Presented at the 6th Annual CMAS Conference, Chapel Hill, NC, October 1-3, 2007

High Time-Resolution Winds and Effects upon Air Quality Modeling A 4KM California August 2006 Case Study

Carlie J. Coats, Jr.* *1,
M. Talat Odman[2]
and Saswatti Datta[1]

[1]Baron Advanced Meteorological Systems, LLC.
[2]Department of Environmental Engineering, Georgia Institute of Technology

Statement of the Problem

Both temporal and spatial resolution are closely tied to the scale of phenomena that may be simulated, as indicated by the *Nyquist–Shannon Sampling Theorem*: a model with spatial scale *dx* or temporal scale *dt* cannot resolve phenomena smaller than *2 dx* or *2 dt*, respectively. One may further add a principle that speed is the transformation factor between spatial and temporal resolution, and arrive at criteria for determining the desired temporal resolution for driving an air quality model with 4 KM resolution. This is somewhat limited by the *actual* spatial and temporal resolution achieved by the driving meteorology model, due to internal smoothing and other effects within the model.

Spectral analysis of spatial variability various mesoscale meteorology models shows that they do not achieve the theoretical *2dx* limit of resolution: MM5 and RAMS do not resolve features smaller than 7 *dx* well; WRF achieves 5 *dx*, whereas Eta is limited to about 10 *dx*. Given MM5 as a driver and a 4 KM model resolution, we will see features of size 28 KM, requiring *dx*=14 KM to resolve. Assuming a "reasonable" top-of-PBL wind speed of 10 m/sec, this corresponds to a temporal resolution *dt*=1400 sec, a little over 20 minutes. Larger time steps for the input meteorology will not resolve atmospheric features actually simulated by the meteorology model. Another issue is *temporal features* in the meteorology, one of the most prominent of which is *gravity waves,* which have observed periods on the order of 10-30 minutes in MM5 simulations and a theoretical limit of the *Brunt-Vaisala Period*, which is about 10 minutes. When these are not resolved correctly, there will be anomalies in the vertical wind components leading to transport and/or conservation errors, when the sampled upward or downward component of the gravity waves are applied for much too long a modeling period.

This failure to resolve meteorology features will result in (among other things) conservation and/or transport failures that can only partially be alleviated by after-the-fact "conservative" advection algorithms in the air quality model.

We selected an August 2006 air quality episode, constructed a nested 36/12/4 KM MM5 domain consistent with the CCOS CAMx domain, and ran MCPL-augmented MM5 for this domain and episode, generating 10-minute time step output compatible with CMAQ and MAQSIP. We constructed a tracer emissions data set with ten time-invariant stack-plumes located at the ten largest NOx emissions sites in the CCOS domain (as determined by the analysis of the CCOS year-2000 episode emissions files), and ran the tracer version of MAQSIP-RT on these data sets

MM5 Set-Up

We constructed a nested 36/12/4 KM MM5 domain using the same 51-level layer definitions as the CCOS MM5, and with at least 5-cell borders around the CCOS atmospheric chemistry domain and around each nest within its parent. Grid dimensions were 42x42 at 36 KM, 78x78 at 12 KM, and 195x195 at 4 KM. This last is shown in Figure 1, below. The

Corresponding author: Carlie J. Coats, Jr., Baron Advanced Meteorological Systems LLC., 920 Main Campus Drive, Suite 101, Raleigh NC 27606

TERRAIN program was run in *Mode 6,* i.e., using 30-arcsecond terrain and land use data for all grids. Input meteorology data were from the GFS model.

MM5 is run with the MCPL output module, giving very flexible windowing on-the-fly to the air quality domain, and directly producing Models-3 I/O API files for input to MAQSIP and CMAQ. The same physics options used in the BAMS operational forecast modeling were used for this run, including particularly:

ICUPA=8,8,1 Kain-Fritsch-2 convection at 36,12 KM
IMPHYS=5,5,5 Reisner-1 microphysics
IBLTYP=5,5,5 MRF PBL

The 36 KM coarse MM5 grid was run from 00 Z on August 1, 2006, through 12 Z on August 4, 2006. The 12KM intermediate MM5 grid started at 06 Z. and the 4 KM fine grid (containing the CCOS grid) started at 12 Z. Note that grid start-up tends to cause "shocks" to the system which take 2-3 hours to settle down, so the MAQSIP-RT runs were started 3 hours later yet, at 15 Z.

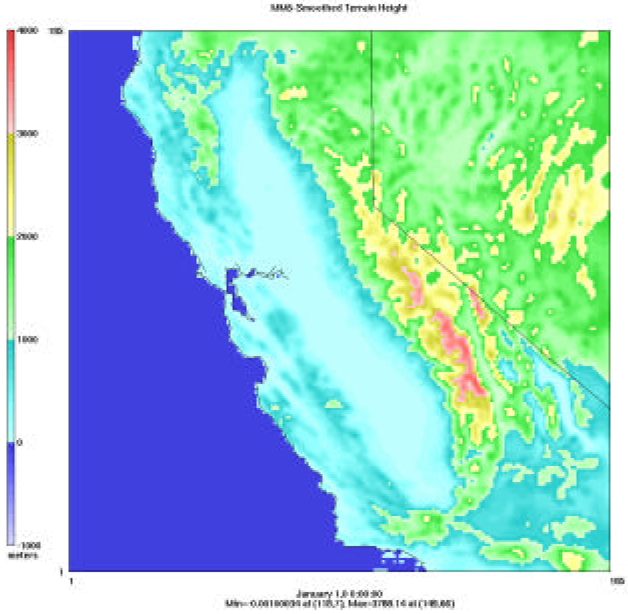

Figure 1 Terrain Elevation for 4KM domain

Output time step for the 4 KM grid was set at 10 minutes, adequate to resolve features reproduced by MM5, while at the same time keeping data volumes from exceeding available resources. (The three-day 4 KM MAQSIP-input file sets amounted to about 90 GB; 5-minute time step output that would have resolved the theoretical 10-minute *Brunt-Vaisala period* for gravity waves would have exceeded available resources. Features that short are not captured by a 4 KM MM5, in any case.). For the same reason, 4 KM run length was limited to three days rather than the hoped-for five days.

We used standard off-the-shelf Models-3 tools **`M3CPLE`** and **`M3INTERP`** to sample the output (the *HTR case*) meteorology files to files with a 1–hour time step and then **`M3TINTERP`** to interpolate the one-hour data back to files with a 10-minute time step for analysis of time-interpolation errors and for input to MAQSIP-RT (the *INTERP* case). These latter files provide a visualizable/analyzable counterpart to the time interpolation that occurs internally within the air quality models.

MAQSIP-RT Set-Up

MAQSIP-RT is an air quality model from the same original code base as CMAQ, but has been substantially restructured, optimized, and parallelized using OpenMP. It has been used for twice-daily air quality forecasts (as well as for regulatory applications) at MCNC and then at BAMS since 1998. Current versions use the Bott version of the Odman-Russel conservative advection scheme; unlike vanilla CAMx it maintains mass consistency between the concentration and dry deposition fi elds (a discrepancy we found in another phase of this project). A nice feature of MAQSIP-RT for this study is that it uses Models-3 I/O API *INTERP3()* functionality to support virtually any regular time step structure on any of its input files (including time-independent data files; the time step granularity is one second) ; moreover, these are independent on a file-by-file basis.

Emissions were constructed with 10 tracer species, each with its own unique source, with locations selected from the top-10 NO_X emissions cells. Each source was an idealized point source with uniform unit emissions for 10 layers in the vertical, with time independent emissions fluxes. MAQSIP-RT was configured tracer-only, on a 185x185 window into the MM5 4 KM grid, with the same vertical structure as the MM5. Dry deposition velocities for ozone were used for all tracers; wet deposition was set to zero, and the full model dynamics (advection and diffusion) and cloud physics were used.

The tracer-MAQSIP-RT was run with both HTR-case and INTERP-case meteorology, started at 15 Z (three hours after nest initialization in MM5), and ran for 66 hours with a 30-minute output time step. **`PAVE`** and **`M3STAT`** analyses were made of both cases and of the differences.

MM5 Analysis

Analysis was performed on the wind fields, that being a primary driver of transport in the air quality models. Qualitatively, this analysis indicates that the interpolation error is concentrated mostly in the mountains, and is mostly weak and disorganized in the San Joaquin Valley. Exceptions to this pattern occur in the 07:00-09:00 AM and PM hours (local daylight time), when there are larger and more organized wind-error patterns there. We conjecture that this is due to the failure of the hourly data to capture transport effects associated with the morning and evening stability transitions. These effects seem to be a major driver to the differences in tracer-species plume trajectories, as well. An example morning vector/tile wind error plot is found in Figure 2 below. Note that error in interpolating from hourly data is zero on the hour, and typically increases to a maximum on the half-hour. Note also that the error is *much* larger at the 12Z start of the MM5 runs, dying off to its "normal" levels by the 15Z time used to start MAQSIP-RT.

Grid-wide statistical and error analysis was performed on selected layers (1, 5, 10, 20) of the wind fields. For each wind component, selected layer, and (10-minute) time step, the grid-maximum and grid-mean of the INTERP-case field and of the interpolated-field vector error were computed. Likewise, the grid-maximum and grid-mean of the magnitude (wind-speed) for the INTERP-case field and for the magnitude of the error-field (which has units M/S) was computed. The time series plot for Layer 1 wind speed and error-magnitude is shown in Figure 3 below. Note that there is a strong diurnal pattern in the magnitude of the interpolation errors. This pattern has a minimum around 3:00 PM local time. Note also that on occasion the maximum error magnitude exceeds the grid mean wind speed (an effect that is even stronger in Layer 5 than in Layers 1, 10, or 20). The magnitude of grid-mean interpolation error typically ranges from 0.2-0.5 M/S at the half-hours for all layers; the magnitude of grid-maximum interpolation error ranges from 1-5 M/S in Layer 1, 2-10 M/S in Layer 5, 2-7 M/S in Layer 10, and 1–5 M/S in Layer 20.

MAQSIP-RT Analysis

We made statistical and graphical analyses of Layer 1 and Layer 5 *HTR Case* and *INTERP Case* and outputs and of their differences, for all ten MAQSIP-RT tracer variables. Treating the 10-minute meteorology time-step HTR Case runs as "reality", and the 1-hour met-step INTERP Case runs as differing from it by errors due to the interpolation of meteorology data, the largest error found in the study was for *TRAC04* at 14:30Z on Aug. 3, 2006 (Figures 4, and 5, below), where a substantial difference in plume placement and down-wind transport caused an error range [–1.68256 to 0.315026]. For comparison, at this time the HTR case and the INTERP case *TRAC04* had ranges [0,1.09999] and [0,2.24491], respectively (comparable in magnitude to the error-range). Generally, the largest plume-errors were found at 02:30-03:30 and 14:30-15:30Z, following the largest met-interpolation errors.

Of the grid-aggregate error statistics, we found the grid-mean statistics least useful, since the grid was dominated by the near-zero tracer concentrations distant from the sources. Time series plots for *TRAC04* concentration maximum and maximum absolute error were most useful. Layer 1 time series are given in Figure 6, below. Typically, maximum absolute error is about one order of magnitude smaller than maximum concentration for all the layers (1-20) studied.

Acknowledgements

This work was funded under the Central California Ozone Study's request for proposals, "Improve Conservation of Mass Module in Air Quality Models". The statements and conclusions of this report are those of tine Investigator, and not necessarily those of the California Air Resources Board, the San Joaquin Valleywide Air Pollution Study Agency, or its Policy Committee, their employees or their members. The mention of commercial products, their source, or their use in connection with material reported herein is not to be construed as actual or implied endorsement of such products.

References

Grell, G., J. Dudhia and D. Stauffer, 1994.A description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5), *NCAR Technical Note: NCAR/TN-398+STR*

Odman, M.T. and A.G. Russell, 2000. Mass conservative coupling of non-hydrostatic meteorological models with air quality models, in *Air Pollution Modeling and its Application XIII*, (S.-E. Gryning and E. Batchvarova, Eds.), New York, Kluwer Academic/Plenum Publishers, pp. 651-660.

Figures

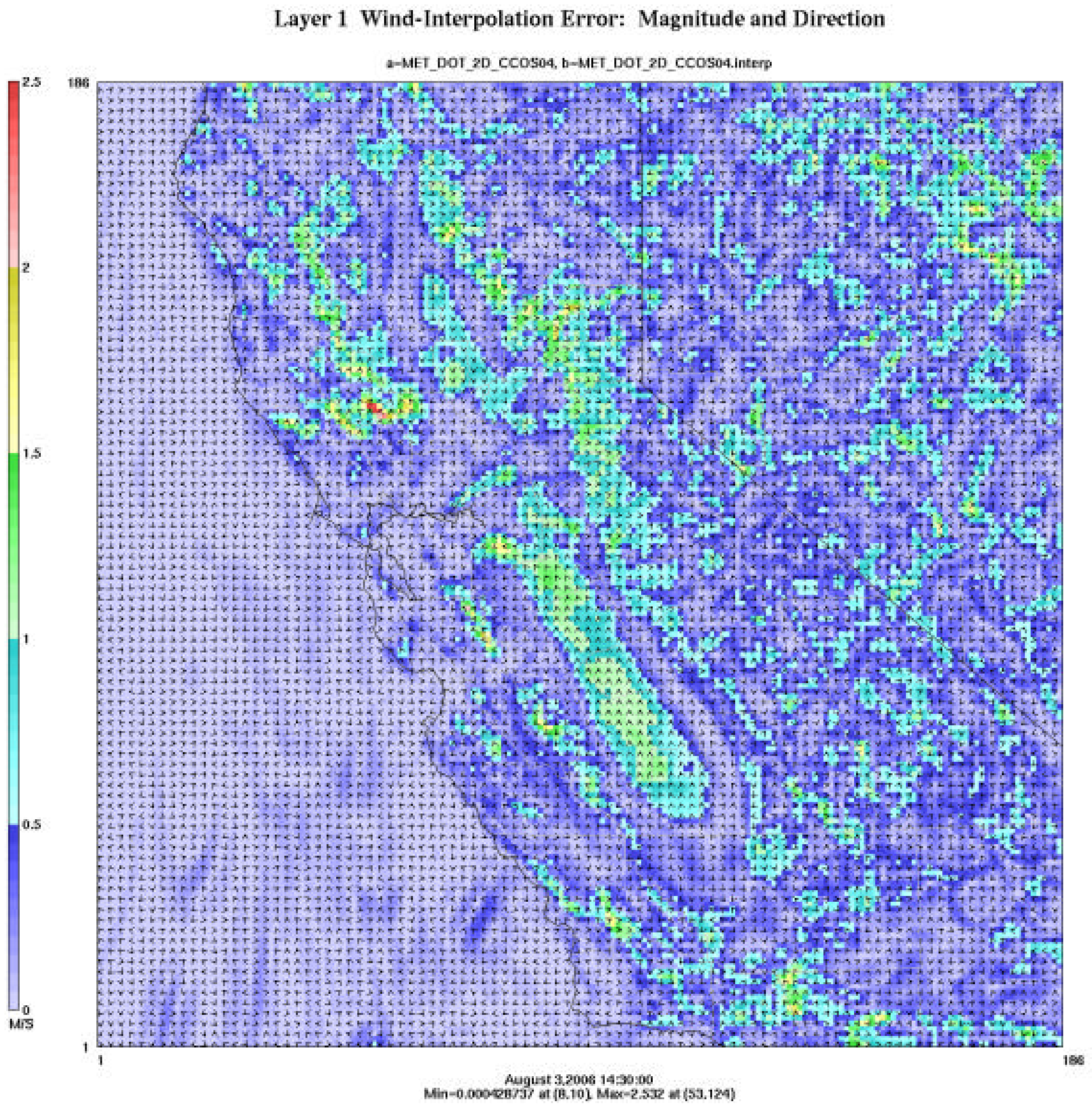

Figure 2: Morning-transition wind interpolation error for Layer 1 at 14:30 Z on August 3, 2006, (local time 7:30 AM PDT). Wind arrows denote the direction, and color denotes magnitude of the error (M/S). Note the organized flow in the south/central San Joaquin Valley. The spatial pattern is typical of 14:30Z, but this may be the most prominent case in the 69-hour run. For related tracer-plumes and their errors at this time, see Figures 4, and 5 below.

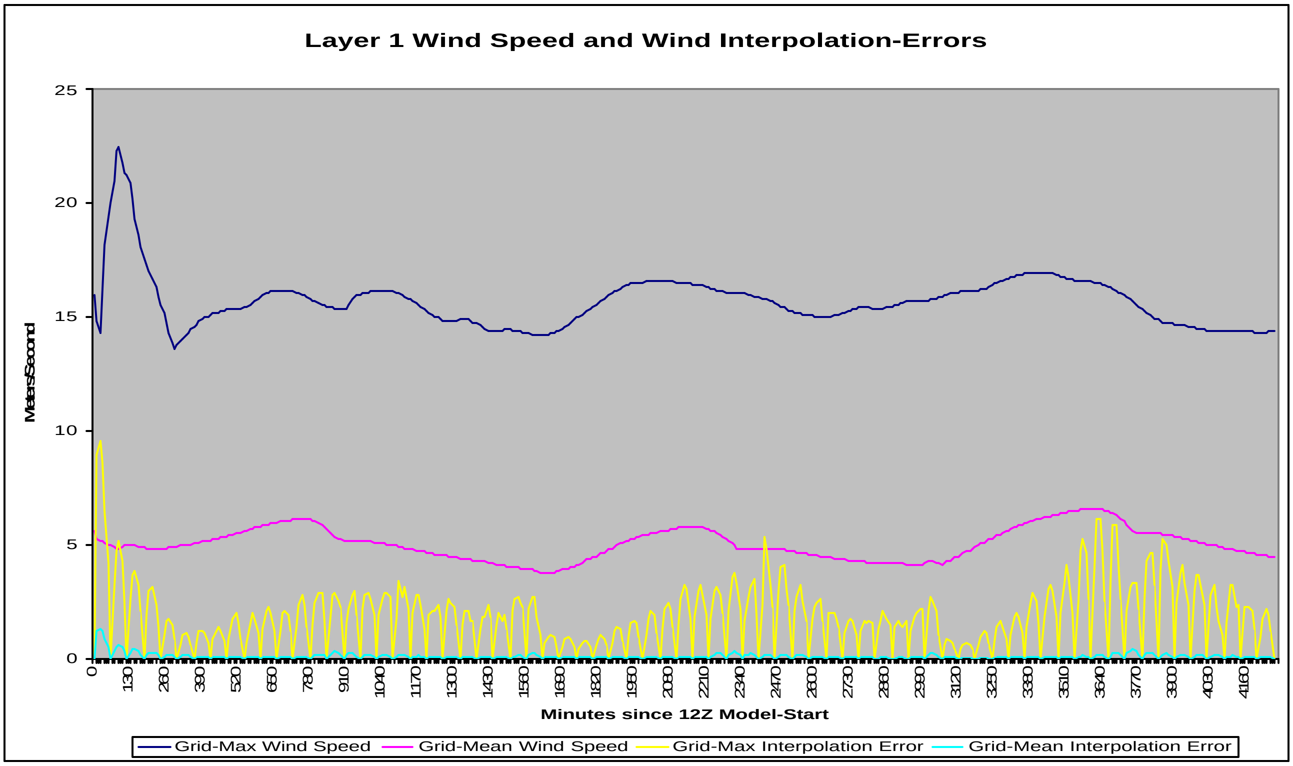

Figure 3: .Grid-mean and grid-maximum wind speed and magnitude of wind error for Layer 1. Note that error is zero on the hour, and is greatest at the half-hour.

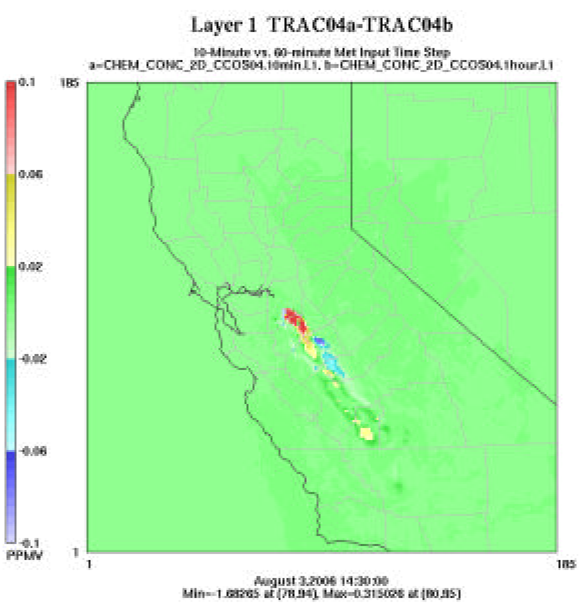

Figure 4: Error in early-morning INTERP-Case tracer plume for *TRAC04* at 14:30Z (07:30 AM PDT, simulation hour 47.5) August 3, 2007. See Figure 2 for the wind-error plots for the same date and time.

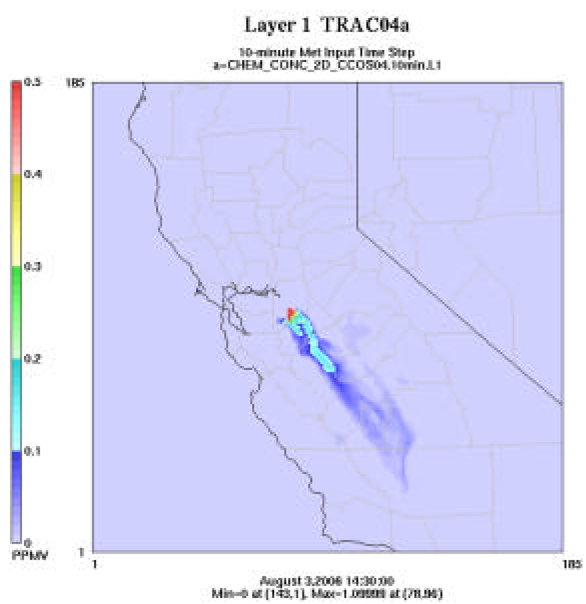

Figure 5: HTR-Case tracer plume for *TRAC04* at 14:30Z August 3, 2007

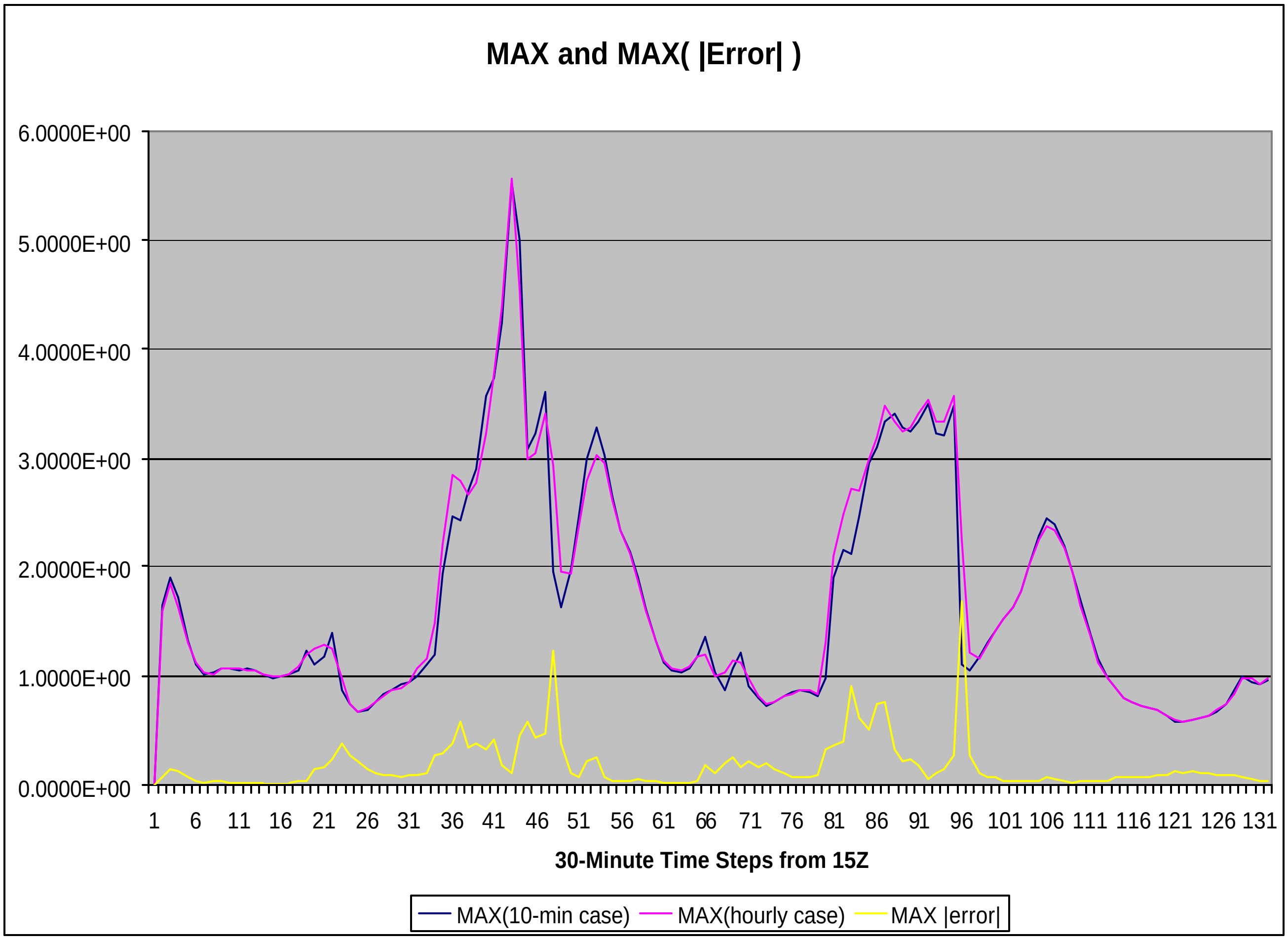

Figure 6: Time series for *TRAC04* maximum HTR Case concentration, maximum INTERP Case concentration, and maximum absolute error.