AN IMPLEMENTATION OF THE TRAJECTORY-GRID ADVECTION ALGORITHM IN CMAQ

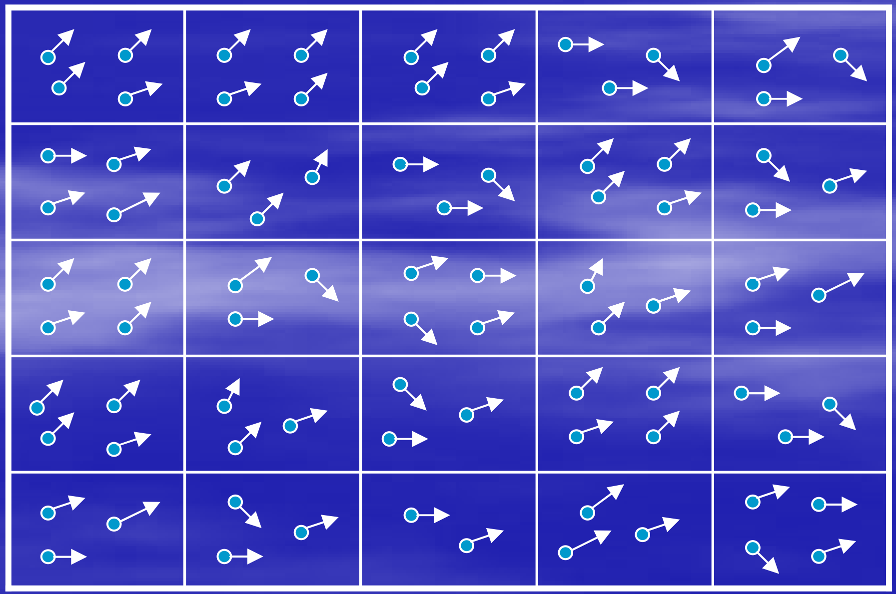
by

Peter B. Percell and Daewon Byun
University of Houston - IMAQS

The Trajectory Grid approach was proposed by David Chock, et al, and has been implemented in CAMx

The TG Approach

- A Lagrangian approach – follows representative air "packets" along trajectories determined by a 3D wind field
- Advection of packets doesn't change air composition
- Perform other process directly on packets, e.g., gas chemistry and dry deposition, when possible
- Use Eulerian grid methods when necessary, e.g., to solve for diffusion
- Packets are distributed at roughly the same resolution as the underlying grid - at most a few packets in each grid cell



Reasons to consider TG advection

- Absence of numerical diffusion from the advection solver
- Not subject to Courant number restriction on time step
- Flexibility in adjusting spatial resolution for simulations
- Potential ability to identify and analyze source-receptor relationships (a possible future application)

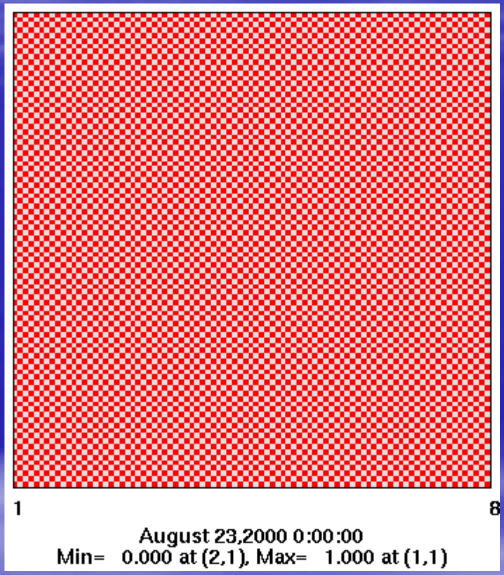
Overview of Implementation

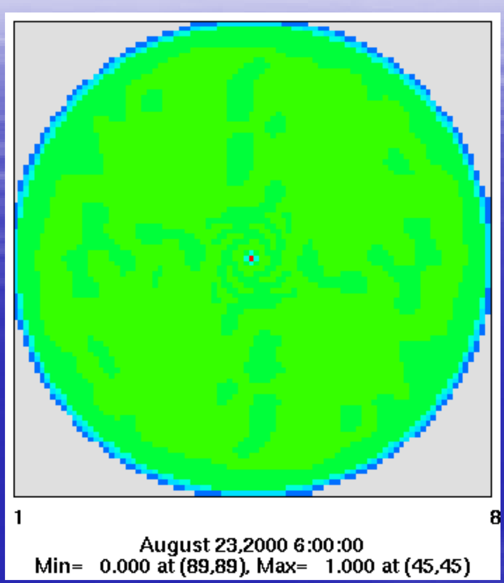
- The current prototype version of CMAQ-TG, based on CMAQ v4.4, supports advection, diffusion, gas chemistry, emissions and dry deposition
- Uses the same meteorology, emissions, initial conditions, boundary conditions, and photolytic rates input as standard CMAQ
- Role of Eulerian Grid
  - Input, such as meteorological data, emissions data, initial conditions and boundary conditions, is all associated with Eulerian grid cells
  - Processes that are potentially global in nature, such as eddy diffusion, do not have satisfactory Lagrangian models at this time and are therefore modeled on a Eulerian grid
  - Grouping packets in the same grid cell together is a convenient way to keep track of which packets are close to each other
  - Output from CMAQ is most easily saved as gridded Models-3 I/O API data and viewed using PAVE
- The advection time step is chosen so that packets cannot “jump over” grid cells – for emissions and trajectory accuracy – and is used as the synchronization time step

Implementation, cont.

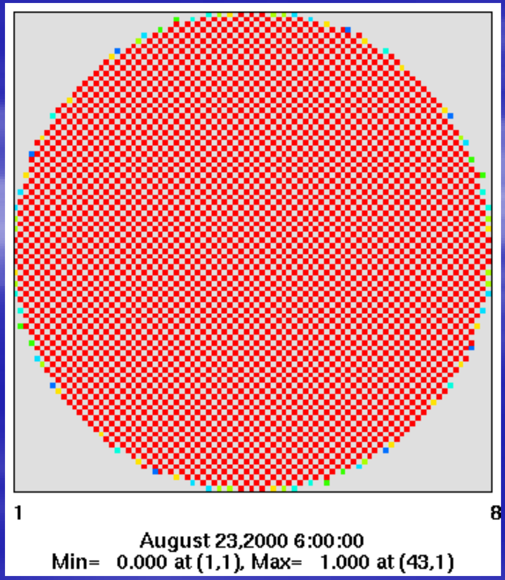
- Packet management, to balance packet density between the needs to cover the solution domain and to limit computational expense, is done as part of the advection process
  - Spawning: When a cell becomes empty, a new packet may be added at its center; its composition is estimated from nearby packets – likely to be somewhat inaccurate and diffusive
  - Pruning: When a cell becomes overpopulated, some of its packets are removed – may lose information
- Diffusion is done using algorithms close to those in standard CMAQ and for cell average mixing ratios gives the same result as standard Eulerian diffusion; however, requirements that the algorithms be positive definite, monotonic and linear at the packet level were more of a challenge than anticipated – can't do Eulerian diffusion for cells and apply cell deltas to packets
- Chemistry is processed for packet mixing ratios instead of grid cell mixing ratios. Otherwise, it is unchanged from standard CMAQ.

Advection of checkerboard by 2-D rotation



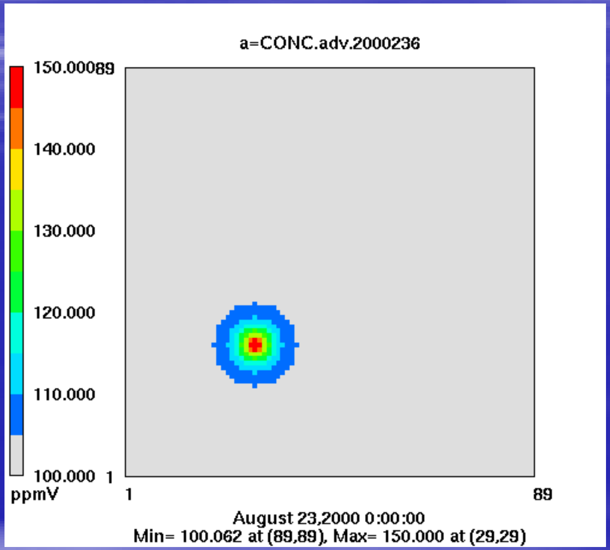


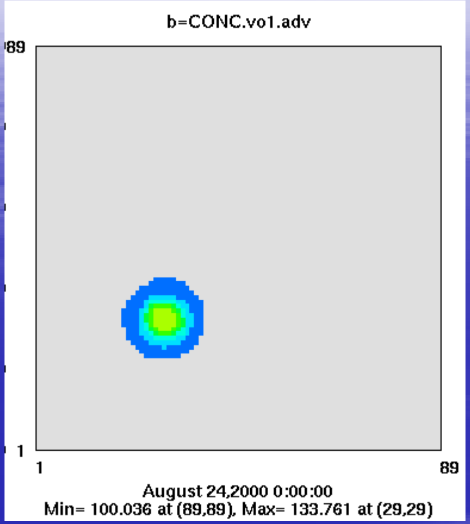
Numerical diffusion from Eulerian advection (PPM) in standard CMAQ



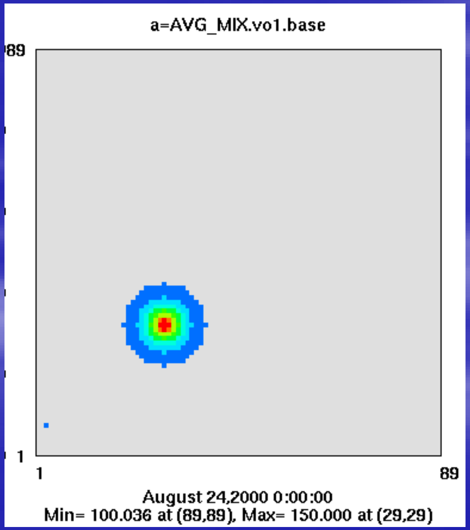
CMAQ-TG preserves the checkerboard pattern almost perfectly

Advection of SPOS mound by 2-D rotation





Standard CMAQ



CMAQ-TG

After 24 hours, standard CMAQ has reduced the peak height by over 30% while CMAQ-TG has preserved the peak

Linearity tests of transport (both advection and diffusion) with a realistic wind field

Uses tracer species available in CMAQ. In both cases the sum of the three concentrations should be zero.

	IC1_BC1 - IC1_BC0 - IC0_BC1	
	CMAQ-TG	**Standard CMAQ**
Layer 1	(-0.0000, 0.0000)	(-0.0190, 0.0238)
Layer 13	(-0.0000, 0.0000)	(-0.2316, 0.1127)
Row 31	(-0.0000, 0.0000)	(-0.0867, 0.0468)
	SPOS_A - SPOS_B - SPOS_C	
	CMAQ-TG	**Standard CMAQ**
Layer 1	(-0.0005, 0.0015)	(-0.3704, 0.3227)
Layer 13	(-0.0010, 0.0013)	(-2.0829, 1.4139)
Row 31	(-0.0028, 0.0021)	(-0.2743, 0.2470)

Linearity of CMAQ-TG transport is excellent

Packet Management Options

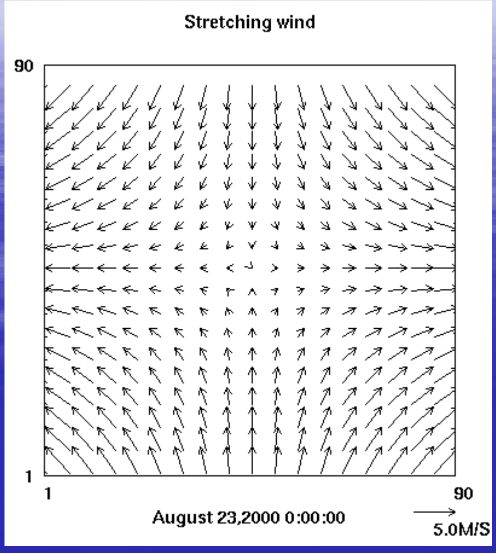
- High Resolution Box
  - Defined by multiplier, N, and a range of columns, rows and layers

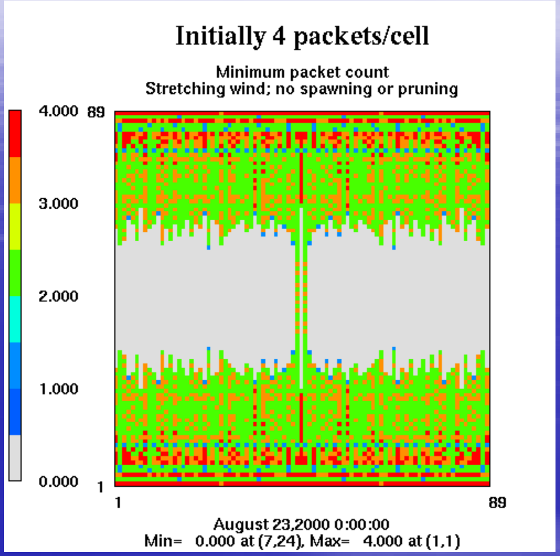
    Cells inside the box are initialized with N^2 uniformly spaced packets; cells outside the box are initialized with just one packet at the center

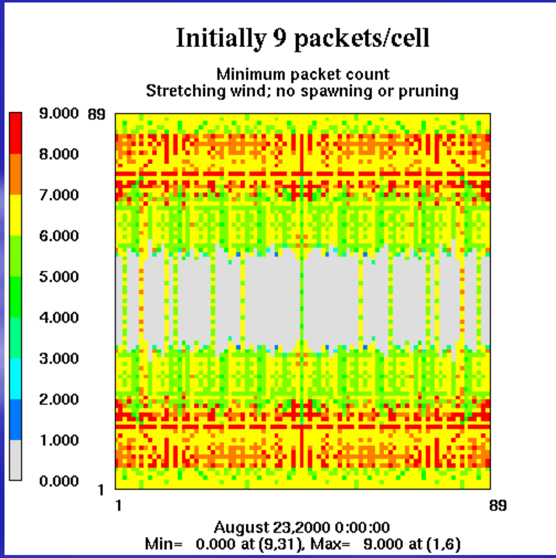
    High resolution cells are never allowed to be empty, except when spawning is turned off
- Spawning options
  - No Fill: never add packets to interior cells, i.e., turn off spawning
  - Fill All: never allow any cell to be empty (default)
  - Sparse Fill: spawn in an interior low resolution cell if it is empty and is surrounded by empty cells
- Pruning options
  - No pruning
  - Keep packets that are closest to center of cell (default)
  - Keep packets that are oldest
  - Parameters:
    - Pruning frequency (number of time steps)
    - Number of packets to keep after pruning
    - Tolerance above number to keep before pruning is triggered

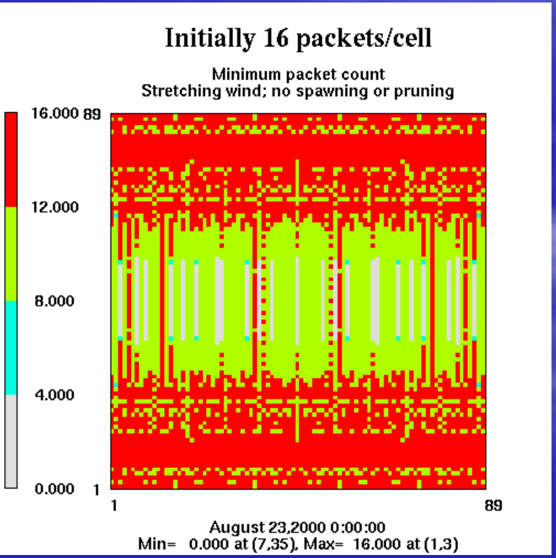
Packet Management Challenge

Even non-divergent flow can be a problem



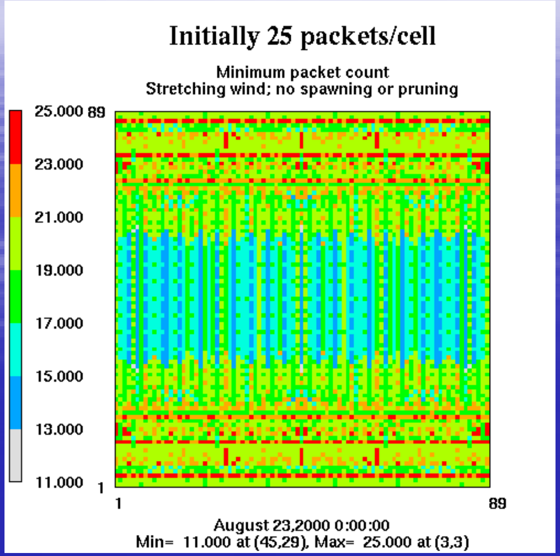


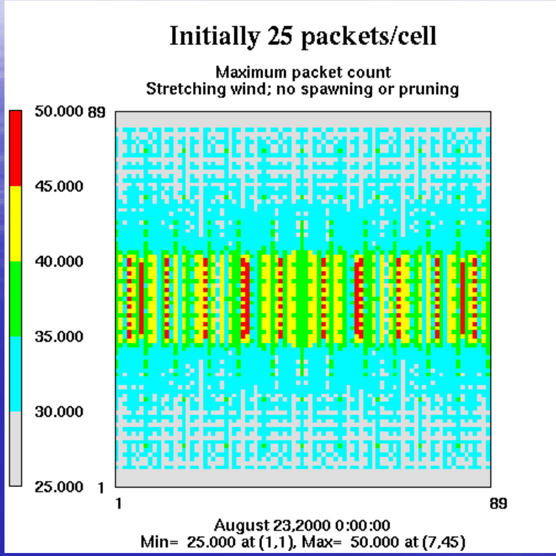




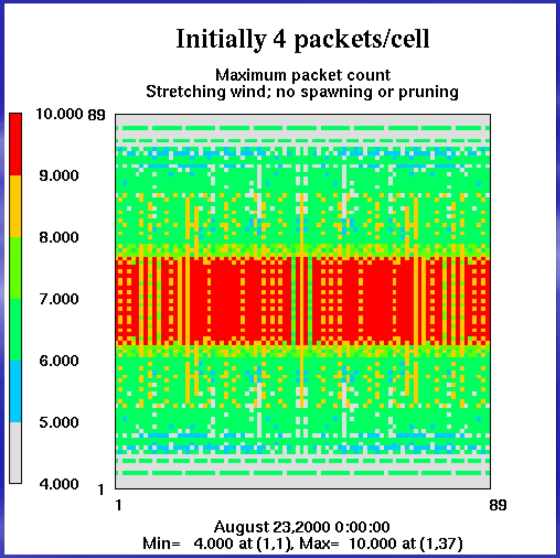
Without spawning, get empty cells even when starting with 16 packets in each cell

Packet Management Challenge, continued



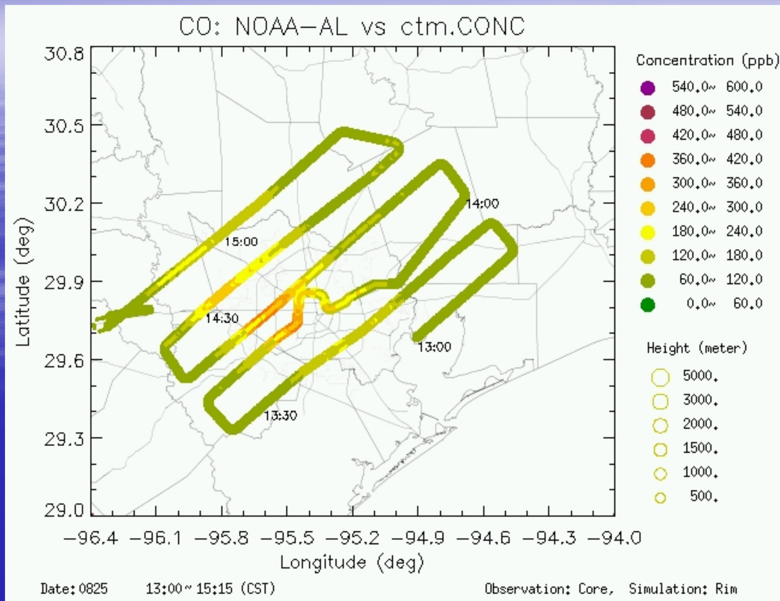


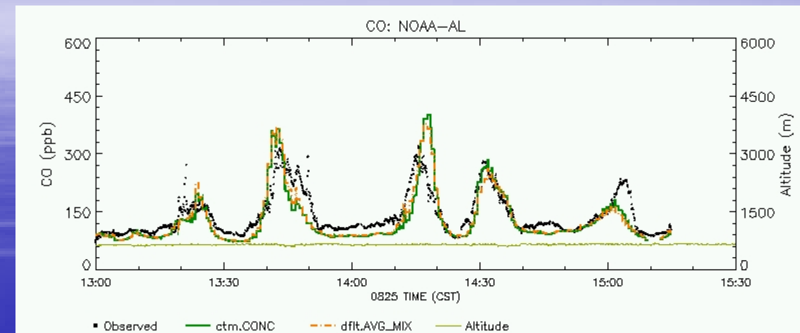
Without spawning, need to start with 25 packets to guarantee every cell always has a packet, but then all cells have too many packets

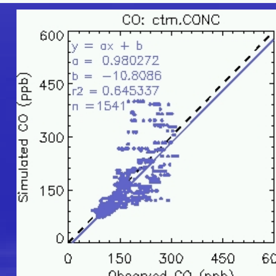


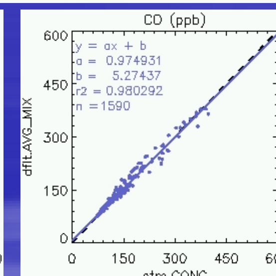
Since chemistry is done for each packet individually, even starting with 4 packets requires pruning for TG to be computationally competitive with an Eulerian method at the same resolution

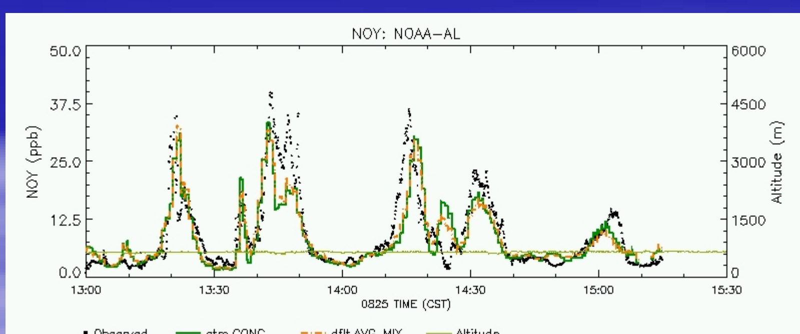
Comparison of CMAQ-TG with Std CMAQ and aircraft observations – high ozone (8/25/2006)

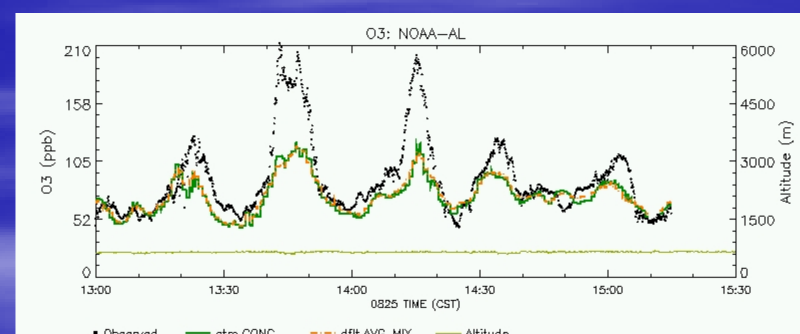


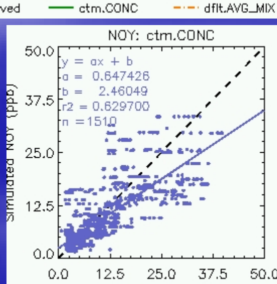


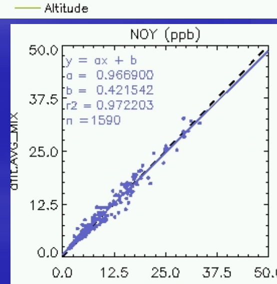


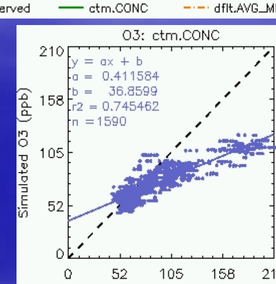


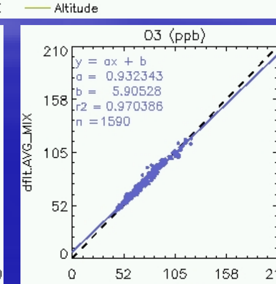




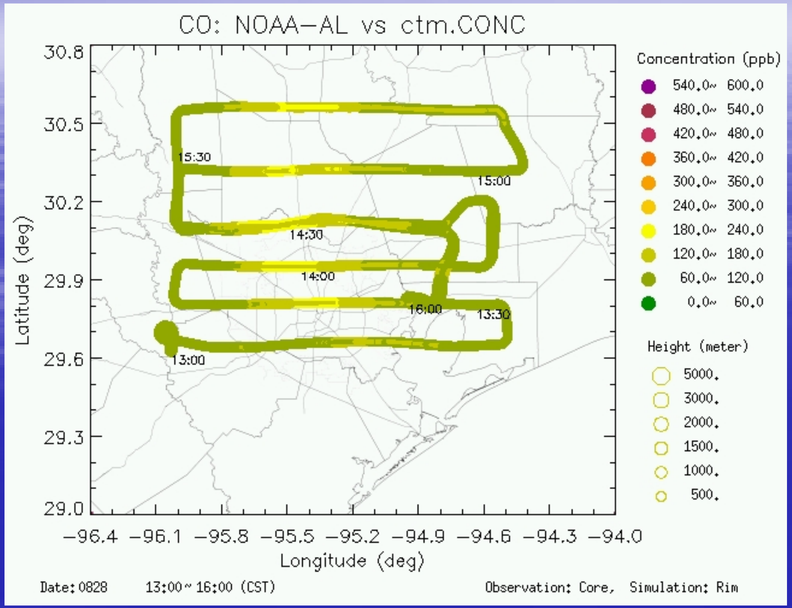


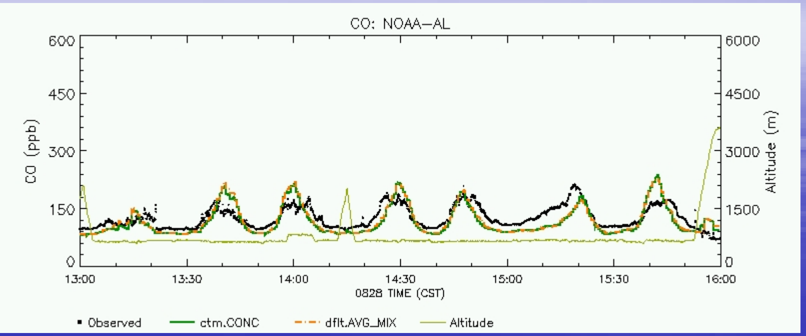


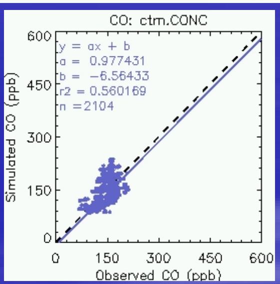


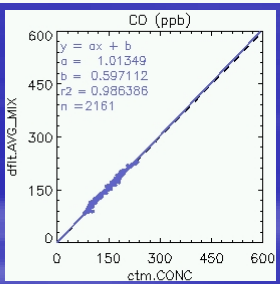


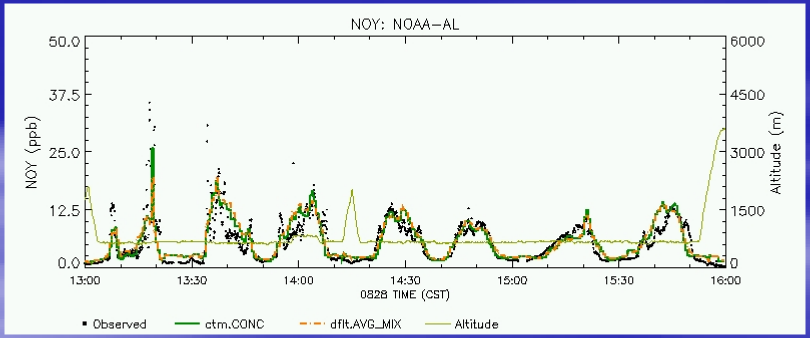
Comparison of CMAQ-TG with Std CMAQ and aircraft observations – simple wind (8/28/2006)

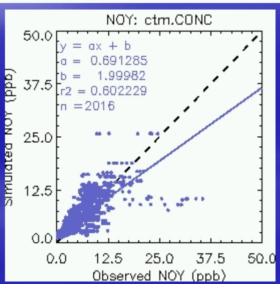


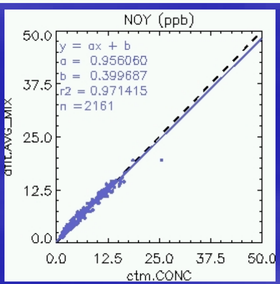


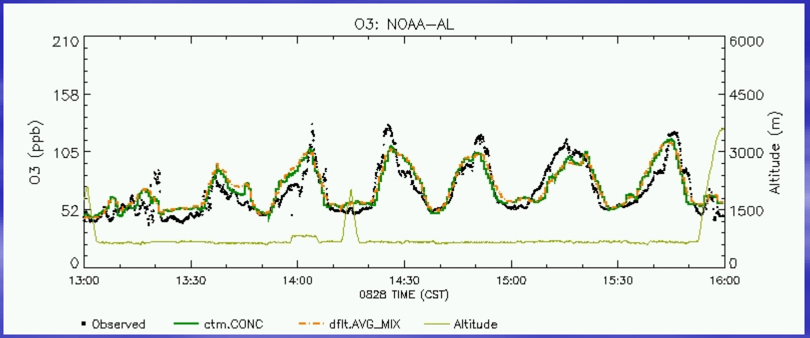


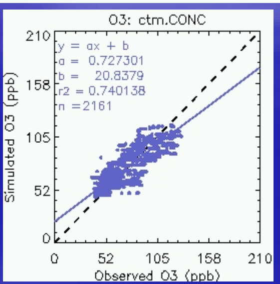


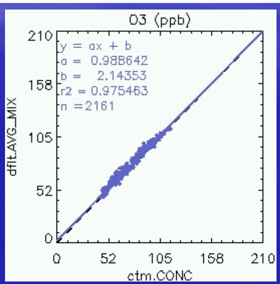




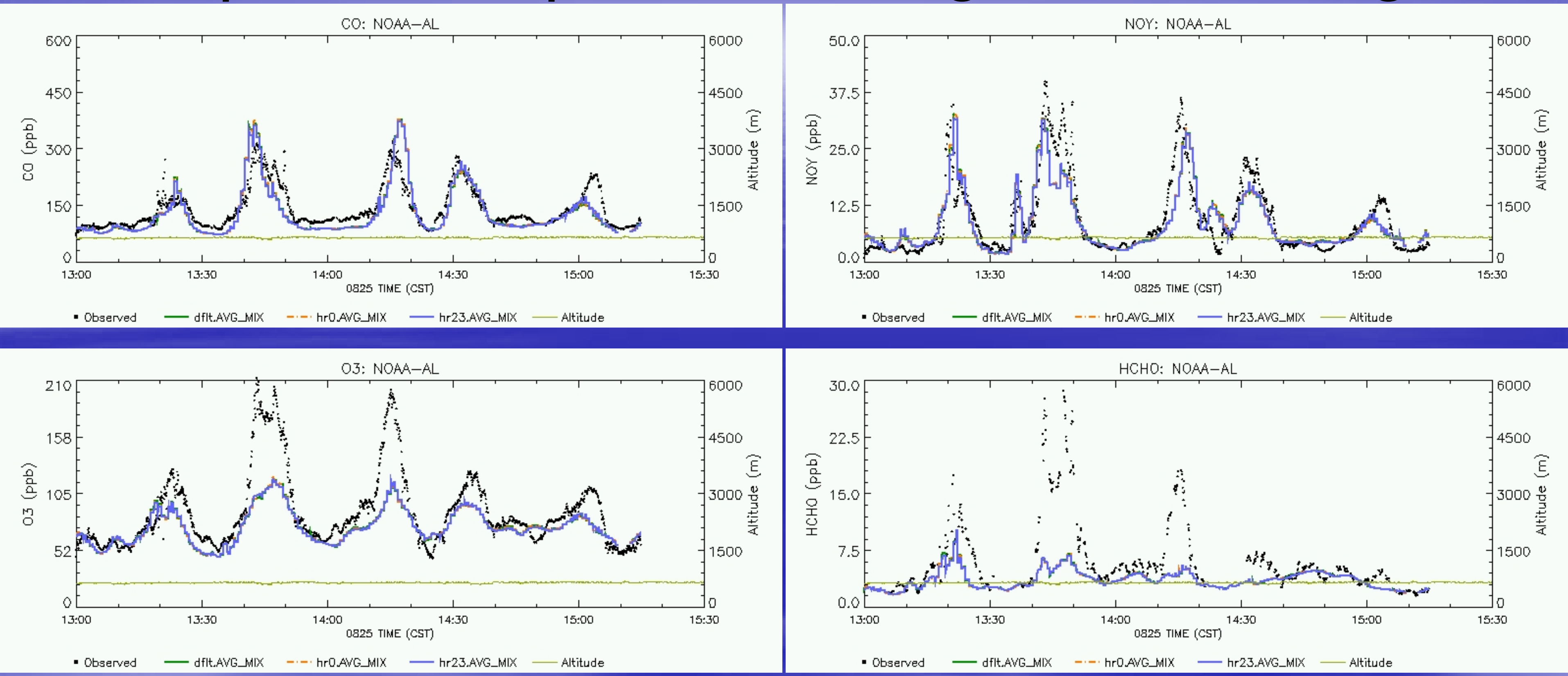








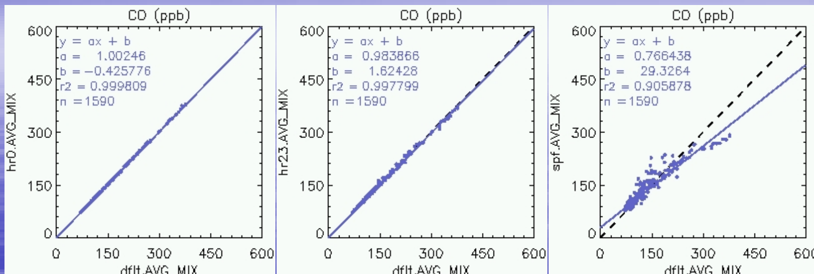
Comparison of packet management strategies

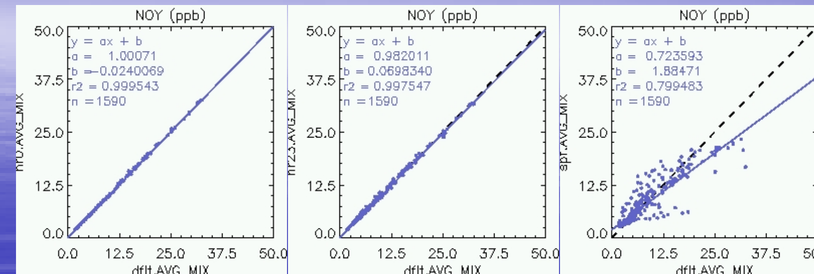


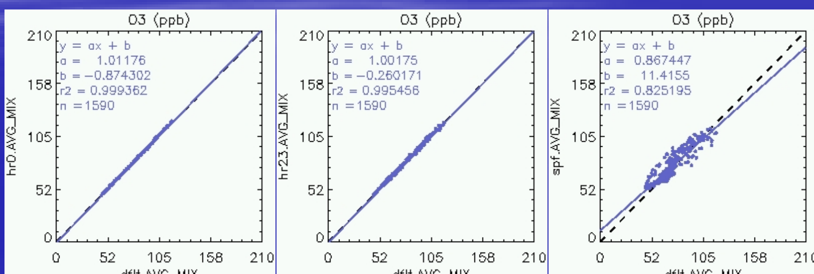
Default: start with 4 packets in each cell in layers 1 & 2, 1 in upper layers
HR0: start with 1 packet per cell in all layers
HR23: start with 4 packets per cell in all layers
(Default spawning rule: never allow any cell to be empty)

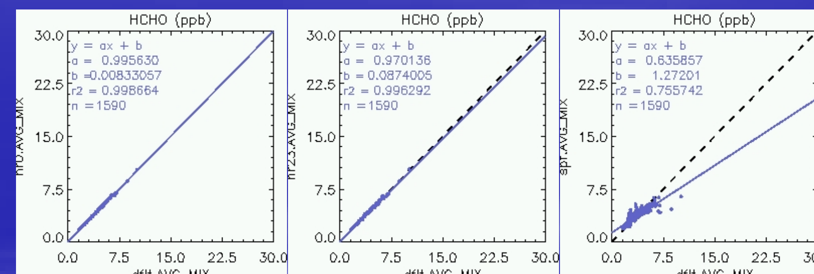
Good agreement between all 3 strategies – starting with 1 packet looks OK

Comparison of packet management strategies









Default: start with 4 packets in each cell in layers 1 & 2, 1 in upper layers; never allow any cell to be empty

HR0: start with 1 packet per cell in all layers; never allow any cell to be empty

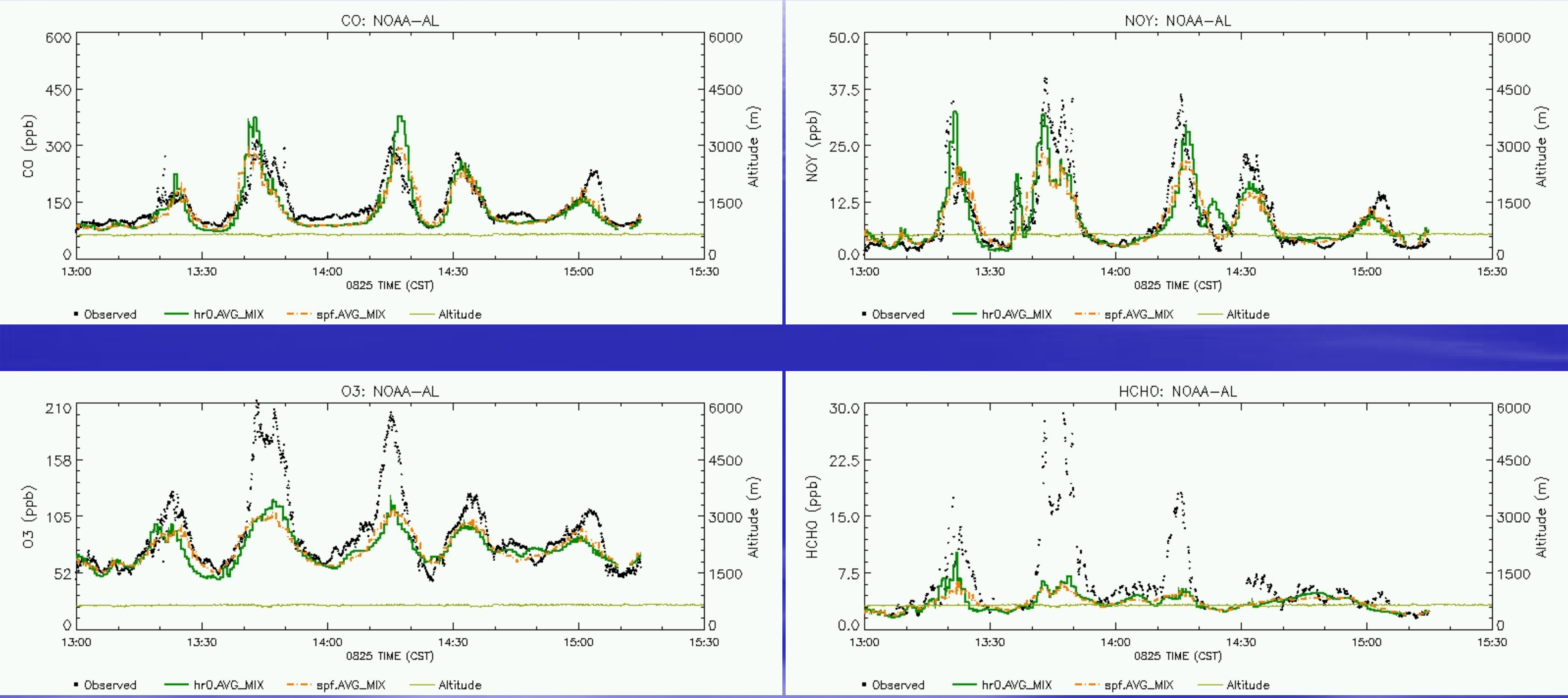
HR23: start with 4 packets per cell in all layers; never allow any cell to be empty

SPF: start with 1 packet in every cell, spawn new packet only when cell and all horizontal neighbors are empty

Good agreement between first 3 strategies – starting with 1 packet looks OK

The last strategy is much faster, but not as accurate

The cheaper, but weaker strategy



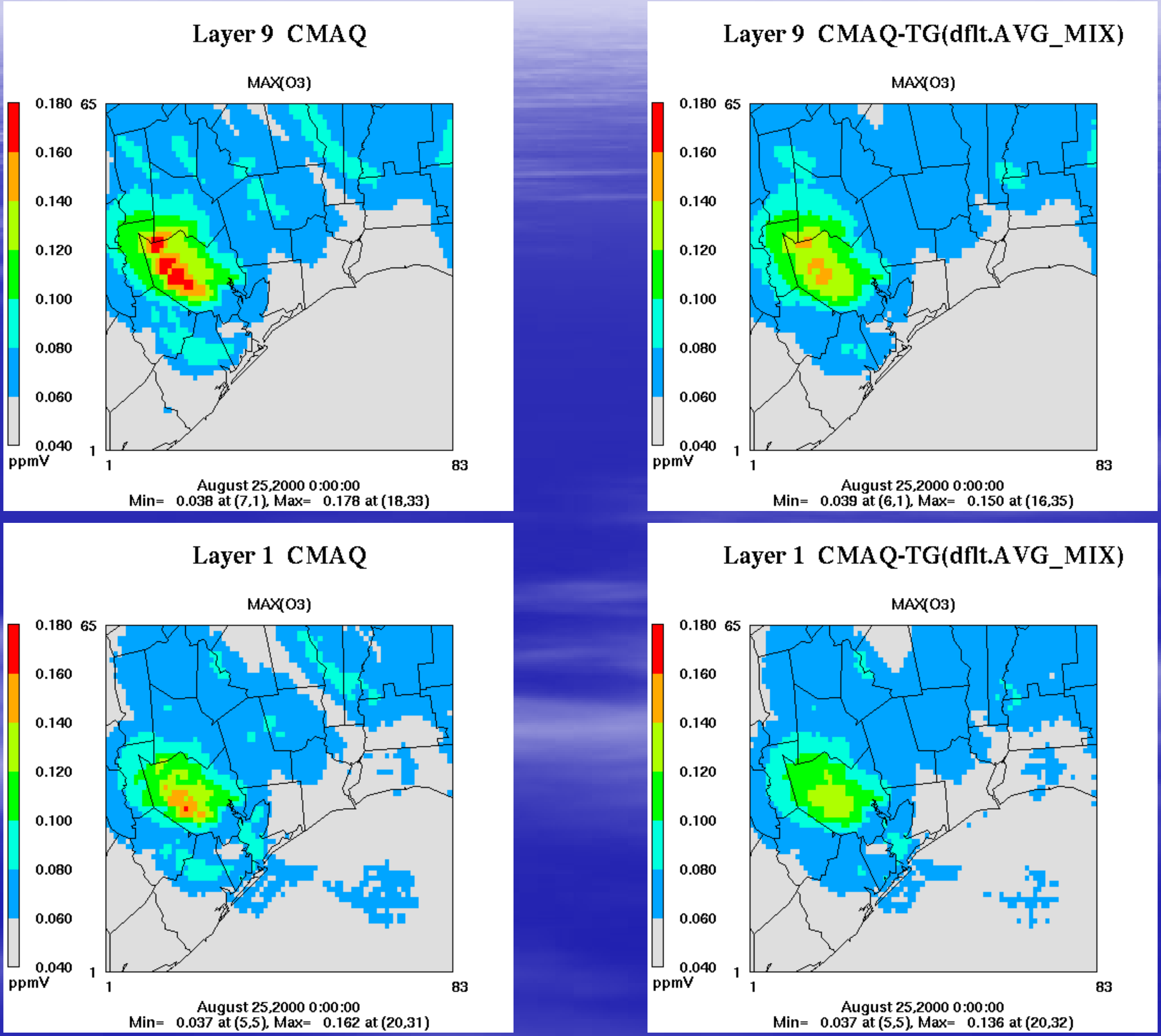
HR0: start with 1 packet per cell in all layers, never allow any cell to be empty

SPF: start with 1 packet in every cell, spawn new packet only when cell and all horizontal neighbors are empty

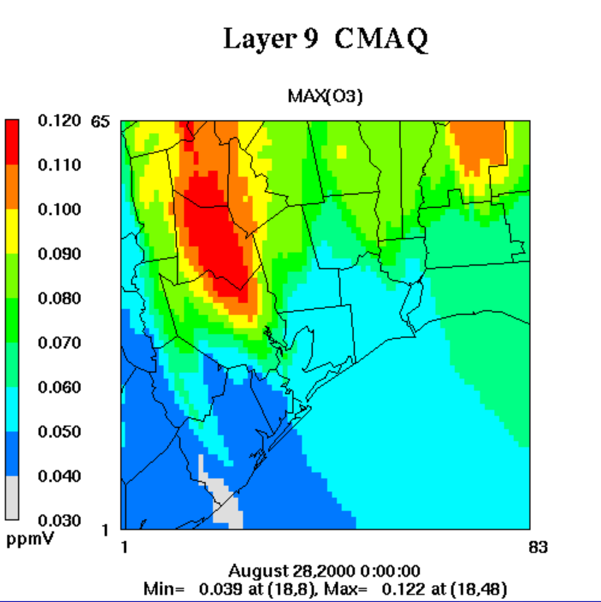
Timing Results

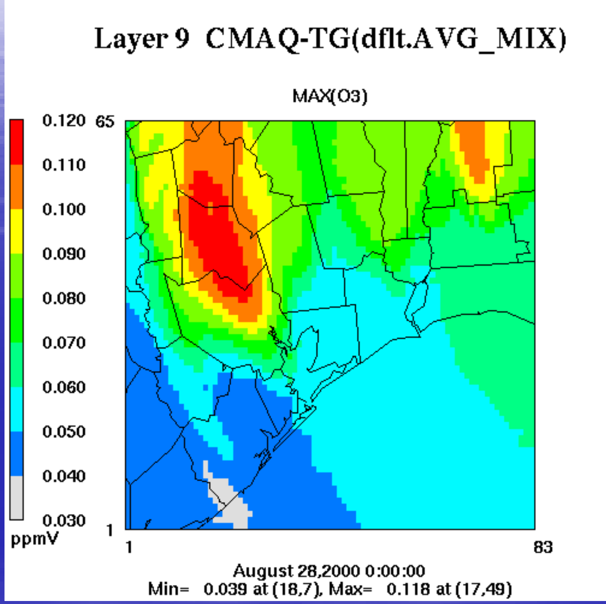
Standard CMAQ (ctm)					
Day	Computation Time (h)	# SyncSteps	# Cells	Time/SyncStep/Cell (10-3 sec)	Time/SyncStep (sec)
8/25/2000	3.67	317	124085	0.336	41.678
8/28/2000	3.6	308	124085	0.339	42.078
CMAQ-TG (124,085 cells): High resolution in bottom 2 layers (default)					
Day	Computation Time (h)	# SyncSteps	# Packets/Cell	Time/SyncStep/Packet (10-3 sec)	Time/SyncStep (sec)
8/25/2000	8.58	643	2.218	0.175	48.037
8/28/2000	7.65	550	2.213	0.182	50.073
CMAQ-TG (124,085 cells): No high resolution layers (hr0)					
Day	Computation Time (h)	# SyncSteps	# Packets/Cell	Time/SyncStep/Packet (10-3 sec)	Time/SyncStep (sec)
8/25/2000	8.31	643	2.128	0.176	46.505
8/28/2000	7.27	550	2.105	0.182	47.582
CMAQ-TG (124,085 cells): High resolution in all layers (hr23)					
Day	Computation Time (h)	# SyncSteps	# Packets/Cell	Time/SyncStep/Packet (10-3 sec)	Time/SyncStep (sec)
8/25/2000	11.94	643	3.636	0.148	66.842
8/28/2000	10.54	550	3.646	0.153	69.014
CMAQ-TG (124,085 cells): No high resolution layers; sparse fill (spf)					
Day	Computation Time (h)	# SyncSteps	# Packets/Cell	Time/SyncStep/Packet (10-3 sec)	Time/SyncStep (sec)
8/25/2000	5.47	643	0.902	0.273	30.612
8/28/2000	4.47	550	0.902	0.261	29.227

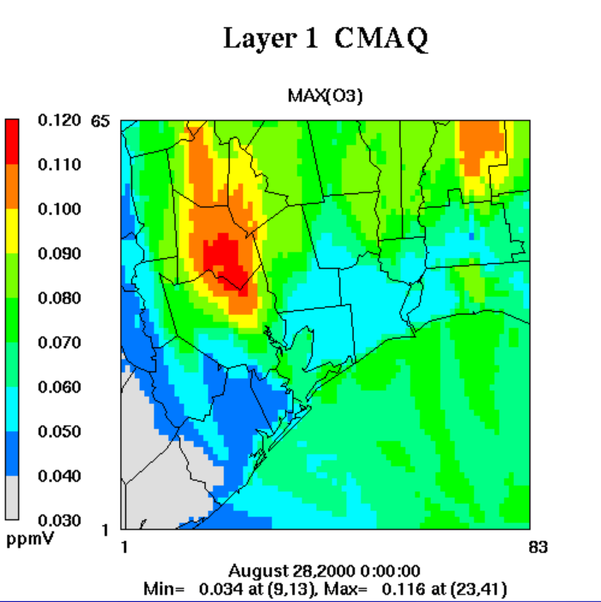
Comparison of daily maximum ozone
August 25, 2000

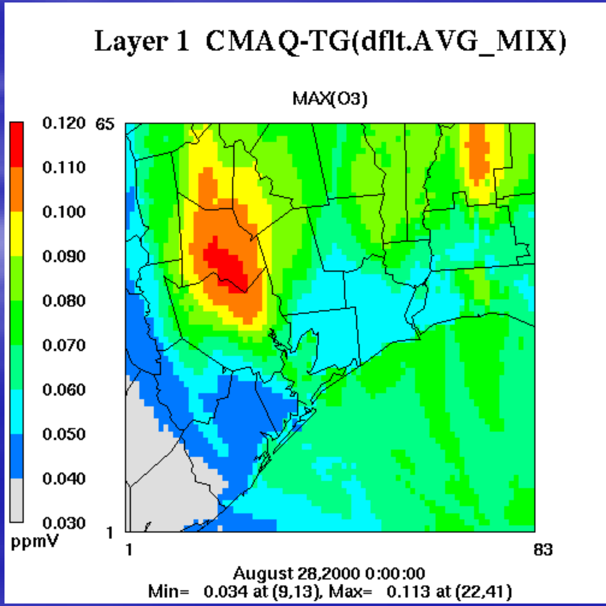


Comparison of daily maximum ozone
August 28, 2000









Conclusions

- CMAQ-TG supports many of the basic physical processes required for a CTM including advection, diffusion, gas chemistry, emissions and dry deposition
- Capable of completely eliminating numerical diffusion from the advection algorithm (depends on spawning and pruning strategies)
- While some comparisons of CMAQ-TG with standard CMAQ validate CMAQ-TG, the comparisons of maximum daily ozone leave unanswered questions
- Packet management strategies and their consequences need further investigation - effective packet management may be the biggest obstacle to CMAQ-TG becoming a competitive approach
- Should improve modeling of physical diffusion and gain a better understanding of possible diffusion caused by spawning and pruning
- Want to add features so that CMAQ-TG can be used for other applications such as identifying source-receptor relations