ATMOS/UrBAT

Regional and Urban Branch Trajectory Model

Version 2.3

Model Description & Model Input Preparation

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ATMOS – UrBAT
Branch Trajectory Model

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Introduction

The ATMOS/UrBAT (Urban Branch Atmospheric Trajectory) model predicts sulfur and particulate deposition and concentrations at regional and urban scale. ATMOS model is a meso-scale three-layer forward trajectory Lagrangian Puff-transport model (Arndt *et al.*, 1997, Arndt, 1997 and Guttikunda *et al*., 2001). The model is a modified version of the USA National Oceanic Atmospheric Administration, Branch Atmospheric Trajectory (BAT) model (Heffter, 1983). This user manual presents technical details on the model operations, parameterization and describes how to run the ATMOS/UrBAT model along with some example datasets.

ATMOS/UrBAT is a Unix/Linux based air pollution dispersion model. The model was primarily developed for sulfur emission and 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). ATMOS model was extensively applied for sulfur and particulate modeling activities in Asia.

- As an analysis tool of sulfur emissions and deposition patterns in Asia (Arndt *et al.*, 1998, and Streets *et al.*, 1995).
- For sulfur control policy implications in Asia (Foell *et al.*, 1995, Arndt, 1997, and Carmichael *et al.*, 1995, Guttikunda *et al.*, 2002).
- For seasonal sulfur deposition and concentration studies in Asia (Guttikunda *et al.*, 2001).
- For Urban Air Quality studies in Asia, e.g., Shanghai (Streets *et al.*, 2001), Chongqing (Adhikary *et al.*, 1998).
- For dispersion modeling of fine particles in Asia and for megacities like Seoul, South Korea, Shanghai, China and Bangkok, Thailand (Dorwart, 2001).

Structure of the Report

This report is divided into four parts. Chapter 2 presents the technical description of ATMOS model, and model parameterization of deposition rates and chemical conversion rates. Chapter 3 describes model installation procedures for Unix and Linux work environments. Chapter 4 explains some of the model parameters and their range of

variability in the utility files like the model initialization file, the model include file, etc. Finally, Chapter 5 demonstrates input and output data file management to execute the model - preparing emissions file, grid description file, Meteorological data and use of extract codes to visualize model outputs.

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Model Description

Air Pollution models that can be used to predict pollution concentrations for periods of up to a month or a year, are generally semi-empirical or analytical approaches based on gaussian plumes or puffs and uses simple surface based meteorological information or diagnostic wind field information.

In ATMOS/UrBAT lagrangian puff transport model, SO_2 and PM emission plumes are modeled as puffs released every 3 hours or every hour respectively, for regional and urban simulation. Each puff is assigned a mass proportional to the source strength. It is assumed to mix uniformly in the vertical throughout an assigned layer and to diffuse along a Gaussian distribution in the horizontal. 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 emission source strength or puffs fall out of the simulation domain. Puffs transported beyond the modeling domain are no longer tracked.

This model uses 2.5° by 2.5° reanalysis meteorological data from the NCEP/NCAR (National Center for Environmental Prediction / National Center for Atmospheric Research) (Kalnay *et al.*, 1996). Meteorological input data include six hourly precipitation, mixing height, and wind vector information.

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 night surface layer extends from ground to 300 meters. 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 (Carmichael and Arndt, 1995).

The model has flexible temporal and spatial resolution and can be run for the periods ranging from days to decades. The model produces hourly average concentrations as output. Similarly, the horizontal spatial resolution of the model can be varied from 5000 meter for an urban scale study to 1° x 1° (approximately 90 km) for a regional scale study. The ATMOS/UrBAT model schematics are presented in Figure 1.

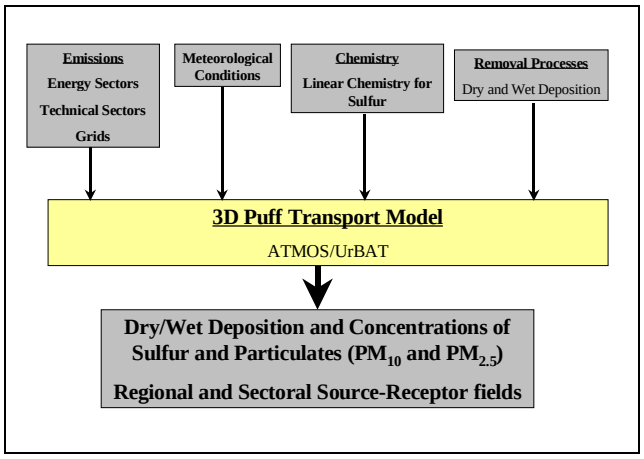

Figure 1: The ATMOS/UrBAT Modeling System

For modeling purposes, emissions are emitted at the center of the grid point for area sources and at the exact locations for elevated sources (in hundredths of a degree). Area emission sources (small industries, incinerators, boilers and mobile sources) are released into the boundary layer during the day and into the surface layer at night, and the elevated sources (large point sources, LPS's) are released into the boundary layer during the day and above the surface layer at night. Volcanic sources are released into the upper layer at all times.

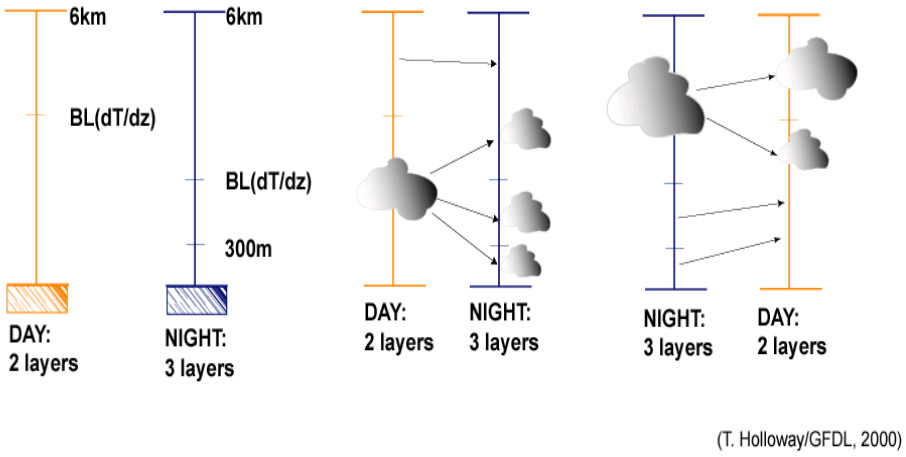

Figure 2: The ATMOS/UrBAT Branching Mechanism

The puff released during daytime or nighttime will be expanded and follows its own trajectory. However, during day to night and night to day transitions the puff branches into multiple puffs. 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. Figure 2 illustrates, the potential branching process during transition. 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 five days or until the trajectories leave the modeling domain as discussed earlier.

For urban studies, the model adopts the "Briggs-urban" formulation for sigma-y and an increased vertical dilution during nighttime over urban areas, by using a modified lower layer of 500 m. As for the elevated point source (LPS's, Volcanoes), 80% of the puff emissions are released into the boundary layer with the remaining 20% entering the urban boundary layer (UBL) during day or into the surface layer during the nighttime. This UBL tends to prevent elevated sources from reaching the urban surface and thus decrease their influence on urban concentration. Furthermore, the UBL acts to trap urban surface emission and magnify their influence. The flow chart in Figure 3 illustrates the order of calculations in the model. The model uses a time-step of 1 hour on which advection and surface processes are calculated and averaged over the desired time period.

ATMOS/UrBAT model is run separately for sulfur and particulate deposition and concentration levels. For sulfur emissions, all the SO_2 emissions are released as a single puff per source. Where as for particulates, due to physical and chemical differences in PM_{10} and $PM_{2.5}$, two separate bins of particles were distinguished: particulates with aerodynamic diameters between 2.5 and 10 micron (the 'coarse fraction') and particles smaller than 2.5μm ($PM_{2.5}$, the 'fine fraction'). If concentrations of PM_{10} (containing particles with aerodynamic diameter smaller than 10μm) are of interest, both size fractions have to be added. In addition, sulfate concentrations obtained from the dispersion calculations of SO_2 emissions are added to the PM10 fraction to reflect the sulfate aerosol component of secondary particles, while nitrate and ammonium components are not considered in this version.

Two removal types are considered in this model – chemical transformation and deposition. Chemical transformation is considered only for SO_2 plumes to sulfate. No chemical or physical transformation is applied to PM plumes. Deposition of pollutants is separated into wet and dry components. A net removal rate at the surface due to dry deposition is calculated using Equation 1:

$$R_d = \frac{V_d}{z} \qquad (1)$$

where, R_d is the removal rate, V_d is the dry deposition velocity, and z is the surface layer height depending on the day/night transitions and stability zones. Similarly, net removal rate at the surface due to wet deposition is calculated using Equation 2:

$$R_w = S_p * p \qquad (2)$$

where R_w is the removal rate , S_p is the precipitation scavenging coefficient and p is the precipitation rate. For more details on removal rates and model parameters refer to Arndt, 1997 and Guttikunda *et al.*, 1999. Dry and Wet Deposition rates utilized in the model are

presented in Table 1 and Table 2. The model uses linear chemical parameterizations for sulfur presented in Table 3.

Table 1: Dry Deposition rates utilized in the ATMOS/UrBAT model

Variable Name	**Deposition Rate (m/sec)**
SO_2 (over land)	= 2.5e-3 for months between May and September (hot season) = 1.25e-3 the rest of the year (cold season)
SO_2 (over water bodies)	= 3.2e-3
SO_4 (over land)	= 2.0e-3
SO_4 (over water bodies)	= 1.0e-3
PM_{10} (over land)	= 7.0e-3
PM_{10} (over water bodies)	= 7.0e-3
$PM_{2.5}$ (over land)	= 2.0e-3
$PM_{2.5}$ (over water bodies)	= 1.0e-3

Table 2: Wet Deposition rates utilized in the ATMOS/UrBAT model

Variable Name	**Scavenging Rate (per sec) (precipitation rate in mm/hr)**
SO_2	= 2.0e-5* precipitation rate
SO_4	= 5.0e-5 * precipitation rate ^ 0.83
PM_{10}	= 7.0e-5 * precipitation rate
$PM_{2.5}$	= 6.0e-5 * precipitation rate ^ 0.83

Table 3: SO_2 -> SO_4 Chemical Conversion rates for utilized in the ATMOS/UrBAT model

Variable Name	**Conversion rate (per sec)**
f_lat	Cos(1.3*lat*π/180)
f_day	Sin((Julian day-80)*2π/365)
rate	1e-5* f_lat + 4e-6*(1-f_lat)*f_day

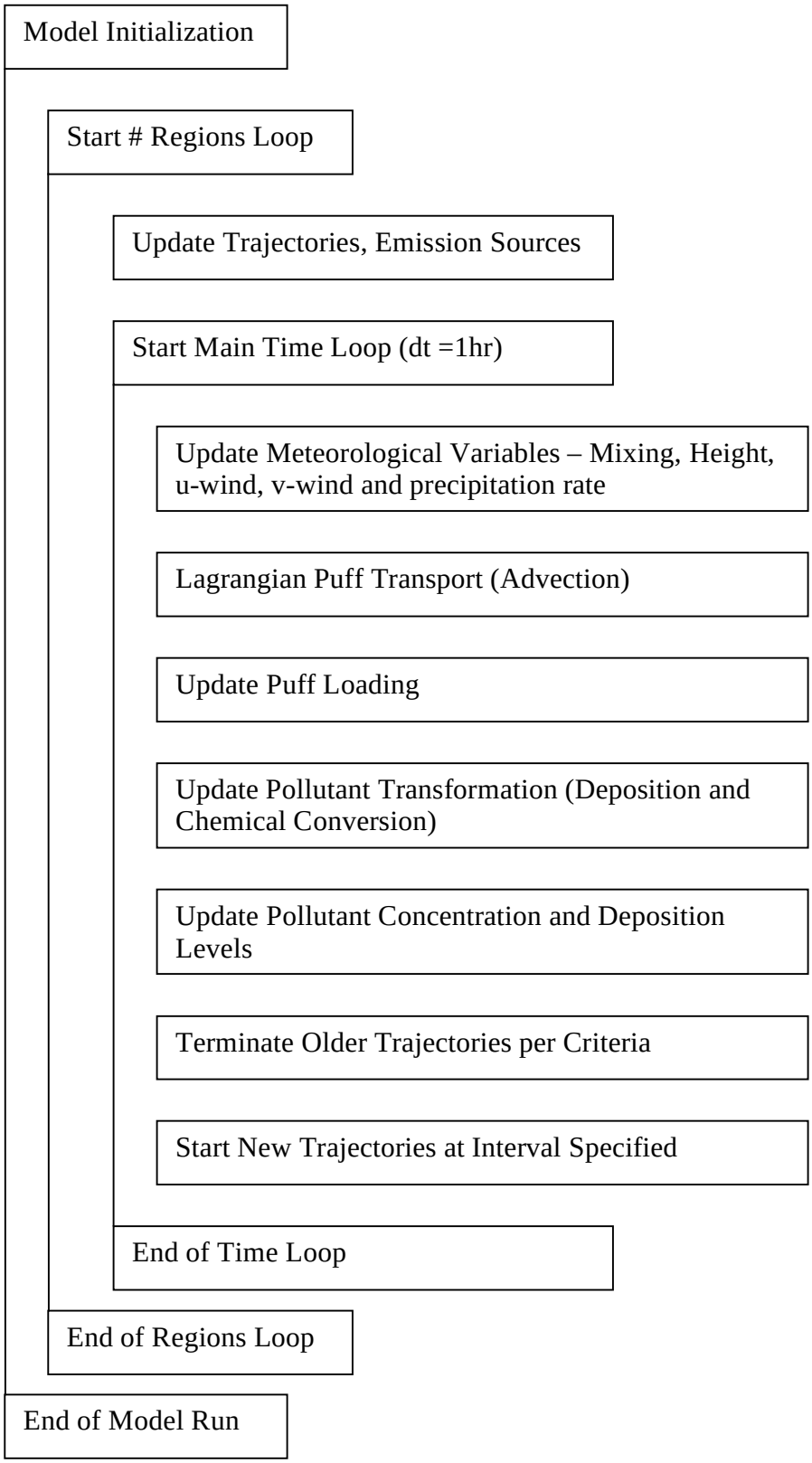

Figure 3: Flow Chart of ATMOS/UrBAT Model

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Model Installation

System Requirements

ATMOS-UrBAT model, the most recent version, works with the following system environments:

1) Unix Operating System
2) Linux Operating System

Download Program and Libraries

1) Unix Operating System:

Download the file atmos-urbat-unix.tar.gz from
http://www.cgrer.uiowa.edu/ATMOS

To use it, you will also need the UCAR/UNIDATA netCDF (http://unidata.ucar.edu/packages/netcdf/index.html) and the NCSA EDSS/Models-3 I/O API (http://envpro.ncsc.org/products/ioapi/index.html) libraries.

2) Linux Operating System:

Download the following files in atmos-urbat-linux folder
http://www.cgrer.uiowa.edu/ATMOS/atmos-urbat-linux

1) Instruction.txt
2) atmos-urbat-linux.tar
3) netcdf-ioapi.tar

Installation

1) Unix Operating System:

- Upon downloading the files, execute the following lines at the command prompt in the directory you want to install the model

    - tar –xvf atmos-urbat-unix.tar

  This will create directories atmos_sulfur and atmos_pm and the following files in each of the directories.

    - Fortran code (advect.f, array.f, atmos2.f, concal.f, branch.f, g2g.f, m3_utils.f, masks.f, meteo.f, output.f, rates.f, setup.f, sigma.f, sources.f, term.f, urban.f, and utils.f)
    - Include file containing parameter declarations and dimensions (atmos2.inc)
    - Input directory containing examples of grid description file (grid.desc), initialization file (atmos2.ini), land-sea mask file (landsea.dat), urban-rural mask file (urbrural.dat), meteorological files (lwind.nc, hmix.nc, prate.nc). **Note:** user should download the meteorological files separately. See the Meteorological data section below.
    - Makefile to compile the atmos code and prepare the executables (atmos2.mak)
    - Run script to run atmos code (run_atmos2)

- To compile the program, enter atmos_sulfur or atmos_pm directories. Check the netCDF and IOAPI library links (see name-list parameters section for description of the libraries and the makefile) in the atmos2.mak file and type the following at the command prompt to generate the executable (atmos2.exe) in the main directory

    - cd atmos_sulfur **or** atmos_pm
    - make –f atmos2.mak

2) Linux Operating System:

- First check whether you got three required file upon download or CD-rom
  - Instruction.txt (this file)
  - atmos-urbat-linux.tar
  - netcdf-ioapi.tar
- Instruction to install libraries file
  - Untar the netcdf-ioapi archive file
    $ tar -xvf netcdf-ioapi.tar

You will get 4 files from this archive (netcdf-3.4.tar, ioapi.tar, libnetcdf.a, and netcdf.inc).

- Install netcdf library;
  You should login as root and go to directory /usr/local
  - Copy netcdf-3.4.tar to /usr/local
  - Untar the archive file:
    # tar -xvf netcdf-3.4.tar
  - Change to the src directory of netcdf-3.4:
    # cd netcdf-3.4/src
  - Run configure to create the proper Makefile:
    # ./configure
  - Compile program:
    # make
    Just ignore the error message during compilation process.
  - You will find all netcdf libraries and include files in
    /usr/local/netcdf-3.4/src/libsrc. Since the bugs during compilation process, please delete libnetcdf.a in /usr/local/netcdf-3.4/src/libsrc and replace w/ libnetcdf.a from the archive file and also copy netcdf.inc to the same directory (/usr/local/netcdf-3.4/src/libsrc)
  - Go to ncdump directory and compile program;
    # cd /usr/local/netcdf-3.4/src/ncdump
    # make
    You will see ncdump executable command (to read netcdf file) after compilation process.
- Instruction to install ioapi library for ATMOS
  You should login as root and go to directory /usr/local
  - Make directory for ioapi
    # mkdir ioapi
    # cd ioapi
  - Copy ioapi.tar to /usr/local/ioapi
  - Untar the archive file:
    # tar -xvf ioapi.tar
    You will have every that need in /usr/local/ioapi/ioapi

Note If you would like to use ioapi for model 3, you need to compile the code go to /usr/local/ioapi/ioapi and edit Makefile by add BIN = Linux2_x86 and change OBJDIR = ../$(BIN) to OBJDIR = ../bin.
See more information http://envpro.ncsc.org/products/ioapi/H.AVAIL.html

- Edit shell script
  - Go to your working directory(Example: /home/chen)
  - Edit shell script (.bashrc)
    $ emacs .bashrc &
  - Add these 3 lines into your shell scipt after fi in your shell script
    export PATH=$PATH:.:
    export NETCDF=/usr/local/netcdf-3.4
    export PATH=$NETCDF/src/ncdump:$PATH

    Example of shell script:

    # .bashrc
    # User specific aliases and functions
    # Source global definitions
    if [-f /etc/bashrc]; then
    . /etc/bashrc
    fi
  - Save your .bashrc and source you shell script by typing
    $ source .bashrc
- Install ATMOS-Urbat
  - Go to your working directory (Example: /home/chen)
  - Copy atmos-urbat-linux.tar to your working directory
  - Un-tar the archive file:
    $ tar -xvf atmos-urbat-linux.tar
  - You will see 3 directories in your home directory (atmos_sulfur, atmos_pm, Metdata)
  - The following files are in atmos_sulfure and atmos_pm directory.

README.txt	readme file
atmos2.f	model source code
atmos2.inc	include file
Makefile	example of compilation script
r_atmos2	example of run script
atmos2.ini	example of initialization file
grids.desc	example of grids definition file
landsea.dat	example of land-sea mask
urbrural.dat	example of urban-rural file
emissions	sub-directory to keep emission data
atmos_out	sub-directory to keep model output
bin	sub-directory to keep executable file
extract_codes	working sub-directory to extract model output

  - Metdata directory consists of three meteorological files.
    (hmix.yyyy.nc, prate.yyyy.nc, and lwind.yyyy.nc)
- To compile the program, enter atmos_sulfur or atmos_pm directories and type "make"
  $make

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Model Input Namelist Parameters

Namelist Parameters

This section describes only some of the parameters utilized in the model, which are variable in nature. For most of the parameters, a brief description is available next to its declaration in every file.

1) Model Include File (atmos2.inc – located in the main directory)

Variable Name	Data Type	Description
maxx_w, maxx_p, maxx_h	integer	Maximum number of longitudinal grids. Fixed at 41. ATMOS model developed for Asia region utilizes NCAR/NCEP meteorological data at 2.5 degree resolution. Model extends from 60 E to 160 E in longitude (41 grids at 2.5° x 2.5° resolution). w = wind (u,v), p = precipation rate, h = mixing height
maxy_w, maxy_p, maxy_h	integer	Maximum number of latitudinal grids. Fixed at 31. ATMOS model developed for Asia region utilizes NCAR/NCEP meteorological data at 2.5 degree resolution. Model extends from -20 N to 55 N in longitude (31 grids at 2.5° x 2.5° resolution). w = wind (u,v), p = precipation rate, h = mixing height
maxx_c, maxy_c	integer	Maximum number of Concentration and Deposition grid cells (Maximum modeling domain size) – can be changed.
maxsrc	integer	Maximum number of sources per sector or region. This depends on operating machine memory.
Max_trajsrc	integer	Maximum number of contemporary trajectories per emitting source equals (Trajectory duration/Transport time step)+1. Equals 41 if puff release time is set every 3 hour, or 121 if puff release time is set every 1 hour
sltop	real	Height of the surface layer (1st layer of the model). Surface layer exists only during the night time and merged into the boundary layer (variable depending on meteorological

		conditions) during the daytime. Fixed at 300. m
ultop	real	Maximum height (top layer height) of the modeling domain. Fixed at 6000. m
allreg	logical	Is "true" if the all regions together flag equals "1" (See the initialization file parameter description)
urban	logical	Is "true" if the urban simulation flag equals "1" (See the initialization file parameter description)
grid2grid	logical	Is "true" if grid to grid calculation outputs are requested by the user. This needs to be activated in the main code (subroutine – setup.f)
col_load	logical	Is "true" if calculation of column total loading in requested by the user. This needs to be activated in the main code (subroutine – setup.f)
lay_load	logical	Is "true" if calculations of mass loading by layer are requested by the user. This needs to be activated in the main code (subroutine – setup.f)
uname, vname, hmixname, pname	character	Variable names for u-wind, v-wind, mixing height, and precipitation rates. This variables are defined for internal purposes. NO need to change the variable names.
c_prefix, dry_prefix, wet_prefix	character	Variable name prefixes for concentrations, dry deposition and wet deposition. This variables are defined for internal purposes. NO need to change the variable names. Model outputs include concentrations, dry deposition and wet deposition (default outputs) of SO2/SO4 if using sulfur version or PM10/PM25 if using particulate version of the model. Output variable names are of the following form concSO2, concSO4, drySO2, drySO4, wetSO2, wetSO4 for sulfur version, and concPM10, concPM25, dryPM10, dryPM25, wetPM10, wetPM25 for particulate version of the model.

2) Model Initialization File (atmos2.ini – located in the inputs directory)

In this file lines starting with the character "!" are comment lines.

Variable Name	**Data Type**	**Description**
Day Month Year Hour	integer	Simulation starting time in the following format (dd mm yyyy hh) Example: 01 01 2000 00 for simulation starting January 1st of year 2000 at hour 00 GMT
Day Month Year Hour	integer	Simulation ending time in the following format (dd mm yyyy hh) Example: 01 01 2000 00 for simulation ending January 1st of year 2000 at hour 00 GMT **Note:** For a year long simulation (starting

		Jan 1st and ending dec 31st) end hour must be 18. Example: 31 12 2000 18. NCAR/NCEP data is only available at 6 hr interval (at 00 06 12 18 hours GMT)
Trajectory duration	integer	In hours. 120 hours by default. Trajectories are discarded after 5 days of tracking unless they are already out of the simulation domain or their puff concentration is already less than 0.1% of the initial puff loading.
Transport time step	integer	In hours. 1 hour by default. Transport calculations are conducted every hour for urban scale and 3 hours for regional scale. Though meteorological data is available only every 6 hours, model uses constant u,v,hmix and prate values for every 6 hours of calculations.
Output Sampling Duration	integer	In hours. Can be changed to output concentrations and depositions every hour (1), every day (24), every month (672) or annual (8766). For monthly outputs use the magic number "672" – number prescribed for monthly outputs in netCDF/IOAPI formats.
Sigma for Area Sources	real	In meters. Initial horizontal sigma (puff diameter) for area sources. As a thumb rule, use any number that lesser or equivalent to simulation grid size. Example: For an urban simulation at 0.1 x 0.1 degree resolution use a value between 8,000. m to 10,000. m as initial sigma. For a regional simulation at 1 x 1 degree resolution use 40,000 m as initial sigma (sigma value used for RAINS-Asia simulation).
Sigma for Large Point Sources	real	In meters. Initial horizontal sigma (puff diameter) for large point sources. As a thumb rule, use a number less or equivalent to the sigma used for area sources. Example: For an urban simulation at 0.1 x 0.1 degree resolution use a value between 4,000. m to 5,000. m as initial sigma. For a regional simulation at 1 x 1 degree resolution use 10,000 m as initial sigma (sigma value used for RAINS-Asia simulation).
% of minimum mass of initial release	real	Fixed at 0.1 %. Trajectories are discarded if the puff mass loading is less than 0.1 % of the initial release, unless puff is already out of the simulation domain or is already 120

		hours older.
Flag to process emitting regions all together or separately	integer	Equals “1” if requested to process all the sectors or regions (see the emission database management section for definitions) together or equals “0” if output is requested in separate files for each sector or region. For either case, check the run_atmos2 file to specify output filenames. For mote details see Input Data File Management section and parameter description for run_atmos2 file.
Flag for Urban Simulation	integer	Equals “1” if it is an urban simulation or equals “0” for a regional simulation.

3) Model Run Script (run_atmos2 – located in the main directory)

In this file lines starting with the character “#” are excluded lines. This file contains links to input files (initialization file, meteorological datafiles, grid description file, emissions file and output filenames.

Setenv Variable Name	**Data Type**	**Description**
OUTDIR	Character	Output directory location. Set to ./outputs in the main directory. By default all the outputs are stored in this directory
INDIR	Character	Input directory location. Set to ./inputs in the main directory. By default all the input files – initialization file, meteorological files, grid description file, emissions files, land-sea mask and urban-rural mask (in case of urban simulation) are located in this directory.
EXEDIR	Character	Executable directory. Upon compiling the code (using atmos2.mak), executable (atmos2.exe) is created in this directory. Set to ./ (main directory). By default executable atmos2.exe is stored in the main directory.
SCENFILE, EXECUTION_ID, IOAPI_CHECK_HEADERS, IOAPI_LOG_WRITE	Character	Required for IOAPI libraries. No need to change any of these.
GRIDDESC	Character	Grid description file (grid.desc) located in the input directory)
INIFILE	Character	Initialization file (atmos2.ini) located in the input directory
URBFILE	Character	Urban-rural mask file (urbrural.dat) located in the input directory. Check

		Input file management section for details.
LANDFILE	Character	Land-sea mask file (landsea.dat) located in the input directory. Check Input file management section for details.
WINDFILE	Character	U-wind and V-wind data file (lwind.2000.nc) located in the input directory. Data is stored every 6hr in netcdf format.
HMIXFILE	Character	Mixing height data file (hmix.2000.nc) located in the input directory. Data is stored every 6hr in netcdf format.
PRECFILE	Character	Precipitation rate file (prate.2000.nc) located in the input directory. Data is stored every 6hr in netcdf format.
FIRSTREG	Integer	Lowest sector number in the emissions file. Check Input file management section for details. By default set at "1".
LASTREG	Integer	Maximum number of sectors allowed in the emissions file. Check Input file management section for details. By default set at "999".
SRCFILE	Character	Emissions data file (emissions.txt) located in the input directory.
OUTFILE**1**	Character	OUTFILE**1** denotes output file for sector or region 1 or output file for all emitting regions or sectors combined. If individual output files for each sector or region is requested (see atmos2.ini variable description table), then number of output filenames equals the number of sectors or regions in the emissions file. Example: If 4 emitting regions or sectors are present in the emissions file starting from 1 to 4 and individual output files are requested (flag = "0"), then user must specify 4 output filenames, viz., OUTFILE1, OUTFILE2, OUTFILE3, OUTFILE4. **Note:** If the region or sector number ranges from 10 to 13, then user must specify 4 output filenames, viz., OUTFILE10, OUTFILE11, OUTFILE12, OUTFILE13. If output for all emitting regions or sectors together (flag = "1") is requested then irrespective of number of regions or sectors in the emissions file, user need to

		specify only one output filename, viz., OUTFILE1. For more details see Input Data File Management section.

4) Model Makefile (atmos2.mak – located in the main directory)

In this file, lines starting with the character "#" are excluded lines.

Setenv Variable Name	**Data type**	**Description**
ROOTDIR	Character	Main directory for ATMOS. Set to ./
NC_INCDIR	Character	NetCDF include directory containing the file netCDF.inc
NC_LIBDIR	Character	NetCDF library directory containing the file libnetcdf.a
IO_INCDIR	Character	IOAPI include directory containing the files PARMS3.EXT, STATE3.EXT, NETCDF.EXT, etc.
IO_LIBDIR	Character	IOAPI library directory containing the file libioapi.a

No need to change the rest of the links.

5

Input and Ouput Data File Management

All the files below are located in the inputs directory.

1) Emissions Data File

The First line start with comment (!) with explanation of each column of data. Examples are provided at the end of each section. (**Note:** This line need be present in the emissions data file. This is for user information only)

The emissions file has the following format:
! Sector# - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release time (hr)

Sector number indicates the user specifications on how to divide the gridded emissions. For example, emissions can be arranged by sector (power, domestic, industrial, agricultural, transport, etc) or by region (provinces in a country, districts in a province or east-west-north-south regions of a city) or by both sector and region.

Longitude and Latitude (in degrees) are the center of the grid for area emissions and precise locations for Large Point Sources (LPS).

Emissions are always read in units of tons/year (of SO_2 for sulfur and PM_{10} or $PM_{2.5}$ for particulates).

Emission type: 0 for area, 1 for LPS and 2 for volcano. Area emission sources (small industries, incinerators, boilers and mobile sources) are released into the well-mixed layer during the day and into the surface layer at night, and for elevated sources (large point sources) are released into the well-mixed layer during the day and above the surface layer at night. Volcanic sources are always released into the well-mixed layer. Since the surface layer height is fixed at 300.m (see atmos2.inc file variable descriptions) only point sources with stack heights of at least 200.m are considered large point sources and given the emission type “1”.

Puff release time (in hours) is interval between two puffs. For regional scale simulations it is set at 3 hr and for urban it is set at 1 hr. See examples below.

Examples:

Type 1: All emissions in the simulation together.

```
! Sector#  - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release  time (hr)
1       120.5   30.5    2000            0       1
1       120.5   31.5    2000            0       1
1       131.4   33.2    10000           1       1
1       132.1   -5.5    10000           1       1
1       80.1    -4.5    20000           2       1
```

This file means there are 5 emitting sources (2 area, 2 LPS, and 1 volcanic) in the simulation domain, all specified under one sector number "1". For this simulation user need to specify only one output filename – OUTFILE1.

Type 2: Emissions separated by type

```
! Sector#  - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release ! time (hr)
1       120.5   30.5    2000            0       3
1       120.5   31.5    2000            0       3
2       131.4   33.2    10000           1       3
2       132.1   -5.5    10000           1       3
3       80.1    -4.5    20000           2       3
```

This file means there are 5 emitting sources (2 area, 2 LPS, and 1 volcanic) in the simulation domain, specified under 3 sectors – 1, 2, and 3. For this simulation, if output format all emitting regions together (flag "1" in atmos2.ini file) is selected, user need to specify only one output filename – OUTFILE1. Otherwise, user needs to specify three output file names – OUTFILE1, OUTFILE2, and OUTFILE3.

Type 3: Emissions separated by sector type (1=industrial, 2=agricultural, 3=boilers, 4=domestic, 5=power, 6=volcano) or by region (1=western province, 2=eastern province, 3=southern province, 4=northern province, 5=LPS, 6=volcano) or by region and sector (1=industry in eastern province, 2=agriculture in eastern province, 3=boilers in western province, 4=domestic in southern province, 5=LPS in northern province, 6=volcano in the western province)

```
! Sector#  - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release ! time (hr)
1       120.5   30.5    2000            0       1
1       120.5   31.5    2000            0       1
2       120.5   30.5    2000            0       1
2       120.5   31.5    2000            0       1
3       120.5   30.5    2000            0       1
3       120.5   31.5    2000            0       1
4       120.5   30.5    2000            0       1
4       120.5   31.5    2000            0       1
5       131.4   33.2    10000           1       1
5       132.1   -5.5    10000           1       1
```

6 80.1 -4.5 20000 2 1

This file means there are 11 emitting sources (8 area, 2 LPS, and 1 volcanic) in the simulation domain, specified under 6 sectors – 1 to 6. For this simulation, if output format all emitting regions together (flag "1" in atmos2.ini file) is selected, user need to specify only one output filename – OUTFILE1. Otherwise, user needs to specify 6 output file names – OUTFILE1, OUTFILE2,… and OUTFILE6.

Type 4: Emissions separated by sector or region as in Type 3, but sector numbers ranging from 10-15 instead of 1-6.

! Sector# - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release ! time (hr)

10 120.5 30.5 2000 0 3
10 120.5 31.5 2000 0 3
11 120.5 30.5 2000 0 3
11 120.5 31.5 2000 0 3
12 120.5 30.5 2000 0 3
12 120.5 31.5 2000 0 3
13 120.5 30.5 2000 0 3
13 120.5 31.5 2000 0 3
14 131.4 33.2 10000 1 3
14 132.1 -5.5 10000 1 3
15 80.1 -4.5 20000 2 3

This file means there are 11 emitting sources (8 area, 2 LPS, and 1 volcanic) in the simulation domain, specified under 6 sectors – 10 to 15. For this simulation, if output format all emitting regions together (flag "1" in atmos2.ini file) is selected, user need to specify only one output filename – OUTFILE1. Otherwise, user needs to specify 6 output file names – OUTFILE10, OUTFILE11,… and OUTFILE15.

Type 5: Emissions separated by sector or region as in Type 3, but sector numbers are random.

! Sector# - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release ! time (hr)

10 120.5 30.5 2000 0 1
10 120.5 31.5 2000 0 1
27 120.5 30.5 2000 0 1
27 120.5 31.5 2000 0 1
32 120.5 30.5 2000 0 1
32 120.5 31.5 2000 0 1
56 120.5 30.5 2000 0 1
78 120.5 31.5 2000 0 1
90 131.4 33.2 10000 1 1
90 132.1 -5.5 10000 1 1
91 80.1 -4.5 20000 2 1

This file means there are 11 emitting sources (8 area, 2 LPS, and 1 volcanic) in the simulation domain, specified under 7 random sectors. For this simulation, if output

format all emitting regions together (flag "1" in atmos2.ini file) is selected, user need to specify only one output filename – OUTFILE1. Otherwise, user needs to specify 7 output file names – OUTFILE10, OUTFILE27, OUTFILE32, OUTFILE56, and so on.

Note: For particulates simulation a similar format for emissions is followed except for the emissions column. For particulate emissions user should input both PM10 and PM2.5 emissions together into the model, following the format below.

Sector# - Longitude - Latitude – PM10 Emission (tons/year) – PM2.5 Emission (tons/year) – Emissions type – Puff release time (hr)

Example:

```
! Sector#  - Longitude - Latitude – Emission (tons/year) – Emissions type – Puff release ! time (hr)
1       120.5  30.5   2000          1000          0       1
1       120.5  31.5   2000          100           0       1
2       131.4  33.2   10000         6000          1       1
2       132.1  -5.5   10000         6000          1       1
3       80.1   -4.5   20000         10000         2       1
```

This file means there are 5 emitting sources (2 area, 2 LPS, and 1 volcanic) in the simulation domain, specified under 3 sectors – 1, 2, and 3. For this simulation, if output format all emitting regions together (flag "1" in atmos2.ini file) is selected, user need to specify only one output filename – OUTFILE1. Otherwise, user needs to specify three output file names – OUTFILE1, OUTFILE2, and OUTFILE3.

2) Land-Sea Mask File

The First line start with comment (!) with explanation of each parameter. See examples.

The Land-Sea Mask File has the following format:
Longitude - Latitude – Grid type

Longitude and Latitude (in degrees) is the southwest corner of the each grid.

Grid type: 0 for water, 1 for land (major portion of the grid)

Example:

```
! Longitude - Latitude land/water(1/0)
120.0   30.0    0
120.0   31.0    0
131.0   33.0    1
132.0   -5.0    1
80.0    -4.0    0
```

This file means that the simulation domain has 5 grid cells (3 water and 2 land). By default, in the model all the grids are assumed land. So, user need not specify land grids in this file.

3) Urban-Rural Mask File

This file is required only if the urban simulation flag is selected in the initialization file (atmos2.ini)

The First line starts with comment (!) with explanation of each parameter. See example.

The Urban-Rural Mask file has the following format:
Longitude - Latitude – Grid type

Longitude and Latitude (in degrees) is the southwest corner of the each grid.

Grid type: 0 for rural, 1 for urban (major portion of the grid)

Example:

```
! Longitude - Latitude urban/rural(1/0)
120.0   30.0    0
120.0   31.0    0
131.0   33.0    1
132.0   -5.0    1
80.0    -4.0    0
```

This file means that the simulation domain has 5 grid cells (3 rural and 2 urban). By default, in the model all the grids are assumed rural. So, user need not specify rural grids in this file.

4) Grid Description File

This file contains the simulation domain description, and meteorological data description. File contains the following lines.

```
! RAINS-ASIA grid systems
'LATLON'         ! "the" lat-lon coord. system
1,  0.0D0, 0.0D0, 0.0D0, 0.0D0, 0.0D0
' '                                          !  end coords
'ATMOS_MET'  ! ATMOS meteo grid
'LATLON',  60.0D0,  -20.0D0,  2.5D0,  2.5D0,  41,  31,  1
'ATMOS_OUT'      ! ATMOS output grid
'LATLON', 119.05D0,  29.05D0,  0.1D0,  0.1D0, 42, 42,  1
' '                                          !  end grids
```

User needs to change only the second last line, which describes the simulation domain dimensions. Second to last line follows the following format (**Note:** All the dimensions are expressed in degrees):

'LATLON', Longitude, Latitude, Longitude grid size, Latitude grid size, # longitudinal grids, # of latitudinal grids, 1

Longitude and Latitude correspond to the center of the southwest corner grid (first grid) of the simulation domain (119.05˚ and 29.05˚ in the example)

Longitude and Latitude grid size in degrees (0.1˚ x 0.1˚ grid resolution in the example)

# of longitudinal and latitudinal grids (42 x 42 grids in this example)

"1" at the end of the line indicates that model uses geographic (lat-lon) coordinate system. **Note:** ATMOS uses only Geographic Coordinate System.

Similarly, line under with 'ATMOSMET' describes the domain for meteorological database. For Asian domain simulations, meteorological data is pre-processed using NCEP reanalysis data for a period of 1-year (example 1990, 1995, 2000, etc) at 6-hour intervals. This statement if fixed for the meteorological data files downloaded from the website indicated below.

Meteorological Data

The model utilizes pre-processed NCAR/NCEP meteorological data at 6-hr interval. Data includes u-wind, v-wind, mixing heights and precipitation rates. NCEP reanalysis project files are available for free at 2.5 x 2.5 degree resolution from NOAA – Climate Diagnostics Center (http://www.cdc.noaa.gov/cdc/data.nmc.reanalysis.html)

Meteorology data is available only in netCDF/IOAPI format. Preprocessed data files for ATMOS model (for Asia only) can be downloaded from (http://www.cgrer.uiowa.edu/ATMOS/metdata) or can be obtained by sending an email to any of the contact persons on page 2.

Upon downloading the preprocessed meteorological files from the above ftp site, user must transfer the files to the "inputs" directory of ATMOS model.

Output Data File Management

Output from the model run is always in netCDF/IOAPI formats. User can download the extract programs to convert IOAPI format output data to text format at this website http://www.cgrer.uiowa.edu/ATMOS/extractcodes