Modeling the effect of high-resolution land-surface heterogeneity and forest structure on emission, chemistry and dispersion of volatile organic compounds and reactant species

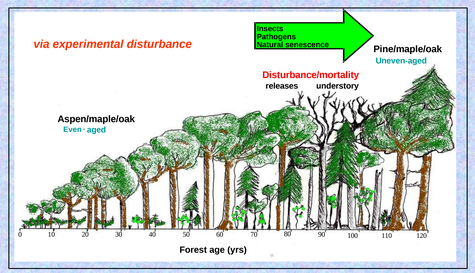
William Kenny, Gil Bohrer; kenny.49@osu.edu & bohrer.17@osu.edu

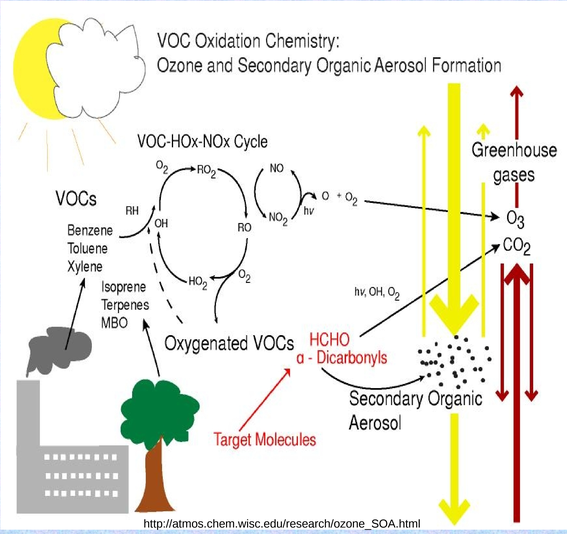
Ohio State University, Dept. of Civil Environmental and Geodetic Engineering, Columbus, OH, USA;

The goal of our work is to produce a simulation tool that can simulate emission, chemistry and dispersion of certain Biogenic Volatile Organic Compounds (BVOC) and their reaction products, focusing on processes within and above forest canopies such as light dependent oxidation of VOCs and NOx reactions. We are working to produce a post-processing model which we will call High resolution VOC Atmospheric Chemistry in Canopies (Hi-VACC) which will be able to resolve the dispersion and chemistry of reacting chemical species given their emission rates from the vegetation and soil and driven by high resolution meteorological forcing and wind fields from various high resolution atmospheric regional and large-eddy simulations. We specifically focus on forested environments and pathways that involve glyoxal and methylglyoxal, which lead to significant formation of Secondary Organic Aerosols (SOA) and affect, particularly in urban-forest interfaces, the levels of tropospheric ozone.

Background:

VOCs, and their reaction products, emitted from forests are highly dependent on forest structure and mixing inside the canopy. Various processes determine the eventual fate of these products which we will study with Hi-VACC





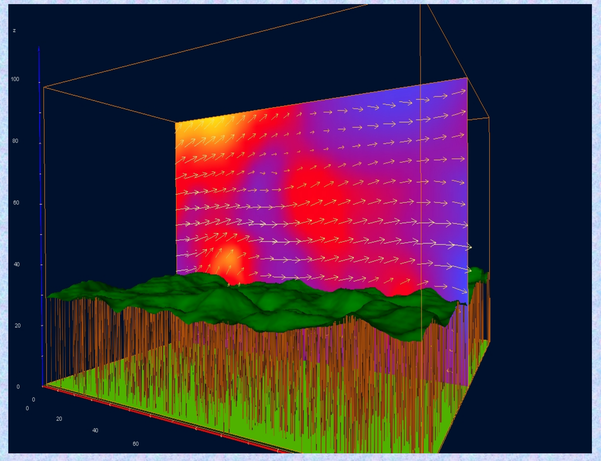
http://atmos.chem.wisc.edu/research/ozone_SOA.html

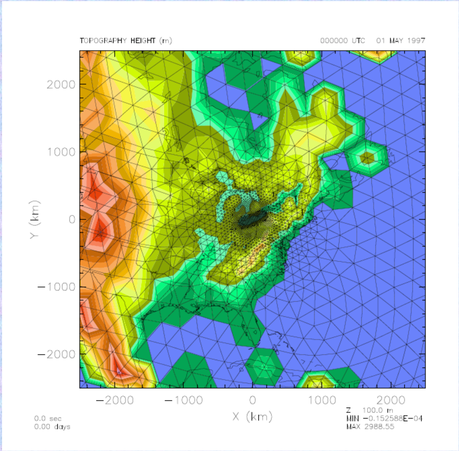
Models:

We will use OLAM and RAFLES as the atmospheric models to drive HI-VACC

RAFLES is a canopy resolving large eddy simulation model. It resolves the wind flow inside and above 3-D heterogeneous tree canopies. The model is initialized and forced with profiles of horizontal wind, temperature and humidity. Here, a synthetic profile, representing a typical dry season day was used. It includes Eulerian-Lagrangian particle dispersion.

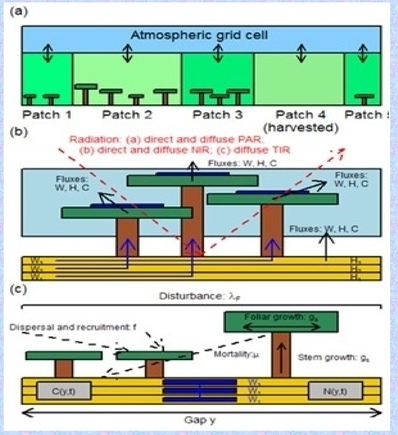
OLAM is a global-regional model with unstructured mess and zoon-in capabilities to extreme high resolution. It includes the same canopy representation and Eulerian-Lagrangian particle dispersion as RAFLES.





Emission:

2nd version of Ecosystem Demography model coupled to OLAM and RAFLES. Utilized to develop Hi-VACC emission functions



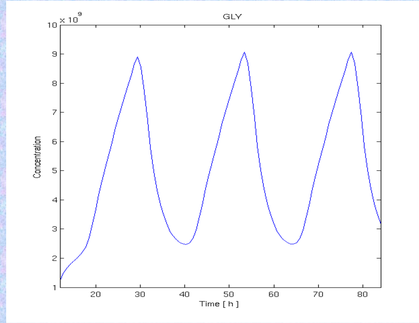
(Medvigy, 2009)

Dispersion:

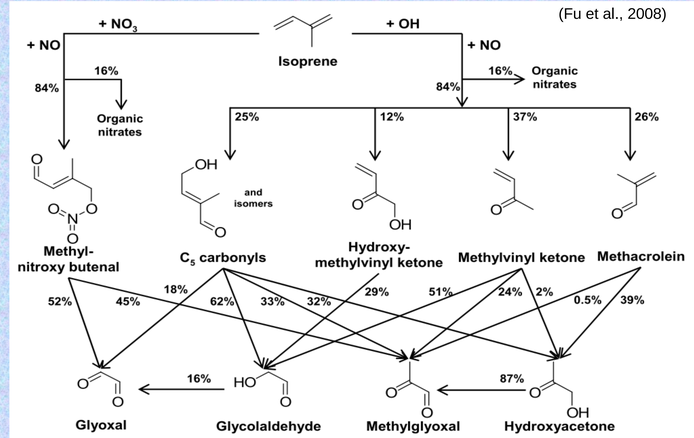
Hi-VACC dispersion developed and tested on a few different RAFLES simulations.

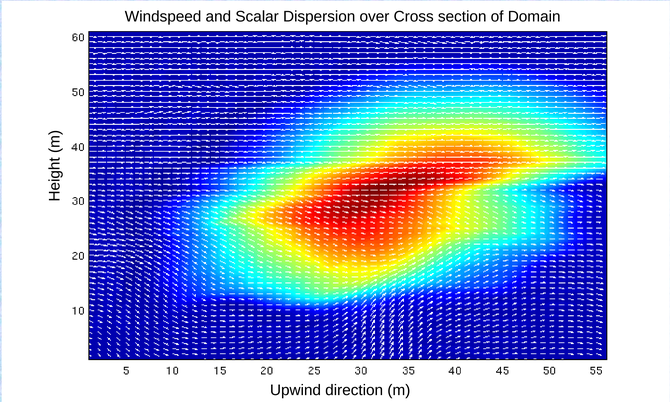
Chemistry:

Generated glyoxal model from Kinetic PreProcessor to be coupled to core of Hi-VACC for handling reactions of interest.

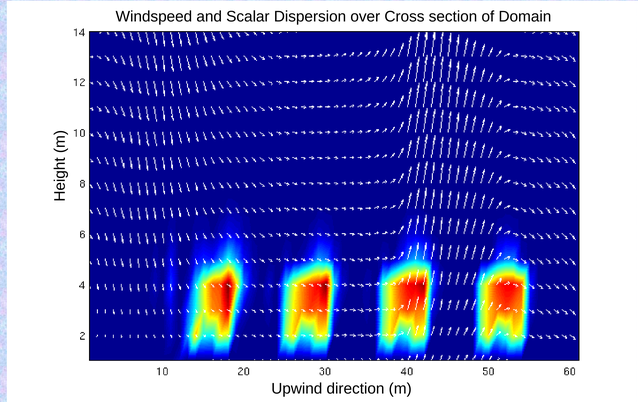


Glyoxal and Methylglyoxal pathways are of particular interest to us. Other mechanisms can be easily developed in KPP and used with KPP





Results from an evaluation simulation of Hi-VACC using forcing fields from a RAFLES simulation of a homogeneous field with weak wind and no vegetation under neutral atmospheric boundary-layer conditions. The initial scalar plume was spherical, and began close to the left edge of the portion of the domain shown.



Results from a Hi-VACC simulation over our experimental domain prescribing a scalar source at the barns using forcing fields from a RAFLES simulation of experimental conditions.

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