Fairbanks North Star Borough $PM_{2.5}$ Non-Attainment Area CMAQ Modeling

Final Report Phase I

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1. Background

On December 18, 2009 the U.S. Environmental Protection Agency (EPA) designated the Fairbanks North Star Borough (FNSB) as a nonattainment area for the 2006 24h-average $PM_{2.5}$ National Ambient Air Quality Standard (NAAQS). This designation led to the obligation to develop an approvable State Implementation Plan (SIP) by December 2012. The SIP must demonstrate attainment by December 2014. To ensure compliance, the State of Alaska's Department of Environmental Conservation (DEC) and the FNSB have been working cooperatively to collect the information needed to educate the public and the Assembly about (1) the causes of Fairbanks' air quality issue and (2) the emission-reduction measures available to attain the NAAQS for $PM_{2.5}$. These activities have encompassed, among other things, the documentation of trends in 24h-average $PM_{2.5}$-concentrations, emissions of $PM_{2.5}$ and its precursors, and the regulatory framework for the SIP-development. This work has included reviewing the current scientific knowledge on (1) what governs particulate formation during winter conditions, (2) the efficiency of various control measures, and (3) air quality models (AQM) to quantify the impact of such control measures on ambient concentrations in future years.

DEC followed EPA guidance for calculating site-specific baseline concentrations in determining the design value for the 2008 base year. This calculation used the average of the three design periods (2006-2008, 2007-2009 and 2008-2010) that straddle the baseline year, and led to a design value of 44.7 $\mu g/m^3$.

Discussions between DEC, FNSB and EPA staff led to the selection of two episodes in the 2008 base year that are to be used for attainment modeling: January 23 – February 10; and November 2–17. In this first phase, we used that first episode to setup a Fairbanks adapted - Community Multiscale Air Quality Modeling System (CMAQ) version, recommend changes to the regulatory CMAQ, and to evaluate the recommended Fairbanks adapted model setup of CMAQ.

Under contact to the EPA Office of Research and Development (ORD), Penn State established a model domain and set up a WRF configuration for Fairbanks. Under that contract Penn State performed simulations of an episode in December 2007 and the January 23 – February 10 episode in 2008 that we used for this first phase. It is likely that Penn State will be contracted to revise the January/February episode WRF-simulation that we used in the work reported about in this document. They may redo the simulations to take advantage of nudging improvements developed under their ongoing work.

Under contract to EPA-ORD, Sierra Research Inc. (Sierra) prepared preliminary emissions inventories for the Fairbanks model domain that was specified by Penn State. These inventories are preliminary in so far as they did not (1) include Motor Vehicle Emission Simulator (MOVES) based emission estimates, and (2) account for source specific activity data that were collected in Fairbanks. Sierra is responsible for preparing the inventories, and for using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System to process source specific emission

estimates into gridded, speciated, hourly emissions. We used this data as input to the CMAQ model. DEC has contracted with Sierra to develop updated gridded temporally resolved emission inventories for both the January/February and November 2008 episodes.

DEC contracted with the University of Alaska Fairbanks (UAF) to adapt and apply the CMAQ system to represent the 24h-average $PM_{2.5}$-concentrations observed in the Fairbanks $PM_{2.5}$ nonattainment area. Note that the State Building site was the only site with measurements in the nonattainment area during the January 23 – February 10, 2008 episode.

This report covers the work contracted for phase I that foresaw to process the aforementioned Fairbanks specific CMAQ inputs from WRF and SMOKE to simulate concentrations for the January/February 2008 episode. This report provides a detailed performance evaluation of the CMAQ model results relative to the available observations including a scientific analysis of CMAQ's performance. It also discusses our recommendations for the model improvements that are needed to meet EPA quality-assurance requirements for use of the modeling in the regulatory context. The key efforts related to air-quality modeling are outlined below.

2. Configuration of CMAQ for the January/February 2008 Episode

2.1 General information

The CMAQ package consists of three primary components: the meteorological modeling system (in our case the Weather Research and Forecasting (WRF)), the emission processing, and the CMAQ chemistry transport mode (CCTM). These components are linked by a set of preprocessors (Fig. 1). The photolysis-rate processor (JPROC) calculates the photolysis rates from tabulated absorption cross-section and quantum-yield data. The meteorology-chemistry interface processor (MCIP) transforms the WRF-input fields to CMAQ's coordinate system (Otte and Pleim, 2010). The outputs from MCIP are further used by the initial and boundary conditions processors (ICON and BCON) that generate the initial concentration of the chemical species and create the boundary conditions for the grid cells surrounding the domain, respectively. Finally, the output files, generated by the preprocessors (JPROC, BCON, ICON, MCIP) and the emission files are used as input for the CCTM. The CCTM provides the concentrations of pollutants, wet and dry deposition rates, aerosol diagnostics, and visibility metrics as output.

The CCTM uses coupled ordinary differential equations (ODEs) to predict the changes in pollutant concentrations throughout a three-dimensional grid that is fixed in space. The continuity equation is used to simulate the change in pollutant concentrations in each grid cell over time

$$\partial C/\partial t = \text{Adv} + \text{Diff} + Rc + Ec - Sc \qquad (1)$$

Where Adv is advection, Diff is diffusion; *Rc* stands for the chemical transformation of specie *C, Ec* and *Sc* describe the source and sinks for the specie *C.*

As stated above we used the Penn State WRF output files and the first (corrected) complete emissions inventory from SMOKE that accounts for Fairbanks specific temporal and spatial variations of emissions.

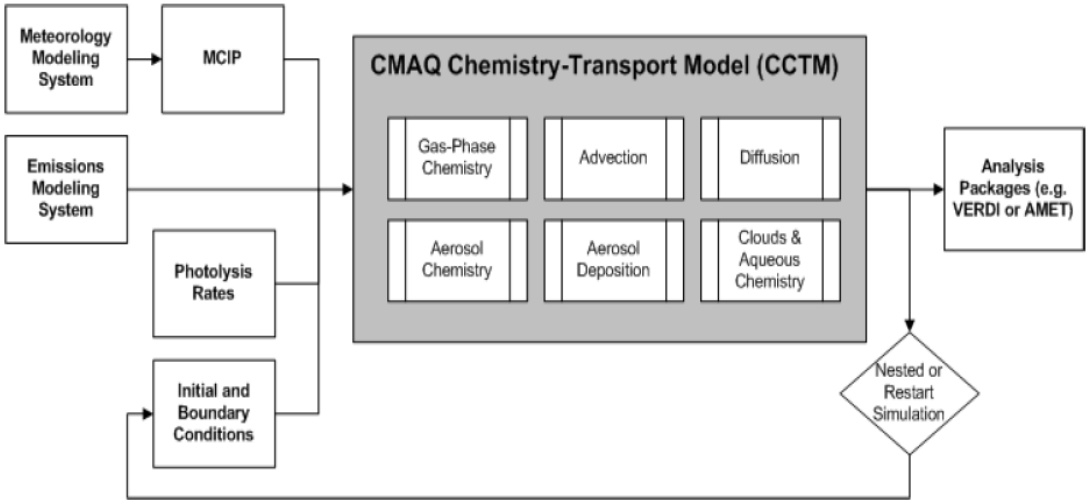


Fig. 1. Schematic view of the CMAQ modeling package: Meteorology modeling system, emission modeling system, chemistry-transport model and associated preprocessors (MCIP, the photolysis processor, initial condition and boundary condition processor). From CMAQ v.4.7.1 Operational Guidance Document (2010).

2.2 Brief description of the input data

The meteorological data are available from January 23, 2008 0000 UTC to February 12, 2008 0000 UTC with a 12 minute and 1333.33m resolution. The map projection is Lambert conformal. The meteorological physical parameterizations used by Penn State are:

Cumulus parameterization:	None
Microphysics:	Morrison 2-moment
Longwave radiation:	RRTMG scheme
Shortwave radiation:	RRTMG scheme
PBL scheme:	Mellor-Yamada-Janjić (Eta) TKE
Surface layer scheme:	Monin-Obukhov (Janjić Eta)
Land-surface scheme:	RUC Land-Surface Model
Urban model:	No urban physics
3D Analysis nudging:	OFF
SFC Analysis nudging:	OFF
OBS Nudging:	ON
Wind coefficient:	$4 \cdot 10^{-4}$ s^{-1}
Temperature coefficient:	$4 \cdot 10^{-4}$ s^{-1}
Moisture coefficient:	$4 \cdot 10^{-4}$ s^{-1}

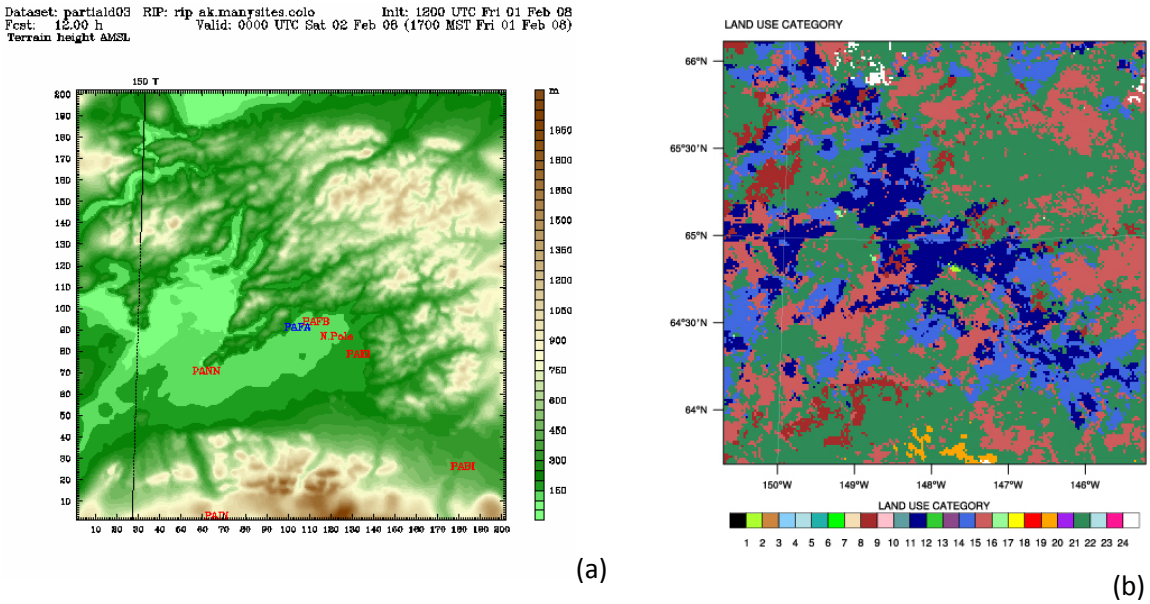
We stored the emission files obtained from Sierra on the archive of UAF's supercomputer. The data that we obtained were emissions of nonpoint, nonroad and onroad sources that were merged into single and 4-layered merged emissions files. Point-source emissions are in the in-line plume rise point source emission file, and the stack parameters are in the stack groups files. The emission data file encompasses December 15, 2007 to February 15, 2008 with an hourly resolution. The emission data is available for 199×199 grid points, i.e. the "emission domain" is one grid cell less on each side than the Fairbanks domain of WRF. The "extra" grid cells on each side of domain 3 act as the boundary buffer (NTHIK). The center of the emission domain is at 64.8N and 148W. The map projection is Lambert conformal, and the grid-cell size of the X and Y-coordinates (XCELL, YCELL) are 1333.33m as the meteorological input data. The X and Y-coordinates for the lower left corner of the grid (XORIG, YORIG) are -130666.125 and -118665.891, respectively. The parameter VGTYP is -1, and the VGLVLS are all zero for both the single and 4-layered merged emission files.

2.3 Installation of the CMAQ package

We installed CMAQ version 4.7.1 and MCIP version 3.6 on the UAF supercomputer. The meteorological data produced by Penn State were obtained from EPA and stored on the supercomputer's archive as well as on a local PC for collaboration with DEC. Penn Stae had generated the meteorological data with the Advanced Research WRF (WRF-ARW) version 3.1 over three one-way nested domains with grid increments of 12 km, 4 km and 1.3 km, respectively (Gaudet and Stauffer, 2010). These domains are called domain 1, 2 and 3, respectively, hereafter. The Fairbanks domain (domain 3) that has a 1.3 km grid increment is centered over the Fairbanks and covers among other things the nonattainment area. This domain is used to simulate the chemical transport of species with CMAQ. The dimension of domain 3 is 201×201 grid points with 38 full vertical layers, and centered at 64.92749N and 147.957W. The elevation and land-use category distributions in domain 3 are shown in Figure 2.

Several changes to the CMAQ package were necessary to get CMAQ running for the episode over the Fairbanks domain. Besides adapting the CCTM, we examined the pre-processors (i.e. JPROC, BCON, ICON and MCIP) used for generating the input data for the CCTM and adapted them for Alaska as necessary. These, among other things, were related to coordinate issues, and looping in the CMAQ code. For instance, for East Coast applications it makes no sense to run a loop on land-use types that only occur at high-latitudes (see details in section 4.1).

We generated initial conditions (IC) and boundary conditions (BC) for the Fairbanks domain, as well as modified the code in JPROC and MCIP to represent the Fairbanks domain.



(a) (b)

Fig. 2. (a) Terrain elevation as used in domain 2 (From Gaudet and Staufer, 2010) and (b) USGS land-use categories in domain 3. The land-use category code is 1 urban and built-up land, 2 dryland cropland and pasture, 3 irrigated cropland and pasture,4 mixed dryland/irrigated cropland and pasture, 5 cropland/grassland mosaic, 6 cropland/woodland mosaic, 7 grassland, 8 shrubland, 9 mixed shrubland/grassland, 10 savanna, 11 deciduous broadleaf forest, 12 deciduous needleleaf forest, 13 evergreen broadleaf, 14 evergreen needleleaf, 15 mixed forest, 16 water bodies, 17 herbaceous wetland, 18 wooden wetland, 19 barren or sparsely vegetated, 20 herbaceous tundra, 21 wooded tundra, 22 mixed tundra, 23 bare ground tundra, 24 snow or ice.

2.3.1 MCIP

The horizontal model grid, vertical layer structure, and model time periods must be consistent across the meteorology data, emissions data, and CCTM. MCIP creates the consistent meteorological data that can be used by the CCTM. MCIP preprocesses the data from the meteorological model, transforms the coordinates, and defines the grid sizes for the chemistry transport domain. To define the horizontal grid domain for the CCTM simulation, the MCIP processor generates the domain based on the domain of the input meteorological field (meteorological domain). The domain generated by the MCIP is automatically given a smaller extent than the meteorological domain with the intention of avoiding the impact of the lateral boundary conditions from the meteorological domain on the air quality simulation in the CCTM.

As pointed out above, the meteorological domain has 201×201 and the emission domain has 199×199 grid points. The boundary trim option ("BTRIM") was used to uniformly trim the grid cells off each of the four lateral boundaries of the input meteorology grid. BTRIM was set to zero (0) to use the maximum extent of the meteorological domain. Two grid cells on each side of the subset domain then act as the boundary buffer (NTHIK). This setting led to the subset domain size of 199×199 grid points, which is the CCTM domain. In addition, the WRF_LC_REF_LAT

parameter was used to force the reference latitude at the center to 64.8 (WRF_LC_REF_LAT = 64.8). The run script for MCIP is attached in Appendix A.

To run MCIP on the Fairbanks domain, we edited the source code of MCIP in the setgriddefs.f file as follows: We commented out six statements per recommendation by G. Pouliot, EPA/ORD (email 12/09/10) so the code works properly with the WRF Fairbanks, Alaska grid domain constraints. Basically, we disabled the forcing of XORIG and YORIG to be offset by half delta-X since the CMAQ grid domain has to be one cell smaller on all boundaries than that of WRF: WRF mandates grid domain "cross points" (#cells + 1) that are evenly divisible by 3 (e.g., 201×201 cross points, 200×200 dot points for the Fairbanks domain). CMAQ/MCIP use an even number of cross points (e.g., 200; T. Carlson email 03/23/2011). Thus, our editions are

```
!     xtemp = xorig_ctm / 500.0
!     ytemp = yorig_ctm / 500.0
!     xtemp = FLOAT(NINT(xtemp))
!     ytemp = FLOAT(NINT(ytemp))
!     xorig_ctm = xtemp * 500.0
!     yorig_ctm = ytemp * 500.0
```

Initially, MCIP failed to generate the emission files and output file. The different grid parameters of emission domains and MCIP output in decimals caused the CCTM to crash. We found and corrected two inconsistencies:

1) Inconsistency from:

XCELL3D	1333.329956054688
XCELL_GD	1333.329956054690
YCELL3D	1333.329956054688
YCELL_GD	1333.329956054650

This inconsistency caused the error message, “file grid sizes do not match CCTM domain definition” when running the CCTM. To remove this error message, the following actions were done:

1.1) The attribute of all input emission files were edited by using following commands:

```
ncatted -a YCENT,global,o,d,64.8000030517578 emission file name
ncatted -a YORIG,global,o,d,-118667.5625 emission file name
ncatted -a YCELL,global,o,d,1333.32995605469 emission file name
ncatted -a XCELL,global,o,d,1333.32995605469 emission file name
```

1.2) The XCELL, YCELL, YORIG and YCENT of GRIDDESC file were edited before use in ICON, BCON and CCTM. Note that the edition is at the decimal place and the edited

decimal numbers are based on the METCRO2D or GRIDCRO2D, which are output of MCIP. The original GRIDDESC file generated by MCIP is shown below:

```
'TEST_GRID'
  2       50.000       70.000     -148.000     -148.000       64.800
'FAIRBANKS'
'TEST_GRID'   -130666.125   -118667.563     1333.330     1333.330 199 199
```

The edited GRIDDESC file is shown below:

```
'TEST_GRID'
  2       50.000       70.000     -148.000     -148.000       64.8000030517578
'FAIRBANKS'
'TEST_GRID'   -130666.125   -118667.5625     1333.32995605469     1333.32995605465
199 199
```

1.3) The source code of the CCTM in the advstep.f was edited to force XCELL3D or YCELL3D to be equal to XCELL_GD or YCELL_GD. The following lines were added before the error message print out as follows:

```
      XCELL3D=XCELL_GD
      YCELL3D=YCELL_GD

     IF ( XCELL3D .NE. XCELL_GD .OR. YCELL3D .NE. YCELL_GD ) THEN
       XMSG = 'File grid sizes do not match CTM domain definition'
       write(6,*)"XCELL3D",XCELL3D
       write(6,*)"XCELL_GD",XCELL_GD
       write(6,*)"YCELL3D",YCELL3D
       write(6,*)"YCELL_GD",YCELL_GD

       CALL M3EXIT( PNAME, JDATE, JTIME, XMSG, XSTAT3 )
     END IF
```

2) Inconsistency in the 4-layer merged emission file

Prior to learning that there is still a problem with the multi-layer emission file, we run tests using the 4-layer merged emission data. When the 4-layer merged emission files were used in the CCTM, we obtained the error message, “Top of plume is less than top of stack for source”. The invalid vertical structure might cause this error message because the attribute of the layered emission file showed that vertical coordinate type (VGTYP) is -1 and vertical coordinate grid levels values (VGLVLS) are all zero. The invalid vertical structure needs to be fixed as suggested by Chris Nolte (RTP, USEPA). At

present, our simulations used single layered merged emission files instead. Sierra is working on fixes for the 4-layer emission files.

Some additional modifications were made to MCIP that did not serve to just get MCIP running for the Fairbanks domain, but to adapt it to the vegetation that exists in the Fairbanks domain. These modifications will be discussed within the framework of the changes to the treatment of dry deposition as these changes were required for this purpose (section 4.1).

2.3.2 ICON, BCON and JPROC

The gas-phase, aerosol, and aqueous-phase chemical mechanisms for the initial conditions, boundary conditions and photolysis rates were set as cb05cl_ae5_aq, carbon-based mechanism including sea salt, aqueous/cloud chemistry and active chlorine in aerosol mechanism for the compiling option. The other configuration options were set as default during the compilation of the ICON and BCON executables. The input files for JPROC, ICON and BCON were based on the ASCII profile files, which come with the CMAQ version 4.7.1 package. The CMAQ package's profile files for the initial condition and boundary conditions are shown in Appendix B. Since the used profile file did not represent the initial and boundary condition for the Fairbanks domain, we created Alaska specific initial and boundary condition for the Fairbanks domain (discussed later).

2.3.3 CMAQ

There are many configuration options in CCTM that can be selected to optimize the model for different applications. For the simulations described in this report, the compilation options were set as follows:

1. ModDriver = ctm_yamo (The generalized coordinate driver module used Yamartino scheme for mass-conserving advection)
2. ModInit = init_yamo (The CCTM time-step initialization module used Yamartino scheme)
3. ModAdjc = // (The mass conservation error adjustment scheme was not set due to using the Yamartino scheme)
4. ModCpl = gencoor (The module used for unit conversion and concentration coupling is the CMAQ generalized coordinate)
5. ModHadv = hyamo (The horizontal advection module calculated by the global mass-conserving scheme)
6. ModVadv = vyamo (The vertical advection module calculated by the global mass-conserving scheme)
7. ModHdiff = multiscale (The horizontal diffusion module used the diffusion coefficient based on local wind deformation)
8. ModVdiff = eddy (The vertical diffusion module used eddy diffusivity theory)
9. ModPhot = phot_inline (Photolysis calculation module considered the aerosol feedback on the photolysis rate)
10. ModChem =ebi_cb05cl_ae5 (use the Euler Backward Iterative solver optimized for the Carbon Bond-05 mechanism with chlorine and extended aerosols)

11. ModAero = module aero5 (used the aerosol module with extensions for sea-salt emissions and thermodynamics and a new formulation for secondary organic aerosol)
12. ModAdepv = module aero_depv2 (The aerosol deposition velocity module used the second-generation CMAQ aerosol deposition velocity routine)
13. ModCloud = module cloud_acm_ae5 (The cloud module used the ACM cloud processor that uses the ACM methodology to compute convective mixing)
14. Mechanism = cb05cl_ae5_aq (The gas-phase, aerosol, and aqueous-phase chemical mechanisms used cb05cl_ae5_aq, i.e. the same as BCON, ICON and JPROC)
15. Tracer = trac0 (No use of tracers in the CCTM)

The run script of the CCTM is attached in Appendix C.

3. First assessment of the installed CMAQ

3.1 WRF/Chem vs. CMAQ

As a first step to assess the original CMAQ's performance, the differences between WRF-CMAQ and WRF/Chem were analyzed as WRF/Chem had showed itself to capture Fairbanks' chemical and meteorological conditions well for winter 2005/06 and winter 2008/09 (Mölders et al., 2011a, b). Note that WRF/Chem is a science (research) model that also had been already used successfully in various emission change scenarios for Alaska (Mölders et al., 2010; Yarker et al. 2010; Tran et al. 2011). WRF-CMAQ is EPA's regulatory model. Same features of WR-CMAQ and WRF/Chem are:

- Both use WRF to simulate the meteorological fields
- Both models assume background concentrations as initial condition at the start of the simulation episode and as boundary conditions throughout the simulation
- Both models take chemical fields of the previous simulation as initial concentration for the next simulation
- Performance skill scores are in the same ballpark for the meteorological quantities (compare Mölders et al., 2010, 2011; Gaudet and Stauffer, 2010)

Differences are:

- WRF/Chem uses Alaska adapted background concentrations (Mölders et al., 2010, 2011), while those of the original CMAQ were valid for the Lower 48 (CMAQ, 2010)
- For the Alaska simulations up to today WRF/Chem used various top-down emission inventories (e.g. Mölders et al., 2010; Tran et al., 2011), while CMAQ uses a bottom-up emission inventory[1] (pers. communication with Dulla in 2009)

[1] An emissions inventory assembled by a top-down approach bases on generalized factors (e.g. total fuel use, total population, total housing units, total number of manufacturing jobs, etc.) as indicators of emissions. Emission factors are derived that assess emissions per unit energy use, person, etc. The product of the emission indicator and emission factor is the emission estimate. The top-down approach is best for global or very large regional scale problems; despite it can be and has been applied to local air pollution questions in applications with as low as 4km grid increments. The bottom-up approach divides the region of interest into relevant sectors. Specific information is gathered for each sector based on the existing industries, residential units, and traffic etc. This information serves to estimate the emissions for each sector. As obvious, the bottom-up approach requires considerably greater efforts than the top-down

- Model domain and increment (4km vs. 1.33km) are different (cf. Mölders et al., 2010, 2011; Gaudet and Stauffer, 2010)
- Advection schemes differ (Peckham et al., 2009; CMAQ, 2010)
- The Alaska adapted WRF/Chem considers feedback of chemistry on meteorology[2] (Peckham et al., 2009), while the WRF-CMAQ package does not (CMAQ, 2010)
- Meteorological options used in WRF and the Alaska adapted WRF/Chem for cloud-microphysics and frequency of calling the radiation scheme (cf. Mölders et al., 2010, 2011; Gaudet and Stauffer, 2010)
- The Alaska adapted WRF/Chem simulations performed for the Fairbanks area correctly apply a cumulus parameterization that is required at their grid increment of 4km, while the WRF runs for CMAQ used in this study are run correctly without use of a cumulus parameterization as at the 1.3km increment, cumulus clouds - should they occur at all - are resolved[3]
- WRF and the Alaska adapted WRF/Chem use different schemes for calculation of shortwave and long-wave radiation (cf. Mölders et al., 2010, 2011; Gaudet and Stauffer, 2010) and calculate radiation with different time steps[4]
- The Alaska adapted WRF/Chem is run in forecast mode, while WRF was run in assimilation mode[5] (cf. Mölders et al., 2010, 2011; Gaudet and Stauffer, 2010)

3.2 Evaluation

We assessed the model performance using the metrics established by Boylan and Russell (2006). Figure 3 shows the evaluation of the first full CMAQ run. Note that this is CMAQ in its original form just setup over Alaska and with the modifications that were technically necessary to get the model running, i.e. without changes to the deposition module or IC/BC, etc.. This plot only serves for comparison to Fig. 17 to demonstrate the improvement made by the Alaska adaption that is described later.

Emissions, advection and diffusion, chemical transformations and deposition can change the predicted concentrations (CMAQ, 2010). Therefore, we examined the impact of the selection of the CCTM module options that include different advection and diffusion schemes as well as photolysis modules. Furthermore, we analyzed the deposition module as the literature documents (e.g. Zhang et al., 2003; Mölders et al., 2010) that deposition over snow requires some special treatment. The results and modifications made are described in this report.

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approach. The data is often more reliable and/or detailed. However, one must be cautious in building emission inventories as an emission inventory cannot be better than the accuracy of the input data.

[2] Recent research shows the under certain meteorological condition, aerosol presence, chemical reactions and aerosol formation can affect the meteorological conditions (e.g. http://www.atmosp.physics.utoronto.ca/SPARC/News21/21_Dethof.html, Yarker et al. 2010).

[3] The theoretical background can be found in all text books on atmospheric modeling, e.g. Pielke (2002)

[4] Differences in the frequency of calling the radiation subroutines and in the radiation schemes may lead to slight differences in calculated photolysis rates.

[5] The idea of data assimilation is to pull the meteorological fields as close as possible to the observations. The idea of running a model in forecast mode for past episodes allows to assess how good a future forecast could be.

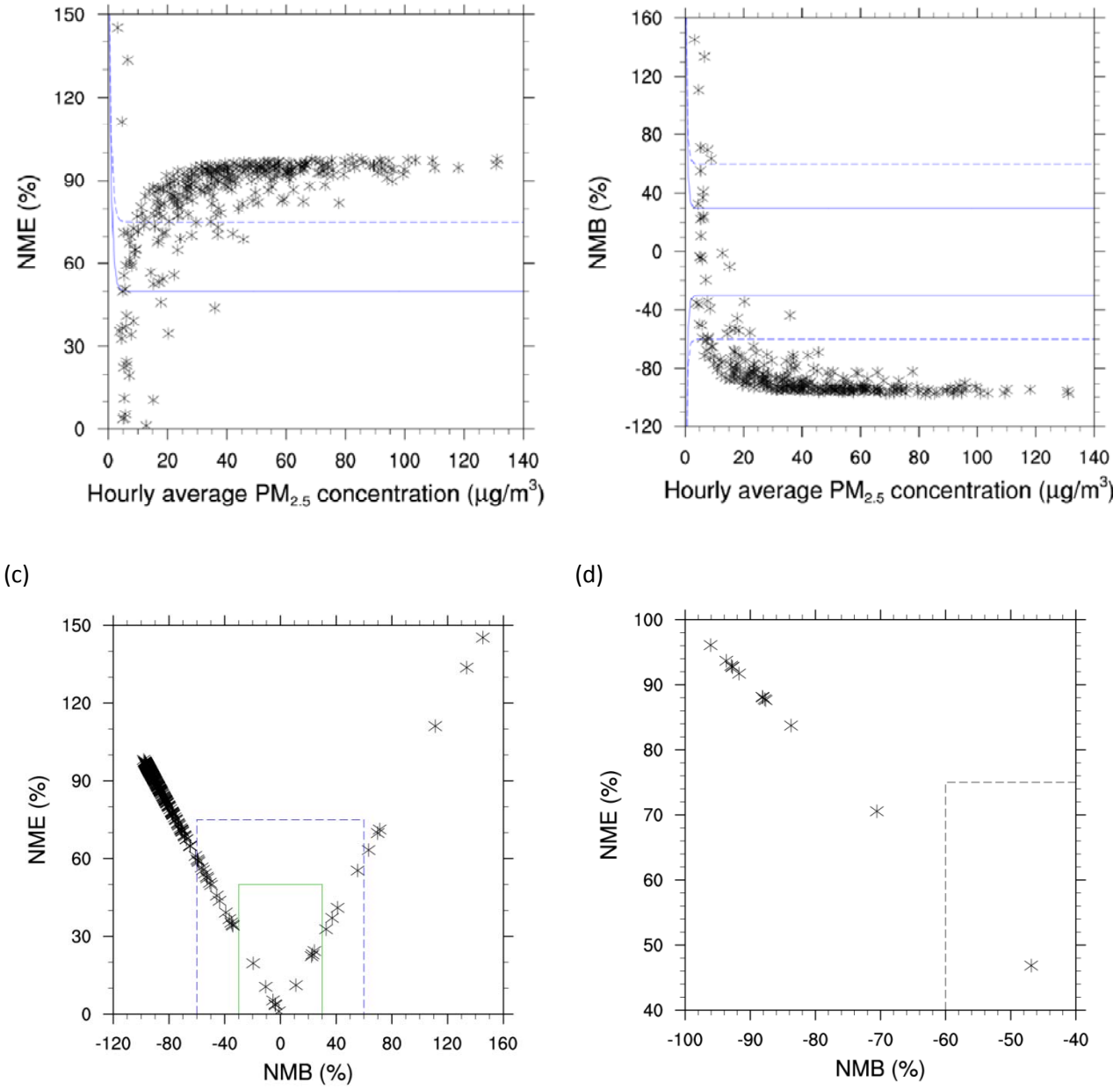


Fig. 3. Performance skill scores as obtained for the original CMAQ simulations with the non-updated EI that had the coordinate offset. (a) bugle plot of hourly $PM_{2.5}$ normalized mean error, (b) bugle plot of hourly $PM_{2.5}$ normalized mean bias, (c) soccer plot of hourly $PM_{2.5}$ normalized mean error and bias, (d) soccer plot of 24h-average normalized mean error and bias. The solid and dashed lines indicate the performance goals and criteria calculated in accord with Boylan and Russell (2006).

3.3 Examination of the emission data

We used the single-layer emission data as it turned out that there were still some problems with the multi-emission layer files that are to be fixed by Sierra for phase II.

After the first successful CMAQ simulations, we compared the simulated $PM_{2.5}$-concentrations to the observations. The comparison showed that CMAQ underestimated the 24h-average $PM_{2.5}$-concentrations tremendously (~ 16 times). Such underestimation can have several reasons that we investigated.

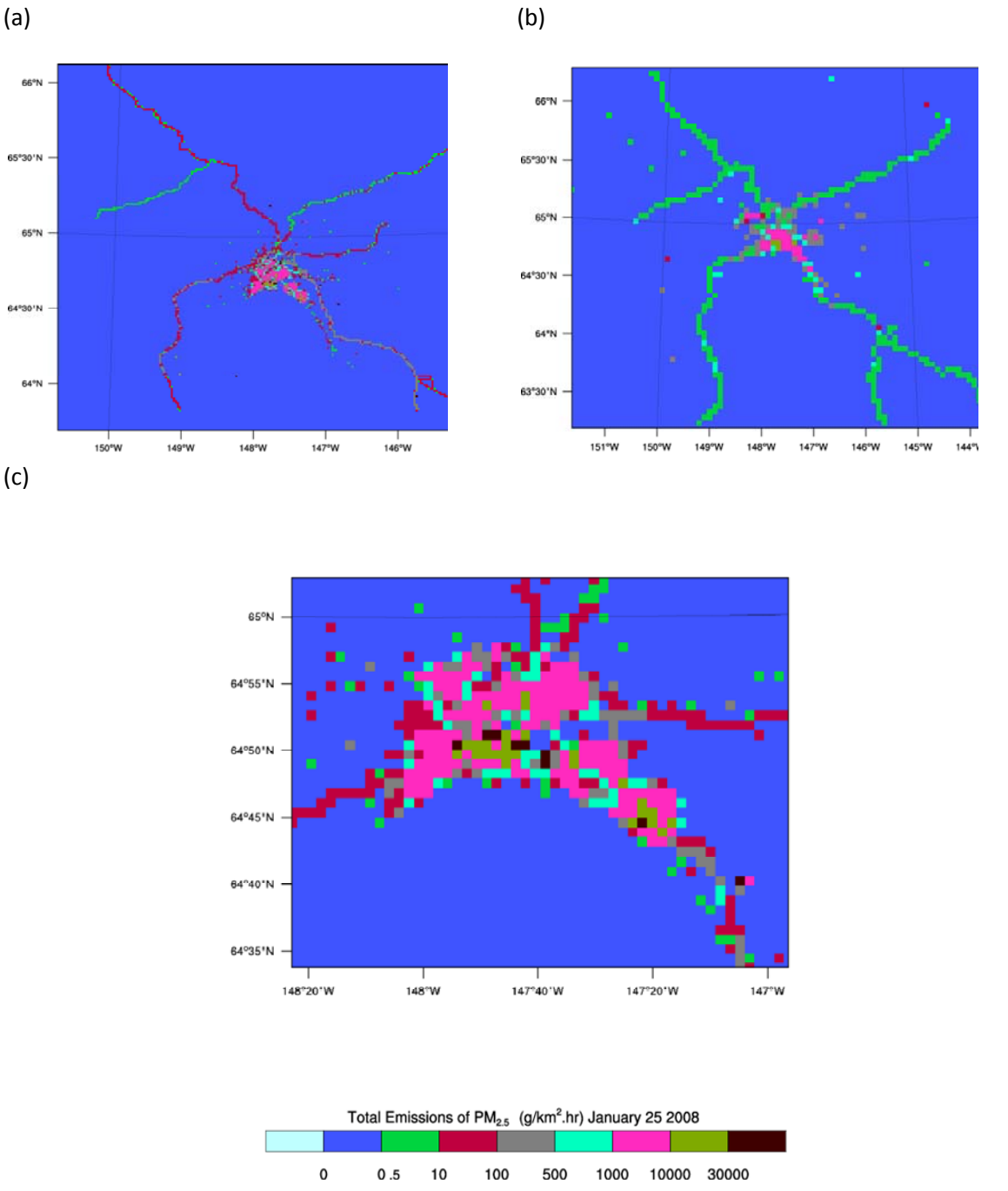


Fig. 4. Exemplary plot of the emissions in the nonattainment area as obtained from the (a) Sierra Research Inc EI as designed for WRF-CMAQ, (b) NEI2008-AkEM as they would be used in WRF/Chem at the WRF/Chem resolution (From: Mölders et al. 2011), and (c) zoom in the corrected EI from Sierra Research Inc for WRF-CMAQ.

To check whether the emission were too low, we downloaded the FNL meteorological analysis data for 1-23-2008 0000 UTC to 2-13-2008 0000 UTC from NCAR (http://dss.ucar.edu/cgi-bin/datasets/getWebList?listAction=doGrMLQuery&dsnum=083.2&startDate=2011-08-15%2000:00&endDate=2011-09-14%2006:00&sort=D&gindex=1) to create the meteorological files required as input for the Alaska Emission allocation Model, AkEM (Mölders, 2010). AkEM needs the WRF meteorological input data (wrfinput) to be able to create emission files from the National Emission Inventory 2008 (NEI2008). Note that this EI is a bottom-down approach. We calculated for each day the total emission of $PM_{2.5}$, SO_2, NO_x, PM_{10}, and NH_3 for the nonattainment area. The data cannot be compared directly 1:1 as the Sierra EI data have a grid of 1.3×1.3km^2 and the emission data derived from NEI2008-AkEM has a grid of 4×4km^2 and the grids have different centers and projections. Thus, we compared the emission totals and found that they have similar order of magnitude (Fig. 4). We found that the area-emission locations were offset. The area emissions were too far south, i.e. in the Tanana Flats where actually no anthropogenic area emission exit. Sierra was notified about this offset and provided a corrected EI (Fig. 4).

4. Modifications and tests of different schemes

4.1 Modification of the dry deposition module

The first simulations with CMAQ showed too high concentrations in remote areas (Fig. 5), where concentrations typically do not exceed 1µg/m^3 except during advection of Asian dust or wildfire events (cf. Cahill, 2003; IMPROVE data). Since it is well known that deposition of precursors may affect their concentration and hence gas-to-particle conversion, we examined the dry deposition module.

Dry deposition of pollutants varies with land-use, surface and atmospheric conditions as well as species in the layer above ground (Wesley et al., 1989; Kramm and Dlugi, 1994; Kramm et al., 1995; Zhang et al., 2003). Alaska has quite different vegetation than found in the Lower 48 and in our simulations large areas are snow-covered. The investigation of the dry deposition model (m3dry.f) showed that no dry deposition was considered by the original CMAQ for any type of tundra. However, huge parts of the Fairbanks model domain are covered by tundra (land-use type 21 in Fig. 2). The do loop in m3dry.f stopped at land-use type 19 so it did not cover the land-use types 20 to 24 of the USGS land-use category. Note that stopping the do loop at land-use type 19 served to save computational time in application over the East Coast where no kind of tundra exists.

We introduced the dry deposition over all USGS-tundra types using the data given in Erisman et al. (1994) by implementing the vegetation parameters for the various tundra types and modifying the source code in m3dry.f so it can represent adequately the deposition onto the land-cover that exists around Fairbanks. Note that the original CMAQ did not include parameters for any type of tundra as these parameters are not required for applications on the East Coast.

We also introduced changes related to dry deposition under cold winter conditions following Zhang et al. (2003) and Mölders et al. (2011). For SO_2, r_{snow} is now taken as a function of temperature with a lower limit of 100s/m and an upper limit of 500s/m (Zhang et al., 2003):

$$r_{snow}(SO_2)=70(2-T) \quad (2)$$

In winter, when temperatures are below -1^oC, r_g and r_{cut} are increased by as much as two times with an upper limit of 2 for the term $e^{0.2(-1-T)}$ of their original value according to a formula similar to Wesely (1989) following (Zhang et al., 2003):

$$r_g(T < -1^oC)=r_g e^{0.2(-1-T)} \quad (3)$$

$$r_{cut}\ (T < -1^oC)=r_{cut} e^{0.2(-1-T)} \quad (4)$$

For wet canopy the stomatal resistance is reduced by half following Zhang et al. (2003)

$$r_{wet}=0.5\times r_{stomata} \quad (5)$$

In the ammonia-bidirectional flux calculation, the minimum SO_2 concentration was lowered to 0.0001ppb to reflect Alaska's relative pristine atmosphere (e.g. IMPROVE 2011).

Buildings and other structures provide additional surfaces in urban areas (due to their walls) for the heterogeneous reaction to occur. Unfortunately, such information is not available for Fairbanks. Therefore, we scaled it to the urban fraction, which is an existing option in CMAQ. The idea of this option is that walls also provide area onto which particles like $PM_{2.5}$ can deposit and hence be removed from the atmosphere. In the original CMAQ version, the extra surfaces were scaled in accord with Svensson et al. (1987). They suggested a typical value of 0.2 for the area to volume ratio (A/V) for buildings in urban environments. In the original version of CMAQ, a maximum value of 0.2 for A/V for buildings was assigned to the grid cell containing the highest urban fraction (variable purb (c,r) in the CMAQ code), i.e., 100. The area-to-volume ratio A/V for buildings for other grid-cells was calculated as purb(c,r)×(0.2/100) where c and r stand for the index of the grid cells counted in south-north and west-east direction, respectively.

Cai et al. (2006) used a value of 1 (total A/V) for their New York study. Since in WRF the strategy of dominant land-use[6] was applied, all grid-cells categorized as urban automatically have a 100% urban fraction. Thus, the land-use data file that was provided with the WRF data was of no help for tackling the problem and applying the option in CMAQ. Therefore, we created a file on the urban fraction (Fig. 11) from the original land-use data that come with the WRF package. Details on this follow later in this report. The use of the strategy of dominant land-use can lead to over- or underestimation of concentrations and deposition; the inhomogeneity at forest edges, for

[6] The strategy of dominant land-use assumes that the dominating land-cover/use type within a grid-cell is representative for the entire grid-cell; it ignores all heterogeneity that exists within the grid-cell. As various studies performed in the last decade showed this assumption can result in huge errors for large numbers of different land-cover/use within the grid-cell and when the surface properties of the dominant land-cover/use and the neglected other land-cover/use types differ strongly (Mölders 2011).

instance, increases the turbulent transports of constituents up to a factor 4 compared to horizontally homogeneous terrain as assumed in the strategy of dominant land-use (Tetzlaff et al., 2002). Inhomogeneity inside an extended stand of trees causes an overall increase of 5–10% with high local extremes, i.e. such an inhomogeneity results to an underestimation of dry deposition at grid-increments like used here. The effects are most pronounced for a wind directions perpendicular to the forest edge (Tetzlaff et al., 2002). The strategy of dominant land-use leads to overestimation of near-surface temperatures in cities located in warm arid regions and underestimation of near-surface temperature in cities located in moderate humid regions (Mölders 2011). Note that the degree of uncertainty various with season and geographic region (Mölders 2011).

In Fairbanks, buildings are typically 2 stories except for downtown (FNSB housing unit data base). Thus, we chose a maximum height of 20m that leads to an A/V of 0.05 and modifies the original CMAQ formulas to

surf_bldg=purb(c,r)×0.002 (6)

to

surf_bldg=purb(c,r)×0.0005 (7)

Furthermore, we changed the pH-value for snow/rain/wet surfaces from 5.0 to 5.2 – an average value found for Interior Alaska (Shaw et al., 1993). Newer data were not available.

The modification made to m3dry.f mainly served to update the module to state-of-the-art findings on deposition on Arctic surfaces, adaptation for the urban conditions of Fairbanks and to include the Alaska vegetation in the dry deposition calculation (test 1). They led to slight difference in simulated $PM_{2.5}$-concentrations (<0.03µg/m^3) in the nonattainment area for the 24h simulated (Table 1, test 1). It is important to note that these modifications were done for adaption to the Fairbanks domain conditions. These modifications are part of the modified code and we continued to use the modified m3dry.f as part of the development for the further tests.

The following changes were necessary in MCIP because dispersion of air pollutants is a function of mixing height and the removal by dry deposition. Overestimation of mixing heights can lead to more vertical mixing of pollutants, and can dilute the pollutants concentrations accordingly. In const_pbl_mod.f90, the constant of the minimum height of the ABL is 50m. We reduced this value to 16m in accord with the observations in Fairbanks (Wendler 1975). According to Wendler, the reason for the low mixing height in Fairbanks is the strong surface radiative forcing. Again no more recent data exist. The minimum stomatal resistance values, which relate to the treatment of dry deposition of gases for the various land-use categories, were edited following Erisman et al. (1994). These values have been found to provide good results in simulations over Alaska with WRF/Chem (e.g. Mölders et al., 2010; 2011; Tran et al., 2011). Note that except for dinitrogen pentoxide (N_2O_5) (Huff et al., 2010) there are no dry deposition measurements for the Fairbanks area at all or for the episode simulated here to do an

evaluation. However, Zhang et al. (2003) found improvements in their simulations over snow. Elbern (person. comm. in 2009) also found improvements for their winter EURAD simulations after introduction of Zhang et al.'s (2003) parameterization.

The default values of resistances in the original CMAQ are as follows:

```
DATA (rstusgs(i),i=1,33)  / 150.0,  70.0,  60.0,  70.0,  80.0,  180.0,  &
                            100.0,  200.0,  150.0,  120.0,  200.0,  175.0,  &
                            120.0,  175.0,  200.0,  9999.0,  164.0,  200.0,  &
                            100.0,  150.0,  200.0,  150.0,  100.0,  300.0,  &
                            100.0,  100.0,  100.0, 9999.0, 9999.0, 9999.0,  &
                            150.0,  140.0,  125.0 /
```

The revised values of resistances are as follows:

```
DATA (rstusgs(i),i=1,33)  / 200.0,  40.0,  40.0,  40.0,  40.0,  70.0,  &
                             40.0,  300.0,  170.0,  70.0,  100.0,  150.0,  &
                            150.0,  125.0,  125.0,  100.0,  40.0,  100.0,  &
                            999.0,  150.0,  150.0,  150.0,  200.0,  999.0,  &
                            100.0,  100.0,  100.0, 9999.0, 9999.0, 9999.0,  &
                           150.0,  140.0,  125.0 /
```

The $PM_{2.5}$-concentrations obtained at the State Building after modifying the "ABL-constants" and resistance values in MCIP are presented in Table 1. These changed constants and values are used in all runs.

Table 1 The first 24h $PM_{2.5}$-concentrations of the simulations for the different 14 tests. All tests used the modified dry deposition module[7].

Test	1	2	3	4	5	6	7	8	9	10	11	12	13	14
IC_BC	ICBC1	ICBC1	ICBC1	ICBC1	ICBC1	ICBC1	ICBC2	ICBC2	ICBC2	ICBC2	ICBC3	ICBC3	ICBC3	ICBC3
Driver	YAMO	PPM	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO	YAMO
Eddy diffusivity	default Kzout=1	Kzout=0.5	Kzout =0.5	PURB	PURB	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ	PURB +half KZ
Vertical diffusion				acm2+ inline	eddy	eddy	eddy	eddy	eddy	eddy	eddy	acm2+ inline	eddy+ inline	eddy+ inline
Photolysis							Phot _inline	Phot _albedo	Phot _inline	Phot _inline	Phot _inline	Phot _inline	Phot _inline	Phot _inline
Vertical advection									Vadv _noop	50%uv	50%uv	50%uv	50%uv	50%uv
Domain	**199**	**199**	**199**	**199**	**199**	**199**	**199**	**199**	**199**	**199**	**66**	**66**	**66**	**199**
	14.9	19.8	19.8	13.9	14.9	19.5	19.5	19.5	18.9	22.6	22.6	15.1	23.5	23.6
	18.8	24.4	24.6	18.1	17.0	23.7	23.7	23.7	21.5	26.2	26.2	25.5	31.6	31.6
	22.6	29.4	29.1	21.0	19.6	27.0	27.0	27.0	26.7	33.1	33.1	30.8	38.5	38.5
	14.0	15.9	15.9	13.3	14.3	16.0	16.0	16.0	15.8	20.1	20.0	18.7	20.5	20.5
	11.6	12.8	12.9	11.8	11.8	12.3	12.3	12.3	12.0	15.4	15.0	16.3	16.1	16.5
	9.1	9.7	9.8	9.1	8.5	8.7	8.7	8.7	8.6	9.9	9.7	11.8	11.4	11.5
	5.3	5.6	5.7	5.2	5.1	5.1	5.1	5.1	4.9	5.9	5.6	6.8	6.5	6.5
	4.1	4.3	4.3	4.0	3.7	3.7	3.7	3.7	3.5	3.9	3.5	4.5	4.1	4.3
	4.5	4.8	4.9	4.4	4.3	4.4	4.4	4.4	4.1	4.8	4.6	5.6	5.3	5.4
	4.6	4.9	5.0	4.5	4.5	4.6	4.6	4.6	4.4	5.3	5.0	5.8	5.7	5.9
	4.3	4.7	4.7	4.2	4.2	4.4	4.4	4.4	4.5	5.0	4.7	5.0	5.1	5.3
	5.1	5.6	5.6	5.0	4.9	5.3	5.3	5.3	5.5	6.0	5.7	5.8	6.0	6.2
	5.5	6.0	6.0	5.4	5.6	6.0	6.0	6.0	5.9	6.7	6.4	6.5	6.7	6.8
	8.9	10.2	10.3	9.0	9.0	10.2	10.2	10.2	9.7	11.1	10.9	10.2	11.3	11.4
	7.0	7.8	7.8	6.9	7.5	7.9	7.9	7.9	8.6	9.1	8.6	9.4	9.5	9.8
	6.2	6.8	6.8	6.2	6.0	6.1	6.1	6.1	6.9	7.0	6.5	8.1	7.7	8.1
	9.8	11.1	11.2	9.8	11.1	11.9	11.9	11.9	12.2	12.8	12.3	13.9	14.2	14.5
	14.4	17.0	17.0	14.5	16.4	18.2	18.2	18.2	18.7	19.7	19.3	19.7	20.3	20.7
	15.2	17.7	17.8	15.5	16.7	18.2	18.2	18.3	19.0	20.4	19.8	20.7	21.0	21.5
	11.6	13.0	13.2	11.4	13.1	13.9	13.9	13.9	13.7	16.6	16.1	17.0	17.1	17.5
	11.2	12.6	12.7	11.0	12.6	13.2	13.2	13.2	13.0	14.5	14.2	15.4	15.2	15.4
	11.2	12.5	12.5	11.1	13.1	13.6	13.6	13.6	13.1	14.8	14.5	15.8	16.2	16.4
	9.5	10.4	10.5	9.4	9.7	9.9	9.9	9.9	9.7	11.2	11.0	12.8	12.2	12.4
	10.3	11.1	11.2	10.1	10.1	10.3			10.1	11.4	11.2	13.2	12.5	12.6
STDEV	4.9	6.5	6.5	4.6	4.8	6.4	6.6	6.6	6.3	7.6	7.7	6.8	8.7	8.6
MEAN	10.0	11.6	11.6	9.8	10.2	11.4	11.5	11.5	11.3	13.1	12.8	13.1	14.1	14.3

[7] Simulations with Kzout=1 were performed for a shorter time and hardly differed.

4.2 Development of Alaska adapted initial and background concentrations

The default initial condition (IC) and boundary condition (BC) profiles in the CMAQ package represent clean air conditions in the eastern-half of the United States (Gipson, 1999). The background conditions in Alaska are cleaner than in the eastern part of the US according to the IMPROVE data (http://views.cira.colostate.edu/web/DataWizard/). To represent the Alaska background condition and use them also as initial conditions, we used data from observations made in Alaska that we found in the literature (Jaeschke et al., 1999; Seinfeld and Pandis, 2006; Porter, 2009). Note that the initial concentrations taken from Porter (2009) have been used in WRF/Chem for prediction $PM_{2.5}$-concentrations (Mölders et al. 2011a, b), and that WRF/Chem and CMAQ consider different species in describing their background atmospheric conditions. This means we could not just take the profiles that we had already researched for WRF/Chem, to adapt CMAQ.

The developed initial concentrations to represent Alaska background concentrations were implemented in the CMAQ-package code. They are used as input for the ICON preprocessor. They also serve as boundary conditions. Previous studies suggested that using background concentrations as boundary conditions is justified for the Fairbanks domain for various reasons. First, Fairbanks is the only major emission source in the area as shown in Figure 5. Furthermore, observations in conjunction with backward trajectories (Cahill et al., 2003) and simulations with WRF/Chem (Tran et al. 2011, Mölders et al. 2011c) showed that the advection of pollutants is marginal.

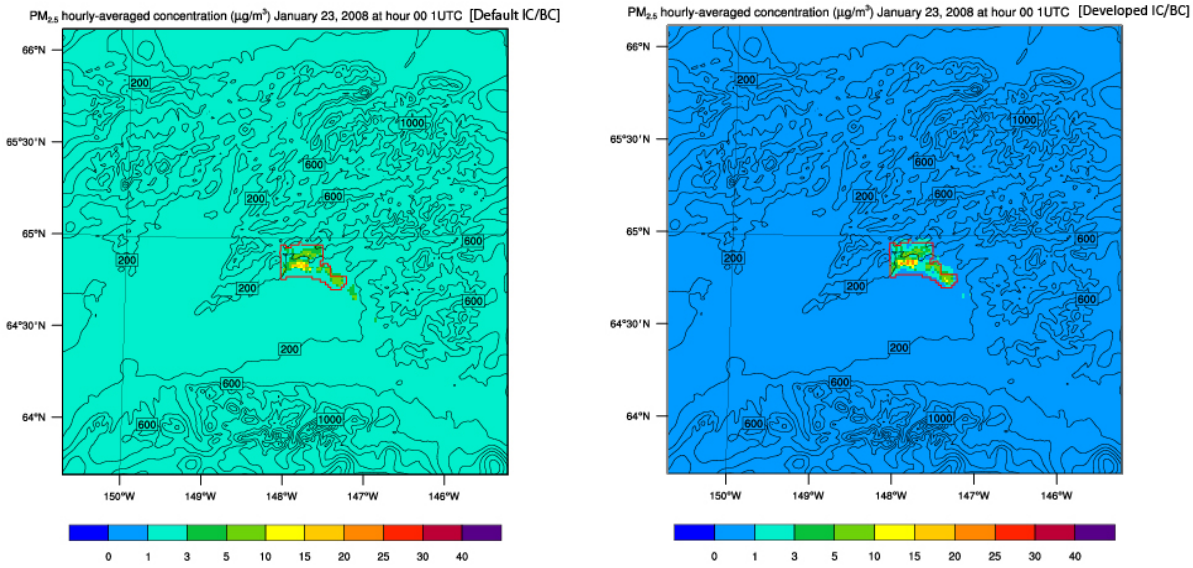


Fig. 5. $PM_{2.5}$-concentration differences at breathing level as obtained with CMAQ using (a) the default IC and BC and (b) the Alaska developed IC and BC. The red polygon indicates the nonattainment area. Note that changing the IC and BC led to slight increases in the nonattainment area.

The vertical profiles of background concentrations of each pollutant as developed for the Alaska adapted CMAQ, the vertical profiles used in the original CMAQ by default, and the vertical

profiles used by the Alaska adapted WRF/Chem (Porter, 2009; Mölders et al., 2010) are presented in Appendix B. Note that the simulation with the final, developed initial chemical concentrations and background concentrations is the ICBC version 3 (ICBC3) in Table 1.

Figure 5 compares the concentrations of $PM_{2.5}$ prior and after introduction of the Alaska adapted IC and BC. As can be clearly seen the $PM_{2.5}$-concentrations outside the nonattainment area decreased from 1-3µg/m^3 to 0-1 µg/m^3. These lower $PM_{2.5}$-concentrations are within the range of what is typically observed in Alaska remote areas (see IMPROVE 2011). The Alaska adapted IC and BC profiles were used the tests described further on.

4.3 Choice of advection schemes

It is well known in the literature that the formulation and order of discretization in advection schemes determine the diffusivity of the schemes (e.g. Pielke, 2002; Jacobson, 2007). The degree and order of discretization may lead to less or more numerical diffusion. The latter is not a physical process, but just a result of that any model development requires to substitute the partial differential equations by differences or finite elements or volumes to solve them on a computer. Therefore, the choice of the advection scheme may yield to higher or lower concentrations as the species experience numerical (artificial) diffusion. A discussion of the consequences is beyond the scope of this report and investigation of the consequences was not to be examined. However, as can be read in the cited textbooks or peer-reviewed literature numerical diffusion can lead to under- or overestimation of concentrations depending on whether a scheme is very diffusive or not (e.g. Pielke, 2002; Jacobson, 2007).

In CCTM, there are three options for dealing with horizontal and vertical advection that can be selected. They are to (1) deactivate horizontal or vertical advection, (2) use the unmodified Piecewise Parabolic Method (PPM) to calculate horizontal or vertical advection, and (3) use the global mass-conserving scheme (YAMO) to calculate horizontal and vertical advection.

The PPM is based on the finite volume subgrid definition of the advected scalar (Colella and Woodward, 1984). In PPM, the subgrid distribution is described by a parabola in each grid interval. The PPM is a monotonic and positive definite scheme to ensure that concentrations will not become negative. The YAMO scheme uses the PPM for horizontal advection together with deriving a vertical velocity component at each grid cell that satisfies the mass continuity equation using the driving meteorology model's air density data. This scheme, of course, is also positive definite.

Deploying the different advection modules yielded slight differences in the simulated $PM_{2.5}$-concentrations in the nonattainment area (Fig. 6). However, the $PM_{2.5}$-concentrations at the State Building site simulated by both modules had differences <1µg/m^3 (Table 1: test 2 and 3). We concluded that the choice of the advection scheme is of marginal relevance for the simulated concentrations.

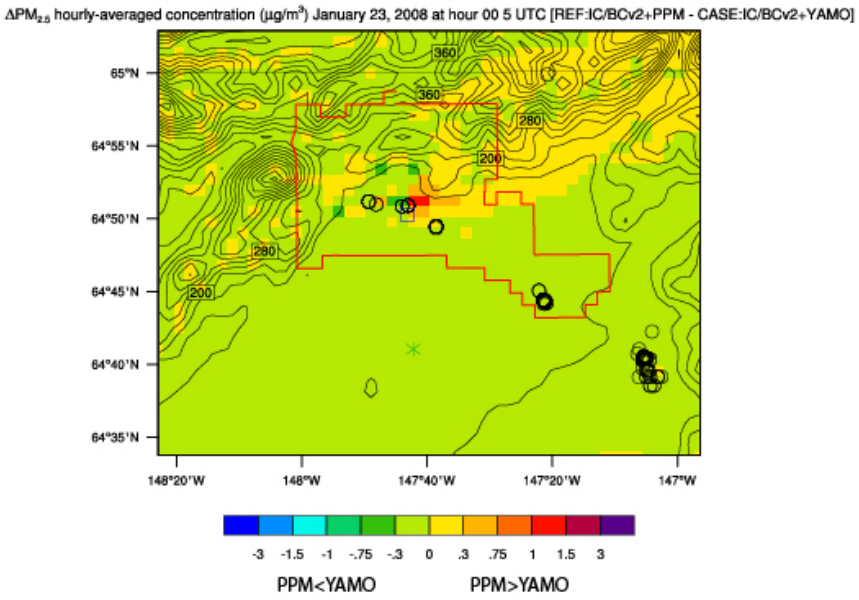


Fig. 6. Zoom-in on the nonattainment area showing the $PM_{2.5}$-concentration differences at breathing level as obtained with CMAQ using the Alaska adapted IC/BC and m3dry.f with PPM (REF) (test 2 in Table 1) and the Alaska adapted IC/BC and m3dry.f with YAMO (test 3). The red polygon, blue rectangle and black circles indicate the nonattainment area, the state building and locations of point sources, respectively. Other times look similar (therefore not shown[8])

Due to the fact that both advection modules did not provide huge differences at the State Building site, we chose to use the YAMO scheme, which uses less CPU time, for the next tests.

4.4 Choice of the diffusion modules

It is well known in the literature that the treatment of diffusion determine the degree of diffusivity of the schemes (e.g. Pielke, 2002; Jacobson, 2007). Often modelers do not consider diffusion at all except in the atmospheric boundary layer (ABL). Except for the ABL, they substitute the physical diffusion by the numerical diffusion that is due to the discretization.

In CCTM there are several options to treat vertical diffusion. Two of them were compared in this study. They are the Asymmetric Convective Method (ACM2) for in-line calculation of emissions and EDDY which uses the eddy diffusivity theory. Changing the treatment of diffusion in the ABL may yield to higher or lower concentrations depending on the parameterization of diffusion used. In the parameterization of diffusion, parameters are used.

[8] We show, on purpose, figures at different times. The reason is that often effects are best visible at different times or not even visible at a given time. This behavior is due to the fact that physical, dynamical and chemical processes vary with time. To optimally elucidate differences, figures are shown for the time at which an effect we want to discuss is most obvious. If we would use the same time for all plots, the reader would most of the time not be able to understand why we made a given change and/or how we came to a certain conclusion.

The EDDY scheme treats turbulent mixing analogously to molecular diffusion, which depends on concentration gradients and happens only between adjacent vertical layers by local mixing (Fig. 7). The ACM2 scheme allows upward turbulent mixing from the surface across non-adjacent layers through the convective boundary layer (CBL) by non-local mixing and slow layer-by-layer downward mixing from the top of the CBL to the surface under convective conditions. ACM2 switches to local-mixing-only during night. Given the fact that during our episode there are only a few hours of day light, local mixing would be the dominant mode in the ACM2 as well.

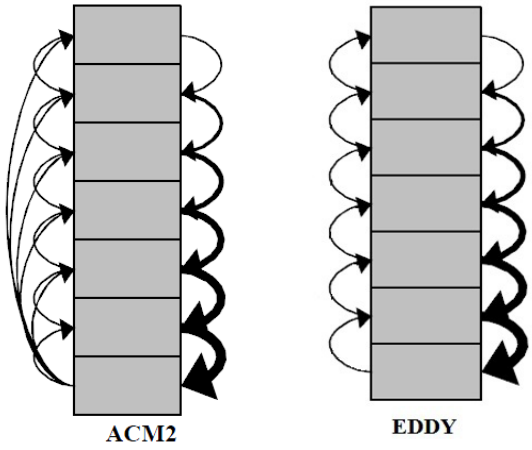


Fig. 7. Schematic illustration of the different concepts of the ACM2-scheme (From: Pleim, 2007) and the Eddy scheme.

Pleim (2007) and Pleim (2006) compared the EDDY and ACM2 schemes in CMAQ. His main findings were that the ACM2 scheme tends to predict larger concentrations of secondary pollutants (ozone) and smaller concentrations of primary pollutants at the surface, and ACM2 has a more well-mixed profile in the ABL than the EDDY scheme. Differences between the simulations with ACM2 and EDDY for the Fairbanks domain and our episode are exemplarily presented in Figure 8. Unfortunately, no data of vertical profiles of $PM_{2.5}$ and/or any chemical species are available for our episode. However, observations in Fairbanks show that most of the winter the ABL is very stable (Wendler and Nicpon, 1975; Bourne et al., 2010; Mölders and Kramm, 2010; Tran and Mölders, 2011). Thus, vertical mixing is low and therefore based on Pleim's findings the EDDY scheme seems to be more appropriate.

Furthermore, the EDDY scheme seems to provide, on average, higher $PM_{2.5}$-concentrations in the nonattainment area (Fig. 9), and its simulated concentrations yield a higher correlation coefficient with the observed data than those obtained by the ACM2 (Fig. 9; Table 1: test 4 and 5). Therefore, EDDY was selected as the diffusion module for the Alaska adapted CMAQ and was used in other following tests.

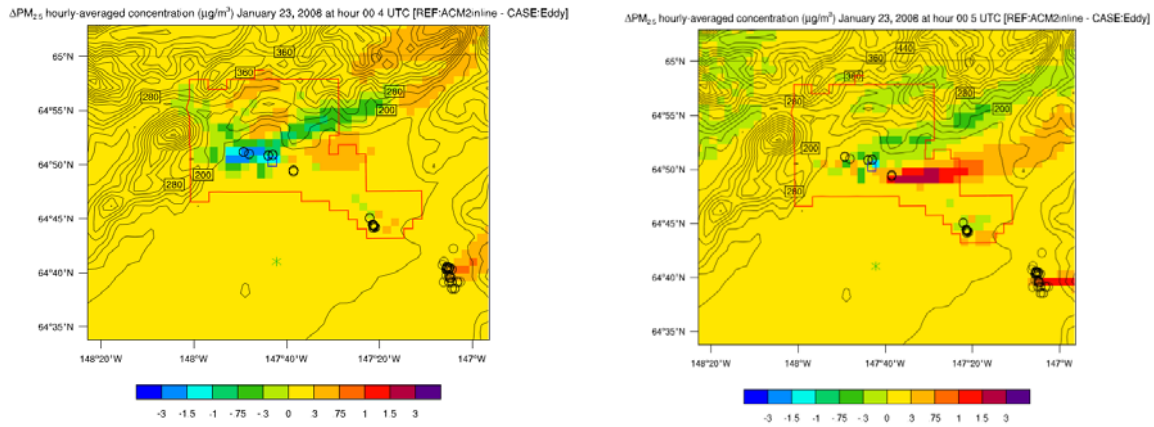


Fig. 8. Zoom-in on the nonattainment area showing exemplarily the $PM_{2.5}$-concentration differences at breathing level as obtained with CMAQ using the ACM2 inline (REF) (test 4) and the EDDY scheme (test 5) for treatment of vertical diffusion at hour 0400 UTC (left) and 0500 UTC of January 23, 2008 (right). The red polygon, blue rectangle and black circles indicate the nonattainment area, the state building and locations of point sources, respectively.

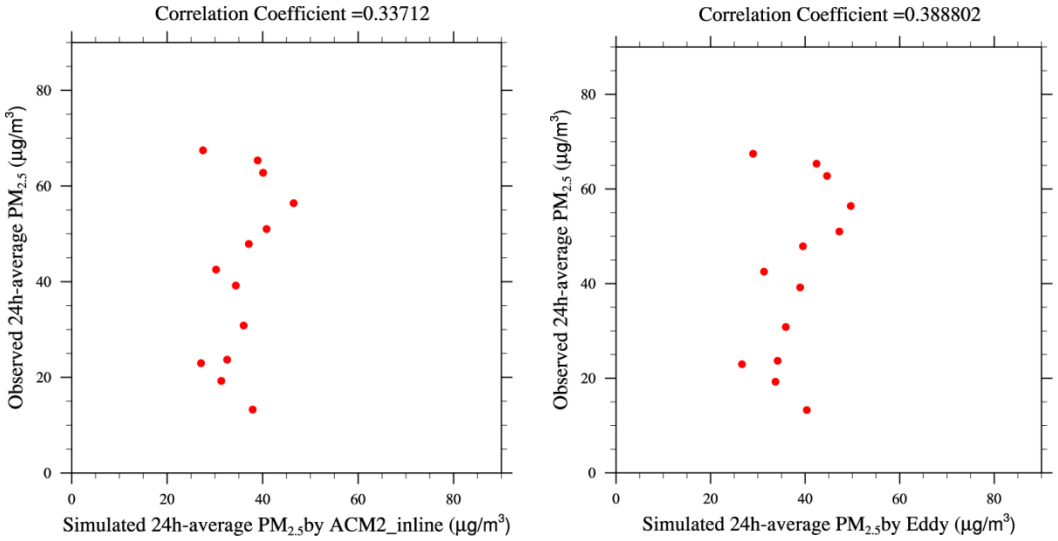


Fig. 9. Scatter plots of observed and simulated $PM_{2.5}$-concentrations at the State Building site as obtained by ACM2_inline and Eddy with the respective obtained correlation coefficients.

4.4.1 Choice of the eddy diffusivity values

As pointed out before, the parameterization of diffusion use various semi-empirical parameters. The value of the minimum diffusivity (Kz_min) plays an important role in the vertical distribution of emissions within photochemical models, especially during nocturnal hours or other periods with stable conditions and limited mixing. Values that are too low/high can lead to unrealistic high/low concentrations of primary species in areas of high emissions. Values that are too high can lead to mixing of species through very deep layers, which is unreasonable in most cases and results in overprediction of ozone at night time in rural area (Tang et al., 2011). The minimum diffusivity values (Kz_min) used in various air quality models range typically between 0.1 and

1.0m^2/s. In the original CMAQ, the default value of Kz_min is 1m^2/s, but CMAQ code provides the option to calculate this value based on the fraction of urban area as given in Eq. (8) (CMAQ v.4.7.1 Operational Guidance Document, 2010).

$$Kz_min = KZL + (KZU-KZL)*UFRAC \quad (8)$$

Where, Kz_min is the minimum diffusivity that has a default value of 1.0m^2/s in the original CMAQ, KZL is the lowest diffusivity coefficient (Kz) with a default value of 0.5m^2/s, KZU is the highest Kz with a default value of 2.0m^2/s, and UFRAC is the fraction of urban land-use.

We modified the source code for Kz_min in eddyx.F, performed simulations with different Kz_min values and compared their results (Fig. 10, Table 1).

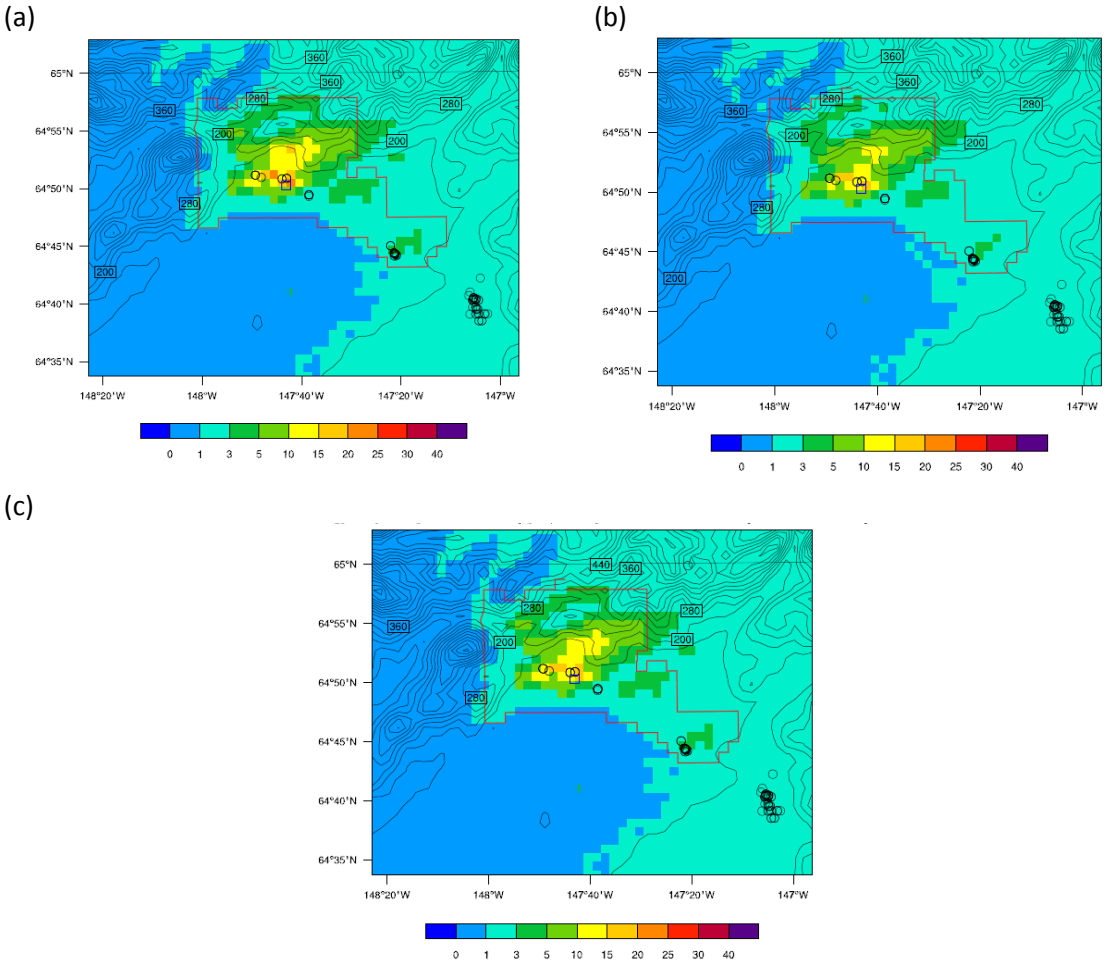


Fig. 10. Zoom-in on the nonattainment area showing the $PM_{2.5}$-concentrations at breathing level for January 23, 2008 0400 UTC as obtained with the Alaska adapted CMAQ for (a) Kz_min=0.5m^2/s (test 1), (b) Kz_min=1.0m^2/s (test 3), and (c) Kz_min calculated according to urban fractional land-use as shown in Figure 11 (test 4). The red polygon, blue rectangle and black circles indicate the nonattainment area, the state building and locations of point sources, respectively.

As shown in Figure 11, $PM_{2.5}$-concentrations in the nonattainment area were affected by the choice of the eddy diffusivity values. Therefore, we selected to use Kz_min based on the urban fractional land-use and we reduced the KZL and KZU to 0.25 and 1.0, respectively for the following tests.

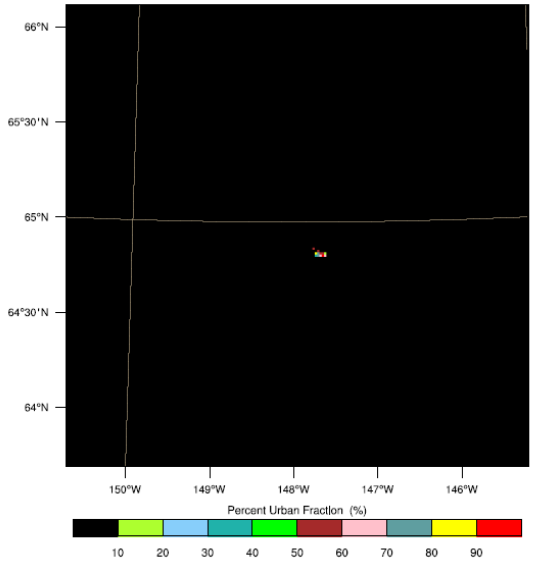


Fig. 11. Percentage of urban land-use in the various grid-cells in the Fairbanks domain as obtained from the high resolution land-use data (2m) that come with the WRF package.

Recall that WRF was run with the strategy of dominant land-use which means that when a land-use type has the highest fraction within a grid-cell this land-use type is assumed to be the representative one for that grid cell and used in the calculation of the exchange of heat, moisture, and momentum at the earth-atmosphere interface. Thus, introducing the consideration of the percentage of urban land-use means that in CMAQ, we consider subgrid-scale heterogeneity. Doing so means an inconsistent treatment between WRF and the CMAQ. However, the method proposed here permits considering dry deposition more realistically.

4.5 Choice of the photolysis modules

CMAQ has several options to calculate photolysis rates – PHO_inline and PHO_table. The latter is a lookup table of photolysis rates, while the former considers the feedback of aerosols on photolysis rates. We corrected the option that uses the lookup table to consider the fact that the ground is snow-covered during our episode. The table contains the surface-albedo values that are used in the calculation of the photolysis rates for UV wavelengths less than 400 nm (Cruickshank, 2008). In the Fairbanks domain, the land-use is mostly categorized as wooded tundra (Fig. 2) so the surface-albedo distributions of the snow-covered land should be about 0.55 instead of 0.05 (e.g. Tanskanen et al., 2007; Mölders, 2011), which is the default value in setalb.f. We set the surface albedo to 0.55 for use in simulations with the Alaska adapted CMAQ for winter episodes.

We run simulations with the PHO_inline module and the modified lookup tables and compared their results. Table 1 (test7 and 8) shows that both options did not yield big differences for the first 24 hours of the simulations. This finding can be explained by the fact that in January, there are only a few hours of sunlight. We expect that the differences will have more impact earlier (October after the first snowfall) and later in the season (e.g. March, April) and for the November episode.

PHO_inline was chosen for the Alaska adapted CMAQ for the following reasons: PHO_inline accounts for the presence of ambient PM and ozone simulated by CMAQ and uses these values to adjust the actinic flux. The simulated concentration profiles should be a better "guess" for the situation over the nonattainment area than the static background concentration. This fact is especially true given the strong variation of light conditions between December 21, March 21 and September 23 in Alaska. Note that in Fairbanks we have 3h, 12.5h and 12h of daylight on these days. A discussion of daylight conditions and the lack thereof on concentrations can be found at http://www.mmm.ucar.edu/wrf/users/workshops/WS2010/abstracts/5B-5.pdf.

4.6 Impacts of turning off the vertical advection, and of reducing wind-speed by 50% in valleys

Due to the very stagnant conditions in Fairbanks (e.g. Tran and Mölders, 2011), vertical advection or the lack thereof may play important role in the Fairbanks domain. CMAQ has an option to switch off the vertical advection (vadv_noop). Note that doing so violates the continuity equation, but using this option was found to provide improved concentrations in the Utah Valley case study (Cruickshank 2011; pers. communication) and was suggested to be tested by EPA region 10. Since the Utah Valley like the Fairbanks Bowl both have stagnant frequent inversion conditions in winter, we deactivated the vertical advection to examine whether doing so has a similar impact for the Fairbanks domain.

It is well known that models have difficulty simulating calm winds accurately. Zhao et al., 2011) reported that WRF had difficulty reproducing weak surface-winds (<1.5m/s) in their long-term 4km-increment simulation over California leading to bias (RMSE) of more than 3m/s (4.5m/s). (Mölders et al. 2011c) reported that in their WRF/Chem simulations for Interior Alaska, the weak winds were associated with stagnation events. Their wind-speed bias (RMSE) was 1.55m/s (2.4m/s) on average over all 23 sites that had data and October 1 2008 to March 31 2009, i.e. an entire winter. In their WRF/Chem study over Interior Alaska for November 1 2005 to February 28 2006, Mölders et al. (2011s) found a wind-speed bias of 1.85m/s based on data of 33 sites.

WRF is known to have a positive wind-speed bias. The WRF-simulations used in our study overestimate the near-surface wind-speeds (Gaudet and Stauffer, 2010). The wind-speed bias may affect the dilution of pollution with consequences for simulated $PM_{2.5}$-concentrations (Mölders et al. 2011c).

Being aware that WRF has this wind-speed bias, we performed a simulation with the so far Alaska adapted CMAQ wherein we reduced the wind-speed by 50% in the Fairbanks Bowl. To examine by how much we had to reduce wind-speed and to which height, we needed a results

from a long-term WRF simulation and compare this wind profile data to radiosonde observations. From other resources results from a WRF/Chem simulation were available that Mölders et al. (2011a) had thoroughly evaluated by radiosonde and SODAR-data. We used this data and assumed that, on average over winter, the wind-speed bias from these WRF/Chem simulations and the WRF simulations that we use for our CMAQ simulation only differ marginally. This assumption can be made (1) as the biases reported by Gaudet and Stauffer (2010) are of similar magnitude than those found for the various simulations with the Alaska adapted WRF and WRF/Chem (e.g. Mölders, 2008; Mölders, 2010; Mölders and Kramm, 2010; Yarker et al., 2010; Mölders et al., 2011a, b, c) and (2) due to the fact that most of the physical packages used are the same.

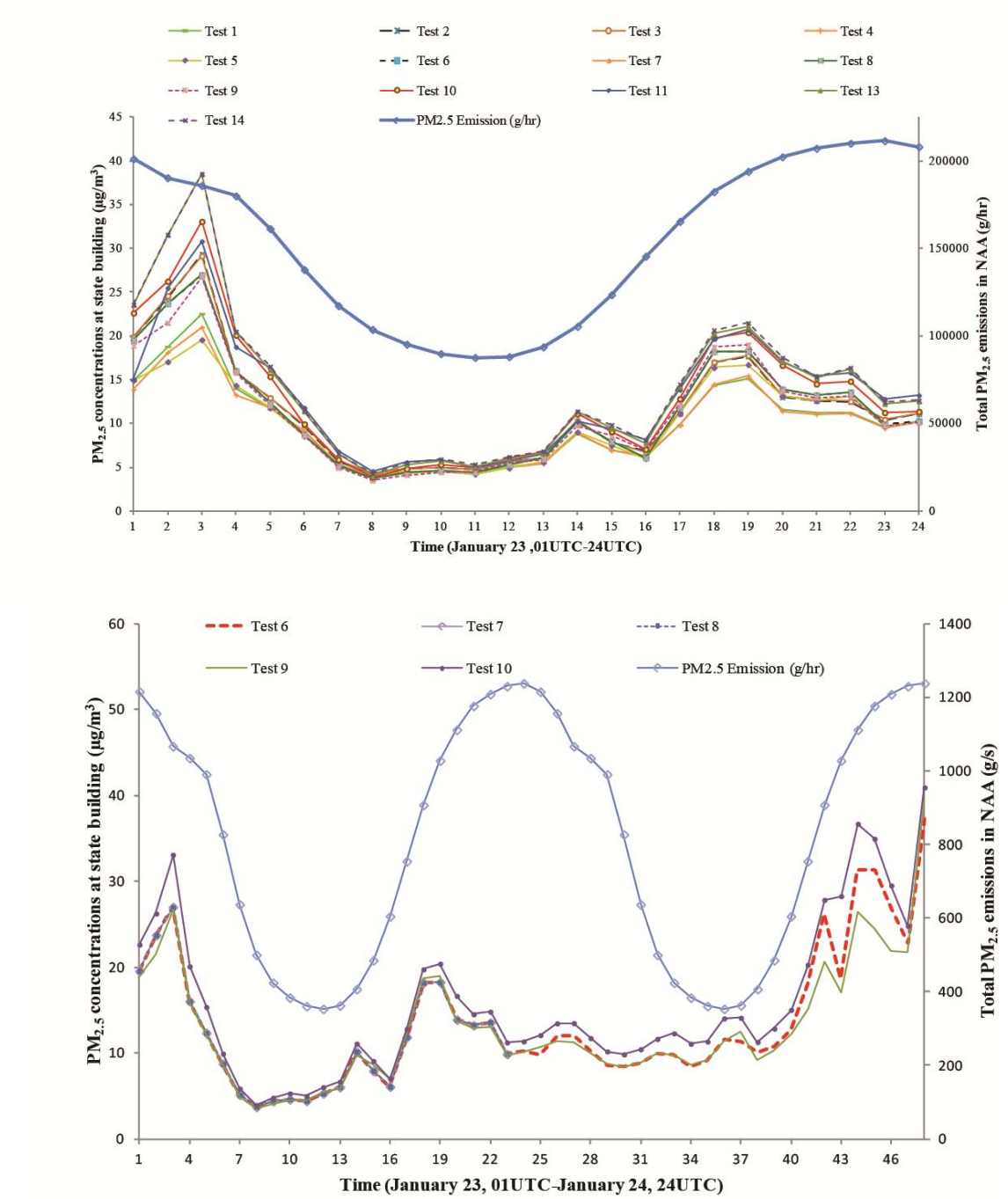
To determine the upper limit to which to do the wind-speed corrections and the reduction factor to correct for WRF's wind-speed bias, we compared the WRF/Chem simulated wind profiles with the radiosonde data for November 1, 2005 to March 1, 2006. This investigation showed that WRF/Chem over-estimated wind in the lower ABL. The ratio between the radiosonde-wind data and the WRF/Chem simulated wind was estimated. The ratio of 0.5 had the highest frequency of occurrences at heights below 3km, which corresponds to layer 20 in CMAQ. To correct for the wind-speed bias of WRF, we edited the MCIP source code in rdwrfem.f90 as follows:

```
!Reduce U and V 50 % for Fairbanks domain <7/28/2011>
 CALL get_var_3d_real_cdf (cdfid, 'U', dum3d_u, nx, nym, nz, it, rcode)
 IF ( rcode == nf_noerr ) THEN
  ua(:,1:nym,:) = dum3d_u(:,:,:)
  ua(:,  ny, :) = ua(:,nym,:)
 ELSE
  WRITE (6,9400) 'U', rcode
  GOTO 1001
 ENDIF
 CALL get_var_3d_real_cdf (cdfid, 'V', dum3d_v, nxm, ny, nz, it, rcode)
 IF ( rcode == nf_noerr ) THEN
  va(1:nxm,:,:) = dum3d_v(:,:,:)
  va(  nx, :,:) = va(nxm,:,:)
      DO ii=10,nx-10
      DO jj=10,ny-10
      IF(scrwnd(ii,jj).eq.0)THEN
      DO kk=1,21
       ua(ii,jj,kk)=ua(ii,jj,kk)*0.5
       va(ii,jj,kk)=va(ii,jj,kk)*0.5
        ENDDO
        ENDIF
        ENDDO
```

```
        ENDDO
        WRITE (*,ifmt1) 'U       ', ua(lprt_metx,lprt_mety,:)
        WRITE (*,ifmt1) 'V       ', va(lprt_metx,lprt_mety,:)
        ELSE
        WRITE (6,9400) 'V', rcode
        GOTO 1001
       ENDIF

IF ( ifw10m ) THEN
  CALL get_var_2d_real_cdf (cdfid, 'U10', dum2d, nxm, nym, it, rcode)
  IF ( rcode == nf_noerr ) THEN
   u10(1:nxm,1:nym) = dum2d(:,:)
   u10(nx,:) = u10(nxm,:)
   u10(:,ny) = u10(:,nym)
  ELSE
   WRITE (6,9400) 'U10', rcode
   GOTO 1001
  ENDIF
  CALL get_var_2d_real_cdf (cdfid, 'V10', dum2d, nxm, nym, it, rcode)
  IF ( rcode == nf_noerr ) THEN
   v10(1:nxm,1:nym) = dum2d(:,:)
   v10(nx,:) = v10(nxm,:)
   v10(:,ny) = v10(:,nym)
   DO ii=10,nx-10
    DO jj=10,ny-10
    IF(scrwnd(ii,jj).eq.0)THEN
     u10(ii,jj)=u10(ii,jj)*0.5
     v10(ii,jj)=v10(ii,jj)*0.5
    ENDIF
   ENDDO
   ENDDO
   WRITE (*,6000) 'U10     ', u10(lprt_metx, lprt_mety), 'm/s'
   WRITE (*,6000) 'V10     ', v10(lprt_metx, lprt_mety), 'm/s'
  ELSE
   WRITE (6,9400) 'V10', rcode
   GOTO 1001
  ENDIF
 ENDIF
```

(a)



(b)

Fig. 12. Temporal evolution of the $PM_{2.5}$-concentrations as obtained for the first 24 hours (a) and 48 hours (b) from the various sensitivity studies for the grid cell holding the State Building. Note that the State Building site is the only site in the nonattainment area with measurements for the January/February episode. However, no data is available for the first day. The blue line shows the total $PM_{2.5}$-emissions in the nonattainment area.

The deactivation of the vertical advection did not improve the simulations, especially during the simulated hours 37-48 (Fig. 13b, test 9), compared with the reduced Kz with modified MCIP line

(Test 6). The reason might be the vertical profile of the Alaska adapted initial and boundary conditions for $PM_{2.5}$ that indicates higher concentrations in the upper than lower ABL. Thus, under subsidence conditions $PM_{2.5}$ is transported downwards. This means that when switching off the vertical advection this marginal advection of $PM_{2.5}$ from above does not occur, leading to lower concentrations at breathing level than we obtain when we consider vertical advection. Therefore, we rejected switching off of the vertical advection from being part of the Alaska adaptation of CMAQ. All further simulations used the vertical advection switched on.

The correction of the simulated wind-speeds (u and v reduced by 50% each) in areas with terrain heights lower than 200m has to be understood as a calibration of the wind-data. It resulted in the biggest improvement in the simulated $PM_{2.5}$-concentrations at the State Building site compared with the observations (Fig. 12b: test 10, Table 1). Hence, the correction of the WRF-simulated u and v-components of the wind was selected as a potential option of the Alaska adapted CMAQ. Note that from a WRF point of view doing so means a violation of the continuity equation. However, from the point of view that the WRF data are just the meteorological data to drive CMAQ one can argue for correcting the wind data (calibration) that are known to be incorrect. The correction suggested here serves to calibrate/adjust the wind data to the observed wind-speeds. Unfortunately, CMAQ needs gridded wind-data and cannot be run with observations. Therefore, we recommend to use the calibrated simulated wind data to obtain better agreement between simulated and observed $PM_{2.5}$-concentrations..

4.7 Trimmed domain

A discussion between DEC, EPA and Sierra Research Inc. personnel led to the conclusion that it would technically be advantageous to reduce the CMAQ domain for the Fairbanks air quality modeling efforts. Future updates of emission data as well as inventories for various emission control strategies will be delivered on the trimmed domain. Future Alaska adapted CMAQ simulations are to use that trimmed domain. Therefore, we used Grid 4M to trim the updated emission data to the new domain size (Table 2) as described in the document obtained from Huff (2011; pers. communication).

In doing so, we edited the MCIP as follows to re-run MCIP to generate the smaller domain:

```
set BTRIM = -1
set X0    = 76
set Y0    = 49
set NCOLS = 66
set NROWS = 66
```

Where BTRIM is the number of boundary points to be removed on each of the four horizontal sides of the MCIP domain. If windowing a specific subset domain of input meteorology, set BTRIM=-1, and BTRIM will be ignored in favor of the specific window information in X0, Y0, NCOLS, and NROWS.

X0 is the x-coordinate of the lower-left corner of the full MCIP cross-point domain. Y0 is the y-coordinate of the lower-left corner of the full MCIP cross-point domain. NCOLS is the number of columns in the output MCIP domain, NROWS is the number of rows in the output MCIP domain. For a definition of cross and dot-points see Pielke (2002), Jacobson (2007) or the CMAQ documentation.

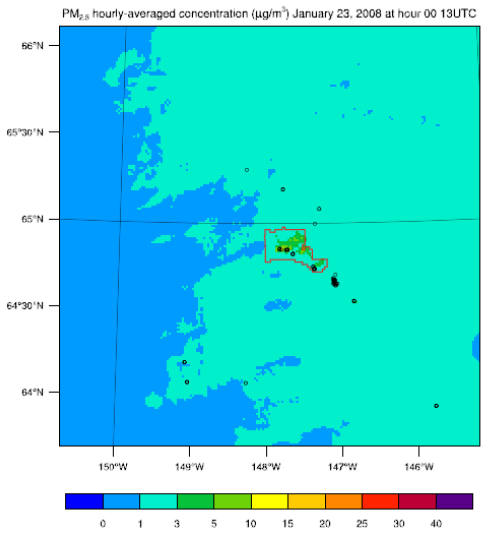
Table 2. Xcells, Ycells, cell size and the coordinates at the corner of the domain grid 4M

									Absolute Corner Coordinates (m)			
						Relative SW Corner (1,1) Point			SW Corner		NE Corner	
Do-main	Cell Size (m)	X Points	Y Points	X Cells	Y Cells	To	X Offset	Y Offset	SW-X	SW-Y	NE-X	NE-Y
Grid 1	12000.00	401	301	400	300	n/a	n/a	n/a	-240000	-180000	+24000	+18000
Grid 2	4000.00	202	202	201	201	Grid 1	156	106	-540000	-540000	+26400	+26400
Grid 3	1333.33	202	202	201	201	Grid 2	103	106	-132000	-120000	+13600	+14800
Grid 4	444.44	202	202	201	201	Grid 3	73	50	-36000	-54667	+53333	+34667
Grid 4M	**1333.33**	**67**	**67**	**66**	**66**	**Grid 4**	**5**	**1**	**-30667**	**-54667**	**+57333**	**+33333**

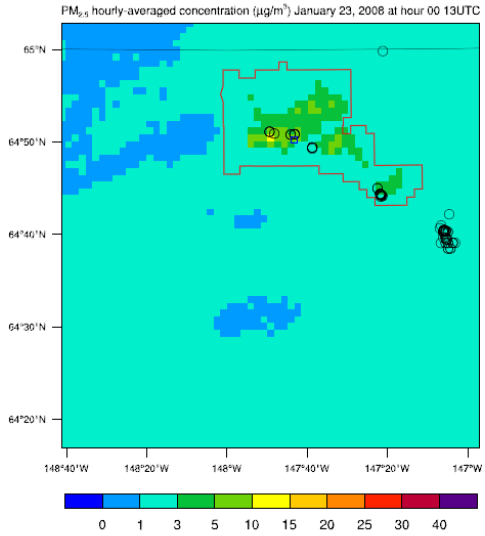
Figure 13 compares exemplarily the simulated $PM_{2.5}$-concentrations in the 199×199 and 66×66 domain. Comparison with the Alaska adapted CMAQ simulations for the 199×199 domain showed that the trimmed domain excludes some point sources. However, trimming the domain did not affect the $PM_{2.5}$-concentrations on average at the State Building site by more than 0.6µg/m^3 (Table 1; tests 10, 11). This value is in the margin of measurement accuracy, and, hence, can be considered as acceptable. The trimmed domain reduced the simulation time from 8 hours to 1-2 hour for a 24 hours simulation and the storage of trimmed domain need less memory only 55 GB compared to the 199 domain which use 607GB.

Though there is less impact of trimming the domain at the State Building site, figures 13b and 13c show small difference in $PM_{2.5}$-concentrations. The effect is due to the boundary being closer to the nonattainment area in the trimmed domain than the 199x199 domain. This effect of boundaries is clearly seen outside the nonattainment area.

(a)



(b)



(c)

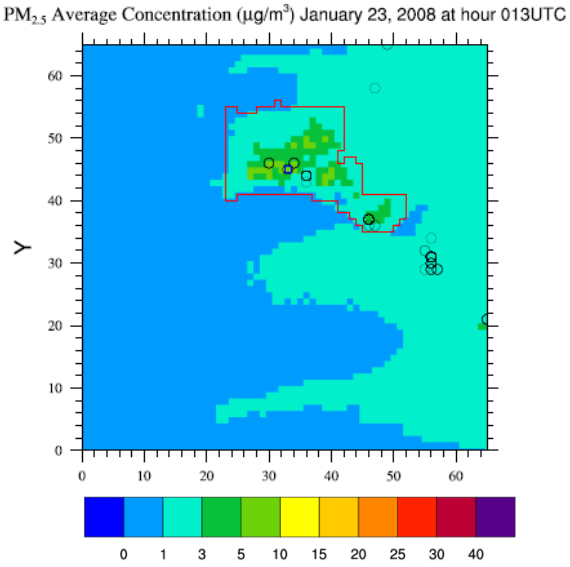


Fig. 13. Simulated $PM_{2.5}$-concentrations at breathing level for January 23, 2008 1300 UTC as obtained (a) for the simulation with the full domain (199×199, nrow x ncol) where (b) displays the zoom-in of the full domain to the same area as the trimmed domain (test 13), and (c) the trimmed domain (66×66) (test 14). The red polygon and black circles indicate the nonattainment area and locations of point sources, respectively.

4.8 Vertical profile and cutting upper vertical layers

To reduce the amount of data that have to be exchanged, handled, and stored, DEC suggested to writing out only the results for the lower-most layers. Doing so required to examine where a cut can be made without risk of missing out valuable information for the attainment question. We determined the variations of hourly $PM_{2.5}$-concentrations in the vertical (Fig. 14). The

variations of $PM_{2.5}$-concentrations seemed to be consistent at heights about 1500m or 850 hPa and independent of lower levels (Fig.14a), and varied again above 3km (Fig.14b) due to the upper wind in the free atmosphere.

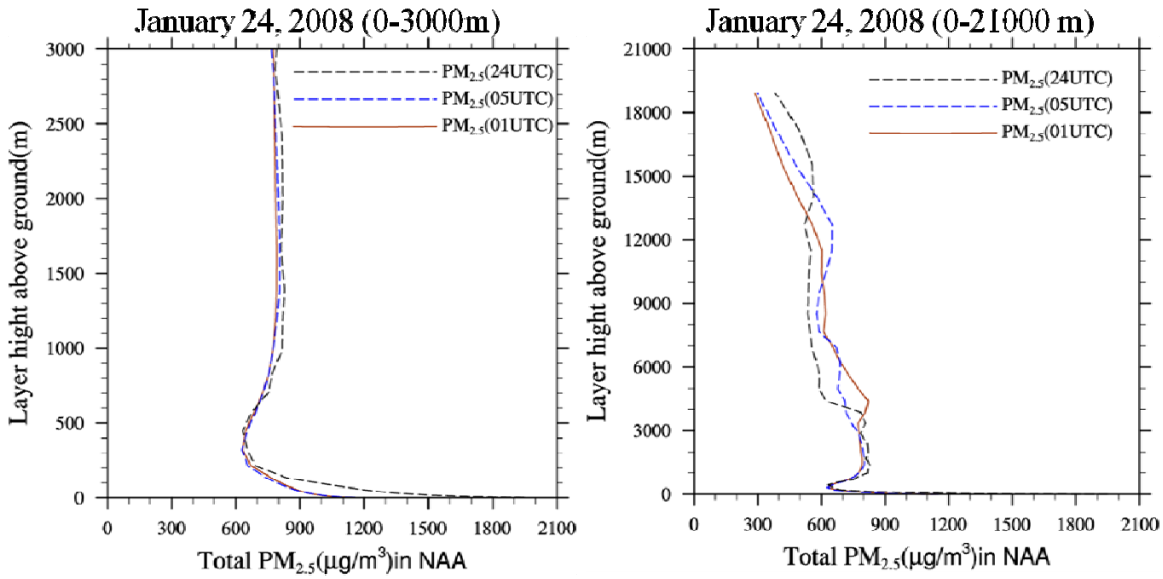


Figure 14 Total simulated $PM_{2.5}$-concentrations in the vertical layers in nonattainment area on January 24, 2008 at 0100, 0500 and 2400 UTC for the heights between (a) 0 and 3000m, (b) 0 and 21000m (test 13).

We suggest that only the results for the lower-most 18 layers (~2000m) are achieved in order to reduce the amount of data that has to be stored, handled and exchanged.

5. Evaluation

The following discussion is the evaluation of the results of the simulation performed with the 66×66 domain with the Alaska adapted CMAQ. Data of 24h-average $PM_{2.5}$-concentrations are available at the State Building from January 29, 2008 to February 10, 2008. This means we have only 13 data points for evaluation. There are 312 hourly values of $PM_{2.5}$-concentrations at the State Building as well.

The CMAQ model performance was assessed with the observed $PM_{2.5}$-concentrations at the Fairbanks official monitoring site located at the State Building (64.838N, 147.716W). The observed hourly $PM_{2.5}$ data were gathered by a Beta Attenuation Monitor and the 1-in-3 day observed $PM_{2.5}$ data with its components were collected by a Super SASS Speciation monitor (Alaska DEC, 2011). The observational datasets were collected by and obtained from the FNSB and the Alaska DEC, respectively. We extracted the simulated data from the CMAQ output file from the integral average of pollutant concentrations at the first layer (CTM_ACONC) for the grid-cell that holds the State Building site.

The statistical metrics used to compare the observed and simulated 24h-average and hourly $PM_{2.5}$-concentrations follow the CMAQ model performance evaluation document (USEPA, 2011).

Fine particle mass was approximated by summing up the Aitken and accumulation mode of species except water as shown below (USEPA, 2011; Appel et al., 2008):

$PM_{2.5}$=ASO4I+ASO4J+ANH4I+ANH4J+ANO3I+ANO3J+AORGCJ+1.167xAORGPAI+1.167xAORGPAJ+ AOLGAJ+AOLGBJ+AECI+AECJ+A25I+A25J+ANAI+ANAJ+ACLI+ACLJ (9)

where ASO4I is the Aitken mode sulfate mass and ASO4J is the accumulation mode sulfate mass, ANH4I is Aitken mode ammonium mass, ANH4J is the accumulation mode ammonium mass, ANO3I is Aitken mode aerosol nitrate mass, ANO3J is the accumulation mode nitrate mass, AORGCJ is the accumulation mode secondary organic mass produced in clouds (Napelenok et al., 2008), AORGPAI is the Aitken mode primary organic mass, AORGPAJ is accumulation mode primary organic mass, AOLGAJ and AOLGBJ are aged secondary organic mass in the accumulation mode (Napelenok et al, 2008), AECI is the Aitken mode elemental carbon mass, AECJ is accumulation mode elemental carbon mass, A25I is the Aitken mode unspecified anthropogenic mass (from soil), and A25J is the accumulation mode unspecified anthropogenic mass. Furthermore, ANAI is the Aitken mode sodium mass, ANAJ is the accumulation mode sodium mass, ACLI is the Aitken mode chloride mass, and ACLJ is the accumulation mode chloride mass. Note that a factor of 1.167 was applied to AORGPAI and AORGPAJ since the CMAQ model assumed the conversion factor between organic carbon to organic mass is 1.2 for primary organic aerosol emission. Appel et al. (2008) and USEPA (2011) recommended a 1.4 factor for the Interagency Monitoring of Protected Visual Environments (IMPROVE) and the Speciation Trends Network (STN) ambient data.

5.1 $PM_{2.5}$-concentrations

Comparison with the observed $PM_{2.5}$–concentrations at the State Building site grid cell showed that CMAQ underestimated the $PM_{2.5}$–concentrations on most days during the January/February episode (Figs. 15, 16). Table 3 lists the performance statistics for the Alaska adapted CMAQ simulated $PM_{2.5}$-concentrations. Based on these performance-skill scores the simulated $PM_{2.5}$-concentrations seem to agree well with the observed values.

Table 3. Performance statistics for the Alaska adapted CMAQ using the observations at the State Building and the CMAQ data simulated in the grid cell holding the State Building.

Fairbanks Official monitoring Site	**#of Observ-ations**	**Mean CMAQ simulations (µg/m^3)**	**Mean Observ-ations (µg/m^3)**	**Ratio of Means (sim/obs)**	**Mean Bias (µg/m^3)**	**Mean Fractional Bias (%)**	**Mean Error (µg/m^3)**	**Mean Fractional Error (%)**	**Correlation Coefficient**
Hourly	312	38.0	41.7	0.66	-3.76	2.82	20.56	57.43	0.33
24h-average	13	38.0	41.7	1.13	-3.76	-0.32	13.13	34.51	0.39

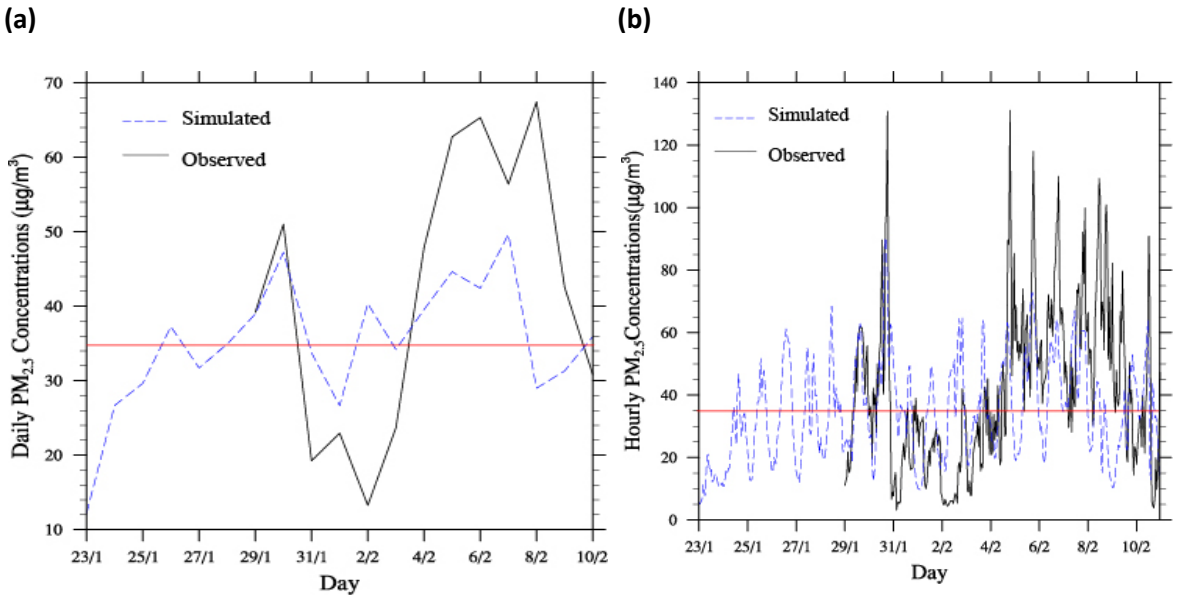


Fig. 15. Time series of CMAQ simulated (blue dashed line) and observed data (black solid line) for (a) 24h-average $PM_{2.5}$-concentrations and (b) hourly $PM_{2.5}$-concentrations (right) during January 23, 2008 (Day 1) to February 10, 2008 (Day 19) at the State Building (test 13).

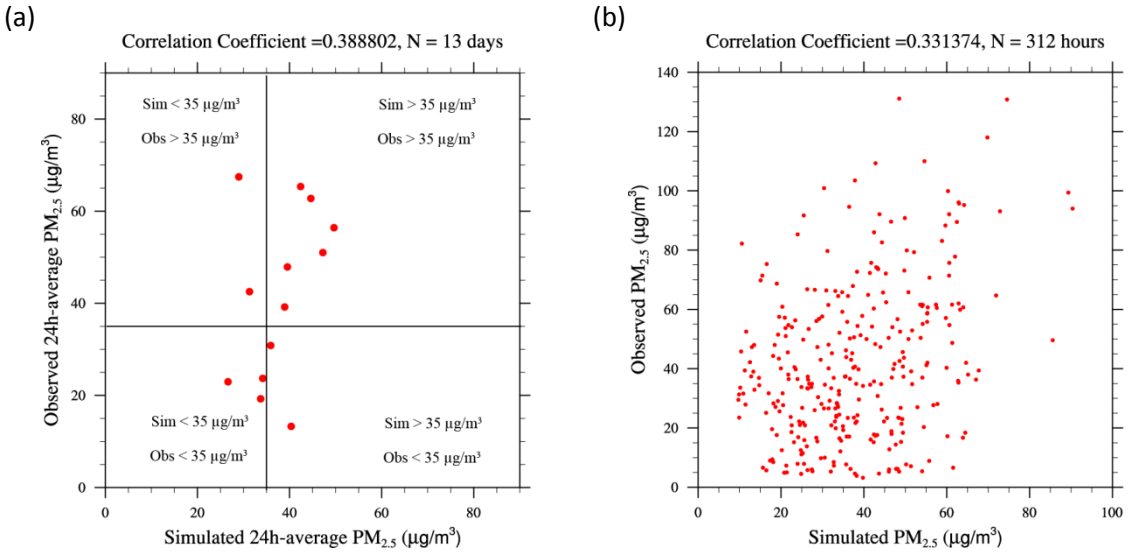
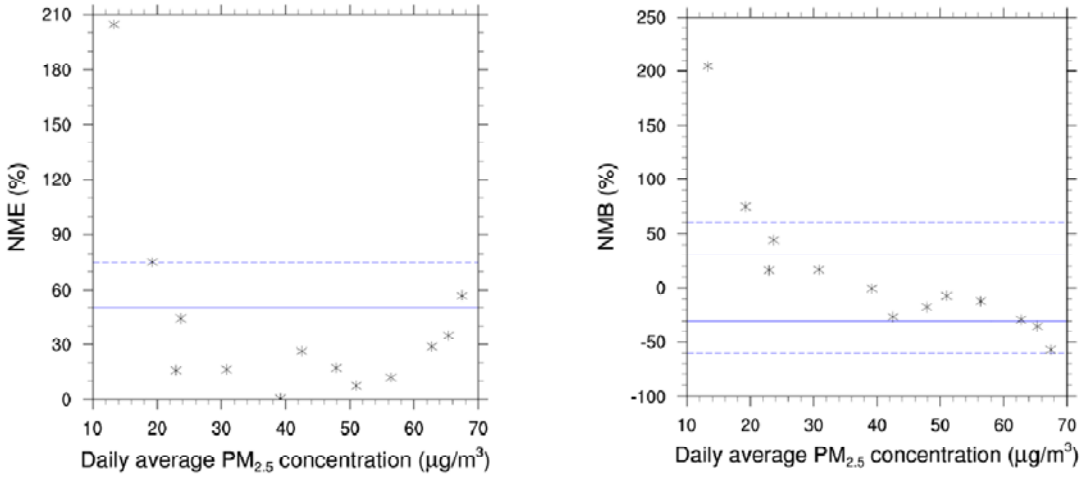


Fig. 16. Scatter plots of (a) 24h-average $PM_{2.5}$-concentrations and (b) hourly $PM_{2.5}$-concentrations during January 29, 2008 to February 10, 2008 at the State Building (test 13).

In a nutshell, there is no statistically significant difference for the hourly data, but there is statistical difference between the simulated and observed 24h-average $PM_{2.5}$-concentrations. This different statistical behavior can be explained by the lower sample number in the case of

the 24h-average data. Recall there are only 13 data points for the observed 24h-average $PM_{2.5}$-concentrations.

(a) (b)



(c)

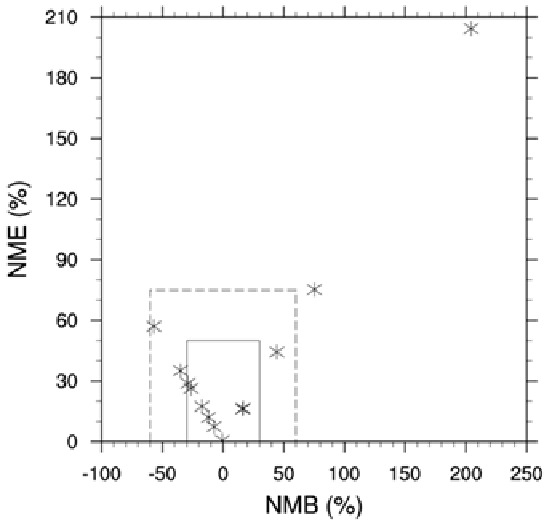


Fig. 17. Bugle plots of normalized mean (a) errors and (b) bias of simulated 24h-average $PM_{2.5}$-concentrations and (c) soccer plot of normalized mean errors and biases all determine with respect to the observations at the State Building site for January 23, 2008 to February 10, 2008 (test 13). The dashed and solid lines indicate the performance criteria and performance goals in accord with Boylan and Russell (2006).The upper most outlier is February 2 and the slight outlier is January 31.

On average, the difference between the simulated and observed 24h-average $PM_{2.5}$-concentrations at the State Building site was -3.76µg/m^3. The minimum and maximum of simulated 24h-average $PM_{2.5}$-concentrations were 26.65 and 49.66µg/m^3, respectively.

Whereas, the minimum and maximum observed were 13.26 and 67.44µg/m^3, respectively. The normalized mean bias and mean error between the simulations and observations were -9% and 31%, respectively. The variance in the simulation was 48.80(µg/m^3)^2 with a standard deviation of 6.98µg/m^3. The variance in the observations was 343.31(µg/m^3)^2 with a standard deviation of 18.53µg/m^3. At the State Building, eight exceedance days were observed during the January/February episode, while eight exceedance days were simulated by the Alaska adapted CMAQ.

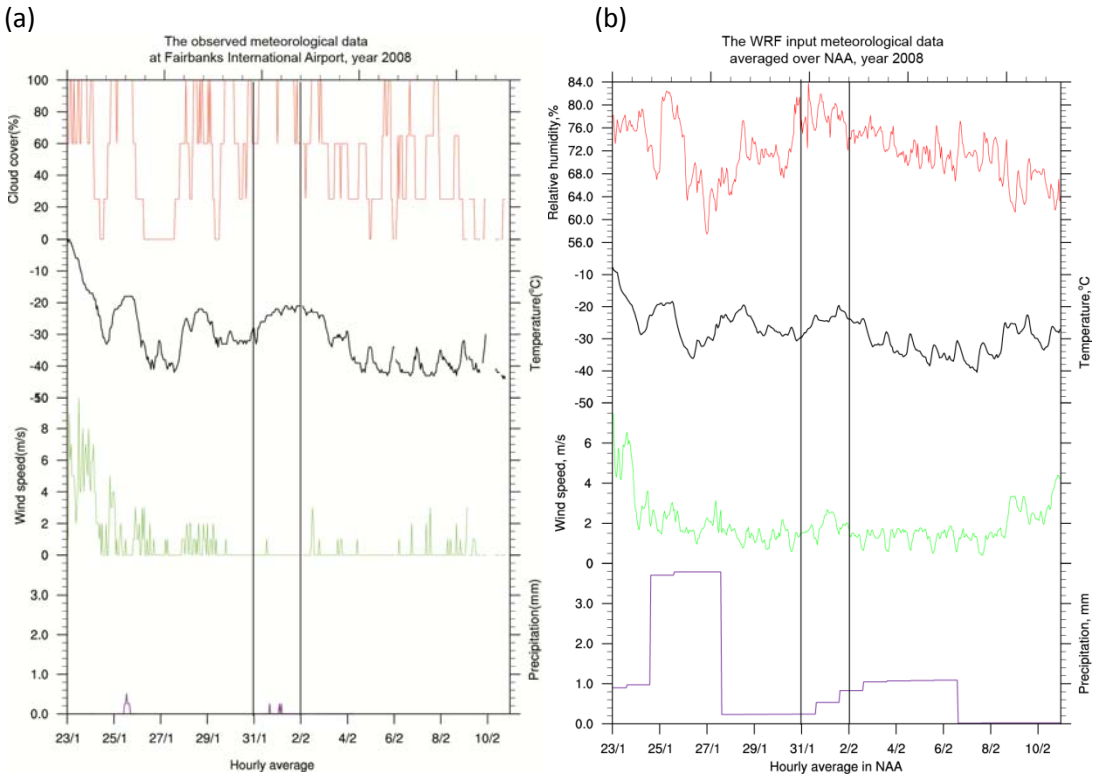


Fig. 18. Meteorological variables (a) as observed at Fairbanks International Airport and (b) as simulated by WRF and averaged over the nonattainment area.

We also evaluated the performances of the Alaska adapted CMAQ by using soccer plots and bugle plots. There are two simulated days on which the Alaska adapted CMAQ fails to meet the performance criteria (Fig. 17). For further investigation of the reasons, we compared the simulated and observed meteorological quantities to assess whether offsets in the WRF simulations are the cause for the weaker performance on February 2 and February 8 2008 (Alaska Standard Time). Mölders et al. (2011a) reported that WRF/Chem-simulated $PM_{2.5}$-concentrations are worse when the timing of frontal passages is offset or the strength of inversions is strongly underestimated. Investigation of the simulated meteorology suggests that there is an air mass exchange simulated for these days. Note that an evaluation of WRF is beyond the scope of our project.

The two outlier points are January 31 and February 2, 2008. We also compared the simulated meteorological conditions in the nonattainment area with those observed at the Fairbanks International airport (Fig. 18). The two outliers from the plots are in the positive values which mean CMAQ model overestimated the 24h-average $PM_{2.5}$-concentrations at the State Building site. The amount of precipitation in the WRF model, which is averaged over the nonattainment area seemed to be too low during January 31 to February 2, 2008 when compared with the observations at the Fairbanks International Airport. To low precipitation can lead to reduced removal of pollutants by wet deposition. Therefore, the simulated $PM_{2.5}$-concentrations at the State Building site are too high compared with the observed data. A detailed process analysis will help in identifying reasons for the outliers and is planned for the future.

5.2 Speciation

There were only six days, for which data on observed $PM_{2.5}$-composition were available, for which a statistic is to be considered with caution. Comparison of the simulated and observed composition of 24h-average $PM_{2.5}$ showed that CMAQ overestimated the percentage of organic carbon in the simulated $PM_{2.5}$ composition (four times out of six data points), but underestimated the percentage of sulfate, nitrate and ammonium. CMAQ simulated elemental carbon was similar to the observed fraction (Figs. 19, 20).

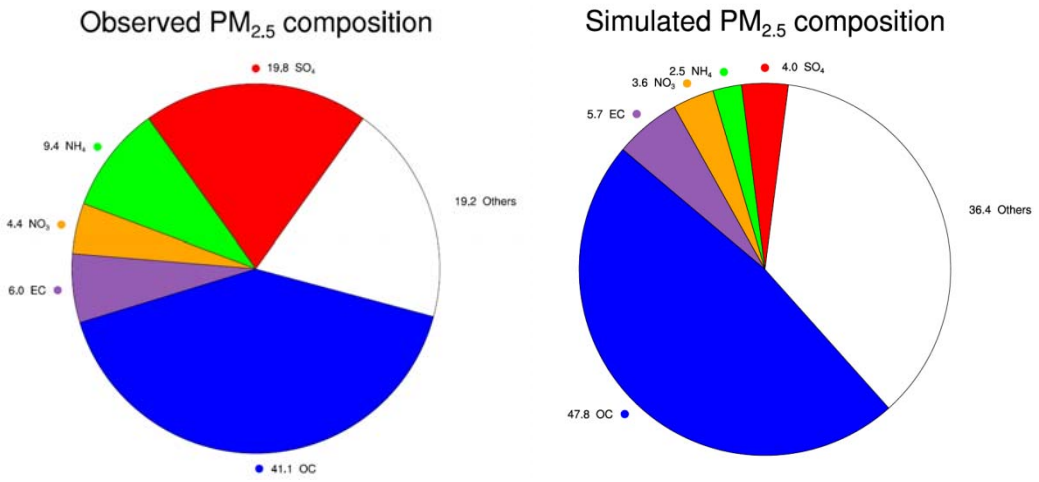


Fig. 19. The composition of observed and simulated 24h-averaged $PM_{2.5}$-concentrations averaged for the six days for which observation data were available at the State Building site. The category "others" in the observed $PM_{2.5}$ composition includes Al, Br, Ca, Na, Cl, Cu, Fe, Pb, Ni, K, Se, Si, S, Sn, Ti, V, Zn, while this category in the simulated $PM_{2.5}$ composition refers to unspecified anthropogenic mass (A25i+A25j). Note that "others" is determined in accord with EPA guidance document (EPA 2007).

We have analyzed and compared the initial condition and boundary condition that used more AORGPAJ than AORGPAI following the behavior of the organic aerosols in the eastern-half of the United States (ICBC2 in Table 2) with the one that used less AORGPAJ than AORGPAI following the behavior of organic aerosol in Alaska (ICBC3 in Table 3). The results show that the simulated

organic carbon fraction was underestimated in both cases, and that they do not cause much difference in the 24h-average $PM_{2.5}$-concentrations at the State Building site. Note that we have only the observed background concentration of organic carbon at the surface, and we used the decreasing factor with height following the vertical profile of $PM_{2.5}$-concentrations (Jaeschke et al., 1999). It might be possible that the emission inventory underestimated the sources of sulfate, nitrate and ammonium.

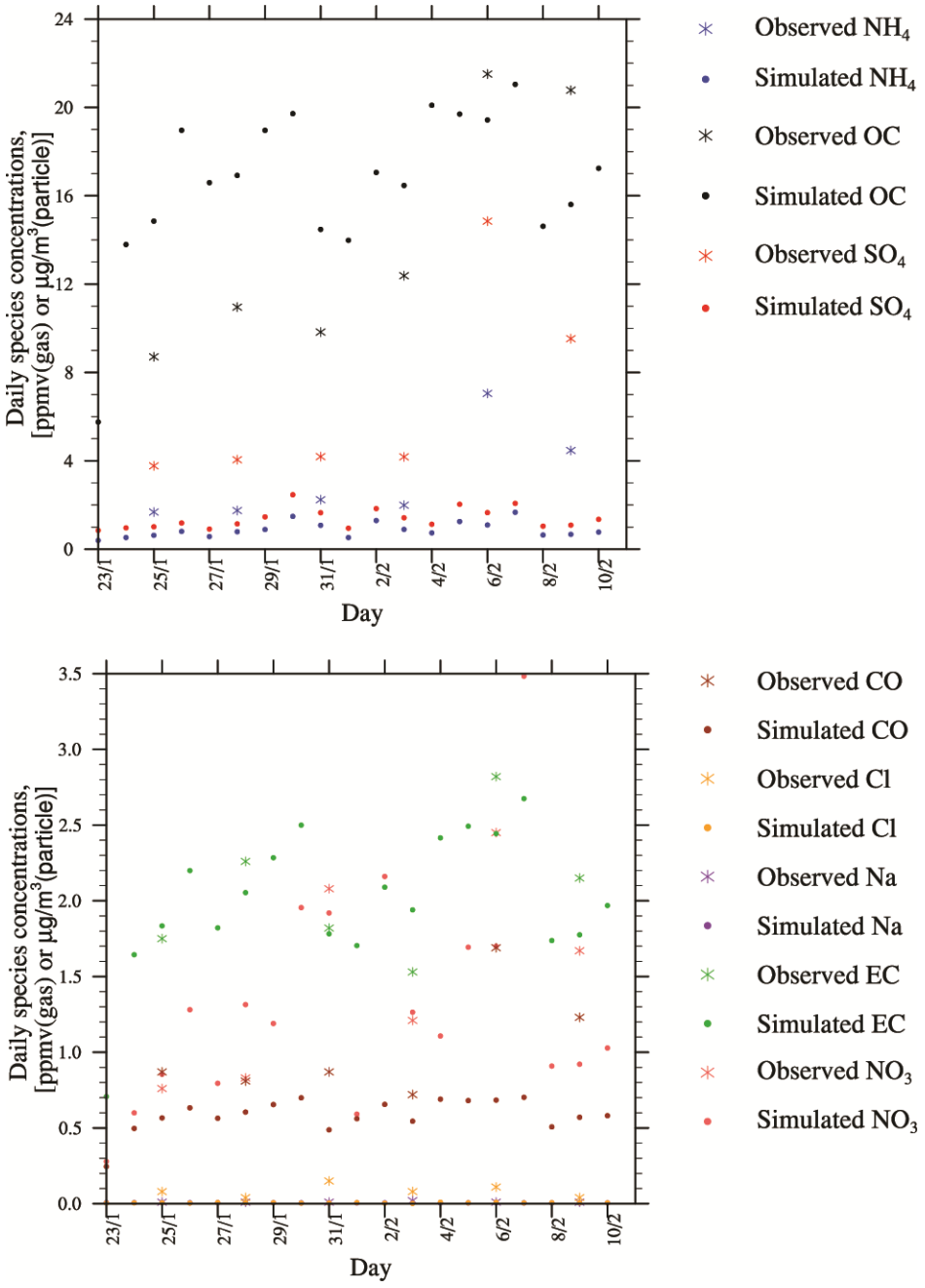


Fig. 20. Time series of the 24h-average $PM_{2.5}$ species and CO during January 23, 2008 to February 10, 2008 at the grid cell that holds the State Building. The stars and circles indicate the observed and simulated values, respectively.

5.3 Spatial distribution

The spatial distribution of $PM_{2.5}$-concentrations in domain 3 is shown in Figure 21. On average over the trimmed domain, the simulated $PM_{2.5}$-concentration was 2.62µg/m^3. The maximum and the minimum daily average were 67.4µg/m^{3}and 14.9µg/m^3, which occurred on Feburuary 7 and January 23, respectively. The grid cell where the maximum simulated hourly-average $PM_{2.5}$-concentration of 67.4µg/m^3 was simulated, was located at X =30 and Y =45 (Fig. 21). The grid cell where the minimum simulated hourly-average $PM_{2.5}$-concentration 0.25 µg/m^3 was simulated, was located at X=50 and Y=65. Low $PM_{2.5}$-concentrations were typically simulated near the boundary of the domain.

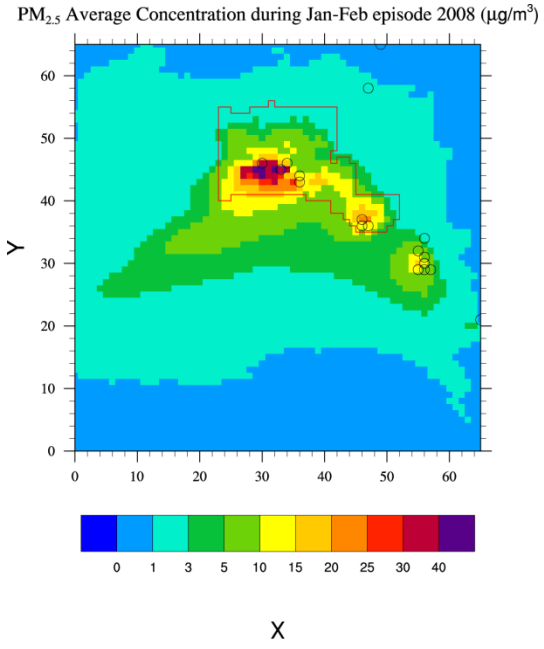


Fig. 21. Spatial distribution of simulated $PM_{2.5}$-concentrations at breathing level averaged over January 23, 2008 to February 10, 2008.

6. Sensitivity tests

6.1 Chemistry on/off sensitivity tests

A sensitivity study was performed wherein the chemistry was switched off to assess the impact of chemistry on the $PM_{2.5}$-concentrations. Preliminarily analysis of the chemistry on/off sensitivity test show that turning off the chemistry leads to a reduction of $PM_{2.5}$-concentrations in the analyzed trimmed domain. This finding indicates that some of the $PM_{2.5}$ is due to chemical processes rather than emitted. Turning off both the gas-phase chemistry and the aerosol chemistry or turning off only the aerosol chemistry lead to similar results (Fig. 22). A detailed analysis will be part of Phase II.

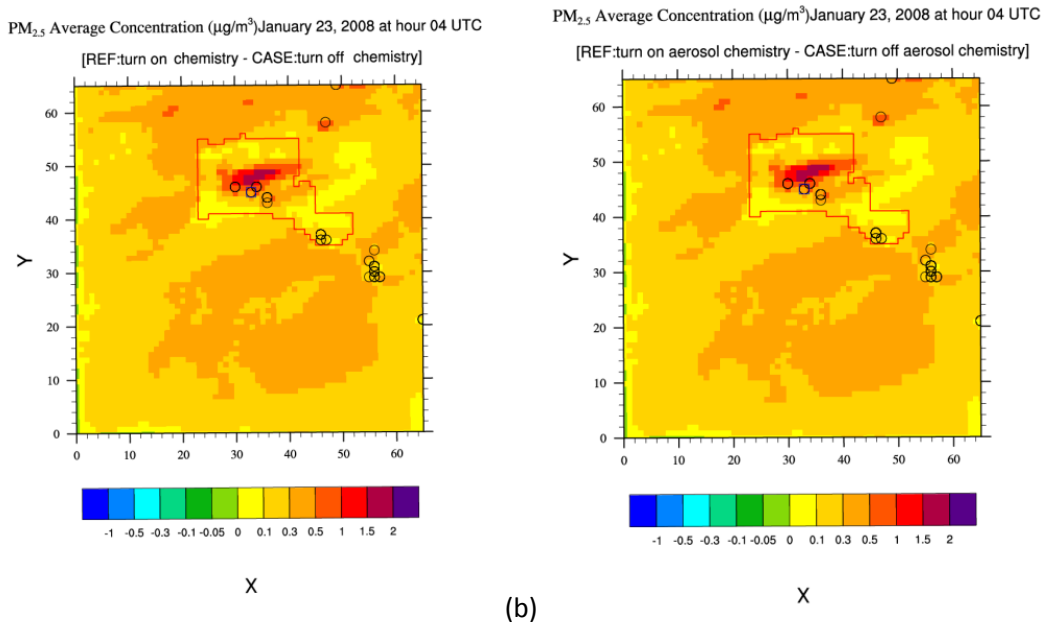


Fig. 22. Exemplary plot of the $PM_{2.5}$-concentration differences at breathing level at 0400 UTC as obtained from the Alaska adapted CMAQ simulation with (a) turned off gas-phase and aerosol chemistry, (b) turned off aerosol chemistry.

6.2 Power plant on/off sensitivity tests and vertical profile

Turning off the emissions from point sources decreased the 24h-average $PM_{2.5}$-concentrations simulated at the State Building site up to 8.2µg/m^3. The average difference in 24h-average $PM_{2.5}$-concentrations from January 23 to February 10 obtained due to switching off the point-source emissions was 3.8µg/m^3 (Table 4). The maximum difference between the Alaska adapted CMAQ simulations with and without consideration of point source emissions occurred in the areas near point sources (Fig. 23).

Note that the average difference between the Alaska adapted CMAQ simulations without and with consideration of point-source emissions is about twice the average response found by WRF/Chem with a 4km increment for switching off point sources for a four month episode in winter 2005/06 (Mölders et al., 2011b). It is common knowledge that a fine resolution typically provides higher average differences than a coarser resolution. Thus, we can conclude that our finding well fit into findings for Fairbanks from other, independent studies (e.g. Mölders et al. 2011b).

7. Summary and conclusions

The CMAQ model has been adapted to simulate 24h-average $PM_{2.5}$-concentrations in the Fairbanks nonattainment area for the first episode January 23 – February 10, 2008. The modifications in the CMAQ model that were conducted to obtain the best representation of the $PM_{2.5}$-concentrations for the State Building site include: the development of Alaska specific initial and background conditions, modification of the dry deposition module to consider Alaska

typical vegetations and conditions, modification of the eddy diffusivity values according to observational evidence, modification of the MCIP code to include a calibration of the WRF simulated wind-speed in the Fairbanks bowl.

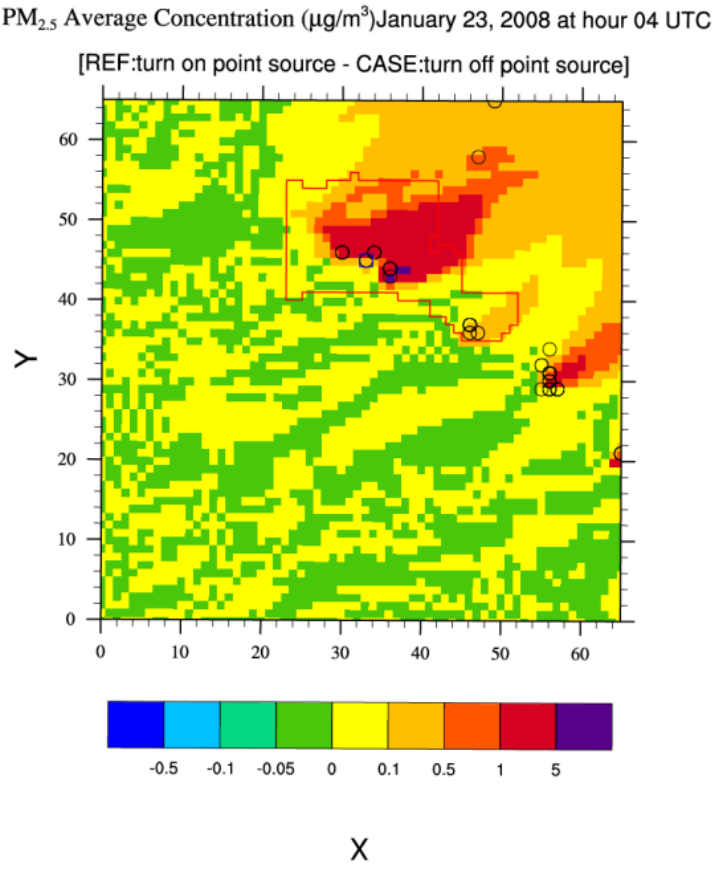


Fig. 23. $PM_{2.5}$-concentration differences at breathing level at 0400 UTC as obtained from the Alaska adapted CMAQ simulations with and without consideration of point source emissions (tests 11, 13).

Various module options have been compared, tested and assessed. Finally, the YAMO scheme was selected to calculate horizontal and vertical advection, eddy scheme was selected to be the diffusion module and PHO_inline was the module to calculate the photolysis rate as these options provided on average the best results and/or were most suitable for the Fairbanks conditions. The results from above CMAQ package set-up resulted in the average 24h-average $PM_{2.5}$-concentrations at the grid cell holding the State Building from January 29, 2008 to February 10, 2008 of 38.0µg/m^3, whereas the episode average of observed 24h-average $PM_{2.5}$-concentrations was 41.7µg/m^3. The correlation coefficient between the observed and simulated 24h-average $PM_{2.5}$-concentrations was 0.39. Due to the lower number of 24h-average observed data, the simulated and observed 24h-average $PM_{2.5}$-concentrations differ statistically significant at the 95% confidence level, but there is no statistically significant difference for the hourly averaged $PM_{2.5}$-concentrations concentrations. This means we may assume that the

Alaska adapted CMAQ is able to simulated the situation of the 24h-average $PM_{2.5}$-concentrations acceptably on average over time. The evaluation the performance of the Alaska adapted CMAQ showed that there were two days on which the simulated 24h-average $PM_{2.5}$-concentrations failed to meet the performance criteria. An evaluation of the meteorological performance would be helpful for assessment of the reasons, but is beyond the scope of our task. However, looking at the observations at the Fairbanks International Airport and WRF's simulation over the nonattainment area suggest that precipitation is underestimated by WRF. Such underestimation of the precipitation in the nonattainment area might lead to too low wet deposition of pollutants and consequently overestimation of $PM_{2.5}$-concentrations.

Table 4. 24-h average $PM_{2.5}$-concentrations at the State Building site as observed data and simulated by the Alaska adapted CMAQ without (B case) and with consideration of emissions from point sources (A case).

	$PM_{2.5}$ conc. at SB (µg/m3)		A =w/o point sources	B=w point sources	B-A
		observed	uv50%,eddy	uv50%,eddy	
Date			66,ICBCv4	66, ICBCV4	
23-Jan	1	-999.00	11.22	12.18	0.96
24-Jan	2	-999.00	25.88	26.69	0.81
25-Jan	3	-999.00	27.67	29.64	1.97
26-Jan	4	-999.00	34.80	37.27	2.47
27-Jan	5	-999.00	30.24	31.71	1.47
28-Jan	6	-999.00	31.61	34.92	3.31
29-Jan	7	39.18	35.81	38.95	3.15
30-Jan	8	51.00	38.08	47.24	9.16
31-Jan	9	19.25	28.07	33.74	5.67
1-Feb	10	22.95	26.28	26.65	0.37
2-Feb	11	13.26	31.26	40.37	9.10
3-Feb	12	23.69	30.56	34.19	3.63
4-Feb	13	47.88	37.43	39.55	2.12
5-Feb	14	62.76	37.43	44.64	7.20
6-Feb	15	65.34	36.98	42.42	5.43
7-Feb	16	56.40	41.43	49.66	8.23
8-Feb	17	67.45	27.66	28.99	1.33
9-Feb	18	42.52	28.67	31.32	2.65
10-Feb	19	30.83	31.77	35.92	4.15
	R		**0.54**	**0.39**	
	Mean		**31.20**	**35.05**	**3.85**
	STDEV	**17.80**	**6.46**	**8.38**	

The investigations on the impact of the choice of the boundary conditions and where the lateral boundaries are located suggested that the lateral boundaries seem to have little impact on the $PM_{2.5}$-concentrations simulated at the grid cell holding the State Building site, but have some impact on the $PM_{2.5}$-concentrations outside the nonattainment area. However, here the concentrations are low for which we may conclude that trimming the domain size does not affect the simulated concentrations in the nonattainment area critically. Due to the marginal differences in the nonattainment are in the runs with domain 3 and the trimmed domain that are moreover less than the accuracy of measurements, it must be concluded that trimming of the domain is justified and reasonable to be able to perform more studies on various mitigation measures.

Preliminarily analysis of the sensitivity tests on the role of gas-phase and aerosol chemistry shows that turning off the chemistry reduces the $PM_{2.5}$-concentrations in the range of 0 to 2$\mu g/m^3$ in the entire trimmed domain. This means one can conclude that gas-to-particle conversion plays a role in the Fairbanks nonattainment area.

The sensitivity study on the impact of point-source emissions on the $PM_{2.5}$-concentrations suggest that point-source emissions contribute up to 8.2$\mu g/m^3$ to the concentrations in the grid cell that holds the State Building site.

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Appendix A

run.mcip

```
set APPL          = 2008024_valleyr
set CoordName = TEST_GRID  # 16-character maximum
set GridName    = FAIRBANKS  # 16-character maximum
set DataPath     =
/import/archive/u1/uaf/tran/EPA_DATA/pennstate_EPA/020612to021200final/d03
set InMetDir     = $DataPath
set InTerDir      = $DataPath
set InSatDir      = $DataPath/goes
set OutDir         = $WRKDIR/INPUT_MET2
set ProgDir        = $cwd/src
set WorkDir       = $OutDir
set InMetFiles   =  ( $InMetDir/wrfout_d03_2008-01-23* \
    $InMetDir/wrfout_d03_2008-01-24* \
    $InMetDir/wrfout_d03_2008-01-25_00:00:00 )
set IfTer           = "T"
set InTerFile     = $ARCHIVE/geogrid/geo_em.d03.nc
set InSatFiles    = ( )
set LDDEP         = 4
set LPV             = 1
set LWOUT        = 1
set LUVCOUT     = 1
set LSAT           = 0
set MCIP_START = 2008-01-24-00:00:00.0000  # [UTC]
set MCIP_END    = 2008-01-25-00:00:00.0000  # [UTC]
set INTVL          = 60 # [min]
set CTMLAYS     = "-1.0"
set MKGRID       = T
#  Setting BTRIM = 0 , use maximum of input meteorology
set BTRIM         = 0
set X0               = default
set Y0               = default
set NCOLS         = default
set NROWS        = default
#-------------------------------------------------------------------------
# Set coordinates for cell for diagnostic prints on output domain.
# If coordinate is set to 0, domain center cell will be used.
#-------------------------------------------------------------------------
set LPRT_COL    = 0
set LPRT_ROW   = 0

set WRF_LC_REF_LAT    = 64.8
# Set up and run MCIP.
set PROG                    = mcip
```

```
date
setenv LOGFILE $WRKDIR/$APPL.log

if ( ! -d $InMetDir ) then
  echo "No such input directory $InMetDir"
  exit 1
endif

if ( ! -d $OutDir ) then
  echo "No such output directory...will try to create one"
  mkdir -p $OutDir
  if ( $status != 0 ) then
    echo "Failed to make output directory, $OutDir"
    exit 1
  endif
endif

if ( ! -d $ProgDir ) then
  echo "No such program directory $ProgDir"
  exit 1
endif

if ( $LSAT == 1 ) then
  if ( ! -d $InSatDir ) then
    echo "No such satellite input directory $InSatDir
    exit 1
  endif
endif
if ( $IfTer == "T" ) then
  if ( ! -f $InTerFile ) then
    echo "No such input file $InTerFile"
    exit 1
  endif
endif

foreach fil ( $InMetFiles )
  if ( ! -f $fil ) then
    echo "No such input file $fil"
    exit 1
  endif
end

if ( $LSAT == 1 ) then
  foreach fil ( $InSatFiles )
    if ( ! -f $fil ) then
      echo "No such input file $fil"
      exit 1
```

```
   endif
  end
endif
#------------------------------------------------------------------------
# Make sure the executable exists.
#------------------------------------------------------------------------

if ( ! -f $ProgDir/${PROG}.exe ) then
  echo "Could not find ${PROG}.exe"
  exit 1
endif

#------------------------------------------------------------------------
# Create a work directory for this job.
#------------------------------------------------------------------------

if ( ! -d $WorkDir ) then
  mkdir -p $WorkDir
  if ( $status != 0 ) then
    echo "Failed to make work directory, $WorkDir"
    exit 1
    echo "Failed to make work directory, $WorkDir"
    exit 1
  endif
endif

cd $WorkDir

#------------------------------------------------------------------------
# Set up script variables for input files.
#------------------------------------------------------------------------

if ( $IfTer == "T" ) then
  if ( -f $InTerFile ) then
    set InTer = $InTerFile
  else
    set InTer = "no_file"
  endif
else
  set InTer = "no_file"
endif

set FILE_GD  = $OutDir/GRIDDESC23Jan
set FILE_HDR = $OutDir/mmheader.${APPL}

#------------------------------------------------------------------------
# Create namelist with user definitions.
#------------------------------------------------------------------------
```

```
set MACHTYPE = `uname`
if ( ( $MACHTYPE == "AIX" ) || ( $MACHTYPE == "Darwin" ) ) then
  set Marker = "/"
else
  set Marker = "&END"
endif

cat > $WorkDir/namelist.${PROG} << !

 &FILENAMES
  file_gd    = "$FILE_GD"
  file_hdr   = "$FILE_HDR"
  file_mm    = "$InMetFiles[1]",
!

if ( $#InMetFiles > 1 ) then
  @ nn = 2
  while ( $nn <= $#InMetFiles )
    cat >> $WorkDir/namelist.${PROG} << !
            "$InMetFiles[$nn]",
!
    @ nn ++
  end
endif

if ( $IfTer == "T" ) then
cat >> $WorkDir/namelist.${PROG} << !
  file_ter   = "$InTer"
!
endif

if ( $LSAT == 1 ) then
  cat >> $WorkDir/namelist.${PROG} << !
  file_sat   = "$InSatFiles[1]",
!
  if ( $#InSatFiles > 1 ) then
    @ nn = 2
    while ( $nn <= $#InSatFiles )
      cat >> $WorkDir/namelist.${PROG} << !
            "$InSatFiles[$nn]",
!
      @ nn ++
    end
  endif
endif

cat >> $WorkDir/namelist.${PROG} << !
```

```
 makegrid   = .${MKGRID}.
$Marker

 &USERDEFS
 lddep     =  $LDDEP
 lpv       =  $LPV
 lwout     =  $LWOUT
 luvcout   =  $LUVCOUT
 lsat      =  $LSAT
 mcip_start = "$MCIP_START"
 mcip_end   = "$MCIP_END"
 intvl     =  $INTVL
 coordnam   = "$CoordName"
 grdnam     = "$GridName"
 ctmlays    =  $CTMLAYS
 btrim      =  $BTRIM
 lprt_col   =  $LPRT_COL
 lprt_row   =  $LPRT_ROW
 wrf_lc_ref_lat = $WRF_LC_REF_LAT
$Marker

 &WINDOWDEFS
 x0        =  $X0
 y0        =  $Y0
 ncolsin    =  $NCOLS
 nrowsin    =  $NROWS
$Marker

#-------------------------------------------------------------------------
# Set links to FORTRAN units.
#-------------------------------------------------------------------------

rm fort.*
if ( -f $FILE_GD ) rm -f $FILE_GD

ln -s $FILE_HDR               fort.2
ln -s $FILE_GD                fort.4
ln -s $WorkDir/namelist.${PROG}  fort.8
if ( $IfTer == "T" ) then
  ln -s $InTerFile             fort.9
endif

set NUMFIL = 0
foreach fil ( $InMetFiles )
  @ NN = $NUMFIL + 10
  ln -s $fil fort.$NN
  @ NUMFIL ++
end
```

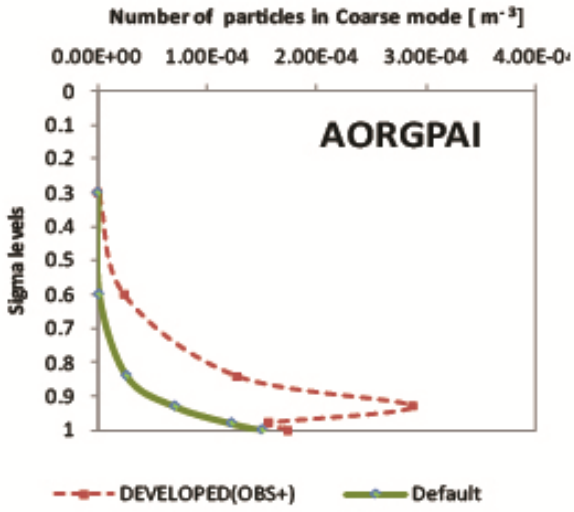
```
#-------------------------------------------------------------------------
# Set output file names and other miscellaneous environment variables.
setenv IOAPI_CHECK_HEADERS  T
setenv EXECUTION_ID       $PROG

setenv GRID_BDY_2D        $OutDir/GRIDBDY2D_${APPL}
setenv GRID_CRO_2D        $OutDir/GRIDCRO2D_${APPL}
setenv GRID_CRO_3D        $OutDir/GRIDCRO3D_${APPL}
setenv GRID_DOT_2D        $OutDir/GRIDDOT2D_${APPL}
setenv MET_BDY_3D         $OutDir/METBDY3D_${APPL}
setenv MET_CRO_2D         $OutDir/METCRO2D_${APPL}
setenv MET_CRO_3D         $OutDir/METCRO3D_${APPL}
setenv MET_DOT_3D         $OutDir/METDOT3D_${APPL}

#-------------------------------------------------------------------------
# Execute MCIP.
#-------------------------------------------------------------------------

$ProgDir/${PROG}.exe

if ( $status == 0 ) then
  rm fort.*
  exit 0
else
  echo "Error running $PROG"
  exit 1
endif
```

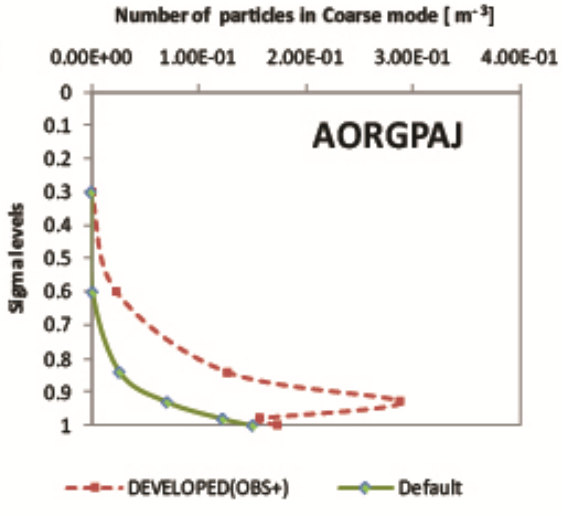
Appendix B

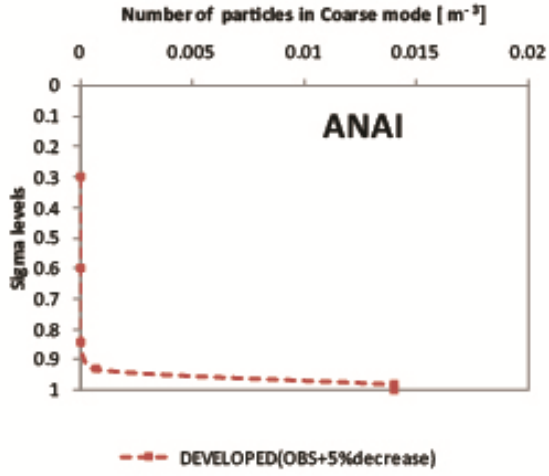
The initial condition and boundary condition of chemical species which is developed for the domain in Alaska

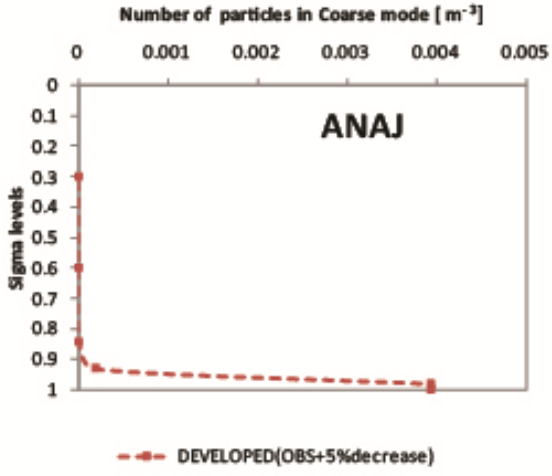
Initial condition for Alaska domain : The vertical coordinate of the model to generate these i.c. is the terrain-following sigma coordinate. The number of sigma layers and defined sigma levels are listed below.

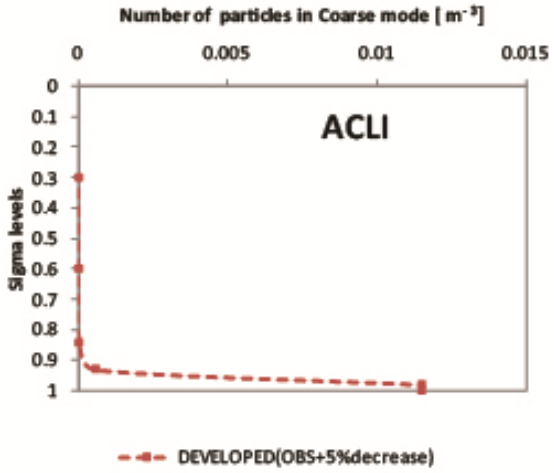
```
      6    35   1.00  0.98  0.93  0.84  0.60  0.30  0.00
1999180  00
"SO2     " 2.000E-05  3.000E-05  6.500E-04  4.000E-05  2.000E-05  1.000E-05
"NO2     " 9.000E-06  9.000E-06  9.000E-06  9.000E-06  9.000E-06  9.000E-06
"NO      " 9.000E-06  9.000E-06  9.000E-06  9.000E-06  9.000E-06  9.000E-06
"O3      " 4.000E-02  5.000E-02  5.500E-02  5.700E-02  1.000E-01  1.500E-01
"HNO3    " 1.000E-04  1.000E-04  1.200E-04  1.500E-04  2.000E-04  1.500E-04
"H2O2    " 2.000E-04  2.000E-04  2.000E-04  2.014E-04  3.707E-04  2.400E-04
"ALD     " 5.000E-05  6.060E-05  1.090E-05  1.450E-04  1.810E-04  1.960E-04
"HCHO    " 6.000E-05  6.000E-05  6.000E-05  9.160E-05  7.360E-05  9.200E-05
"OP1     " 1.000E-04  1.000E-04  1.000E-04  1.430E-04  3.130E-04  2.820E-04
"N2O5    " 1.949E-08  1.127E-08  8.449E-09  6.997E-09  1.340E-08  3.221E-08
"NO3     " 1.949E-08  1.127E-08  8.449E-09  6.997E-09  1.340E-08  3.221E-08
"PAN     " 4.125E-04  3.375E-04  5.250E-04  3.375E-04  3.375E-04  3.750E-04
"HC3     " 1.150E-10  2.460E-09  2.600E-07  3.310E-06  4.610E-05  1.500E-04
"HC5     " 1.150E-10  2.460E-09  2.600E-07  3.310E-06  4.610E-05  1.500E-04
"CO      " 4.400E-02  4.400E-02  4.400E-02  4.400E-02  4.400E-02  4.400E-02
"OL2     " 1.710E-05  1.710E-05  1.710E-05  1.710E-05  1.710E-05  1.710E-05
"HNO4    " 2.559E-06  2.357E-06  1.811E-06  7.869E-07  1.212E-07  5.702E-08
"ISO     " 1.000E-24  1.000E-24  1.000E-24  1.000E-24  3.540E-07  7.930E-07
"HO      " 3.460E-07  1.812E-07  4.928E-08  3.098E-08  2.459E-08  2.056E-08
"HO2     " 2.026E-06  2.750E-06  3.565E-06  5.196E-06  8.296E-06  1.296E-05
"ASO4I   " 2.210E-01  8.350E-01  1.230E+00  1.300E+00  8.450E-01  1.040E+00
"ASO4J   " 7.540E-03  2.850E-02  4.200E-02  4.440E-02  2.880E-02  3.560E-02
"ANH4I   " 5.010E-02  3.780E-01  3.430E-01  3.690E-01  3.500E-01  1.580E-01
"ANH4J   " 1.240E-03  9.370E-03  8.490E-03  9.150E-03  8.670E-03  3.920E-03
"ANO3I   " 1.170E-02  5.720E-02  6.910E-02  5.720E-02  1.130E-01  8.110E-02
"ANO3J   " 3.520E-03  1.720E-02  2.080E-02  1.720E-02  3.410E-02  2.430E-02
"NUMATKN " 5.193E+06  4.674E+06  8.593E+06  3.777E+06  7.082E+05  9.440E+03
"NUMACC  " 1.888E+07  1.699E+07  3.123E+07  1.373E+07  2.574E+06  3.430E+04
"NUMCOR  " 5.736E+03  5.162E+03  9.490E+03  4.171E+03  7.821E+02  1.040E+01
"AORGPAI " 1.736E-01  1.563E-01  2.873E-01  1.263E-01  2.368E-02  3.157E-04
"AORGPAJ " 1.736E-04  1.563E-04  2.873E-04  1.263E-04  2.368E-05  3.157E-07
"ANAI    " 1.400E-02  1.400E-02  7.020E-04  3.510E-05  1.750E-06  8.770E-08
"ANAJ    " 3.940E-03  3.940E-03  1.970E-04  9.850E-06  4.930E-07  2.460E-08
"ACLI    " 1.150E-02  1.150E-02  5.760E-04  2.880E-05  1.440E-06  7.200E-08
"ACLJ    " 3.540E-03  3.540E-03  1.770E-04  8.840E-06  4.420E-07  2.210E-08
```

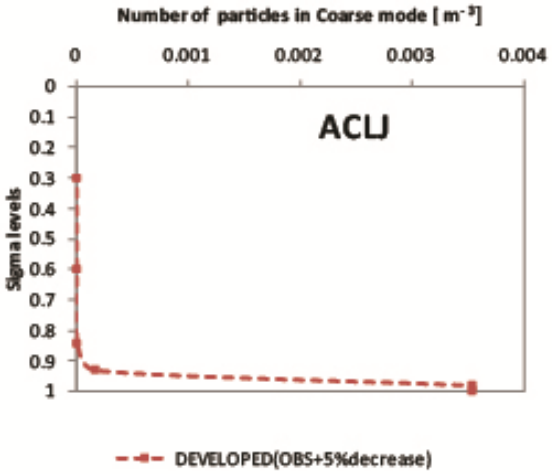

Number of particles in Coarse mode [m-3]
0.00E+00
1.00E-04
2.00E-04
3.00E-04
4.00E-04
AORGPAI
Sigma levels
DEVELOPED(OBS+)
Default

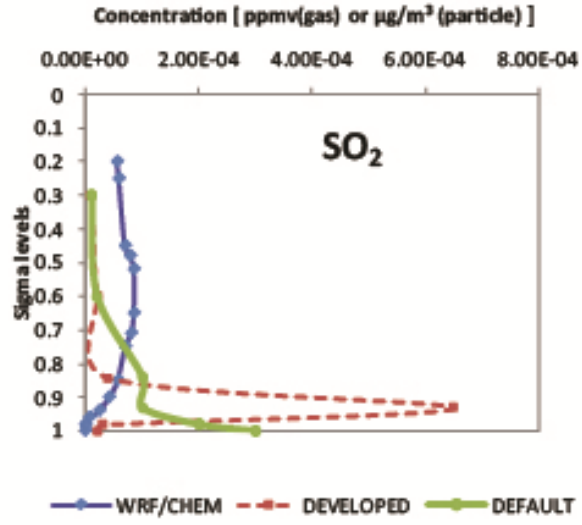

Number of particles in Coarse mode [m-3]
0.00E+00
1.00E-01
2.00E-01
3.00E-01
4.00E-01
AORGPAJ
Sigma levels
DEVELOPED(OBS+)
Default

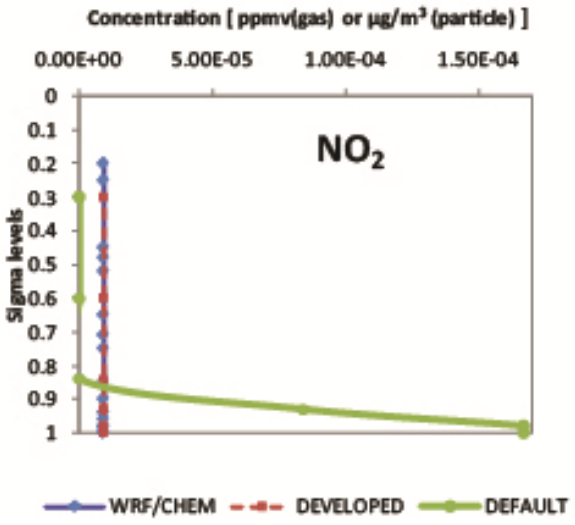

Number of particles in Coarse mode [m-3]
0
0.005
0.01
0.015
0.02
ANAI
Sigma levels
DEVELOPED(OBS+5%decrease)

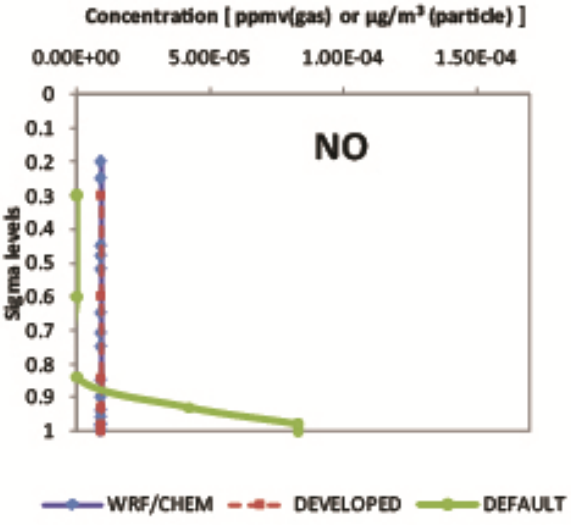

Number of particles in Coarse mode [m-3]
0
0.001
0.002
0.003
0.004
0.005
ANAJ
Sigma levels
DEVELOPED(OBS+5%decrease)

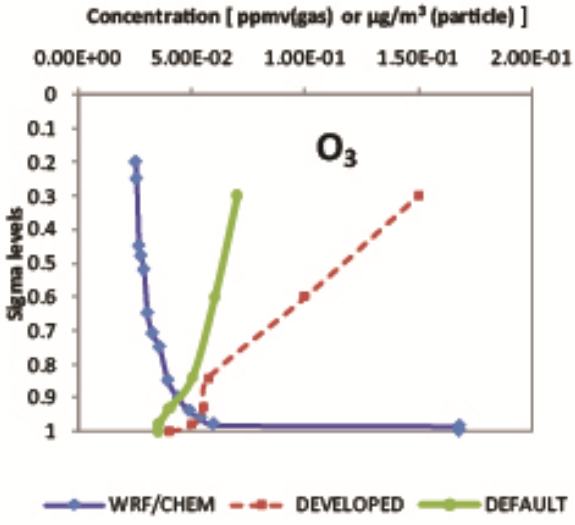

Number of particles in Coarse mode [m-3]
0
0.005
0.01
0.015
ACLI
Sigma levels
DEVELOPED(OBS+5%decrease)

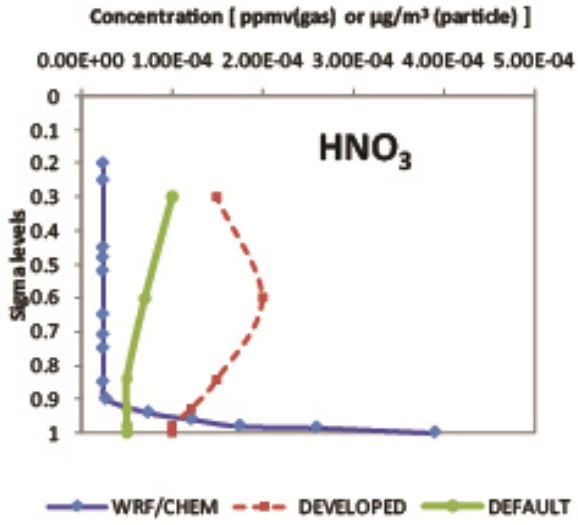

Number of particles in Coarse mode [m-3]
0
0.001
0.002
0.003
0.004
ACLJ
Sigma levels
DEVELOPED(OBS+5%decrease)

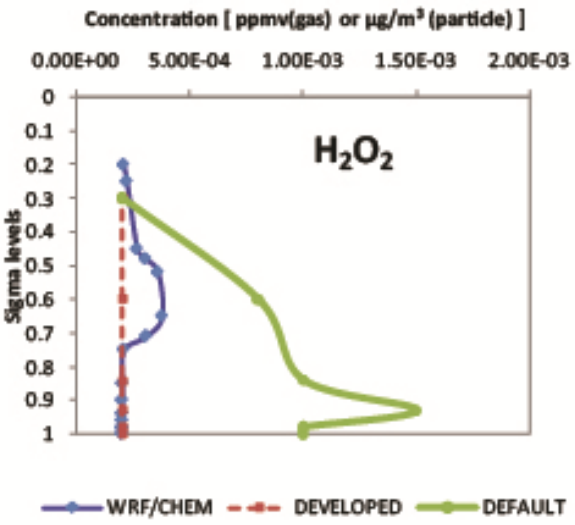

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 2.00E-04 4.00E-04 6.00E-04 8.00E-04
SO2
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

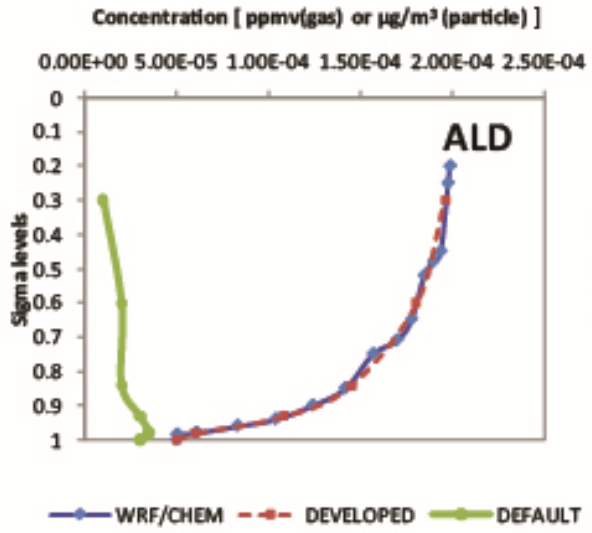

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04
NO2
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

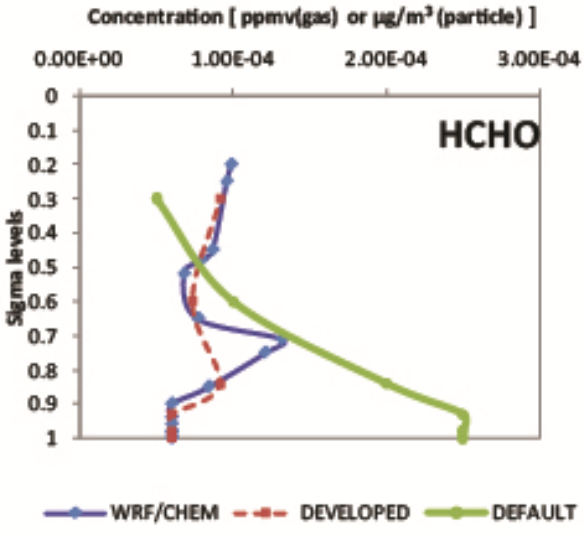

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04
NO
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

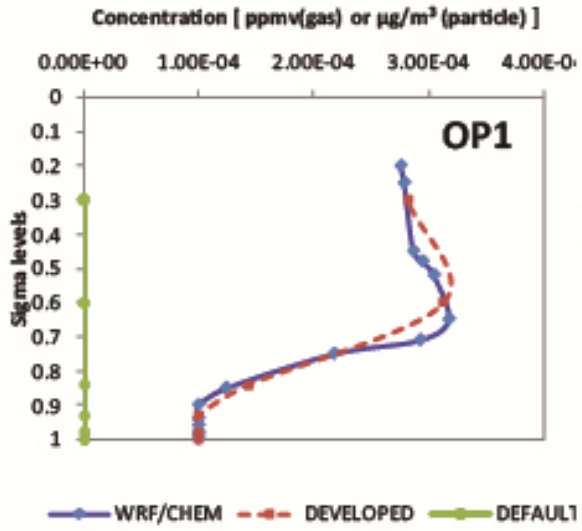

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-02 1.00E-01 1.50E-01 2.00E-01
O3
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

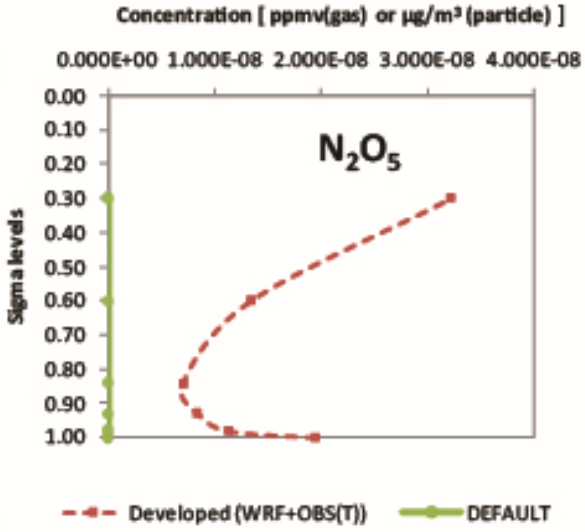

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 1.00E-04 2.00E-04 3.00E-04 4.00E-04 5.00E-04
HNO3
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

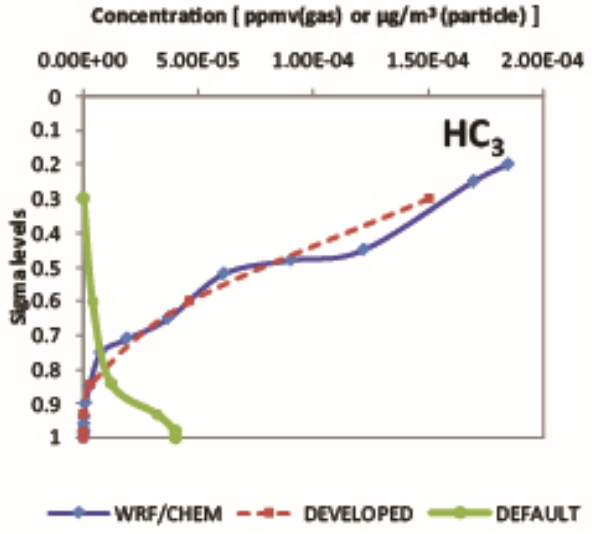

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-04 1.00E-03 1.50E-03 2.00E-03
H2O2
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM DEVELOPED DEFAULT

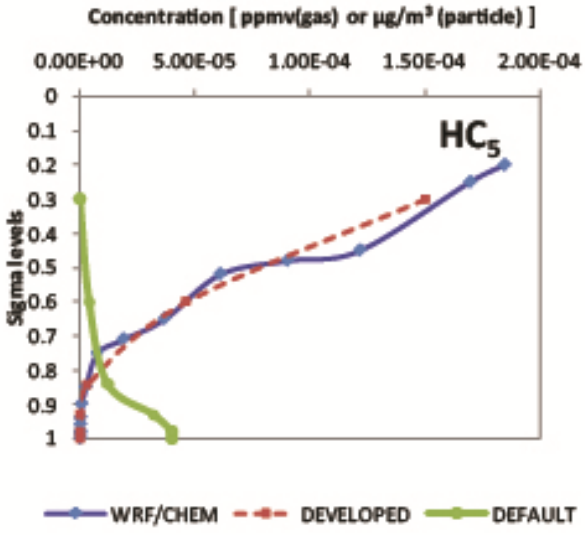

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04 2.00E-04 2.50E-04
ALD
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM
DEVELOPED
DEFAULT

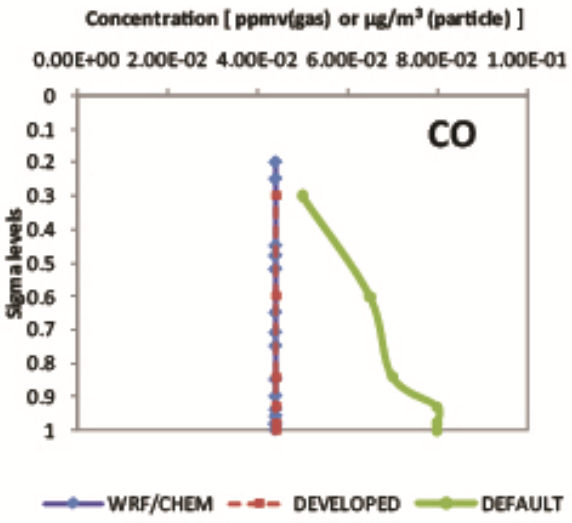

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 1.00E-04 2.00E-04 3.00E-04
HCHO
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM
DEVELOPED
DEFAULT

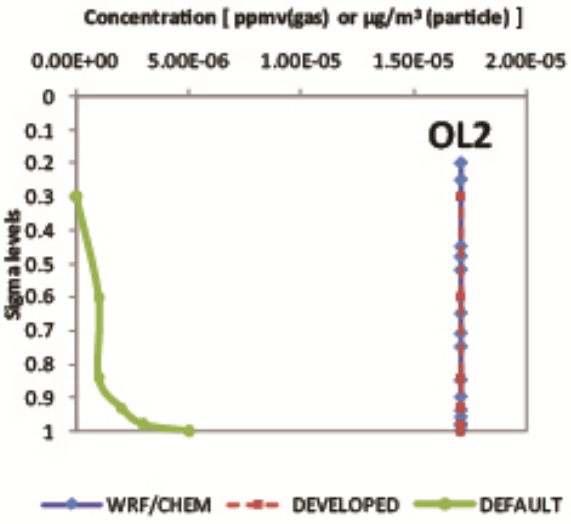

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 1.00E-04 2.00E-04 3.00E-04 4.00E-0
OP1
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM
DEVELOPED
DEFAULT

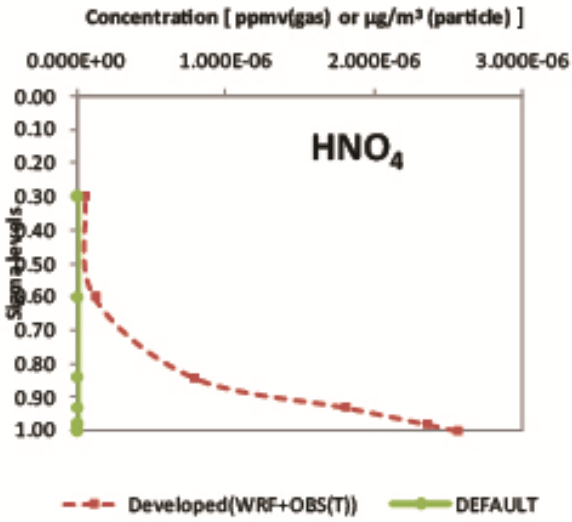

Concentration [ppmv(gas) or µg/m³ (particle)]
0.000E+00 1.000E-08 2.000E-08 3.000E-08 4.000E-08
N2O5
Sigma levels
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.00
Developed (WRF+OBS(T))
DEFAULT

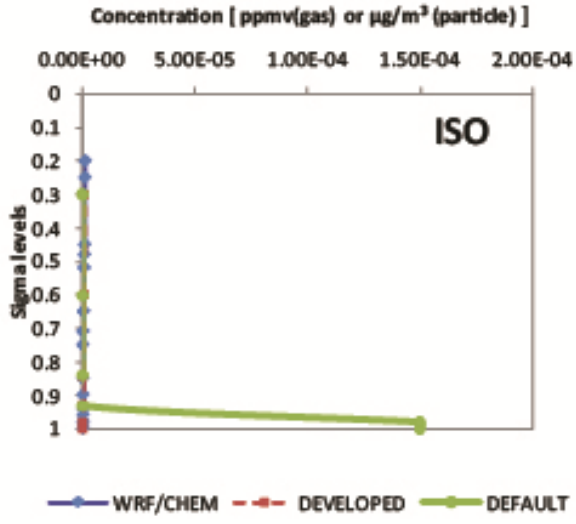

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04 2.00E-04
HC3
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM
DEVELOPED
DEFAULT

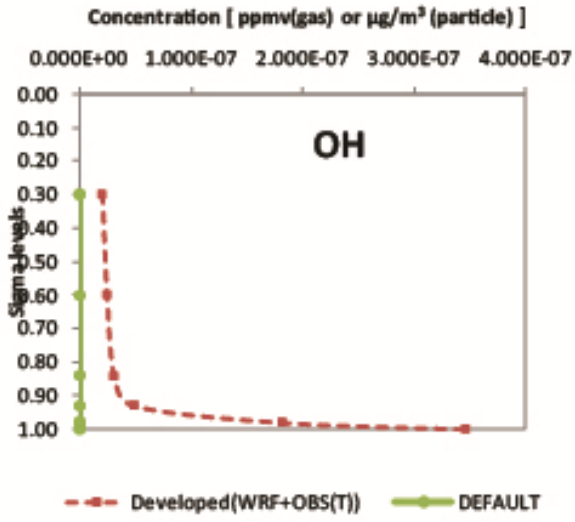

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04 2.00E-04
HC5
Sigma levels
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
WRF/CHEM
DEVELOPED
DEFAULT

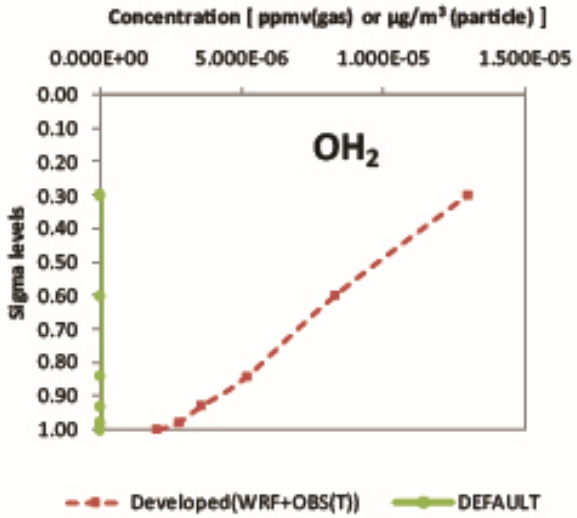

Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 2.00E-02 4.00E-02 6.00E-02 8.00E-02 1.00E-01
CO
Sigma levels
WRF/CHEM
DEVELOPED
DEFAULT


Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-06 1.00E-05 1.50E-05 2.00E-05
OL2
Sigma levels
WRF/CHEM
DEVELOPED
DEFAULT


Concentration [ppmv(gas) or µg/m³ (particle)]
0.000E+00 1.000E-06 2.000E-06 3.000E-06
HNO4
Sigma levels
Developed(WRF+OBS(T))
DEFAULT


Concentration [ppmv(gas) or µg/m³ (particle)]
0.00E+00 5.00E-05 1.00E-04 1.50E-04 2.00E-04
ISO
Sigma levels
WRF/CHEM
DEVELOPED
DEFAULT


Concentration [ppmv(gas) or µg/m³ (particle)]
0.000E+00 1.000E-07 2.000E-07 3.000E-07 4.000E-07
OH
Sigma levels
Developed(WRF+OBS(T))
DEFAULT


Concentration [ppmv(gas) or µg/m³ (particle)]
0.000E+00 5.000E-06 1.000E-05 1.500E-05
OH2
Sigma levels
Developed(WRF+OBS(T))
DEFAULT

Appendix C

run.cctm

```
set APPL          = eddy199
 set CFG          = e1a
 set EXEC         = CCTM_${CFG}_Linux2_x86_64pg
 setenv NPCOL_NPROW "4 4"; set NPROCS   = 16
#> Set the working directory:
 set BASE     = $HOME/CMAQ/scripts/cctm
 cd $BASE; date; cat $BASE/cfg.e1a_Linux2_x86_64pg; echo "    "; set echo

#> timestep run parameters

 set STDATE       = 2008024      # beginning date
 set STTIME       = 000000       # beginning GMT time (HHMMSS)
 set NSTEPS       = 240000       # time duration (HHMMSS) for this run
 set TSTEP        = 010000      # output time step interval (HHMMSS)

#> set log file [ default = unit 6 ]; uncomment to write standard output to a log
 setenv LOGFILE $WRKDIR/$APPL.log

#> max sync time step (sec) (default is 720)
setenv CTM_MAXSYNC 720

#> min sync time step (sec) (default is 60)
setenv CTM_MINSYNC 120

#> top sigma level thru which sync step determined [0.7]
setenv SIGMA_SYNC_TOP 0.7

#> aerosol diagnostic file [ T | Y | F | N ] (default is F|N)
 setenv CTM_AERDIAG Y

#> sea-salt emissions diagnostic file [ T | Y | F | N ] (default is F|N)
 setenv CTM_SSEMDIAG N

#> Calculate surface HONO interactions. This option is ignored if CTM_ILDEPV is turned off.
setenv CTM_SFC_HONO N

#setenv CTM_DEPV_FILE Y

#setenv CTM_PT3DEMIS Y

#setenv PROMPTFLAG F

#setenv PT3DDIAG N  # optional 3d point source emissions diagnostic file [N]
```

```
#setenv LAYP_STDATE $STDATE
#setenv LAYP_STTIME $STTIME
#setenv LAYP_NSTEPS $NSTEPS
#setenv STK_GRPS_01  #/import/wrkdir1/leelasak/stack_groups.CMAQ_GRID3.2008030.sierra.ncf
#setenv STK_EMIS_01  /import/wrkdir1/leelasak/inln.sierra.CMAQ_GRID3.cb05.2008030.ncf
#setenv CTM_EMLAYS 38
#> stop on inconsistent input file [ T | Y | F | N ]
 setenv FL_ERR_STOP F
#error related to PURB so set KZMIN False April 04
 setenv KZMIN T
#> remove existing output files?
 set DISP = delete

#> output files and directories
 set OUTDIR   = $WRKDIR/Jan23T26eddy/199
 if ( ! -d "$OUTDIR" ) mkdir -p $OUTDIR
 set CONCfile  = CTM.$APPL.CONC.ncf            # CTM_CONC_1
 set ACONCfile = CTM.$APPL.ACONC.ncf           # CTM_ACONC_1
 set CGRIDfile = CTM.$APPL.CGRID.ncf           # CTM_CGRID_1
 set DD1file   = CTM.$APPL.DRYDEP.ncf          # CTM_DRY_DEP_1
 set WD1file   = CTM.$APPL.WETDEP1.ncf         # CTM_WET_DEP_1
 set WD2file   = CTM.$APPL.WETDEP2.ncf         # CTM_WET_DEP_2
 set SS1file   = CTM.$APPL.SSEMIS1.ncf         # CTM_SSEMIS_1
 set AV1file   = CTM.$APPL.AEROVIS.ncf         # CTM_VIS_1
 set AD1file   = CTM.$APPL.AERODIAM.ncf        # CTM_DIAM_1
 set PA1file   = CTM.$APPL.PA_1.ncf            # CTM_IPR_1
 set PA2file   = CTM.$APPL.PA_2.ncf            # CTM_IPR_2
 set PA3file   = CTM.$APPL.PA_3.ncf            # CTM_IPR_3
 set IRR1file  = CTM.$APPL.IRR_1.ncf           # CTM_IRR_1
 set IRR2file  = CTM.$APPL.IRR_2.ncf           # CTM_IRR_2
 set IRR3file  = CTM.$APPL.IRR_3.ncf           # CTM_IRR_3
 set RJ1file   = CTM.$APPL.RJ_1.ncf            # CTM_RJ_1
 set RJ2file   = CTM.$APPL.RJ_2.ncf            # CTM_RJ_2

#> set ancillary log file name extensions
 setenv CTM_APPL $APPL

#> set floor file (neg concs)
 setenv FLOOR_FILE $BASE/FLOOR_${APPL}

#> horizontal grid defn; check GRIDDESC file for GRID_NAME options
 setenv GRIDDESC  $WRKDIR/Test9/GRIDDESC23

 setenv GRID_NAME FAIRBANKS

#> layer range for standard conc; if not defined, export for all layers
setenv CONC_BLEV_ELEV " 1 38"
```

```
#> species for integral average conc
#setenv AVG_CONC_SPCS "O3 NO CO NO2 ASO4I ASO4J NH3"
 setenv AVG_CONC_SPCS "ALL"

#> layer range for integral average conc
 setenv ACONC_BLEV_ELEV " 1 1"
#> input files and directories

set OCEANpath            =$WRKDIR
set OCEANfile            = surfzone.FAIRBANKS.ncf

set EMISpath              = $WRKDIR/SMOKE/output
set EMISfile             = emis_mole_all_sources_${STDATE}_CMAQ_GRID3_cb05_REF.ncf

set GC_ICpath            = $WRKDIR/Jan23T26eddy/199
set GC_ICfile            = CTM.eddy199e2008033.CGRID.ncf

 set GC_BCpath           = $WRKDIR/INPUT_MET3_199
 set GC_BCfile           = BCON_2008023_199_FAIRBANKS_profile

 set METpath             = $WRKDIR/INPUT_MET2
 set extn                = Jan24_valleyr
 set GC2file   = GRIDCRO2D_${extn}
 set GD2file   = GRIDDOT2D_${extn}
 set MC2file   = METCRO2D_${extn}
 set MD3file   = METDOT3D_${extn}
 set MC3file   = METCRO3D_${extn}
 set MB3file   = METBDY3D_${extn}

 set TR_DVpath = $METpath
 set TR_DVfile = $MC2file

#> 7-level photolysis data w/ file header
 set JVALpath  = $WRKDIR/jprocdata
 set JVALfile  = JTABLE_${STDATE}

 set AE_ICpath = $GC_ICpath
 set NR_ICpath = $GC_ICpath
 set TR_ICpath = $GC_ICpath
 set AE_ICfile = $GC_ICfile
 set NR_ICfile = $GC_ICfile
 set TR_ICfile = $GC_ICfile

 set AE_BCpath = $GC_BCpath
 set NR_BCpath = $GC_BCpath
 set TR_BCpath = $GC_BCpath
 set AE_BCfile = $GC_BCfile
 set NR_BCfile = $GC_BCfile
```

```
 set TR_BCfile = $GC_BCfile

#> input and output files and directories (boilerplate)
 source in_out.q
 if ( $status ) exit 1

#> for the run control ...

 setenv CTM_STDATE      $STDATE
 setenv CTM_STTIME      $STTIME
 setenv CTM_RUNLEN      $NSTEPS
 setenv CTM_TSTEP       $TSTEP
 setenv CTM_PROGNAME    $EXEC

env

 ls -l $BASE/$EXEC; size $BASE/$EXEC

#> Executable call for serial executable, uncomment to invoke
#time $BASE/$EXEC
mpdboot -v -f $PBS_NODEFILE
#> Executable call for multiple PE, set location of MPIRUN script
# set MPIRUN = /share/linux/bin/mpich-ch_p4/bin/mpirun
# set MPIRUN = /home/uaf/tran/MPICH2/bin/mpirun
#./bin/csh -f
  set MPIRUN = /u1/uaf/leelasak/MPICH2/bin/mpiexec
# set TASKMAP = $BASE/machines8
# cat $TASKMAP
# time $MPIRUN -v -machinefile $TASKMAP -np $NPROCS $BASE/$EXEC
 time $MPIRUN -n $NPROCS $BASE/$EXEC

 date
 exit
```