentration. *Atmos. Chem. Phys.* **2008**, *8*, 141–158.
- Valari, M.; Menut, L. Transferring the heterogeneity of surface emissions to variability in pollutant concentrations over urban areas through a chemistry-transport model. *Atmos. Environ.* 2010, 44, 3229–3238.
- 64. Cassiani, M.; Vinuesa, J.F.; Galmarini, S.; Denby, B. Stochastic fields method for sub-grid scale emission heterogeneity in mesoscale atmospheric dispersion models. *Atmos. Chem. Phys.* **2010**, *10*, 267–277.
- 65. Arunachalam, S. Multiscale Simulations and Analyses of Impacts of Aviation Emissions on Ambient Air Quality. In *Proceedings of the OMEGA International Conference on Airport Air Quality*, London, UK, October 2008.
- 66. Davis, N.; Arunachalam, S. A Hybrid CMAQ and AERMOD Approach to Investigate the Impact of Airports on Local Air Quality. In *Proceedings of the 8th Annual Models-3/CMAS Users Conference*, Chapel Hill, NC, USA, October 2009.

- 67. Karamchandani, P.; Santos, L.; Sykes, I.; Zhang, Y.; Tonne, C.; Seigneur, C. Development and evaluation of a state-of-the-science reactive plume model. *Environ. Sci. Technol.* **2000**, *34*, 870–880.
- 68. Seigneur, C.; Tesche, T.W.; Roth, P.M.; Liu, M.-K. On the treatment of point source emissions in urban air quality modeling. *Atmos. Environ.* **1983**, *17*, 1655–1676.
- 69. Reynolds, S.D.; Roth, P.M.; Seinfeld, J.H. Mathematical modeling of photochemical air pollution-I: Formulation of the model. *Atmos. Environ.* **1973**, *7*, 1033–1061.
- 70. Morris, R.E.; Yocke, M.A.; Myers, T.C.; Kessler, R.C. Development and Testing of UAM-V: A Nested-Grid Version of the Urban Airshed Model. In *Proceedings of the AWMA Specialty Conference: Tropospheric Ozone and the Environment II*, Atlanta, GA, USA, November 1991.
- 71. Sillman, S.; Logan, J.A.; Wofsy, S.C. A regional scale model for ozone in the United States with subgrid representation of urban and power plant plumes. *J. Geophys. Res.* **1990**, *95*, 5731–5748.
- 72. Myers, T.C.; Guthrie, P.D.; Wu, S.-Y. *The Implementation of a Plume-in-Grid Module in the SARMAP Air Quality Model (SAQM)*; SYSAPP-96/06; Systems Applications International, Inc.: San Rafael, CA, USA, 1996.
- 73. Chang, J.S.; Jin, S.; Li, Y.; Beauharnois, M.; Lu, C.-H.; Huang, H.-C. *The SARMAP Air Quality Model*; Final Report; Atmospheric Sciences Research Center: Albany, NY, USA, 1997.
- 74. Kumar, N.; Russell, A.G. Development of a computationally efficient, reactive subgrid-scale plume model and the impact in the northeastern united states using increasing levels of chemical detail. *J. Geophys. Res.* **1996**, *101*, 16737–16744.
- 75. Gillani, N.V.; Godowitch, J.M. Plume-in-Grid Treatment of Major Point Source Emissions. In Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, EPA-600/R-99/030; Byun, D.W., Ching, J., Eds.; U.S. Environmental Protection Agency: Washington, DC, USA, 1999; Chapter 9.
- Godowitch, J. Simulations of Aerosols and Photochemical Species with the CMAQ Plume-in-Grid Modeling System. In *Proceedings of the 3rd Annual CMAS Models-3 User's Conference*, Chapel Hill, NC, USA, October 2004.
- 77. Gillani, N.V. Ozone Formation in Pollutant Plumes: Development and Application of a Reactive Plume Model with Arbitrary Crosswind Resolution; EPA-600/S3-86-051; U.S. Environmental Protection Agency: Research Triangle Park, NC, USA, 1986.
- 78. Karamchandani, P.; Seigneur, C.; Vijayaraghavan, K.; Wu, S.-Y. Development and application of a state-of-the-science plume-in-grid model. *J. Geophys. Res.* **2002**, *107*, 4403.
- 79. Karamchandani, P.; Vijayaraghavan, K.; Chen, S.-Y.; Seigneur, C.; Edgerton, E.S. Plume-in-grid modeling for particulate matter. *Atmos. Environ.* **2006**, *40*, 7280–7297.
- ENVIRON. *CAMx (Version 5.30) User's Guide*; ENVIRON International Corporation: Novato, CA, USA, 2010; Available online: http://www.camx.com/files/CAMxUsersGuide_v5.30.pdf (accessed on 17 August 2011).
- Karamchandani, P.; Vijayaraghavan, K.; Zhang, Y.; Chen, S.-Y. Development of a Plume-in-Grid Version of Global-through-Urban WRF/Chem. In *Proceedings of the 9th Annual CMAS Conference*, Chapel Hill, NC, USA, October 2010.

- Korsakissok, I.; Mallet, V. Subgrid-scale treatment for major point sources in an eulerian model: A sensitivity study on the European Tracer Experiment (ETEX) and chernobyl cases. *J. Geophys. Res.* 2010, 115, D03303.
- 83. Korsakissok, I.; Mallet, V. Development and application of a reactive plume-in-grid model: Evaluation over Greater Paris. *Atmos. Chem. Phys.* **2010**, *10*, 8917–8931.
- Alvarado, M.J.; Wang, C.; Prinn, R.G. Formation of ozone and growth of aerosols in young smoke plumes from biomass burning: 2. Three-dimensional eulerian studies. *J. Geophys. Res.* 2009, 114, D09307.
- 85. Yano, A.; Garcia-Menendez, F.; Hu, Y.; Odman, M.T.; McRae, D.S.; Achtemeier, G.L. Modeling Biomass Burnings by Coupling a Sub-Grid Scale Plume Model with Adaptive Grid CMAQ. In *Proceedings of the 9th Annual CMAS Conference*, Chapel Hill, NC, USA, October 2010.
- 86. Sykes, R.I.; Parker, S.F.; Henn, D.S.; Lewellen, W.S. Numerical simulation of anatex tracer data using a turbulence closure model for long-range dispersion. *J. Appl. Meteorol.* **1993**, *32*, 929–947.
- 87. Sykes, R.I.; Henn, D.S. Representation of velocity gradient effects in a gaussian puff model. *J. Appl. Meteorol.* **1995**, *34*, 2715–2723.
- 88. Vijayaraghavan, K.; Karamchandani, P.; Seigneur, C. Plume-in-grid modeling of summer air pollution in central California. *Atmos. Environ.* **2006**, *40*, 5097–5109.
- Karamchandani, P.; Vijayaraghavan, K.; Chen, S.-Y.; Balmori-Bronson, R.; Knipping, E.M. Development and application of a parallelized version of the Advanced Modeling System for Transport, Emissions, Reactions and Deposition of Atmospheric Matter (AMSTERDAM): 1. Model performance evaluation and impacts of plume-in-grid treatment. *Atmos. Pollut. Res.* 2010, *1*, 260–270.
- 90. Karamchandani, P.; Vijayaraghavan, K.; Seigneur, C. Detailed Treatment of Power Plant Plumes in the Regional Modeling of Atmospheric Mercury. In *Proceedings of the 8th International Conference on Mercury as a Global Pollutant*, Madison, WI, USA, August 2006.
- 91. Vijayaraghavan, K.; Karamchandani, P.; Seigneur, C.; Balmori, R.; Chen, S.-Y. Plume-in-grid modeling of atmospheric mercury. *J. Geophys. Res.* **2008**, *113*, D24305.
- 92. Vijayaraghavan, K.; Balmori, R.T.; Chen, S.-Y.; Karamchandani, P.; Seigneur, C. Modeling of Atmospheric Nitrogen Deposition to the Escambia Bay and Watershed in the Southeastern United States. In *Proceedings of the 6th Annual CMAS Conference*, Chapel Hill, NC, USA, October 2007.
- Vijayaraghavan, K.; Zhang, Y.; Seigneur, C.; Karamchandani, P.; Snell, H.E. Export of reactive nitrogen from coal-fired power plants in the U.S.: Estimates from a plume-in-grid modeling study. *J. Geophys. Res.* 2009, *114*, D04308.
- 94. Karamchandani, P.; Lohman, K.; Seigneur, C. Using a sub-grid scale modeling approach to simulate the transport and fate of toxic air pollutants. *Environ. Fluid Mech.* **2009**, *9*, 59–71.
- 95. Karamchandani, P.; Vijayaraghavan, K.; Chen, S.-Y.; Balmori-Bronson, R.; Knipping, E.M. Development and application of a parallelized version of the Advanced Modeling System for Transport, Emissions, Reactions and Deposition of Atmospheric Matter (AMSTERDAM): 2. Source region contributions. *Atmos. Pollut. Res.* 2010, *1*, 271–279.
- 96. Kemball-Cook, S.; Johnson, J.; Yarwood, G. *Modeling Northeast Texas Ozone for Summer 2005*; ENVIRON International Corporation: Novato, CA, October 2006.

97. U.S. EPA. Primary National Ambient Air Quality Standards for Nitrogen Dioxide; Final Rule. *Federal Register, Vol. 75, No. 26, Rules and Regulations, 40 CFR Parts 50 and 58, 9 February* 2010; Available online: http://www.epa.gov/ttn/naaqs/standards/nox/fr/20100209.pdf (accessed on 17 August 2011).

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