Numerical Errors in Chemistry-Transport Models

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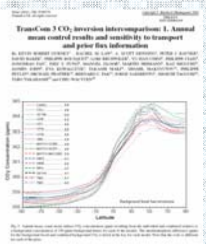
What is the Problem?

One expectation we have, when solving the chemistry-transport equations for atmospheric trace species, is that there should be a single, correct answer.

If we include the correct physics, refine our numerical methods, and increase the resolution, then the model will converge to this correct answer. With this optimism, the authors began a series of numerical experiments under the auspices of the NASA Global Modeling Initiative (GMI) to demonstrate that independent chemistry-transport models (CTMs) developed at UC Irvine and NASA Goddard could achieve this same answer.

After considerable effort to ensure that both CTMs simulated the same physical processes, we failed to produce two similar answers. We conclude that considerable uncertainty in the CTM simulation of trace species remains due to the choice of numerical methods, and we have not yet ruled out structural differences as the source of this error.

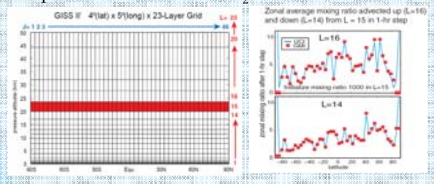
Why do we care?



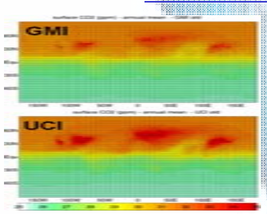
Consider the TransCom3 (T3) effort to use the atmospheric variations in CO_2 abundance to deduce the deduce the pattern of fossil-fuel emissions The differences among the dozen or so CTMs in simulating atmospheric CO2 gradients from a prescribed fossil-fuel pattern become a major source of uncertainty in the inverse calculation. *(K.R. Gurney et al., 2002, Nature 415, 626-630; 2003, Tellus 55B, 555-579).*

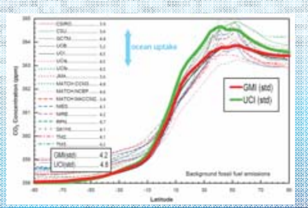
These T3 results were due to a wide range in meteorological fields ***and*** numerical methods. Using modern tracer-transport algorithms and the same met fields, we assumed that we could eliminate at least the errors in tracer transport. This optimism was short-lived. After correcting several minor "bugs" in both CTMs, ensuring that we interpreted the emissions and meteorological fields in the same manner, the differences were uncomfortably large: not significantly less than the original T3 model spread; comparable to the amplitude of the oceanic CO_2 sink.

TEST:
GISS GCM II' met fields, 4°lat x 5°long x 23 layers, 1-hr advection step with tracer only in L=15.
excellent, except at poles.



Surface CO_2, how bad can it be?

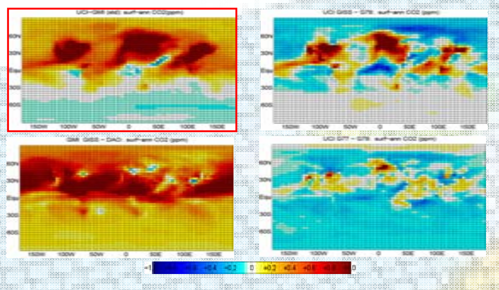




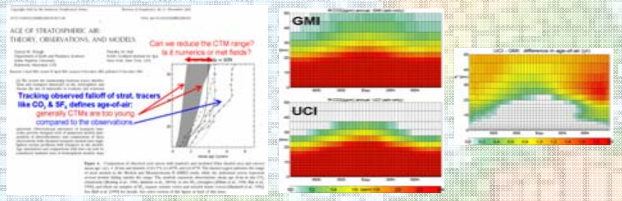
UCI-GMI Grades for Surface CO_2 mixed:

Tropics & S. Hemisphere: **A**
N. Hem. & Source Regions: **C-**

UCI – GMI differences in N. Hem, ***using the same met fields***, (upper left panel below) are comparable to one CTM running different met fields.



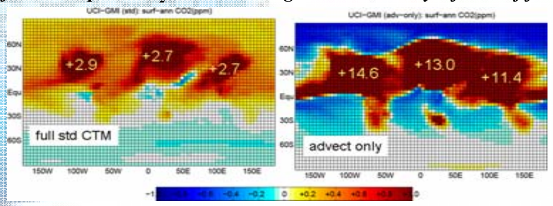
Stratospheric age-of-air, how bad can it be?



The age-of-air in the stratosphere (defined as the time since it was last in the troposphere) describes the stratospheric circulation and time-scales of chemical perturbations. It is measured directly from nearly inert trace gases that are increasing linearly in the troposphere (CO_2, SF_6). ***CTMs show a very wide range, as does the UCI – GMI comparison (figures above).*** The year-10 zonal average of stratospheric CO_2 shows surprisingly large differences, corresponding to more that 1 yr in age. GMI is more diffusive, and the problem is not obviously related to differing polar treatment.

the Advection Algorithm

Multiple tests with both UCI and GMI CTMs showed that the age-of-air was barely influenced by wet convection or boundary layer mixing. Thus we continued with only advection of tracer by the winds resolved on the original 4x5 grid. The surface CO_2 differences were greatly reduced by convection/boundary-layer mixing: ***when only advection was used, the difference in peak CO_2 over source regions increased by a factor of four.***



Global rms differences (ppm): **1.6** (original CTMs), **0.6** (corrected CTMs), **2.8** (advection only CTMs)

Is there a Correct Answer?

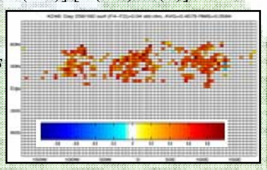
Since tracer advection is represented physically (rather than parametrically), errors due to calculation on a finite grid and should disappear as the resolution increases.

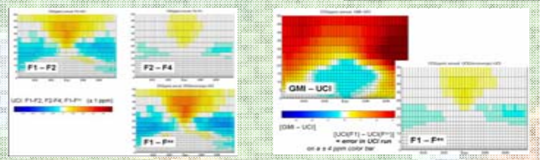
With the UCI CTM we pursued a "doubling to convergence" approach: from F1 (original resolution Δ: 72x46x23) to F8 (Δ/8: 576x354x184). The series of calculated abundances (A) at any location and time obtained through Δ-halving converges (i.e. Aitken's):

$$A^{true} = A(\Delta) + A(\Delta/2) - A(\Delta) + A(\Delta/4) - A(\Delta/2) + A(\Delta/8) - A(\Delta/4) + \ldots$$
$$= A(\Delta) + A(\Delta/2) - A(\Delta) / (1 - k_{421}),$$

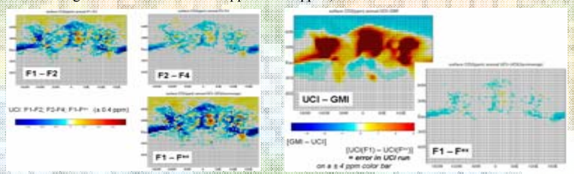
where the convergence factor $k_{421} = [A(\Delta/4) - A(\Delta/2)]/[A(\Delta/2) - A(\Delta)]$

Using a 2-month simulations with Δ, Δ/2, Δ/4, and Δ/8 and surface CO_2 abundances on day 62 (Sep 1), we calculate
$k_{421} = 0.46 \pm 0.17$ & $k_{842} = 0.46 \pm 0.06$
(see Wild & Prather, 2006, JGR D111, D11305).





Convergence of UCI CTM (F1=>F2=>F4) for stratospheric CO_2 in year 10 is shown as differences F1 - F2, F2 - F4, and extrapolated error F1 - F^{ex}. The error is at most ± 0.4 ppm, much less than UCI-GMI differences.
(Note the change in color scale from ± 1 ppm to ± 4 ppm.)



Surface CO_2 in year 10 shows similar convergence, and once again, the UCI errors are much smaller than the UCI-GMI differences.

Do both Numerical Methods get the same Answer?

Correcting the UCI CTM reduces the UCI-GMI differences, by at most 10%, suggesting that tracer advection errors using the GMI algorithm are much larger than those with the UCI algorithm and to first-order are represented by the GMI-UCI differences.

As of now, the GMI CTM has been able to complete only a single case with doubled vertical layers (23 to 46) and no change in horizontal resolution. The UCI-GMI differences are somewhat reduced (see figure), but closure on this topic awaits the full F2 and F4 GMI simulations.