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SIMULATION OF HAZARDOUS ATMOSPHERIC RELEASES USING OMEGA

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SUMMARY

The Operational Multiscale Environment model with Grid Adaptivity (OMEGA) is a new atmospheric simulation system that merges state-of-the-art computational fluid dynamics techniques with a comprehensive non-hydrostatic equation set. Based upon an unstructured triangular prism grid, OMEGA permits simulation of hazardous releases at all scales with horizontal grid resolution ranging from 100 km down to 1 km and a vertical resolution from a few tens of meters in the planetary boundary layer to 1 km in the free troposphere.

I. INTRODUCTION AND OVERVIEW

Numerous natural and anthropogenic activities can lead to the atmospheric release of hazardous materials. This can range from a localized accidental release of radioactivity or a hazardous chemical (*e.g.*, Chernobyl and Bhopal, respectively) to the intentional widespread release of atmospheric pollutants (*e.g.*, the Kuwait oil field fires). Our ability to understand the impact of these releases on both the environment, and upon human activity depends critically upon our ability to simulate the near and far field transport and diffusion of the pollutant. The accurate simulation of the transport and diffusion of an aerosol or gas in the atmosphere in turn depends critically upon the accurate simulation of the wind and turbulence fields.

Aerosol transport and diffusion models typically use large scale observed or analyzed wind fields to transport the aerosol. As an alternative, they may use the results from a mesoscale meteorological model which has been saved at some spatial resolution at pre-determined times. While this approach has been sufficient for many studies to date, the data requirements grow as the inverse cube of the grid resolution. Improving aerosol transport capability by increasing the grid resolution from roughly 100 km to 1 km increases the data handling requirements of the model by roughly one million times.

The goal of creating an operational aerosol and gas dispersion model with horizontal resolution down to 1 km and vertical resolution down to a few tens of meters determines a number of requirements imposed upon the model. It must be fully non-hydrostatic, three dimensional, and contain extensive surface and PBL physics packages. OMEGA was built to meet these requirements (Table 1). Two key features are the use of an unstructured triangular grid and the incorporation of **embedded** transport and diffusion models.

The unstructured grid used in OMEGA is naturally scale spanning and adaptable. The OMEGA grid can readily adapt to fixed surface or terrain features, or dynamic features in the evolving weather. OMEGA can provide enhanced grid resolution in localized regions such as urban areas, airports, air route corridors, or sources of pollution or potential hazardous release locations such as chemical plants and accident sites. Finally, the grid generator for OMEGA produces these adapted grids **automatically**.

The embedded dispersion models in OMEGA permit the simulation of transport and diffusion to proceed with full access to all of the meteorological variables **at each timestep** without the burden of writing all of this data.

II. OMEGA GRID STRUCTURE

The great bulk of releases occur near the surface, are restricted to the PBL, and are strongly influenced by the surface features.[1,2] These situations require the highest possible resolution of both the atmospheric state as well as the aerosol concentration.

OMEGA is based on an unstructured triangular prism computational mesh.[3] This mesh is unstructured in the *horizontal* dimension and structured in the *vertical* dimension. The rationale for this mesh is the physical reality that the atmosphere is roughly decorrelated horizontally but correlated vertically. While completely unstructured three-dimensional meshes have been used for other purposes,[4] the benefit of having a structured vertical dimensional is a reduction of three orders of magnitude in the computational requirements of the model.

An OMEGA grid element is shown in Figure 1. These elements are stacked vertically in such a fashion that all of the cells in a column have the same projection onto the surface of the Earth (Figure 2). This common projected footprint considerably simplifies the grid generation and provides an extremely simple framework for the radiation transport model. The scalar quantities are defined at the

Table 1. OMEGA overview

Governing equations	Fully non-hydrostatic equation set
Dimensionality	3D
Grid structure	Unstructured and adaptive triangular prisms. Horizontal resolution from 100 km down to 1 km; vertical resolution from 20 m (near surface) to 1000 m (near tropopause).
Grid Adaptivity	Static adaptation to topography, land/water boundary, fixed surface features (*e.g.* airports, power plants). Dynamic adaptation to evolving atmospheric circulation.
Coordinate system	Rotating Cartesian coordinate framework
Numeric	Finite volume based upon Smolarkiewicz
Surface roughness	Specified over land, predicted over water
Soil surface	Based on the force-restore rate method
PBL	Planetary boundary layer is treated separately as viscous sublayer, surface layer, and transition layer
Turbulence closure	*First order closure*: O'Brien K-profile for unstable conditions; Blackadar local K-profile for stable conditions. *1.5 order* κ-ε *closure*: Based on turbulent kinetic energy and its dissipation
Cumulus parameterization	Modified Kuo scheme
Microphysics	Extensive bulk-water microphysics
Radiation	Shortwave absorption by water vapor and longwave emissivities of water vapor and carbon dioxide and computationally efficient technique of Sasamori
Initialization	Based on 4D data assimilation
Transport and diffusion	Embedded Eulerian and Lagrangian aerosol dispersion algorithms

geometric center of each grid element; the components of the velocity are defined at the center of the top face.

The major advantage of OMEGA over current state-of-the-art models includes the ability to resolve the surface terrain down to scales of 1 km by using the flexibility of the unstructured grid to place vertices only where required. This allows OMEGA to resolve microscale events while being fully consistent and providing the large scale forcing which is required to ensure the proper simulation of the atmosphere. In order to accomplish this, however, it is necessary to include all of the physical parameters and processes which affect the local flows. These include not only the topography, but also the land use, the land/water composition, the vegetation, the soil moisture, the snow cover (if appropriate), and the surface moisture and energy budgets. This additional physics, some of which is appropriate only because of the increased spatial resolution, represents an additional advance in the state-of-the-art.

OMEGA represents a significant advance for emergency response to atmospheric releases. Current operational systems are scale-specific and have a limit to their resolution caused by their fixed rectangular grid structure. OMEGA is naturally scale spanning and its unstructured grid permits the addition of grid elements at any point in space and time. Therefore OMEGA can readily

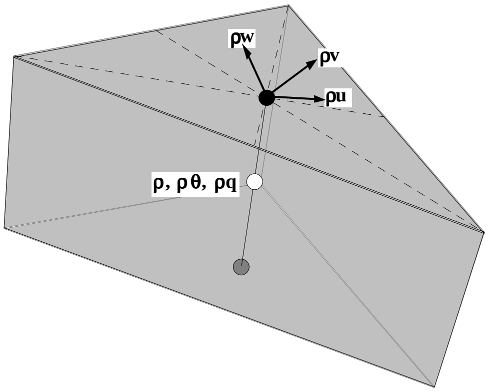


Figure 1. OMEGA grid element

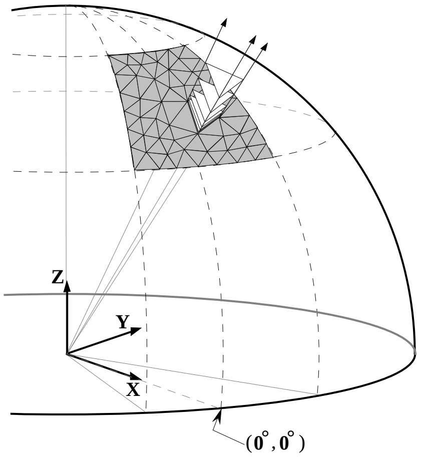


Figure 2. OMEGA coordinate system and vertical alignment of OMEGA grid.

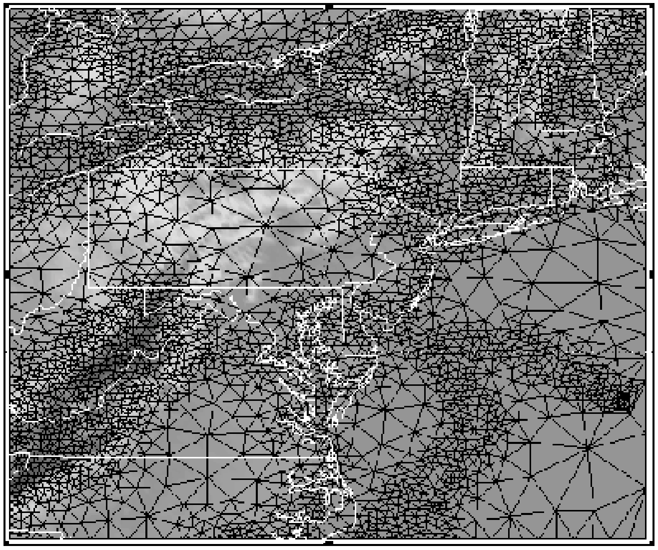


Figure 3. OMEGA grid generated for the Nor'Easter of 1992. The grid was created by adapting to topography, land/water interface, and the weather existing at the beginning of the OMEGA simulation.

adapt its grid to fixed surface or terrain features (*e.g.* potential hazardous release sites such as chemical plants), or dynamic features in the evolving weather. In addition, OMEGA can provide enhanced grid resolution in localized regions such as in the vicinity of an aerosol cloud. OMEGA can resolve orographic and land/water boundary features improving the fine scale meteorological simulation and, in turn, the simulation of the aerosol transport. This is especially important in such situations as aerosol transport in complex terrain and near land/water boundaries.

Figure 3 shows a grid generated for the Nor'Easter of 1992. This grid was built by adapting to the gradient in elevation (thereby capturing the mountains with high resolution), adapting to the gradient in the land/water index (thereby placing higher resolution in the coastal regions), and adapting to an artificial field that represents the surface temperature gradient. The final grid contains 6835 triangles. The shortest edge length is roughly 4 km while the longest is roughly 140 km. More significantly, over 90% of the edges are less than 30 km in length. By contrast, it would require over 250,000 square cells in order to achieve this 4 km horizontal grid resolution using a standard, uniform, structured grid.

A final example of the flexibility of the OMEGA grid is seen in Figure 4. This figure shows an OMEGA grid generated to provide higher resolution in the vicinity of emission sources. In this case, the grid adapted to a subset of the 1990 Regional Interim Emissions Inventory (sources producing more than 25,000 TPY of SO_2). Future versions of OMEGA could adapt not only to the location of the emission source, but provide higher resolution depending on the strength of the source.

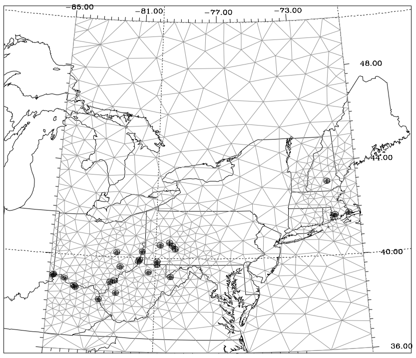


Figure 4. OMEGA grid adapting to the 1990 Regional Interim Emissions Inventory sources producing more than 25,000 TPY of SO_2.

III. EMBEDDED DISPERSION ALGORITHMS

Most current atmospheric transport and diffusion models create a wind field (from either data or simulation) and then transport the aerosol or gas in that wind field. This, for example, is the paradigm for Models-3, the next generation air quality model of the US Environmental Protection Agency (EPA).[5] This approach has some merit when the meteorological component of the modeling system is going to be re-used many times over. (A typical EPA study may vary emissions assumptions and alter the atmospheric chemistry package for fixed atmospheric conditions in order to develop an understanding of the driving factors in that particular air quality situation and to aid in the development of control strategies.) Under this paradigm, a meteorological modeling system is used to create a wind field which is output at selected times; the transport model then transports the aerosol and/or gas in this wind field. The Models-3 program will use the NCAR/Penn State University MM5 model coupled to the Alpha Prototype Chemistry-Transport package (a new chemistry and transport model); other similar systems include the Colorado State University Regional Atmospheric Modeling System (RAMS) coupled to a particle dispersion model.[6]

A major drawback to this approach is the large amount of data that must be output by the meteorological model and ingested by the particle transport model. As higher and higher resolution is implemented, this method quickly becomes bound by its input/output requirements. OMEGA overcomes this problem by incorporating the aerosol and gas dispersion **into** the meteorological model. OMEGA has both Eulerian (grid based) and Lagrangian dispersion models. These models have the benefit of the full simulation fields (temperature, moisture, wind, turbulence, *etc.*) at **each** timestep. In addition, the flexible grid structure of OMEGA permits the use of high resolution where it is naturally needed (in regions of complex terrain, near land/water boundaries, near emission sources) without burdening the model with high resolution everywhere. Next to the use of an unstructured grid, the embedding of the aerosol and gas dispersion routines into OMEGA represents a key departure from conventional techniques.

The OMEGA Eulerian dispersion is intended for use in situations involving a large scale dispersal and also for situations with extensive chemistry which is more easily treated in an Eulerian based system. The Eulerian dispersion algorithm uses the same conservation equation used for the water substance transport in the meteorological simulation part of OMEGA. This is given by:

$$\frac{\partial(\rho \mathrm{q}_i)}{\partial t} = -\nabla\cdot(\rho \mathrm{q}_i \mathrm{v}) + \nabla\cdot(\kappa\nabla\rho \mathrm{q}_i) + S \qquad (1)$$

where S represent the source and sink terms.

The Lagrangian dispersion is more useful for resolving very near source transport and diffusion issues as well as in tracking very diffuse highly localized tracer trajectories such as those in most hazardous transport situations. The Lagrangian dispersion operates in two modes: a particle and a Gaussian puff mode. In particle mode, the dispersion of pollutants in the atmosphere is simulated by means of a large ensemble of particles moving with *pseudo*-velocities composed of a mean transport velocity and a semi-random turbulent component.

$$\left.\begin{aligned} x(t+\Delta t) &= x(t) + \left[\overline{u}(t) + u'(t)\right]\Delta t \\ y(t+\Delta t) &= y(t) + \left[\overline{v}(t) + v'(t)\right]\Delta t \\ z(t+\Delta t) &= z(t) + \left[\overline{w}(t) + w'(t)\right]\Delta t \end{aligned}\right\} \qquad (2)$$

where $\overline{u}$, $\overline{v}$, and $\overline{w}$ are the mean wind components obtained directly from the highly resolved OMEGA prognostic wind field, and u', v', and w' are the corresponding subgrid scale turbulent velocity fluctuations whose statistics are derived from the boundary layer formulations used in the OMEGA model. The particle turbulent velocity fluctuations are calculated using a Markov chain scheme:

$$\left.\begin{aligned} u'(t+\Delta t) &= R_{u'}(\Delta t)\,u'(t) + r_{u'}(t+\Delta t) \\ v'(t+\Delta t) &= R_{v'}(\Delta t)\,v'(t) + r_{v'}(t+\Delta t) \\ w'(t+\Delta t) &= R_{w'}(\Delta t)\,w'(t) + r_{w'}(t+\Delta t) \end{aligned}\right\} \qquad (3)$$

where $r_{u'}$, $r_{v'}$, and $r_{w'}$ are purely random uncorrelated turbulent velocity components. Distributions of these turbulent velocity components are Gaussian with zero mean (*i.e.*, they are completely characterized by the variances).

The Lagrangian turbulent statistics in each of the three component directions need to still be determined. The required turbulent statistics are related to the OMEGA simulated turbulent kinetic energy using the relationship reported by Mellor and Yamada.[7]

IV. SIMULATION OF TRANSPORT IN A SEA BREEZE

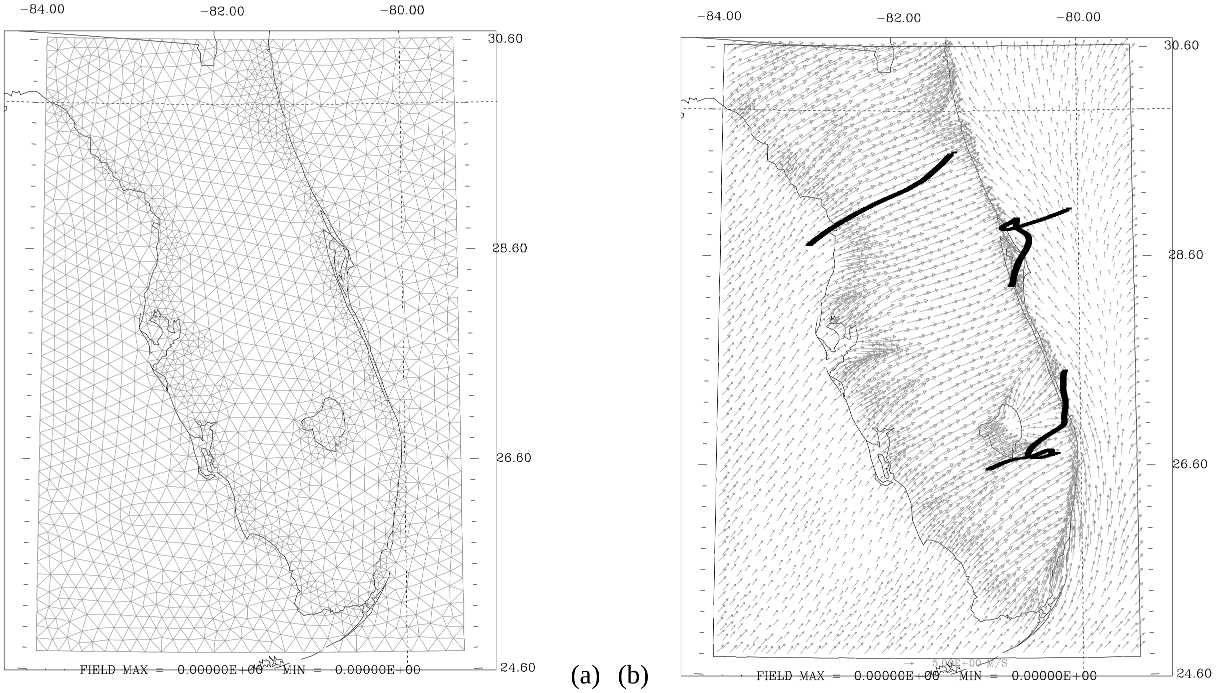
For operational uses, OMEGA is initialized from rawinsonde and surface observations and/or from analyzed gridded data from either the National Meteorological Center or the Fleet Numerical Meteorological and Oceanographic Center. In this mode, the OMEGA preprocessor performs an optimal interpolation of the data onto the unstructured OMEGA grid. For this test problem, however, an idealized flow was used.

A southwesterly flow of 6.0 m/s was used in this simulation for a typical summer day under the assumption that neither frontal nor tropical systems were present. The model domain contained 23 vertical levels with the model top at 6.5 km. The horizontal domain (about 600 km by 700 km) included 3929 unstructured grid cells with a high resolution in the vicinity of coastlines, surface property boundaries, and areas with a high potential for convective initiation. The grid had a variable effective size (defined by the square root of the area of the triangle) ranging from roughly 4 to 40 km (Figure 5a).

This 12 hour OMEGA simulation was initialized at 7 am local time. At 10 am local time, the background flow had not been significantly modified by the surface heating. By 1 pm, the effects of surface heating were seen as evidenced by the bending of the horizontal wind fields in the coastal regions, around Lake Okeechobee, and Cape Canaveral. The sea breeze formed in the Cape Canaveral area translated northward the plume which earlier had headed eastward. Also, a region of convergence was seen northeast of Lake Okeechobee, which is indicative of a normal southern Florida feature that initiates afternoon thunderstorm activity. Then by 4 pm (Figure 5b), the full effect of the Florida sea breeze could be seen. The three plume configurations clearly shows the influence of the enhanced sea breeze. The rather curlicue plumes seen in both the Cape Canaveral area and the Lake Okeechobee area are the result of the sea breeze convergence lofting the later plume to higher altitudes where it is not as affected by the sea breeze formed near the surface.

V. CONCLUSIONS

The high resolution in the coastal areas, made possible by the adaptive unstructured mesh, leads to a significant improvement in the resolution of the sea breeze and its impact on the larger scale circulations. The scale spanning grid of OMEGA resolves the large scale flow simultaneously with the small scale flow created by the bays and inlets improving the overall model fidelity. The vertical lofting caused by the sea breeze convergence is obviously important for any hazardous release situation.



(a) (b)

Figure 5. Simulation of the evolution of a Florida sea breeze using OMEGA. A uniform Southwesterly flow was initialized at 7 am local time. Shown are: (a) the grid used for the simulation and (b) the wind field and plume centroid (for three continuos releases) at 4 pm.

OMEGA represents a significant change in aerosol transport and diffusion modeling. For the first time, advanced numerical methods developed for computational fluid dynamics have been applied to atmospheric simulation. This has permitted the development of an extremely high resolution atmospheric simulation tool. In addition, by embedding the aerosol transport and diffusion model into the atmospheric simulation, the maximum benefit is derived. As seen in the application of OMEGA to the transport of an aerosol in the complex flow created by a sea breeze, this high resolution transport tool has a range of non-academic applications. This provides a unique platform for emergency response simulation.

ACKNOWLEDGEMENTS

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