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Large eddy simulations as a parameterization tool for canopy-structure X VOC-flux interactions

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We have been working to develop a new post-processing model - High resolution VOC Atmospheric Chemistry in Canopies (Hi-VACC) - which resolves the dispersion and chemistry of reacting chemical species given their emission rates from the vegetation and soil, driven by high resolution meteorological forcing and wind fields from various high resolution atmospheric regional and large-eddy simulations. Hi-VACC reads in fields of pressure, temperature, humidity, air density, short-wave radiation, wind (3-D u, v and w components) and sub-grid-scale turbulence that were simulated by a high resolution atmospheric model. This meteorological forcing data is provided as snapshots of 3-D fields. We have tested it using a number of RAMS-based Forest Large Eddy Simulation (RAFLES) runs. This can then be used for parameterization of the effects of canopy structure on VOC fluxes. RAFLES represents both drag and volume restriction by the canopy over an explicit 3-D domain. We have used these features to show the effects of canopy structure on fluxes of momentum, heat, and water in heterogeneous environments at the tree-crown scale by modifying the canopy structure representing it as both homogeneous and realistically heterogeneous. We combine this with Hi-VACC's capabilities to model dispersion and chemistry of reactive VOCs to parameterize the fluxes of these reactive species with respect to canopy structure. The high resolution capabilities of Hi-VACC coupled with RAFLES allows for sensitivity analysis to determine important structural considerations in sub-grid-scale parameterization of these phenomena in larger models.