Modeling Tools for DC3 Analysis

The Players:

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Models

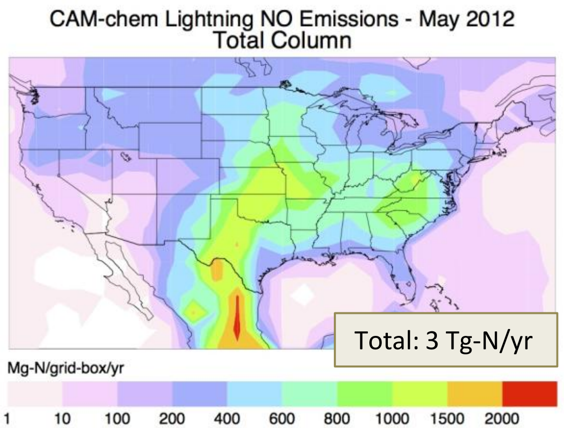
- **CAM-Chem** – global chemistry transport model
- **WRF-Chem** – regional chemistry+meteorology
- **WRF** – electrification, lightning and lightning-NO_x
- **Box models** – Lagrangian perspective
- **Steady-state chemistry** models (?)
- **Back trajectories** (?)

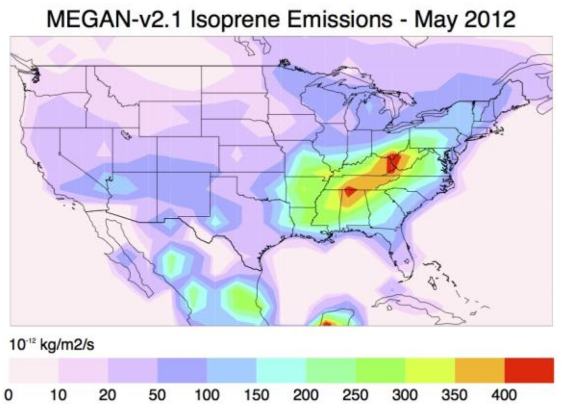
CAM-chem for DC3

Louisa Emmons, Mijeong Park - NCAR/ACD

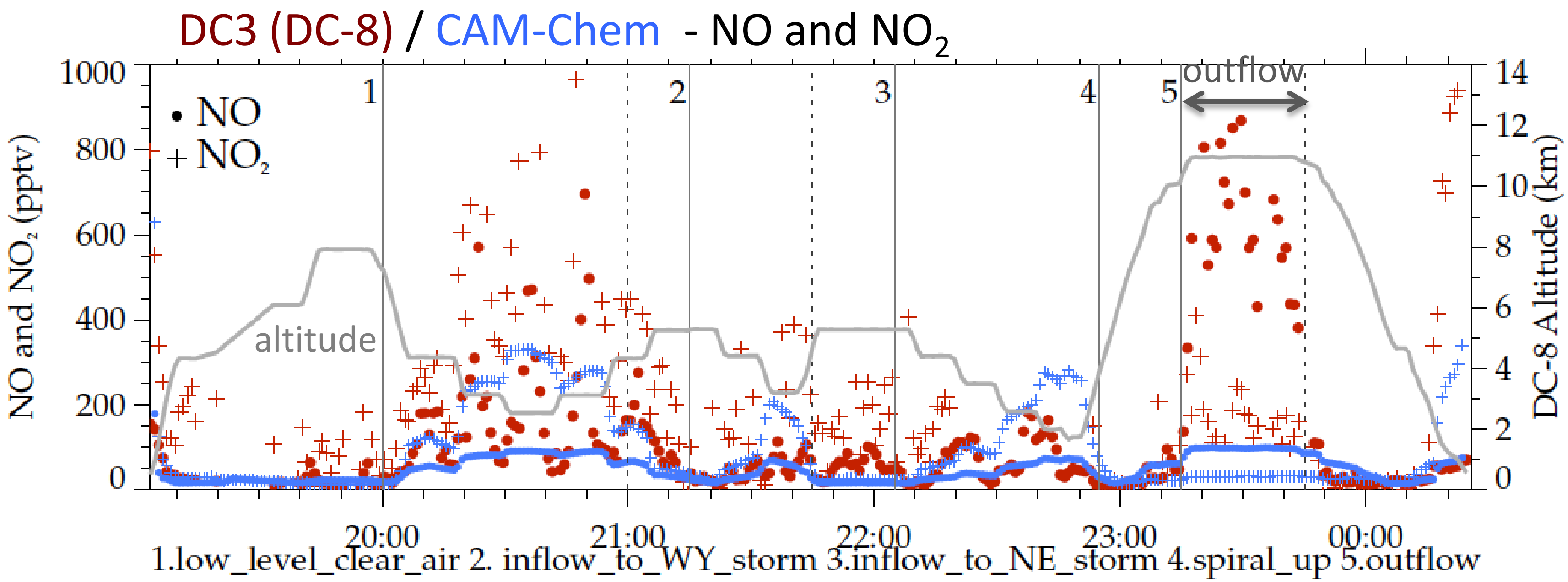
- **CAM-chem**: Community Atmosphere Model with Chemistry, component of NCAR CESM (Community Earth System Model), driven by GEOS-5 met.
- **Anthropogenic emissions**: Streets ARCTAS-v1.2 inventory (for 2008; includes US NEI 2002)
- **Lightning NO emissions**: Price et al. [1997] with vertical distribution as in DeCaria et al. [2006]; CG=IC [Ridley et al., 2005]
- **Biogenic emissions**: MEGAN-v2.1 online (in Community Land Model)
- **Fire emissions**: FINN-v1
- **Configuration**:

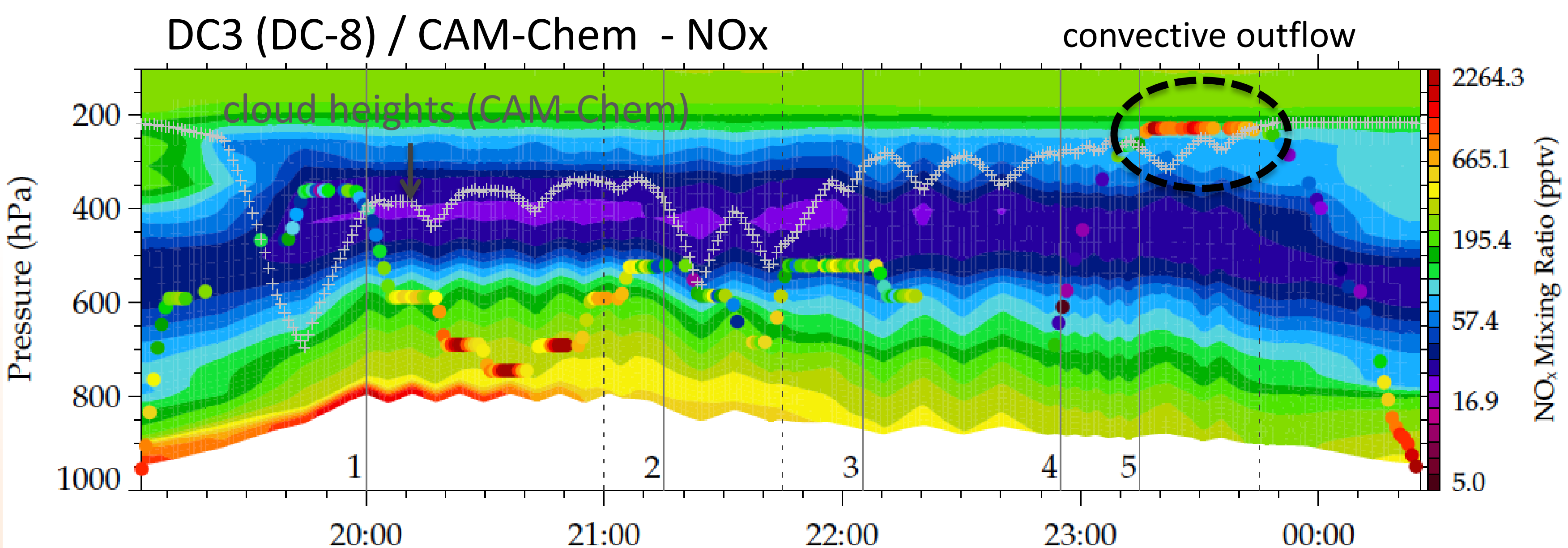
  1.9° x 2.5° (lat-lon), 56 levels up to 3 hPa





May 18, 2012 (Colorado Convection)





CAM-chem for DC3

Louisa Emmons, Mijeong Park - NCAR/ACD

Analysis plans and possibilities:

- Evaluation of large-scale influence of lightning NO_x on UT distributions (see Louisa & Frank's poster)
- Evaluation of lightning NO vertical distribution in model versus observations
- Convection and chemical evolution of biogenic emissions
- Impact of fires on DC3 observations
- Boundary conditions for regional model simulations

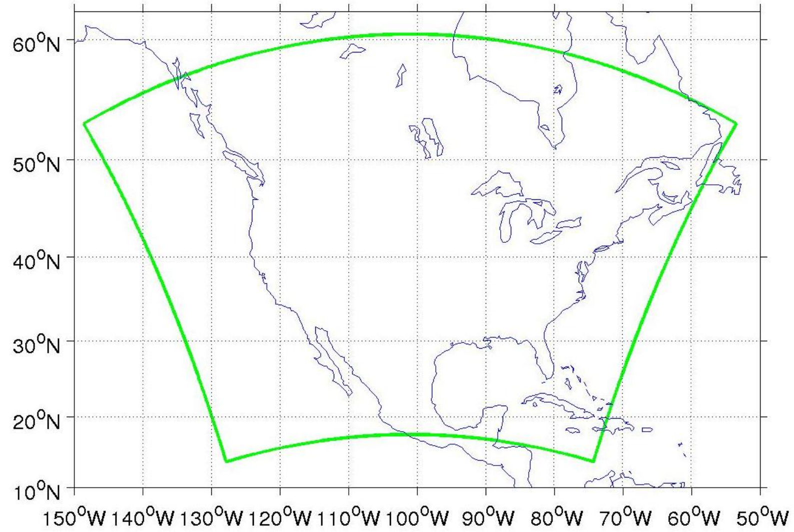
Additional simulation(s) at 0.5° resolution

WRF-Chem

Megan Bela (U. Colorado), Mary Barth (NCAR), Kristin Cummings (U. Maryland), Ken Pickering (NASA), Yunyao Li (U Maryland)

- Anthropogenic emissions: EPA NEI 2005 projected to 2012; aircraft (Baughcum, 1999)
- Lightning NO emissions:
  - Parameterized convection: Price et al. [1997] with vertical distribution as in Ott et al. [2010]; [Wong et al., 2012, GMDD]
  - Cloud resolving: flash rate = f(updraft volume), DeCaria et al. [2005] placement both vertically and horizontally
- Biogenic emissions: MEGAN-v2.04 online (in NOAH Land Model)
- Fire emissions: FINN-v1
- Configuration:

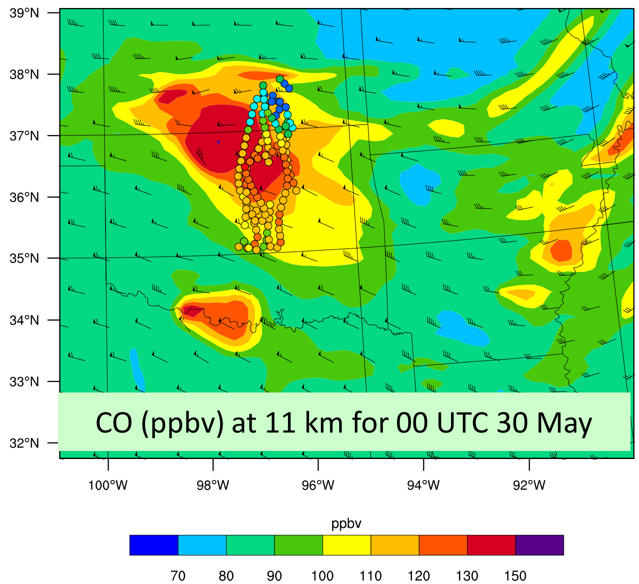
  Δx = 15 km, 40 vertical levels to 50 hPa



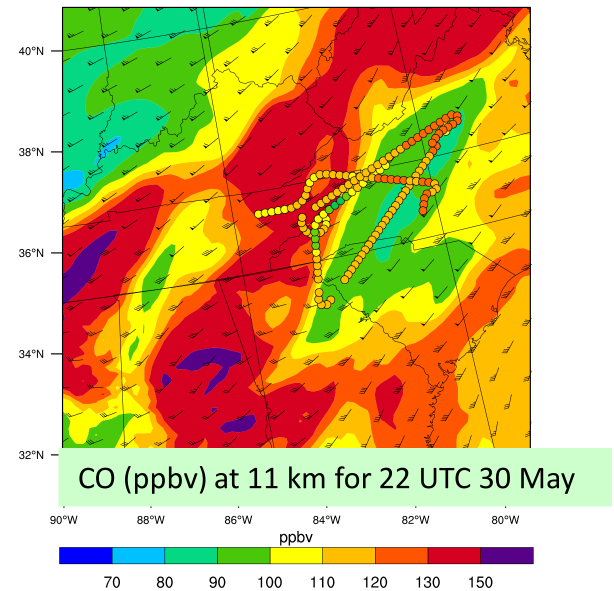
WRF-Chem

Megan Bela (U. Colorado), Mary Barth (NCAR), Kristin Cummings (U. Maryland), Ken Pickering (NASA), Yunyao Li (U Maryland)

29-30 May 2012 Oklahoma case and downwind



CO (ppbv) at 11 km for 00 UTC 30 May



CO (ppbv) at 11 km for 22 UTC 30 May

Science plans:

- Convective transport; Scavenging of soluble trace gases
- Production of NO_x from lightning; flash rate – storm parameter relationships
- Production of O_3 downwind of convection

Future possibilities:

- Processing of aerosols by convection; effect of aerosols on convection

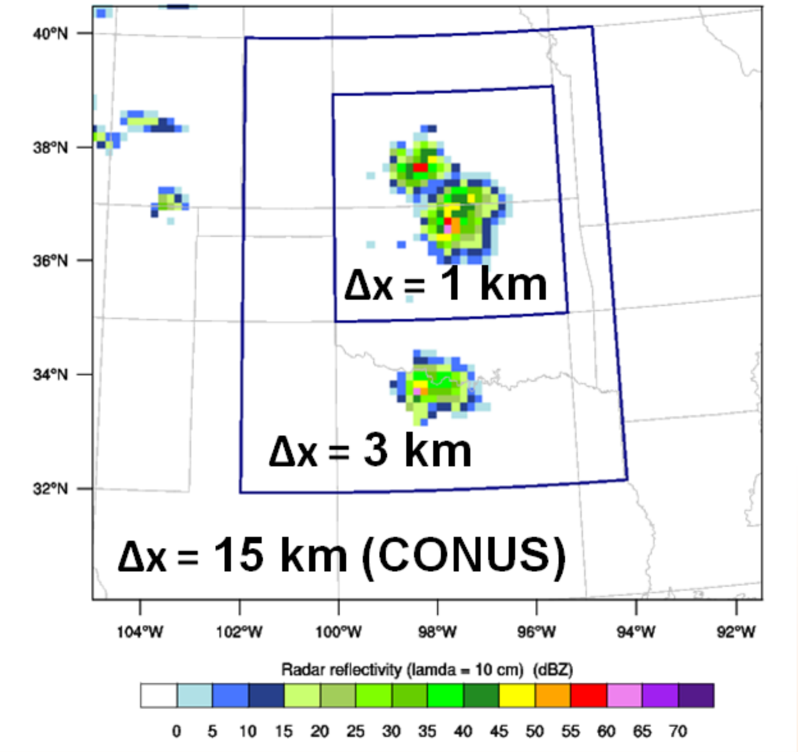
WRF-Chem

Megan Bela (U. Colorado), Mary Barth (NCAR), Kristin Cummings (U. Maryland), Ken Pickering (NASA), Yunyao Li (U Maryland)

Domains and grid spacing plans:

Run for most/all DC3 cases: Δx = 15 km, 40 vertical levels to 50 hPa

Run specific cases at cloud resolving grid spacing:



Other case studies of focus:

21 May 2012 Alabama case

6 June 2012 Colorado case

22 June 2012 Colorado case with BB

WRF

Ted Mansell (NOAA/NSSL)

- Cloud-resolving ($\Delta x \leq 4$ km) simulations of electrification and lightning in WRF
  - Noninductive charge separation schemes
  - MacGorman et al. (2001) lightning parameterization
- Lightning NO_x parameterization
  - Barthe et al. (2007) JGR based on lightning flash length
- Future: assimilate radar data with EnKF and use LMA data to inject lightning-NO_x

NASA Langley Lagrangian Box Model

Jennifer Olson, Jim Crawford (NASA/LaRC)

<u>Description:</u>

Detailed HO_x-NO_x-CH_4-NMHC chemical mechanism:
Explicit C_2H_6, C_3H_8 and C_2H_4 chemistry
Lumped C_4+ alkanes and C_3+ alkenes.
Explicit Isoprene chemistry, based on MIM2 (Taraborelli et al., 2009).

Clear sky photolysis rates calculated using TUV (DISORT 8 streams) and can be normalized to account for reflectance/attenuation by clouds.

Lagrangian mode provides loss of all (or selected) constraining precursor species, and production/loss of radical species after initialization. The model is run to a background steady state, and then an "injection" of species (i.e. BL or inflow air) is imposed and followed in a Lagrangian mode.

Dilution with background air can be parameterized.

NASA Langley Lagrangian Box Model

(Jennifer Olson, Jim Crawford: LARC)

Proposed uses for DC3:

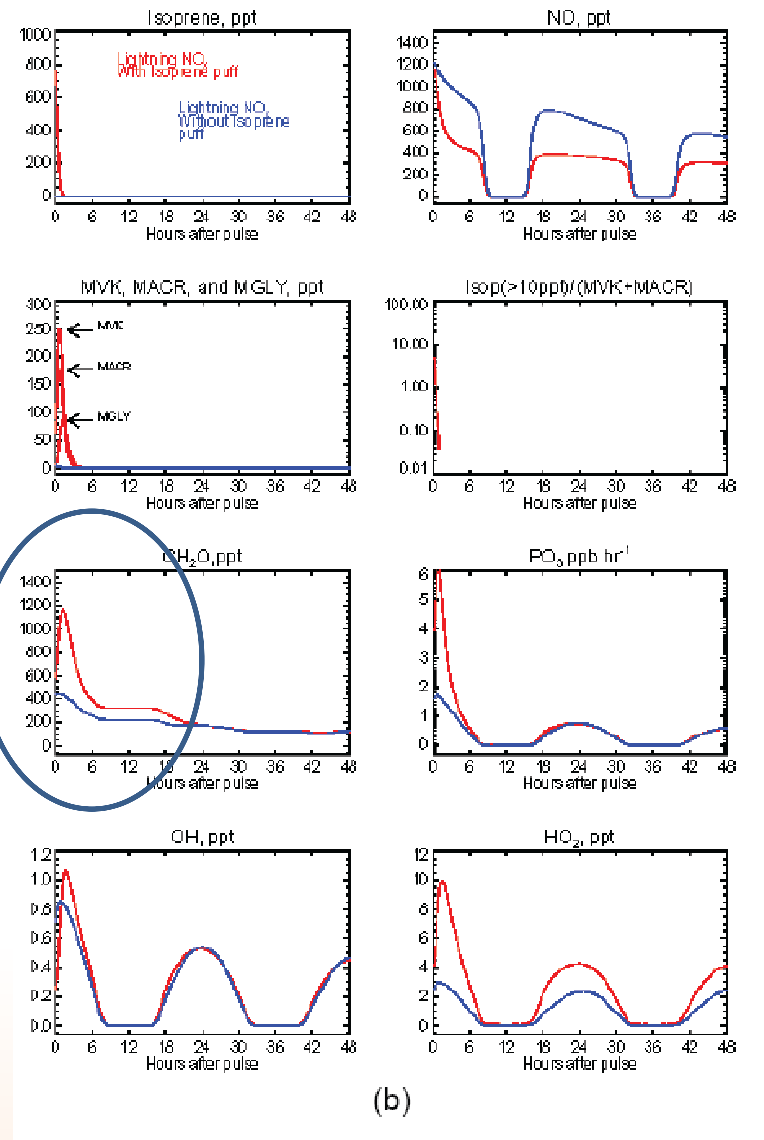
- UT chemical evolution analysis (e.g., 24-hour sampling flights)
- Convective injection chemical analysis (Following evolution of injection of inflow concentrations)
- Budget analysis (e.g. identification of production terms for CH_2O)

Relevant previous studies (Lagrangian mode analysis of flight data):

Apel, et al., Impact of the deep convection of isoprene and other reactive trace species on radicals and ozone in the upper troposphere, Atmos. Chem. Phys., 12, 1135-1150, 2012.

Fried et al., Detailed Comparisons of Airborne Formaldehyde Measurements with Box Models during the 2006 INTEX-B Campaign: Evidence for Unmeasured and Multi-Generation Hydrocarbon Oxidation Processing, Atmos. Chem. Phys., 11, 13181-13199, 2011.

Apel et al., 2012



(Example of CH_2O produced from convected isoprene under high NO_x conditions)

Discussion Topics for Group

- Emissions inventory
- Need for back trajectories
- Synergistic activities among models