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Key Processes in Canadian Oil Sands Gas and Aerosol Chemistry Identified through Model Evaluation Against Monitoring Network and Aircraft-Based Data

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Multiple simulations were conducted using Environment and Climate Change Canada's Global Environmental Multiscale-Modelling Air-quality and CHemistry (GEM-MACH) in order to evaluate the model's predictive capabilities for concentrations, height of plume emissions, and deposition for regions within and downwind of the Canadian Oil Sands. The innermost domain of the nested setup was 1350x1345 km in extent, centered on the Canadian provinces of Alberta and Saskatchewan, with a grid-cell size of 2.5 km. Successive model science updates were carried out in a series of 15-month simulations covering the period August 1, 2017 through October 31, 2018. The simulations were compared to local (Wood Buffalo Environmental Association, Lakeland Industry and Community Association, Peace River Area Monitoring Program), provincial (Alberta Precipitation Quality Monitoring Program (APQMP)), and national (National Air Pollution Surveillance (NAPS) and Canadian Air and Precipitation Monitoring Network (CAPMoN)) monitoring network data for the entire period, as well as to aircraft and ground-based measurement intensive data from August 2017, April 2018 and June to July 2018.

The series of simulations included successive updates to the model's gas-phase chemistry, secondary organic aerosol formation, photolysis rate calculations, particle speciation, plume rise, inorganic heterogeneous chemistry, cloud processing of gases and aerosols, gas reactions on particle surfaces, the addition of a tracer for the emissions, transport and deposition of total organic carbon gas, the addition of H_2S as a transported species, and numerous updates to the model's input emissions making use of inventory and observation-based emissions. While the model evaluation is still underway, the evaluation thus far has identified key chemical and physical processes relevant to the Oil Sands area, which will be highlighted in this presentation, including:

(1) Concentrations of particulate base cations are dominated by fugitive dust, , and exhibit strong seasonality (higher in summer than winter). This seasonality can be reasonably well simulated by the model if coarse mode emissions of fugitive dust are shut off at temperatures slightly below the freezing point of water;

(2) Low biased model surface ozone predictions from January through April are potentially due to insufficient simulated Troposphere / Stratosphere exchange, in turn identifying the process as a driver for springtime ozone in the area;

(3) The concentrations of NO_2, particulate matter and nitric acid are all linked via a combination of surface reactions transforming NO_2 to HONO and HNO_3, and inorganic heterogeneous chemistry, with the former reaction probabilities being highly uncertain;

(4) Aircraft-based estimates of total organic carbon gas emissions and deposition used as a tracer within the model suggest high molecular mass hydrocarbons are emitted as gases from OS facilities and are being deposited in the surrounding area. Conventional gas-phase deposition algorithms may not explain observed deposition rates; absorptive partitioning to landscape surfaces is presented as a possible alternative pathway for deposition.

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