# The Implications of Acetone Condensation on Remote Conditions

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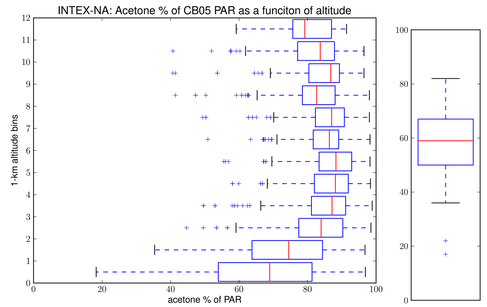
## MOTIVATION

Global background ozone ($O_3$) is increasingly relevant for policy, but condensed chemical mechanisms are designed to predict $O_3$ in urban environments. The tightening standards and increasing background $O_3$ decreases the policy relevant margin, which necessitates better modeling of the background $O_3$. Background and urban $O_3$ production occur under distinct environmental conditions (e.g., temperature and pressure) with different primary precursors. The relative importance of organic precursors determine which species can be condensed. This poster highlights the influence of distinct conditions by illustrating the importance of acetone in rural and remote conditions as modeled by the Carbon Bond mechanism. The next version (VI) of Carbon Bond has addressed many of these concerns, and we make the case for using the updated version when rural and remote conditions are a primary research focus.

## PAR VS. ACETONE

| Property | PAR[*Gery and Whitten*, 1988] | Acetone |
|---|---|---|
| $k_{PAR+HO^{\cdot}}$ | 1200 $ppm^{-1}$ $min^{-1}$: urban average of 23 alkanes | $2 \times 206$ $ppm^{-1}$ $min^{-1}$ primary carbons |
| $RNO_3$ Yield | based on primary and secondary oxidation channels | primary only |
| Photolysis | N/A | $j = f(\text{pressure}, \text{temperature})$ |

## OBSERVED ACETONE / PAR




(a) INTEX-NA (b) OZIE

Figure 1: INTEX-NA [*Singh et al.*, 2006] and OZIE [*Wiedinmyer et al.*, 2005] observed acetone as a fraction of PAR.

## A FIRST APPROXIMATION

**PROBLEM:** High % acetone and over-estimated $RNO_3$ yield causes $RNO_3$ high bias [*Henderson et al.*, 2010]

**GOAL:** Characterize magnitude and spatial distribution of bias associated with overproduction of organic nitrate.

**METHOD:** Reduced direct yield of $XO_2N$ from 13% to 3%

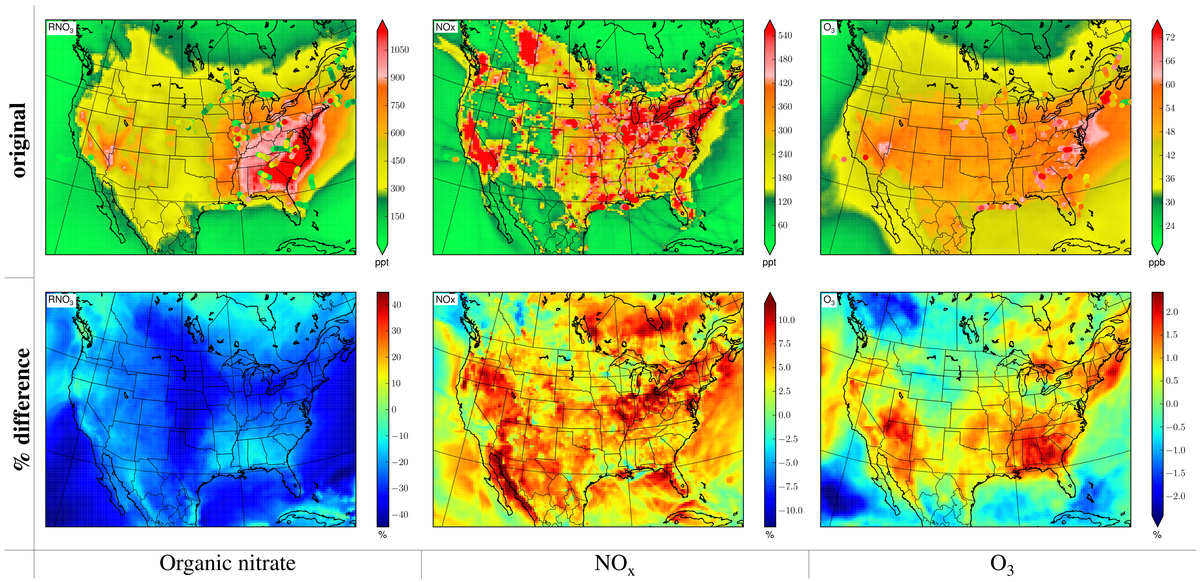
| | |
|---|---|
| Original | $PAR + HO^{\cdot} \longrightarrow .87XO_2 + .13XO_2N + .76ROR + \ldots$ |
| Adjusted | $PAR + HO^{\cdot} \longrightarrow .97XO_2 + .03XO_2N + .76ROR + \ldots$ |

**Simulations**

- Continental June to August with lightning NO [*Allen et al.*, 2010]
- CMAQ Hemispheric development test-case for April

## CONTINENTAL MODELING

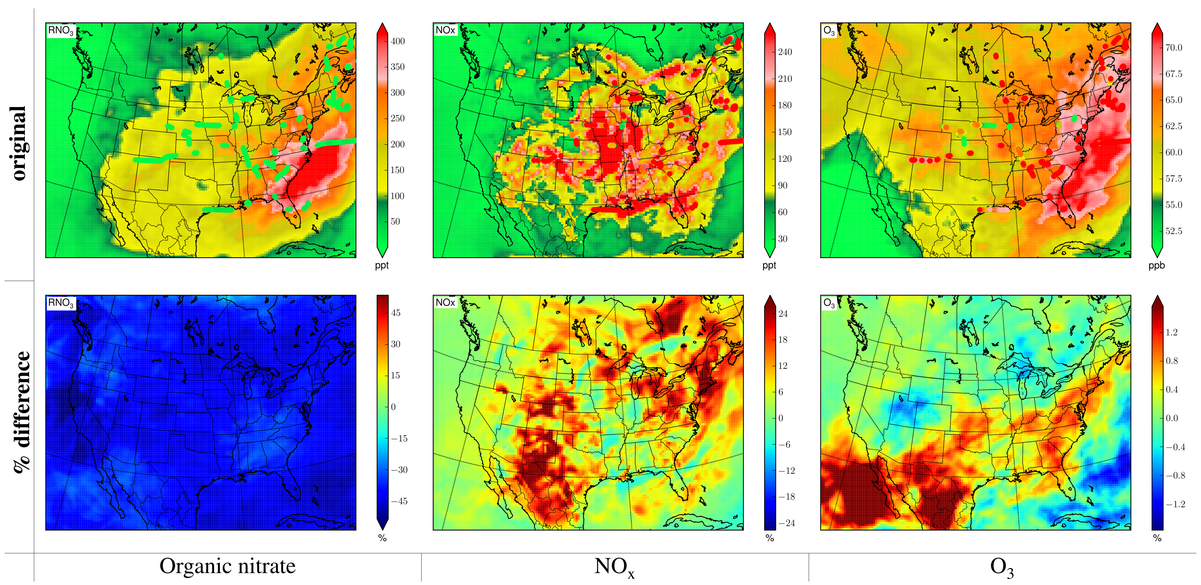
### Planetary Boundary Layer Results




Organic nitrate $NO_x$ $O_3$

Figure 2: INTEX-NA observations (dots) over mean predicted mixing ratios from the standard model (top row) and percent difference from updates (bottom row) in the planetary boundary layer (0 - 1.9 km) at 1700 UTC.

### Upper Troposphere Results




Organic nitrate $NO_x$ $O_3$

Figure 3: Same as Figure 2 for the upper troposphere (7.5 - 9.3 km) at 1700 UTC.

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## HEMISPHERIC MODELING

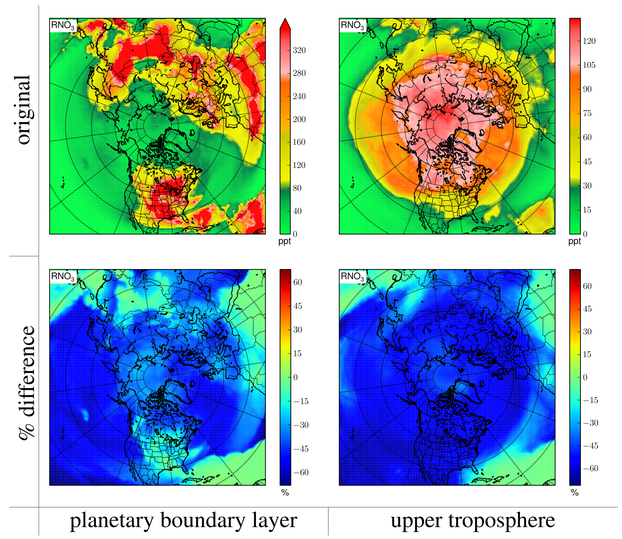


Figure 4: Organic nitrate in the planetary boundary layer (0 - 2.1 km) and upper troposphere (7.7 - 9.7 km) at 1700 UTC.

## SUMMARY

Condensed mechanisms provide computational efficiency that is necessary for large scale applications, but assumptions used for condensing may be specific to certain environments (e.g., urban). For instance, the assumptions required to lump ketones with alkanes have not been explicitly evaluated for remote and rural conditions that provide background mixing ratios to regulatory modeling. The results shown here illustrate the potential magnitude and spatial distribution of bias due to overestimating organic nitrate yield from acetone. Carbon Bond VI makes acetone explicit and creates a lumped ketone species; the updated mechanism should be used as soon as possible.

### References

Allen, D., K. Pickering, B. H. Henderson, R. Pinder, and T. Pierce, An evaluation of upper tropospheric NOx/O3 chemistry during the INTEX-A period using CMAQ and an adjusted CB05 chemical mechanism., *11th Science Conference of the Int'l Global Atmos. Chem.*, 2010.

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Wiedinmyer, C., et al., Ozarks isoprene experiment (ozie): Measurements and modeling of the "isoprene volcano,", *J. Geophys. Res*, *110*(D18307), doi:10.1029/2005JD005800, 2005.

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