www.sim-air.org

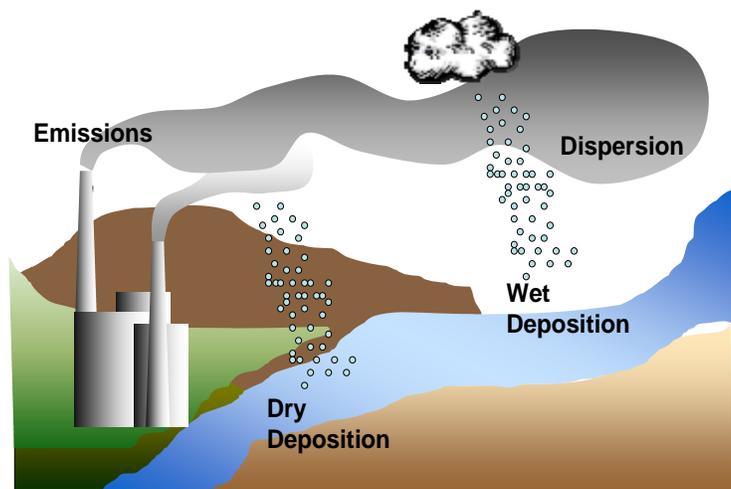# Simplified Atmospheric Transport Modeling System (ATMoS-4.0) for the SIM-air tool

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December, 2009

Emissions

Dispersion

Wet Deposition

Dry Deposition

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Simplified Atmospheric Transport Modeling System (ATMoS-4.0) for the SIM-air tool

Part 1: Dispersion model to generate source-receptor transfer matrix

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The SIM-air (Simple Interactive Models for better air quality) is an MS Excel based analytical tool for air pollution modeling, which enable the user to collate the available information on energy and emissions in a city and build an emissions inventory, followed by air quality modeling, health impact analysis and optimization among a possible array of the management options.

Scope of this Paper

In the SIM-air tool, all the calculations, including the conversion of emissions to concentrations, are conducted in Excel, using the source-receptor transfer matrix (SRTM). The transfer matrix, which enables the conversion of emissions to concentrations, is based on a dispersion model, which is not included the Excel analytical tool. This part of the calculations (generating the SRTM) is conducted outside the SIM-air tool and then transferred into Excel to enable further analysis to health impacts and optimization.

A number of dispersion models are available to support the development of SRTM; some are free for use with some technical support and some are available at commercial level. As usual, the dispersion models are very data intensive and need substantial training, before using the models for analysis.
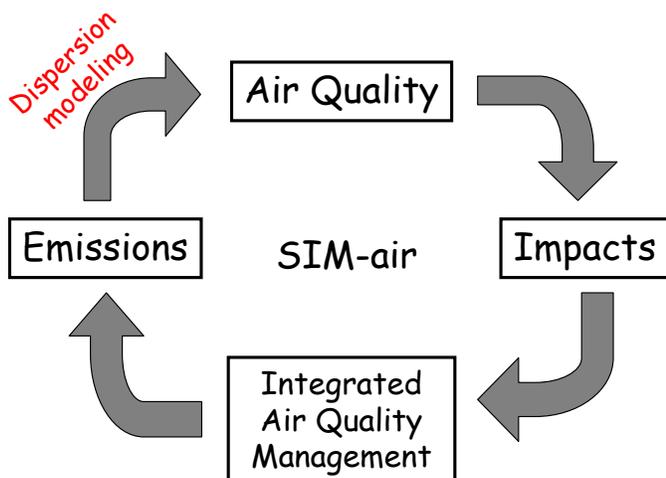

Figure 1: Outline for the SIM-air analytical tool

At the training events, there was one question which was asked repeatedly is "*access to a dispersion model, when the data available is minimum, experience is limited, and yet there is need for some rapid assessment*". While we supplemented the need for a dispersion model with SRTM concept, the generation of the SRTM based on a dispersion model is now available.

This paper describes a simplified dispersion model ATMoS-4.0 to generate SRTM using minimum data inputs for direct use in SIM-air for urban applications (see **Annex 1**).

Source-Receptor Transfer Matrix

The source-receptor transfer matrix presents the incremental change in concentrations due to an incremental change in emissions and defined as "change in concentrations in a receptor grid per ton/year change in emissions in the source grid". For the scenario analysis in urban cases, when the only variable changing is emissions, this methodology helps with the rapid assessment[1].
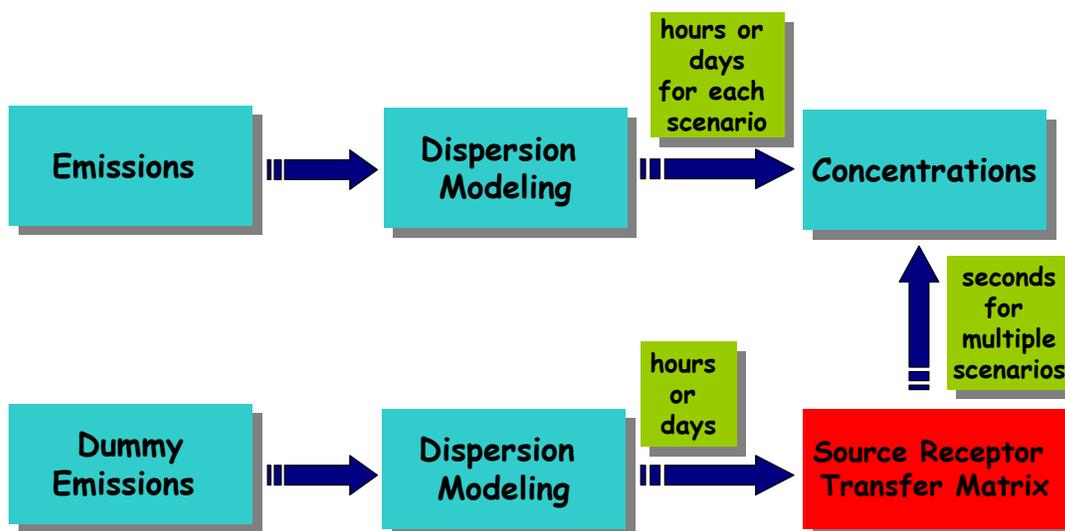

Figure 2:Use of the source receptor transfer matrix in SIM-air

Mathematically, it is represented as $C_{kl} = \sum_{ij} Cb_{kl} \dfrac{E_{ij}}{Eb}$

where
- Eb = base case emission rate of used to generate the transfer matrix (3,000 tons/yr)
- E_{ij} = actual emission rate at the source cell (i, j)
- C_{kl} = calculated mass concentration of the pollutant at the receptor cell (k, l)
- Cb_{kl} = modeled mass concentration at the receptor cell (k, l) due to "Eb"
- l, i   = maximum number of horizontal cells
- k, j   = maximum number of vertical cells

One matrix doesn't fit all. This should be developed separately for each city, using local meteorological conditions. All the matrix calculations need calibration and validation before using for multiple scenario analysis. The output of the ATMoS-4.0 model is **a source-receptor transfer matrix** and for use in the SIM-air tool ONLY.

An example Excel file is included along with the dispersion model.

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[1] Note that this methodology is applicable for linear pollutants like PM (with some assumptions for secondary pollutants like sulfates and nitrates), but NOT SUITABLE for secondary pollutants like Ozone, which is a result of a complex set of chemical reactions between a number of primary pollutants like NOx and VOCx and numerous radical species.

Air Pollution Dispersion Modeling

Air pollution dispersion models are computerized representations of the atmospheric processes, such as physical and chemical transformation of a mix of pollutants at urban, regional, and global level. The models simulate the atmosphere in varying degree of detail by mathematically representing emissions; initial and background concentrations of chemical species; the chemical reactions of the emitted species and their products; and the local meteorology such as sunlight, wind, and temperature.

The physical transformation includes advection of the pollutants, depending on the local terrain and meteorological conditions, and dry and wet deposition of the pollutants. The deposition schemes vary for the pollutants depending on the chemical composition. The chemical transformation depends on the intensity and mix of the emissions, local meteorology affecting the mix of the pollutants via advection. For example, Ozone which is a secondary pollutant is a result of a series of chemical interactions between two primary pollutant emissions, e.g., Nitrogen Oxides (NO_x), Volatile Organic Compounds (VOC) and Carbon Monoxide (CO). All three pollutants have a large transport sector contribution and the Ozone pollution tends to be higher along the transport corridors (during the day time). The Ozone and CO are also known to contribute not only to regional signatures, but also to the intercontinental transport.
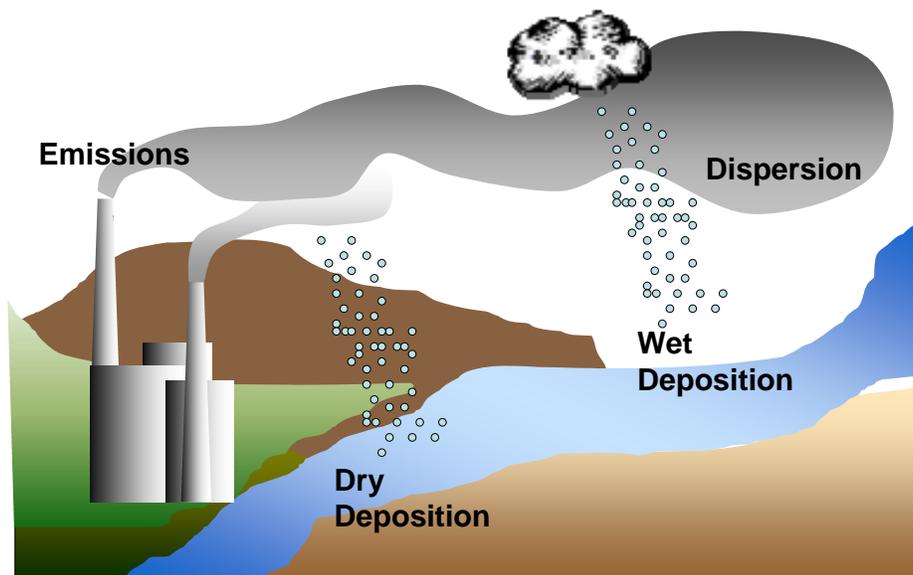

Figure 3: Physical schematics of atmospheric dispersion

A pollutant which is very pertinent to the urban centers is Particulate Matter (PM). The mix of PM pollution is also complex, with contribution from the primary emissions, such as black carbon, soil dust, and sea salt, and the secondary. The secondary contribution is a result of chemical transformation of the primary emissions, such as sulfates from sulfur dioxide (SO_2), nitrates from NO_x, and secondary organic aerosols due to oxidation of VOCs. Understanding the mix of the PM pollution is critical to substantiate contributions from

various sources and the ability to control the same. The dispersion models with defined chemical mechanisms can help study these physical and chemical transformations.

The mathematical representation of the dispersion models varies depending on the depth of information available for modeling and computational facilities. The models range from easy to use simplified Box models to complex 3D Eulerian models with full fledged chemical mechanisms. A comparative description of the dispersion models is provided in **Table 1**. There are benefits for using any of the available models, depending on the model output requirements. For example,

- The Box models can be very advantageous in rapid assessment of the emissions and studying the chemical mechanisms
- The Gaussian plume models have been in use for evaluating the impacts of point sources (e.g., industrial stacks)
- The Eulerian models are very data and computationally intensive and known to provide modeling flexibilities at urban, regional, and global scales

Table 1: Comparative description of the dispersion models

	Box	Plume	Eulerian
Complexity	*	**	****
Data requirement	*	**	****
Pollutant chemistry	*	**	****
Advection of pollutants	*	**	****
Ease of operations	****	**	*
Computational requirements	*	**	****
Results – level of detail	*	**	****

Criteria for Model Selection

Given the complexities of the models available, the selection of a dispersion model primarily depends on

- Information: The models vary on the intensity of data requirements and it is important to understand the level of information available. A general thumb rule is "garbage in – garbage out". The confidence levels and the accuracy of the models depend entirely on the input information and it is important that a model is chosen to support the information available.
- Computational Facilities: The intensity of the modeling varies from the box models to Eulerian models. The Box models can simulated even in a MS Excel format, while the 3D Eulerian models are data intensive and require Linux or UNIX operating environment for ease of data manipulation. The latter are also time consuming – for the preparation of the input fields and computational times. So, depending on the technical expertise and computational facilities available, a model is chosen to support necessary modeling objectives.
- Modeling Objectives: Each of the models available is capable of performing a set of similar calculations, but the levels of details vary. A model should be chosen

depending on the objective. For example, if the objective is evaluate point sources and not the interactions of pollutants, and then a Gaussian plume model will suffice. However, for the later a Eulerian model is better suited.

An output from a dispersion model is advantageous in many ways. The output can used to study the spatial distribution of the pollution over a city or region; to better understand the pollution hot spots and assist in the allocation of monitoring networks; to study the influences of the local terrain and meteorological conditions on pollution chemistry; and to evaluate the possible pollution scenarios for the future.

This paper presents a simplified dispersion model, with modifications to support low-level computational facilities and **for direct use in the SIM-air analysis tool[2]**.

ATMOS-4.0 Model Description

The Atmospheric Transport Modeling System (ATMoS) is a UNIX/Linux based air pollution dispersion model. The model was primarily developed for sulfur pollution dispersion modeling as part of the Regional Air Pollution Information System for Asia (RAINS-Asia – software developed and distributed by the International Institute of Applied Systems Analysis (IIASA), Laxenburg, Austria), which was later updated to support PM and Nitrate pollution[3].
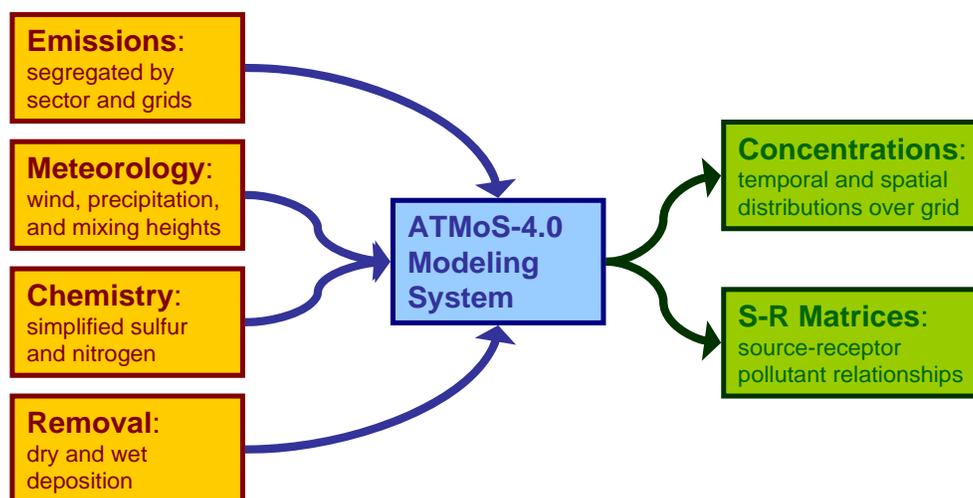

Figure 4: Input and output schematics of ATMoS-4.0

The ATMoS-4.0 model is modified from the original format (**Figure 4**), while keeping the physical and chemical mechanisms intact, to predict the pollutant deposition and concentrations at urban scale. The ATMoS is a meso-scale three-layer forward trajectory Lagrangian Puff-transport model[4]. The model is a modified version of the USA National

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[2] SIM-air, Simple Interactive Models for Better Air Quality @ www.sim-air.org
[3] See Annex for model applications
[4] See an application example in SIM-air Working Paper No.19, "Impact of Brick Kiln Emissions on Air Quality in Dhaka, Bangladesh" @ http://www.urbanemissions.info/simair/simseries.html

Oceanic Atmospheric Administration, Branch Atmospheric Trajectory (BAT) model (Heffter, 1983). **This paper presents a technical explanation of the model operations, parameterization, and the simplifications made to support low-tech operations.**

The main advantages of the model are
- Since the model uses the puff transport methodology, illustrated in **Figure 5**, this allows for segregated analysis of the pollutant concentrations by grid or by sector, depending on the input details.
- The modeling can be conducted for individual grids or all grids combined.
- The model has flexibility in grid size resolution and the number of grids (domain size to be modeled). However, for the simplifications to suite urban analysis, the maximum domain size is fixed in this version (details in the next section).
- All the modeling calculations are conducted on a Linux or UNIX platform and the outputs are formatted for direct input in MS Excel worksheet or GIS platforms for further analysis.
- The ATMoS-4.0 has been simplified, especially for the meteorological pre-processors, to reduce computational time and input requirements (details in the next section).
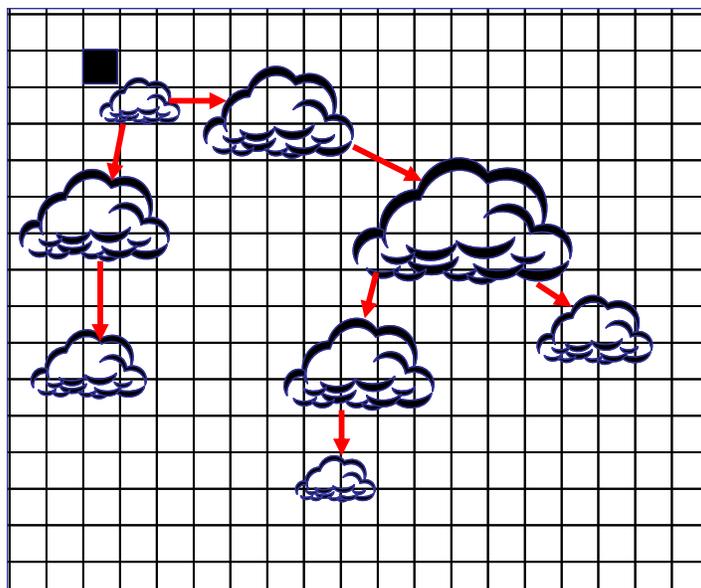- The output format is fixed for monthly and yearly time frames.

Figure 5: Lagrangian puff transport of the pollutants in ATMoS-4.0

Spatial and Temporal Scales

The ATMoS-4.0 is a grid based model defined in "*degrees*" of latitudes and longitudes. For the ease of operations, the maximum number of grids is limited to 25 x 25 for latitudes and longitudes, for a maximum grid resolution of 0.1° for latitude and longitude[5]. The maximum restriction is VERY important for the model application and this is based on the assumption that within the urban domain selected, the observed wind patterns are similar. If the domain size goes beyond the maximum of 2.5° resolution, the assumption doesn't hold true, leading to false results.

The dispersion model is "*modified for urban settings*", in which the emission plumes are modeled as puffs released every 3 or 6 hours. Each puff is assigned a mass proportional to the source strength. It is assumed the emission puff mixes uniformly in each layer (vertically) and diffuses along a Gaussian distribution in the horizontal (as illustrated in **Figure 5**).

Individual emission puffs are tracked for 120 hours (5 days) or until the mass falls below a cut-off value of 0.1 percent of the original emission source strength or puffs fall out of the simulation domain. Puffs transported beyond the modeling domain are no longer tracked. However, for buffering purposes, an additional 5 grids (pre-defined in the model) are added in all four directions to the user defined domain size. For example, if the modeling domain is defined as 20 x 20 grids, then the simulations are conducted for 30 x 30 grids. However, the output is displayed for the original 20 x 20 grids (see **Figure 6**).
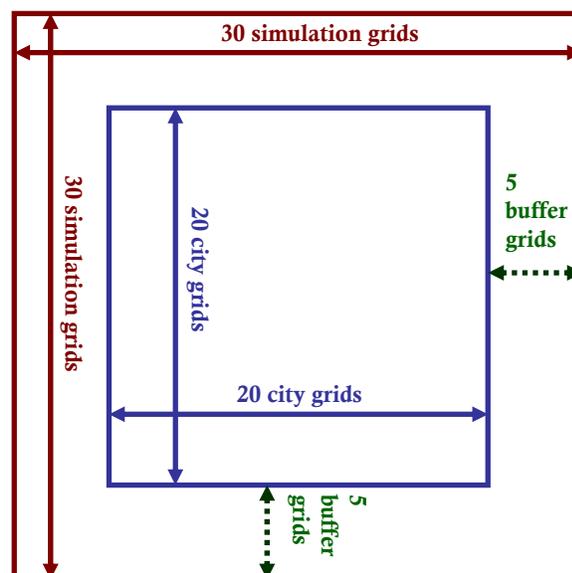
The model has flexible temporal and spatial resolution and can be run for the periods ranging from months to a year. The model produces monthly average concentrations as output and then converted to seasonal and yearly averages for further analysis. The user can define the period for which the transfer matrix is to be generated (details in the model input file).

Figure 6: An example representation of the model grid assignments

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[5] Applications of the previous versions of the model were conducted at 1 degree resolution for national or regional studies and ~0.05 degree resolution for urban scale studies

Meteorological Data

The previous ATMoS model utilized 2.5° by 2.5° reanalysis meteorological data from the NCEP/NCAR[6]. Meteorological input data included six hourly precipitation, mixing height, and wind vector information (speed and direction).

In the modified version 4.0, the same meteorological parameters are utilized, but the input is simplified to a single windrose data for the city. This is under the assumption that anywhere in the city limits (defined by the user) the meteorological conditions are similar.
The model utilizes
- U, horizontal x-wind component
- V, horizontal y-wind component
- MH, mixing layer height
- Precipitation

Most often the meteorological data is available in the form of wind speed and wind direction. The equation in **Figure 7** is used to convert the wind speed and wind direction into u and v parameters. Hence, the model meteorological input fields include
- Wind speed (m/sec)
- Wind direction (origin, as shown in **Figure 7**) (degrees)
- MH, mixing layer height (m)
- Precipitation (mm/hr)

$$u = -Ws * \sin(\frac{\pi}{180} * \varphi_{met}(\deg))$$

$$v = -Ws * \cos(\frac{\pi}{180} * \varphi_{met}(\deg))$$
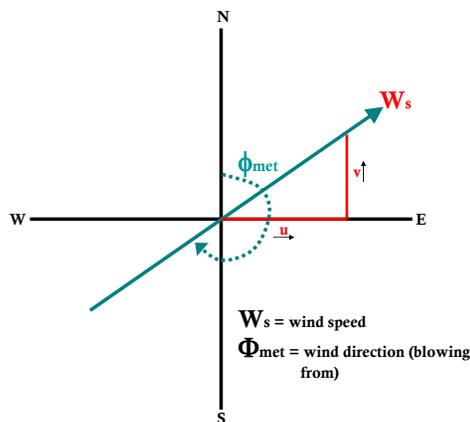
Ws = wind speed
Φmet = wind direction (blowing from)

Figure 7: Converting wind speed and wind direction to u & v

The data time interval is flexible to the available time intervals. However, when data is not available for the every time step, the data points are repeated from the previous available time step. For example, if the data is available for hours 6 and 12, and the time step for calculations is very hour, then for hours 7 to 11, the data values for hour 6 are repeated as shown in **Figure 8**.

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[6] National Center for Environmental Prediction / National Center for Atmospheric Research (NCEP/NCAR) - Kalnay et al., 1996 (see Annex 1). The gridded data file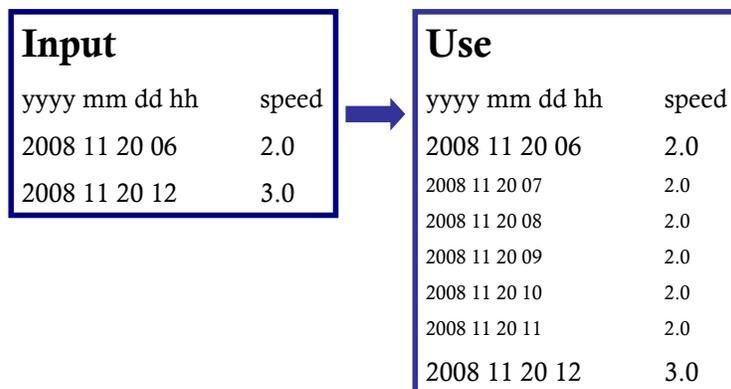s for the global domain are available for free to download @ http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.html

Input		Use	
yyyy mm dd hh	speed	yyyy mm dd hh	speed
2008 11 20 06	2.0	2008 11 20 06	2.0
2008 11 20 12	3.0	2008 11 20 07	2.0
		2008 11 20 08	2.0
		2008 11 20 09	2.0
		2008 11 20 10	2.0
		2008 11 20 11	2.0
		2008 11 20 12	3.0

Figure 8: An example of translation of meteorological input data in ATMoS-4.0

The precipitation field is utilized for wet scavenging of the pollutants from all layers of the model. The rates of wet deposition are pre-defined. However, user has an option to modify in the model's input file.

Emission Processing

There is **no input** required for the emissions. A dummy emission value of 3,000 tons/year for each pollutant is released from each grid point as area and point source (separately) to build the source receptor transfer matrix (**Figure 9**). All the emissions are treated as puffs and advected utilizing the meteorological data (as illustrated in **Figure 3**).
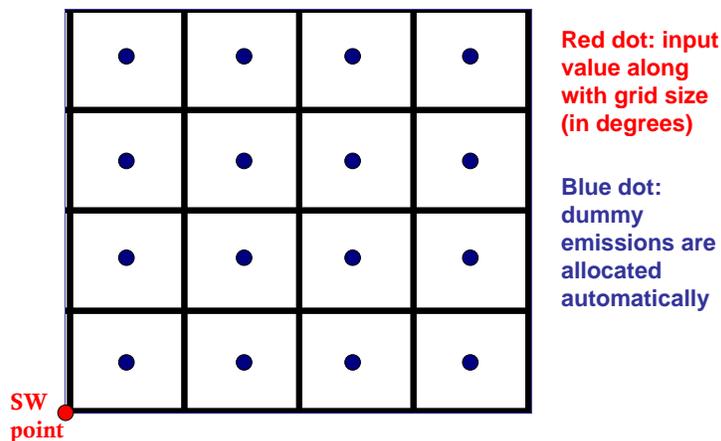
Red dot: input value along with grid size (in degrees)

Blue dot: dummy emissions are allocated automatically

SW point

Figure 9: An example input for the emissions field

Area sources are released into the boundary layer during the day and into the surface layer at night, and the point sources are released into the boundary (second) layer at all times.

The model separates the vertical dimension into two layers during the day and three layers at night. The day layers are the boundary and upper layer. The night layers are the surface, boundary, and upper layers. The surface layer is fixed at 300 meters to calculate the ground level concentrations followed by the mixing layer. The boundary and upper layers are

separated by the critical inversion, which determined from the vertical temperature profile. The maximum height for the model is 6000 meters.

The puff released during daytime or nighttime expands and follows its own trajectory. However, during day to night and night to day transitions the puff branches into multiple puffs (**Figure 10**). This action is performed to simulate vertical wind shearing of the puff. Up to 32 branches of the original puff may be tracked simultaneously after which branching ceases.
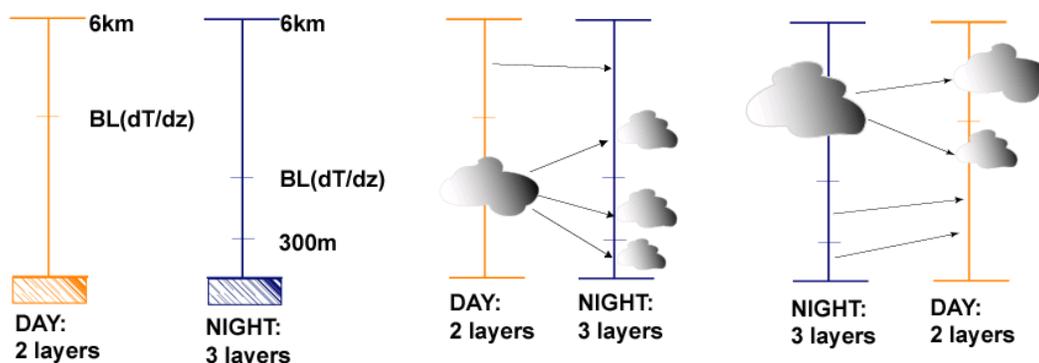
(T. Holloway/GFDL, 2000)

Figure 10: Distribution of emission puff during advection in vertical direction

During a day to night transition a puff in boundary layer will branch into all night three layers while a puff in the upper layer will stay in the same layer during nighttime. During night to day transition a puff in the surface layer will go to boundary layer, a puff in the boundary layer will stay in the same layer during daytime, and the growing boundary layer will cause a puff in the upper layer to branch into the two layers. This continues for 5 days (120 hours) or until the trajectories leave the modeling domain as discussed earlier.

For urban studies, the model adopts the "Briggs-urban" formulation for horizontal expansion of the puffs and an increased vertical dilution during nighttime, by using a fixed lower layer of 300 m. As for the elevated point source, 80% of the puff emissions are released into the boundary layer with the remaining 20% into the surface layer during the nighttime. This tends to prevent elevated sources from reaching the urban surface immediately and thus decrease their influence in the vicinity of the source.

Multi-pollutant Processing

The PM pollution, which is critical for the urban centers, is a result of contributions for multiple sources and multiple pollutants. **Figure 11** presents an approximation of chemical species present in PM fractions. The ATMoS model allows for multi-pollutant analysis for PM in which each of the primary emissions are modeled separately and aggregated at the end. This includes SO_2 to sulfates and NO_x to nitrates. If the emissions for black carbon (BC) and organic carbon (OC) (partly secondary organic aerosols from VOCs), then the model can evaluate them separately – this is not included in this version of the model. The chemical transformation to sulfates and nitrates is simplified using linear reactions. These

rates are specified in the model input file and user has an option to either use the default value or change it accordingly. No chemical transformation is applied to direct PM emissions.
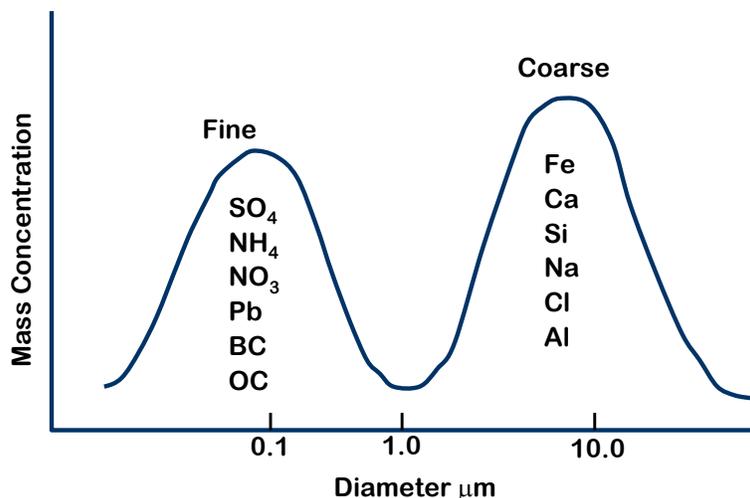

Figure 11: Approximate chemical distribution in PM fractions

Modeling each of the sub-fractions is very important due to the differences in physical and chemical differences in PM_{10} and $PM_{2.5}$. In the model, besides the sub-fractions, the direct PM emissions are also simulated in two bins – distinguished as PM with aerodynamic diameters between 2.5 and 10 micron meters (the 'coarse fraction') and particles between 0 and 2.5 micron meters (the 'fine fraction').

At the end of the simulations, the total PM_{10} concentrations comprise of all the sub-fractions ($PM_{coarse}+PM_{fine}+SO_4+NO_3$) while the total $PM_{2.5}$ comprise of the finer sub-fractions ($PM_{fine}+SO_4+NO_3$), thus providing a multi-pollutant aspect to the PM pollution.

Removal Processing

While the chemical transformation of the species provides a form of removal of the PM emissions, two physical processes are included – dry and wet deposition. The wet deposition scheme is activated only during the precipitation period.

A net removal rate at the surface due to dry deposition is calculated using the equation $R_d = \dfrac{V_d}{z}$ where, R_d is the dry removal rate (per sec), V_d is the dry deposition velocity (m/sec), and z is the surface layer height (m). Constant dry deposition rates are prescribed in the model. Similarly, net removal rate at the surface due to wet deposition is calculated using the equation $R_w = S_p * P$ where R_w is the wet removal rate (per sec), S_p is the precipitation scavenging coefficient and p is the precipitation rate (mm/hr). The rates are average numbers and the methodology of calculation is flexible, depending on the available local information. An average set of dry and wet deposition rates are presented in the input file of ATMoS-4.0 and user has the option to either keep the defaults or change.

Model Calculations

The flow chart in **Figure 12** illustrates the order of calculations in the model.
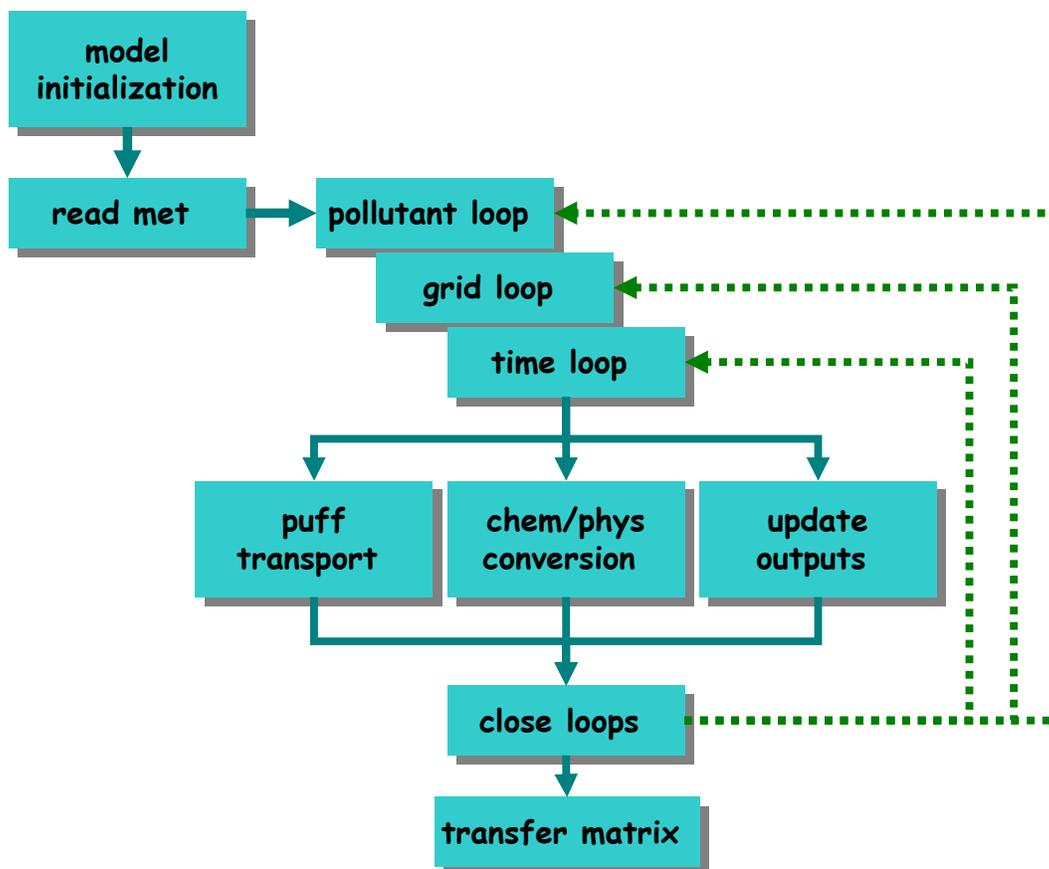

Figure 12: ATMoS-4.0 dispersion model simulation cycle

The output is in text format and easy to import into MS Excel for further calculations. See the attached example MS Excel file. The output files include the following 8 output

pmc.point.matrix; pmc.larea.matrix;
pmf.point.matrix; pmf.larea.matrix;
so4.point.matrix; so4.larea.matrix;
no3.point.matrix; no3.larea.matrix;

The segregation allows for calculating the individual contributions and further apportionment for controls and impacts analysis. The time period of the matrix is defined by the user – with option to generate individual monthly or seasonal or yearly average matrices.

Limitations

This is a model and needs calibration, like any other model.

User can play with the deposition and reaction rates using appropriate and available literature.

The dispersion depends on the meteorological data. The model is set-up to use only one meteorological data point, hence applicable for a city level analysis only.

The output is 8 files containing grid-grid source-receptor matrix using a dummy emission of 3,000 tons/yr for each grid. The output must be divided by 3,000 and follow the equation presented in **Page 2** and the example excel file.

This is a first cut analysis to demonstrate how the dispersion calculations can be conducted and an alternative for rapid analysis. If more detailed modeling is required, for example, adding ozone analysis to the model, then ATMoS-4.0 is not capable of doing so.

User is responsible for the final results.

ATMoS-4.0 Model Installation & Requirements

The model and the test run results are available for download
@ www.urbanemissions.info/simair/atmos.html

The code is written in FORTRAN language and do not need any external libraries, except for a FORTRAN compiler.

IMPORTANT NOTE: This model, in its current form, is suitable for developing source-receptor transfer matrix for an urban setting and the output is formatted for use in SIM-air tool framework.

Installation and Use in Linux/Unix Environment

Download the zipped file and then type

> gunzip atmos40.tar.gzip
> tar –xvf atmos40.tar

This will create 13 files in the current directory.

1. **atmos40.f** – main program
2. **atmos40.inc** – is an include file with data/array specifications (no need to change any of the values, unless the user wishes to)
3. **atmos40.ini** – this is the initial file, which requires **user input**
4. **test.meteo.dat** – provides an example meteorological file (**user input**). The meteorological file format is described in **Annex 2**.
5. 8 example output files
   test.pmc.point.matrix; test.pmc.larea.matrix;
   test.pmf.point.matrix; test.pmf.larea.matrix;
   test.so4.point.matrix; test.so4.larea.matrix;
   test.no3.point.matrix; test.no3.larea.matrix;
6. **SIM-air-test-case** – An excel file using the test case transfer matrices for calculations

Depending on available fortran complier, compile the program. For example

> g95 atmos40.f
Or
> pgf90 atmos40.f
Or
> ifort atmos40.f
Or
> f95 atmos40.f

This will create an executable called "**a.out**" in the same directory.

Make the "**meteo.dat**" file using local data (you can name the file anything)

Edit the "**atmos40.ini**" file for local domains – follow the maximum limit rules specified

> ln –s meteo.dat meteofile
Or
> ln –s "your met file name" meteofile

> ln –s atmos40.ini inifile

The names meteofile and inifile are fixed filenames used by the atmos40 program.

To run the program type

> ./a.out

The output files will be placed in the same directory. The model will create 8 output files

pmc.point.matrix; pmc.larea.matrix; pmf.point.matrix; pmf.larea.matrix;
so4.point.matrix; so4.larea.matrix; no3.point.matrix; no3.larea.matrix;

Total PM_{10} = pmc + pmf + so4 + no3
Total $PM_{2.5}$ = pmf + so4 + no3

The user is responsible for renaming the files and storing after every simulation. These names are locked in the program; the same files are replaced with new model run data.

Run time - approximately 10 minutes per pollutant per sector for a 10x10 domain on an eight-core workstation (and the time will vary depending on the machine CPU).

Take the output files into Windows, open in excel for further use. An example calculation of using the transfer matrix is presented in the attached MS Excel file "**SIM-air-test-case**".

To use the transfer matrices for analysis,
- copy and paste the transfix matrices into appropriate worksheets (as shown in the example case)
- enter gridded emissions inventories for PMC (PM-Coarse = PM_{10}-$PM_{2.5}$), PMF (PM-Fine = $PM_{2.5}$), SO2 and NOx in tons/year
- enter gridded population data

If the number of grids are different from 10x10, then user needs to re-do the emission assignments and matrix multiplications in the 'calculations' sheet.

All the results are displayed in the "Summary" sheet.

Annex 1: ATMoS Model Applications and References

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Annex 2: Meteorological Input File

An example, meteorological file looks like the following

Month Day Hour "Wind speed" "Wind direction" "mixing height" "Precipitation"

1	1	6	2.0	130.0	800.0	0.004
1	1	12	2.0	230.0	800.0	0.004
1	1	18	2.0	30.0	800.0	0.004
1	1	24	1.0	80.0	800.0	0.004
1	2	6	1.0	50.0	800.0	0.004
1	2	12	1.0	83.0	800.0	0.004
1	2	18	1.0	130.0	800.0	0.004

and so on (see the example file)

Corresponding units are

Wind speed   - m/sec
Wind direction   - degrees (blowing from)
Mixing height   - meters
Precipitation   - mm/hr