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Short Communication

Implementation of the Unified Post Processor (UPP) and the Model Evaluation Tools (MET) for WRF-chem evaluation performance

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RESUMEN

Este trabajo se centra en la descripción detallada de varias modificaciones realizadas a las versiones más recientes de los paquetes informáticos Unified Post Processor (UPP) y Model Evaluation Tools (MET), las cuales son necesarias para incorporar especies químicas importantes y parámetros meteorológicos al proceso de verificación. Los cambios realizados en ambos programas se ejemplifican con un episodio de altas concentraciones de ozono, comparando simulaciones del modelo Weather Research and Forecasting-chemistry (WRF-chem) con datos observacionales de la Red Automática de Monitoreo Atmosférico correspondientes a un fin de semana en la Zona Metropolitana de la Ciudad de México. El modelo WRF-chem se alimentó con datos formateados del Inventario Nacional de Emisiones (2006). Se proporcionan ejemplos de resultados y gráficas que contemplan la adición de nuevas especies químicas al proceso de verificación, con el objeto de explicar el tipo de mediciones de verificación y gráficas que el MET podría aportar en la actualidad. Por último, las modificaciones realizadas a diferentes archivos de los paquetes UPP y MET podrían ser de interés en particular para los usuarios y desarrolladores del modelo WRF-chem preocupados por el pronóstico o la investigación de episodios con mala calidad del aire urbano.

ABSTRACT

This study focuses on a detailed description of several modifications made in both the Unified Post-Processor (UPP) and the Model Evaluation Tools (MET) release packages, which are necessary in order to incorporate relevant chemical species and meteorological parameters into the verification process. The changes made in UPP and MET are illustrated with a high ozone concentration episode, comparing the Weather Research and Forecasting-chemistry (WRF-chem) simulations against observational data from the Red Automática de Monitoreo Atmosférico (Automatic Atmospheric Monitoring Network) during a weekend in the Mexico City Metropolitan Area. National Emission Inventory (2006) formatted data was supplied to the WRF-chem model. Examples of statistical results and plots contemplating the new chemical species added to the verification process are given, with the aim to illustrate the kind of verification measurements and plots that MET could provide now. Finally, The modifications made over different files in UPP and MET packages could be of particular interest for users and developers of the WRF-chem model concerned about the forecast of the analysis episodes related with poor urban air quality.

Keywords: WRF-chem, evaluation, UPP, MET.

1. Introduction

Improving air quality in many large cities requires a better understanding of the sources and transformation of pollutants in the atmosphere. The air quality models constitute a major tool to carry out this task. However, the process of verifying the model results can be even more important.

The Weather Research Forecast (WRF) model was developed at the National Center for Atmospheric Research (NCAR). Grell et al. (2005) and Fast et al. (2006) updates incorporated into the WRF the chemical transformations, complex gas-phase chemistry, photolysis, and aerosols, creating in this way the WRF-chem model. In order to work with the WRF-chem model outputs, there are several computing packages: NCL (NCAR, 2015); GrADS (COLA, 2015); NetCDF (UNIDATA, 2015); and the Unified Post-Processor (UPP), developed at NOAA (DTC, 2015). All of them are very useful to visualize and extract information. Also, there are statistical tools that serve to evaluate the performance of model simulations, in some cases comparing the simulation results against observations.

Recently, the Model Evaluation Tools (MET) (Gotway et al., 2014), a state-of-the-art suite of verification tools, was released by the Developmental Testbed Center (DTC) (http://www.dtcenter.org/met/users/index.php). It can perform a set of standard verification scores by comparing gridded model data with point-base observations and with gridded observations, among others. This kind of software provides useful information to the model users in order to improve the model performance by testing different model configuration setups, to improve the forecast and the decision making, and to identify forecast weakness and strengths. MET reads the output from UPP. In turn, the UPP code take in WRF output files (wrfout*) in NetCDF format. The original configuration of UPP can read several fields (eg, U, V, T, albedo) (see Baldwin *et al*., 2012, chapter 7, table 2). However, as far as we have seen, the chemical species oriented to the study of air quality are not included in these fields. Therefore, changes were made in the UPP source code and the MET configuration file to add new fields for air quality modeling evaluation.

In this document, a detailed description of modifications made in both UPP and MET is provided. These changes must be included to incorporate relevant chemical species (NO, NO_2, SO_2, CO, particulate matter, O_3) and meteorological parameters into the verification process. These modifications have been tested in the UPPV3.1 (http://www.dtcenter.org/upp/users/) and METv5.2 releases, under a Linux 86-64 cluster with the corresponding Fortran, C and C++ Intel compilers. A script is given in Appendix B that allows controlling the desired flow through MET. However, the process to perform the evaluation is similar to the procedure described in the WRF-NMM users page for UPP and MET.

A specific episode of high weekend ozone concentration to illustrate the verification process is considered, where MET is used to verify agreement between simulated species concentrations and data form the Red Automática de Monitoreo Atmosférico (Automatic Atmospheric Monitoring Network, RAMA) in Mexico City. The episode corresponds to the "ozone weekend effect" reported in Stephens *et al*. (2008), which occurs when vehicular traffic emissions decrease during the weekend; the amount of ozone measured in the monitoring stations remains approximately the same or higher that during the weekdays.

2. UPP modifications

Modifications are needed in order to incorporate new chemical species in the post-processing data from the WRF-chem model. It is essential to modify the following files:

DEALLOCATE.f, INITPOST.F , MDLFLD.f, ALLOCATE_ALL.f, RQSTLD.f , VRBLS3D_mod.f and wrf cntrl.parm. Specific line codes for each file are presented in Appendix A.

To place data in a standard grib format, run the UPP tool unipost.exe provided script in UPP (run_unipost). The WRF-Chem considers the ARW core therefore the utility *copygb* was not used.

3. MET modifications

MET reads gridded forecast data for both gridded and point observations. The tools interpolate gridded fields to a point observation using user specified options. Point observations may be supplied in PREPBUFR or ASCII format. In our case the ASCII observation files are re-formatted by the ascii2nc tool to create an intermediate NetCDF file for point statistics evaluation by using the Point-Stat tool. The output NetCDF file can contain meteorological and chemical variables.

Example of variables that can be incorporated in the input file for ascii2nc:

```
ADPSFC  76201  20130101_000000   19.635
-98.912  2240.  11 776. -9999.  1   284.150
ADPSFC  76201  20130101_000000   19.635
-98.912  2240.  33 776. -9999.  1    -0.618
ADPSFC  76201  20130101_000000   19.635
-98.912  2240.  34 776. -9999.  1     0.329
ADPSFC  76201  20130101_000000   19.635
-98.912  2240.  52 776. -9999.  1    58.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 180 776. -9999.  1  2000.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 148 776. -9999.  1  1500.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 232 776. -9999.  1  6000.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 141 776. -9999.  1 23000.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 142 776. -9999.  1 30000.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 156 776. -9999.  1   127.000
ADPSFC  76201  20130101_000000   19.635
-98.912  2240. 157 776. -9999.  1 -9999.000
```

The names particle matter (coarse) and particle matter (fine) are used for PM_{10} and $PM_{2.5}$, respectively. The chemical variables are set up in different parameter table versions (ON388, 2013) as shown in Table I. For the chemical variables CO, NO_2, NO and SO_2 the table version 141 has to be explicit. In order to do the comparison between model and observations in the configuration file (PointStatConfig) the following lines has to be modified. For meteorological variables temperature, u wind, v wind and relative humidity there is no need to set the grib table:

```
field = [
      {
        name       = "TMP";
        level      = [ "L1" ];
       cat_thresh = [  >273, >288, >293 ];
      },
      {
        name       = "UGRD";
        level      = [ "L1" ];
        cat_thresh = [ >=2 ];
      },
      {
        name       = "VGRD";
        level      = [ "L1" ];
        cat_thresh = [ >=2 ];
      },
      {
        name       = "RH";
        level      = [ "L1" ];
        cat_thresh = [ >=30 ];
      },
```

for chemical compounds and particles, O_3, NO, NO_2, CO, SO_2, PMTC and PMTF :

```
      {
        name       = "OZCON";
        level      = [ "L1" ];
        cat_thresh = [ >=50, >=110 ];
         GRIB1_ptv  = 129;
      },
     {
        name       = "NO";
        level      = [ "L1" ];
```

Table I. Chemical species description and grib table version and code

Version	Code	Parameter	Units	Abbrev
129	156	Particulate matter (coarse)	mg m^{-3}	PMTC
129	157	Particulate matter (fine)	mg m^{-3}	PMTF
129	180	Ozone concentration	µl m^{-3}	OZCON
141	141	Nitrogen oxide	µl m^{-3}	NO
141	142	Nitrogen dioxide	µl m^{-3}	NO_2
141	148	Carbon monoxide	µl m^{-3}	CO
141	166	Formaldehyde	µl m^{-3}	FORM
141	232	Sulfur dioxide	µl m^{-3}	SO_2

Note: µl m^{-3} = ppb.

```
    cat_thresh = [ >=105, >=210 ];
         GRIB1_ptv  = 141;
  },
  {
    name       = "NO2";
    level      = [ "L1" ];
    cat_thresh = [ >=105, >=210 ];
         GRIB1_ptv  = 141;
  },
  {
    name       = "CO";
    level      = [ "L1" ];
    cat_thresh = [ >=5500, >=11000 ];
         GRIB1_ptv  = 141;
  },
  {
    name       = "SO2";
    level      = [ "L1" ];
    cat_thresh = [ >=65, >=130 ];
         GRIB1_ptv  = 141;
  },
 {
   name      ="PMTF";
    level      = [ "L1" ];
    cat_thresh = [ >=65, >=130 ];
     GRIB1_ptv  = 129;
 },
 {
   name      ="PMTC";
    level      = [ "L1" ];
    cat_thresh = [ >=65, >=130 ];
         GRIB1_ptv  = 129;
    }
  ];
```

For a demonstrative purpose, gas pollutants categorical threshold values were set on the 1-h average air quality standard (upper value) and half of the standard (lower value).

4. Results

A high weekend ozone episode was considered to show a comparison between model and observed data by using MET and UPP modified codes. The episode took place in Mexico City from 06:00 LT on April 13, 2007 through 03:00 LT on Apr 15, 2007. During that period, measurements of criteria pollutants were made by RAMA. Although it is possible to extract the model formaldehyde concentrations during this episode, this compound was not measured.

WRF-chem was configured to use the chemical mechanism RADM2 as the chemical module (Stockwell *et al*., 1990). The emissions inventory was gridded based on the National Emission Inventory for the Mexico City Metropolitan Area (MCMA) for the year 2006 (SMA, 2015). These emissions were updated to fill in a 3-km spatial resolution and simulations were carried out for a 40-h time period. Finally, the observational data, required by MET, is provided by the MCMA monitoring stations (RAMA). Figures 1 and 2 show examples where simulations are compared against monitoring stations data.

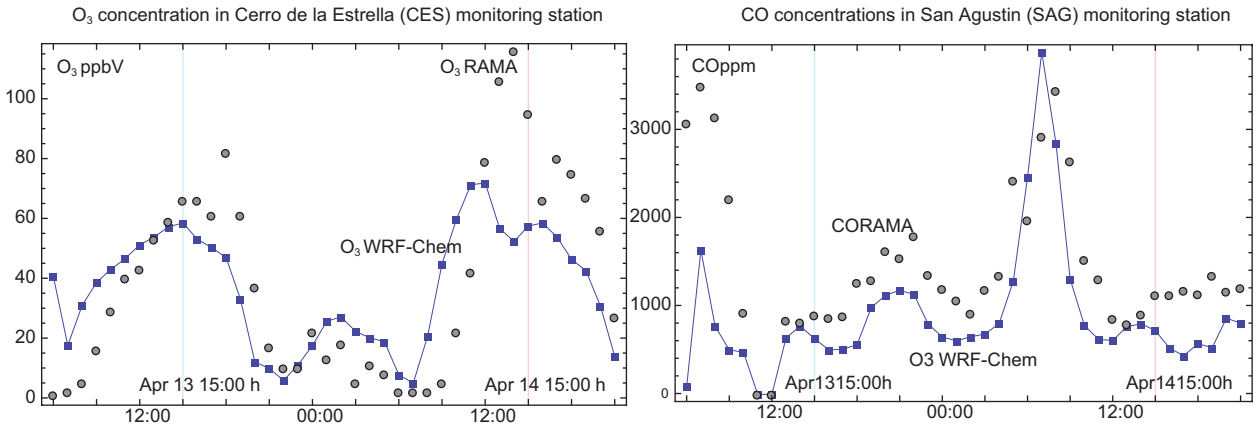

Fig. 1. Simulated and observed fields in ground based stations in Mexico City, from April 13, 2007 at 6:00 LT to April 14 at 03:00 LT. Filled circles correspond to measurements from the ground-based Air Quality Monitoring Network (RAMA) in the MCMA and lines (filled squares) are the simulations made with WRF-chem model

The Point-Stat tool computes several statistics to evaluate the forecast performance in monitoring stations. Figure 1 shows the simulated and observed concentrations of O_3 and CO in ground-base stations. To the left, the ozone concentration in the Cerro de la Estrella (CES) monitoring station is shown. The simulations (continuous line with fill squares) fit well with the observation data (filled circles) in most of the time domains, except for the high ozone concentration time interval, where the simulations underestimate the ozone peak (Apr 14, 15:00 LT). Conversely, illustrated on the right side of Figure 1, the simulated CO concentrations at San Agustín (SAG) monitoring station are well fitted in the high measured ozone concentrations. The CO simulated concentrations systematically underestimate the measurements, but almost follow the same observed data pattern, which could indicate that the emission inventory should be modified in that case. Also it is possible that MET computes the grid average of fields; the Stat-Analysis tool provides verification statistics for a matched forecast and observation grid.

Figure 2 shows the point averages of the observations and simulations, the simulated variables (continuous line with fill squares) are compared against the average of all RAMA stations (filled circle). On the left in figure 2, the average ozone concentration against RAMA data is shown. The maximum ozone concentration occurred at 15:00h Apr 14 (Saturday) and is pretty close to 140 μL m^{-3} (ppbv), this value is bigger than the previous day maximum Apr 13 (Ozone weekend effect). The ozone numerical simulation concentrations underestimate the second ozone peak; the model concentration value is approximately 42% of the measured value. This pattern is presented in other monitoring stations indicating that the model underestimates the ozone concentration. In figure 2 (right panel) the average SO_2 concentration for model and observations is shown. This chemical species is well reproduced by the model especially in the first hours of the high concentration episode.

Ambient concentrations depend on the emissions and weather conditions. In the studied episode, primary pollutants (CO and SO_2) concentrations have a better agreement with the measurements than secondary pollutants (O_3). The O_3 concentration depends on primary pollutants like NO_2 and Volatile Organic Compounds (VOC), and the highest ambient concentration is reached downwind from its precursor emissions. Because CO and SO_2 concentrations from the model are in agreement with measurements, and they are primary pollutants that depend on local emissions, the high O_3 concentrations on April 14 suggest that this pollutant was transported from elsewhere.

Additionally, Table II shows examples of several verification measurements for SO_2, including the normal and bootstrap lower and upper confidence limits (NCL, BCL, NCU and BCU). In this case the threshold concentration were 130 ppb in order to compute the categorical statistics. The first parameter shown on this table correspond to the accuracy

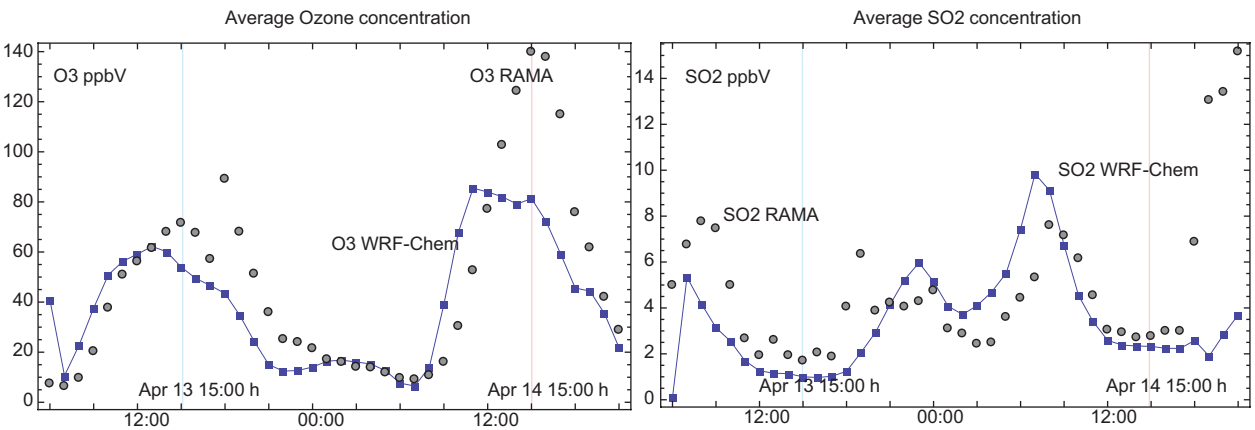

Fig. 2. Simulated and observed averaged fields, from April 13, 2007 at 6:00 LT to April 14 at 03:00 LT, in Mexico City. Continuous line represents the average field calculated with the WRF-chem model, and filled circles represent the average measured field from RAMA in the MCMA.

Table II. Statistical analysis results for SO_2 evaluation. Accuracy (ACC), Hansen-Kuipers Discriminant (HK) and Heidke Skill Score (HSS) for 662 total observations.

ACC	0.883	HK	0.624	HSS	0.680
ACC_NCL	0.843	HK_NCL	0.578	HSS_BCL	0.582
ACC_NCU	0.914	HK_NCU	0.671	HSS_BCU	0.765
ACC_BCL	0.848	HK_BCL	0.520		
ACC_BCU	0.918	HK_BCU	0.718		

(ACC) contingency parameter. In our simulation ACC = 0.883, meaning the fraction of forecast that was correct, ACC ranges from 0 to 1, perfect forecast has an ACC value of 1.

The two other parameters are the Hanssen-Kuipers Discriminant (HK) and the Heidke Skill. Its values range from –1 to 1. A perfect forecast has HK = 1, and a value of 0 indicates no skill. HSS is a skill score based on accuracy with values ranging from $-\infty$ to 1. A perfect forecast will have an HSS = 1. For a more comprehensive description of these and other verification measurements, see Appendix C, Verification measures on the MET Users Guide v5.2.

5. Conclusions

The modifications made in the UPP code can provide files that include pollutant concentration variables (i.e., O_3, CO, SO_2, PM_{10} and $PM_{2.5}$, among others); these files can be used by MET in order to evaluate objectively the model performance with a set of statistical parameters. A demonstration of the functionality of the code modifications was presented through its application in the case study, which showed that CO and SO_2 model concentrations have a better agreement than O_3 when compared to measured values. In the case of O_3, the first day presents a good agreement, but for the second day its concentrations could indicate that it comes from elsewhere.

These code additions can reduce the time for data analysis and standardize the evaluation procedure for chemical and meteorological variables by using a state-of-the-art suite of verification tools.

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References

Baldwin M., H.-Y. Chuang, L. Bernardet, D. Jovic, R. Rozumalski, W. Ebisuzaki and L. Nance, 2012. User‘s cuide for the NMM core of the Weather Research and Forecast (WRF) modeling system version 3. Chapter 7. Post Processing Utilities. NCAR/MMM, 2012.

COLA, 2015. Grid Analysis and Display System (GrADS). Available at: http://www.iges.org/grads/.

DTC, 2015. Developmental Testbed Center. Available at: http://www.dtcenter.org (last accessed on June 10, 2017).

Fast J.D., W.I. Gustafson, R.C. Easter, R.A. Zaveri, J.C. Barnard, E.G. Chapman, G.A. Grell and S.E. Peckham, 2006. Evolution of ozone, particulates, and aerosol direct radiative forcing in the vicinity of Houston using a fully coupled meteorology-chemistry-aerosol model. J. Geophys. Res.-Atmos. 111. DOI: 10.1029/2005JD006721

Gotway J. H., R. Bullock, P. Oldenburg, T. Jensen, L. Holland, B. Brown, T. Fowler, D. Ahijevych and E. Gilleland, 2014. Model Evaluation Tools Version 3.0.1 (METv3.0.1). Development Testbed Center, Boulder, Colorado.

Grell G.A., S.E. Peckham, R. Schmitz, S.A. McKeen, G. Frost, W.C. Skamarock and B Eder, 2005. Fully coupled “online” chemistry within the WRF model. Atmos. Environ. 39, 6957-6975.

NCAR, 2015. The NCAR Command Language (NCL). Available at: http://www.ncl.ucar.edu/overview.shtml.

ON388, 2013. Parameters and UNITS Table 2. Available at: http://www.nco.ncep.noaa.gov/pmb/docs/on388/table2.html.

SMA, 2015. Inventario de Emisiones de Contaminantes de la Zona Metropolitana del Valle de Mexico 2008. Secretaría de Medio Ambiente, Mexico City. Available at: http://www.aire.df.gob.mx/.

Stephens S., S. Madronich, F. Wu, J. Olson, R. Ramos, A. Retama and R. Muñoz, 2008. Weekly patterns of Mexico City’s surface concentrations of CO, NO_x,

PM_{10}, and O_3 during 1986-2007. Atmos. Chem. Phys. Discuss. 8, 8357-8384. doi: 10.5194/acp-8-5313-2008

Stockwell W.R., P. Middleton, J.S. Chang and X. Tang, 1990. The second-generation regional acid deposition model chemical mechanism for regional air quality modeling. J. Geophys. Res. 95, 343-16,367.

UNIDATA, 2015. Network Common Data Form. Available at: http://www.unidata.ucar.edu/software/netcdf/.

Appendix A. Specific modifications for UPP files

A1 VRBLS3D_mod.f
After line 27

```
   ! Add GFS fields
         ,O3(:,:,:),O(:,:,:),O2(:,:,:)&
        ,NO(:,:,:),NO2(:,:,:),SO2(:,:,:),-
CO(:,:,:) &
       ,HCHO(:,:,:),PMTC(:,:,:) ,PMTF(:,:,:)
```

A2 ALLOCATEALL.f
After line110

```
   !GFS FIELD
       allocate(o3(im,jsta_2l:jend_2u,lm))
         ...
       allocate(NO(im,jsta_2l:jend_2u,lm))
      allocate(NO2(im,jsta_2l:jend_2u,lm))
      allocate(SO2(im,jsta_2l:jend_2u,lm))
       allocate(CO(im,jsta_2l:jend_2u,lm))
      allocate(HCHO(im,jsta_2l:jend_2u,lm))
      allocate(PMTC(im,jsta_2l:jend_2u,lm))
      allocate(PMTF(im,jsta_2l:jend_2u,lm))
```

A3 RQSTFLD.f
After line 1611

```
! GFS fields Chemistry Add

       DATA IFILV(510),AVBL(510),IQ(510),I
S(510),AVBLGRB2(510) &
      &                      /1,'SO2 ON MDL
SFCS     ',232,109,&
      &                            'SO2 con-
centration ppb'/       !table 141  232
       DATA IFILV(511),AVBL(511),IQ(511),I
S(511),AVBLGRB2(511) &
      &                       /1,'CO ON MDL
SFCS      ',148,109,&
      &                           'CO concen-
tration ppb'/         !table 141  148
       DATA IFILV(512),AVBL(512),IQ(512),I
S(512),AVBLGRB2(512) &
      &                         /1,'HCHO ON
MDL SFCS    ',166,109,&
      &                              'Formal-
dehyde conc ppb'/      !table 141  166
       DATA IFILV(513),AVBL(513),IQ(513),I
S(513),AVBLGRB2(513) &
      &                       /1,'O3 ON MDL
SFCS      ',180,109,&
      &                         'Ozone conc.
ppb     '/        !table 129  180
       DATA IFILV(514),AVBL(514),IQ(514),I
S(514),AVBLGRB2(514) &
      &                       /1,'SURFACE O3
CONC     ',180,100,&
      &                          'Ozone surf
conc ppb '/         !table 129
      DATA IFILV(515),AVBL(515),IQ(515),IS
(515),AVBLGRB2(515)  &
       &                         /1,'PMTC ON
MDL SFCS    ',156,109,&
      &                          'PM 10 conc
ug/m3    '/         !table 129 156
      DATA IFILV(516),AVBL(516),IQ(516),IS
(516),AVBLGRB2(516)  &
     &                       /1,'PMTF ON MDL
SFCS    ',157,109, &
     &                           'PM 2.5 conc
ug/m3   '/          !table 129 157
       DATA IFILV(517),AVBL(517),IQ(517),I
S(517),AVBLGRB2(517) &
      &                         /1,'NO ON MDL
SFCS      ',141,109,&
      &                          'NO concen-
tration ppb  ' /      !table 141  141
       DATA IFILV(518),AVBL(518),IQ(518),I
S(518),AVBLGRB2(518) &
      &                       /1,'NO2 ON MDL
SFCS     ',142,109,&
      &                            'NO2 con-
centration ppb' /      !table 141  142
```

A4 DEALLOCATE.f
Include the following lines after line 111:

```
!GFS FIELD
      deallocate(O3)
      deallocate(NO)
      deallocate(NO2)
      deallocate(SO2)
      deallocate(CO)
      deallocate(HCHO)
      deallocate(PMTC)
      deallocate(PMTF)
```

A5 INITPOST.F

After line 48.

```
      use vrbls3d, only: t, u, uh, v, vh,
wh, q, pmid, t, omga, pint, alpint,&
            qqr, qqs, qqi, qqg, qqni,qqnr,
cwm, qqw, qqi, qqr, qqs, extcof55,&
              f_ice, f_rain, f_rimef, q2,
zint, zmid, cfr, REF_10CM, &
          o3,co,no,no2,so2,pmtf,pmtc,hcho
```

After line 341. (Because WRF-chem model has gas concentrations in ppm a conversion to ppb is made multiplying by 1000 only gas chemical variables).

```
      print*,'finish reading mixing ratio'
! For Particulate Matter (Coarse) PM10
       VarName='PM10'
        call getVariable(fileName,DateStr,-
DataHandle,VarName,DUM3D, &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             PMTC( i, j, l ) = dum3d ( i,
j, l )
  end do
        end do
       end do
! For Particulate Matter (Fine) PM2.5
       VarName='PM2_5_DRY'
        call getVariable(fileName,DateStr,-
DataHandle,VarName,DUM3D, &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             PMTF( i, j, l ) = dum3d ( i,
j, l )
         end do
        end do
       end do
      print*,'finish reading PM10 and PM2.5
concentrations'
! For Ozone O3
       VarName='o3'
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             O3( i, j, l ) = dum3d ( i, j,
l )*1000.
         end do
        end do
       end do
! For Nitrogen Oxides NO
       VarName='no'
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             NO( i, j, l ) = dum3d ( i, j,
l )*1000.
         end do
        end do
       end do
! For Nitrogen Dioxide NO2
       VarName='no2'
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
            NO2( i, j, l ) = dum3d ( i, j,
l )*1000.
         end do
        end do
       end do
! For Sulfur Dioxide SO2
       VarName='so2'
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
            SO2( i, j, l ) = dum3d ( i, j,
l )*1000.
         end do
        end do
       end do
! For Carbon Monoxide CO
       VarName='co'
```

```
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             CO( i, j, l ) = dum3d ( i, j,
l )*1000.
         end do
        end do
       end do
! For Formaldehyde HCHO
       VarName='hcho'
      call getVariable(fileName,DateStr,Da-
taHandle,VarName,DUM3D,        &
        IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
       do l = 1, lm
        do j = jsta_2l, jend_2u
         do i = 1, im
             HCHO( i, j, l ) = dum3d ( i,
j, l )*1000.
          end do
        end do
       end do
      print*,'*** Finish reading gas chem-
ical concentrations'
```

A6 MDLFLD.f

After line 82

```
      use vrbls3d, only: zmid, t, pmid, q,
cwm, f_ice, f_rain, f_rimef, qqw, qqi,&
           qqr, qqs, cfr, dbz, dbzr, dbzi,
dbzc, qqw, nlice, nrain, qqg, zint, qqni,&
             qqnr, uh, vh, mcvg, omga, wh,
q2, ttnd, rswtt, rlwtt, train, tcucn,&
               o3, rhomid, dpres, el_pbl,
pint, icing_gfip, icing_gfis, REF_10CM,&
             co,no,no2,so2,pmtf,pmtc,hcho
```

After line 2049

```
! Nitrogen Oxide (NO) ON MDL SURFACES.
          IF (IGET(517).GT.0) THEN
          IF (LVLS(L,IGET(517)).GT.0) THEN
           LL=LM-L+1
           ID(1:25) = 0
           ID(2)=141
!$omp parallel do private(i,j)
          DO J=JSTA,JEND
            DO I=1,IM
             GRID1(I,J)=NO(I,J,LL)
            ENDDO
          ENDDO
               if(grib=="grib1") then
          CALL GRIBIT(IGET(517),L,GRID1,IM,-
JM)
               else if(grib=="grib2" )then
                 cfld=cfld+1
                          fld_info(cfld)%i-
fld=IAVBLFLD(IGET(517))
                  fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(517))
!$omp parallel do private(i,j,jj)
                 do j=1,jend-jsta+1
                   jj = jsta+j-1
                   do i=1,im
                         datapd(i,j,cfld) =
GRID1(i,jj)
                   enddo
                 enddo
               endif
  ENDIF
 ENDIF
! Nitrogen Dioxide (NO2) ON MDL SURFACES.
          IF (IGET(518).GT.0) THEN
          IF (LVLS(L,IGET(518)).GT.0) THEN
           LL=LM-L+1
           ID(1:25) = 0
           ID(2)=141
!$omp parallel do private(i,j)
          DO J=JSTA,JEND
            DO I=1,IM
             GRID1(I,J)=NO2(I,J,LL)
            ENDDO
          ENDDO
               if(grib=="grib1") then
          CALL GRIBIT(IGET(518),L,GRID1,IM,-
JM)
               else if(grib=="grib2" )then
                 cfld=cfld+1
                          fld_info(cfld)%i-
fld=IAVBLFLD(IGET(518))
                  fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(518))
!$omp parallel do private(i,j,jj)
                 do j=1,jend-jsta+1
                   jj = jsta+j-1
```

```
                  do i=1,im
                        datapd(i,j,cfld) =
GRID1(i,jj)
                  enddo
                enddo
               endif
  ENDIF
 ENDIF
!              Sulfur Dioxide (SO2) ON MDL
SURFACES.
          IF (IGET(510).GT.0) THEN
          IF (LVLS(L,IGET(510)).GT.0) THEN
           LL=LM-L+1
           ID(1:25) = 0
           ID(2)=141
!$omp parallel do private(i,j)
          DO J=JSTA,JEND
            DO I=1,IM
             GRID1(I,J)=SO2(I,J,LL)
            ENDDO
          ENDDO
               if(grib==”grib1”) then
          CALL GRIBIT(IGET(510),L,GRID1,IM,-
JM)
               else if(grib==”grib2” )then
                 cfld=cfld+1
                          fld_info(cfld)%i-
fld=IAVBLFLD(IGET(510))
                  fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(510))
!$omp parallel do private(i,j,jj)
                do j=1,jend-jsta+1
                  jj = jsta+j-1
                  do i=1,im
                        datapd(i,j,cfld) =
GRID1(i,jj)
                  enddo
                enddo
               endif
  ENDIF
 ENDIF
!              Carbon Monoxide (CO) ON MDL
SURFACES.
          IF (IGET(511).GT.0) THEN
          IF (LVLS(L,IGET(511)).GT.0) THEN
           LL=LM-L+1
           ID(1:25) = 0
           ID(2)=141
!$omp parallel do private(i,j)
          DO J=JSTA,JEND
            DO I=1,IM
             GRID1(I,J)=CO(I,J,LL)
            ENDDO
          ENDDO
               if(grib==”grib1”) then
          CALL GRIBIT(IGET(511),L,GRID1,IM,-
JM)
               else if(grib==”grib2” )then
                 cfld=cfld+1
                          fld_info(cfld)%i-
fld=IAVBLFLD(IGET(511))
                  fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(511))
!$omp parallel do private(i,j,jj)
                do j=1,jend-jsta+1
                  jj = jsta+j-1
                  do i=1,im
                        datapd(i,j,cfld) =
GRID1(i,jj)
                  enddo
                enddo
               endif
  ENDIF
 ENDIF
!           Formaldehyde (HCHO) ON MDL SUR-
FACES.
          IF (IGET(512).GT.0) THEN
          IF (LVLS(L,IGET(512)).GT.0) THEN
           LL=LM-L+1
           ID(1:25) = 0
           ID(2)=141
!$omp parallel do private(i,j)
          DO J=JSTA,JEND
            DO I=1,IM
             GRID1(I,J)=HCHO(I,J,LL)
            ENDDO
          ENDDO
               if(grib==”grib1”) then
          CALL GRIBIT(IGET(512),L,GRID1,IM,-
JM)
               else if(grib==”grib2” )then
                 cfld=cfld+1
                          fld_info(cfld)%i-
fld=IAVBLFLD(IGET(512))
                  fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(512))
```

```
!$omp parallel do private(i,j,jj)
                  do j=1,jend-jsta+1
                    jj = jsta+j-1
                    do i=1,im
                          datapd(i,j,cfld) =
GRID1(i,jj)
                    enddo
                  enddo
                endif
  ENDIF
 ENDIF
!            OZONE (O3) ON MDL SURFACES.
           IF (IGET(513).GT.0) THEN
           IF (LVLS(L,IGET(513)).GT.0) THEN
            LL=LM-L+1
            ID(1:25) = 0
            ID(2)=129
!$omp parallel do private(i,j)
           DO J=JSTA,JEND
             DO I=1,IM
              GRID1(I,J)=O3(I,J,LL)
             ENDDO
           ENDDO
                if(grib==”grib1”) then
           CALL GRIBIT(IGET(513),L,GRID1,IM,-
JM)
                else if(grib==”grib2” )then
                  cfld=cfld+1
                           fld_info(cfld)%i-
fld=IAVBLFLD(IGET(513))
                   fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(513))
!$omp parallel do private(i,j,jj)
                  do j=1,jend-jsta+1
                    jj = jsta+j-1
                    do i=1,im
                          datapd(i,j,cfld) =
GRID1(i,jj)
                    enddo
                  enddo
                endif
  ENDIF
 ENDIF
!            PMTC (PM10) ON MDL SURFACES.
           IF (IGET(515).GT.0) THEN
           IF (LVLS(L,IGET(515)).GT.0) THEN
            LL=LM-L+1
            ID(1:25) = 0
            ID(2)=129
!$omp parallel do private(i,j)
           DO J=JSTA,JEND
             DO I=1,IM
              GRID1(I,J)= PMTC(I,J,LL)
             ENDDO
           ENDDO
                if(grib==”grib1”) then
           CALL GRIBIT(IGET(515),L,GRID1,IM,-
JM)
                else if(grib==”grib2” )then
                  cfld=cfld+1
                           fld_info(cfld)%i-
fld=IAVBLFLD(IGET(515))
                   fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(515))
!$omp parallel do private(i,j,jj)
                  do j=1,jend-jsta+1
                    jj = jsta+j-1
                    do i=1,im
                          datapd(i,j,cfld) =
GRID1(i,jj)
                    enddo
                  enddo
                endif
  ENDIF
 ENDIF
!            PMTF (PM2.5) ON MDL SURFACES.
           IF (IGET(516).GT.0) THEN
           IF (LVLS(L,IGET(516)).GT.0) THEN
            LL=LM-L+1
            ID(1:25) = 0
            ID(2)=129
!$omp parallel do private(i,j)
           DO J=JSTA,JEND
             DO I=1,IM
              GRID1(I,J)= PMTF(I,J,LL)
             ENDDO
           ENDDO
                if(grib==”grib1”) then
           CALL GRIBIT(IGET(516),L,GRID1,IM,-
JM)
                else if(grib==”grib2” )then
                  cfld=cfld+1
                           fld_info(cfld)%i-
fld=IAVBLFLD(IGET(516))
                   fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(516))
```

```
!$omp parallel do private(i,j,jj)
                  do j=1,jend-jsta+1
                    jj = jsta+j-1
                    do i=1,im
                          datapd(i,j,cfld) =
GRID1(i,jj)
                    enddo
                  enddo
                endif
  ENDIF
 ENDIF
!
! ---- ADD GOCART FIELDS

A7 wrf cntrl.parm

Additional lines to be add.
  (O3 ON MDL SFCS      ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (NO ON MDL SFCS      ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (NO2 ON MDL SFCS     ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (SO2 ON MDL SFCS     ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (CO ON MDL SFCS      ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (HCHO ON MDL SFCS    ) SCAL=( 4.0)
   L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (SURFACE O3 CONC     ) SCAL=( 4.0)
   L=(00000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000
00000)
  (PMTC ON MDL SFCS    ) SCAL=( 4.0)
 L=(10000 00000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
  (PMTF ON MDL SFCS    ) SCAL=( 4.0)
 L=(10000 00000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
```

Appendix B Scripts to run MET

B1 This is the main script to run MET

```
#!/bin/bash
echo  “WRF-chem statistics analysis”
#
#  The following directories have to be set
#  DIRFCT    - Forecast/model output from UPP
#   fobservado - Observational data from
ascii2nc
#  fconfig    - Configuration file to extract
met, chem variables
export DIR=/media/Disco2
export  DIRFCT=/media/DOMAINS/abr_2007/
postprd
export fobservado=${DIR}/met/out/ascii2nc/
ramaApr2007.nc
export  fconfig=${DIR}/met/scripts/config/
PointStatConfig_Apr
#
#  Data extraction and comparison
#
    n=1
   for file in ${DIRFCT}/WRFPRS_d01.0?
   do
     echo $file
    if [ $n -lt 10 ]; then
   bin/point_stat $file $fobservado $fconfig
-outdir out/point_stat -v 2 >& fe_0$n.log
    else
   bin/point_stat $file $fobservado $fconfig
-outdir out/point_stat -v 2 >& fe_$n.log
    fi
  (( n++ ))
   done
```

B2 Script to run the stat module from MET

```
ecaim_stat.sh
#!/bin/sh

echo
echo “*** Running STAT-Analysis for Ecaim
***”
/tmpu/agr_g/agr/met/bin/stat_analysis \
   -config ./STATAnalysisConfig_ecaim \
   -lookin ./out/point_stat \
    -out  ./out/stat_analysis/stat_analy-
sis_ecaim.out \
   -v 2
```

B3 Additions in the point stat configuration file

```
PointStatConfig_Apr
field =[
      {
        name       = “TMP”;
        level      = [ “L1” ];
        cat_thresh = [  >298 ];
      },
      {
        name       = “OZCON”;
        level      = [ “L1” ];
       cat_thresh = [ >=60, >=95, >=110 ];
         GRIB1_ptv  = 129;
      },
     {
        name       = “NO”;
        level      = [ “L1” ];
        cat_thresh = [ >=105, >=210 ];
              GRIB1_ptv  = 141;
      },
      {
        name       = “NO2”;
        level      = [ “L1” ];
        cat_thresh = [ >=105, >=210 ];
              GRIB1_ptv  = 141;
      },
      {
        name       = “CO”;
        level      = [ “L1” ];
        cat_thresh = [ >=550, >=1100 ];
              GRIB1_ptv  = 141;
      },
      {
        name       = “SO2”;
        level      = [ “L1” ];
        cat_thresh = [ >=65, >=130 ];
              GRIB1_ptv  = 141;
      },
     {
       name      =”PMTF”;
```

```
    level      = [ "L1" ];
    cat_thresh = [ >=65, >=130 ];
     GRIB1_ptv  = 129;
},
{
  name      ="PMTC";
    level      = [ "L1" ];
    cat_thresh = [ >=45, >=90 ];
     GRIB1_ptv  = 129;
}]
```

B4 Additions in the stat analysis configuration file

```
"-job aggregate_stat -fcst_var OZCON -line_type MPR -out_line_type CTC -out_fcst_thresh >=95.0 -out_obs_thresh >=95.0 -dump_row ./out/stat_analysis/job3_eca_aggr_stat_mpr.stat -interp_pnts 4",
"-job aggregate_stat -fcst_var NO -line_type MPR -out_line_type CTC -out_fcst_thresh >=105.0 -out_obs_thresh >=105.0 -dump_row ./out/stat_analysis/job4_eca_aggr_stat_mpr.stat -interp_pnts 4",
"-job aggregate_stat -fcst_var NO2 -line_type MPR -out_line_type CTC -out_fcst_thresh >=105.0 -out_obs_thresh >=105.0 -dump_row ./out/stat_analysis/job5_eca_aggr_stat_mpr.stat -interp_pnts 4",
"-job aggregate_stat -fcst_var CO -line_type MPR -out_line_type CTC -out_fcst_thresh >=550.0 -out_obs_thresh >=550.0 -dump_row ./out/stat_analysis/job6_eca_aggr_stat_mpr.stat -interp_pnts 4",
"-job aggregate_stat -fcst_var SO2 -line_type MPR -out_line_type CTC -out_fcst_thresh >=100.0 -out_obs_thresh >=100.0 -dump_row ./out/stat_analysis/job7_eca_aggr_stat_mpr.stat -interp_pnts 4",
```