A New Framework for Modelling Wildfire Smoke Aerosol Concentration

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Introduction

Wildfire smoke is a primary source of particulate matter (PM) pollution. It is impractical to include more than a handful of organic aerosol precursors in partitioning schemes for PM forecasts due to the sheer number of species emitted.

Understanding the interplay between secondary organic aerosols and parcel dilution at a more detailed level is required to improve representation of wildfire emissions.

We present a setup combining observed emissions data, the F0AM 1D Lagrangian chemical box model, a new 2D-Lumping Framework, and the AIOMFAC thermodynamic model, to predict total PM concentration in a smoke plume.

Step #1: Emission Factors

We compiled a **dataset of emission factors** from biomass-burning observational sources.

The dataset is a mix of single plume, field campaign, and gas/aerosol laboratory measurements.

Where necessary, emission factors (g/kg) are converted to emission ratios (ppb/ppm CO) using a simple conversion factor.

The SMILES for each species is obtained, and the saturation vapor pressure estimated using the **UManSysProp** facility.

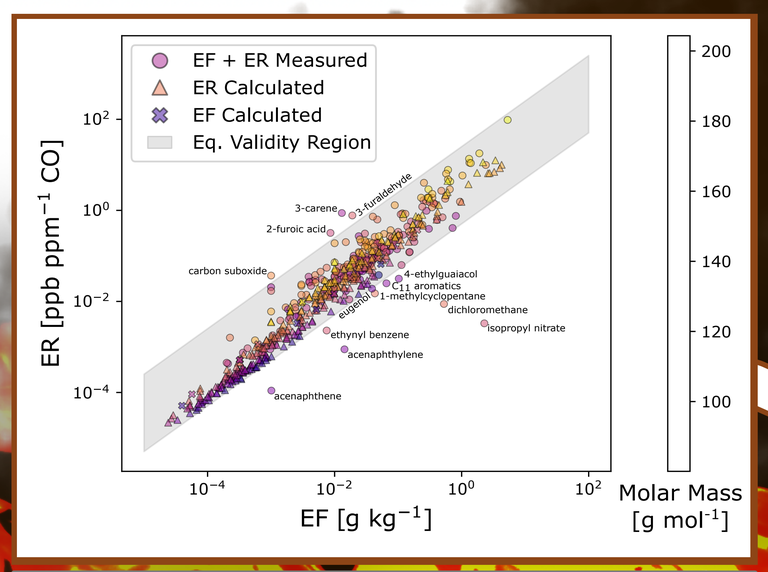

Figure 1: Comparison of reported and calculated emission ratios against emission factors for species from the datasets used.

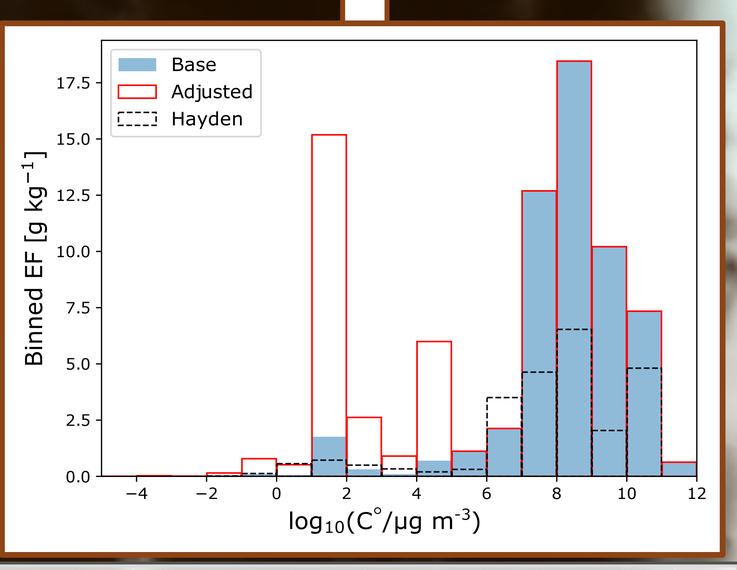

Figure 2: Volatility distributions of the compiled dataset (blue) and the non-VOC adjusted dataset (red) compared against an observed distribution by Hayden et al. (2022).

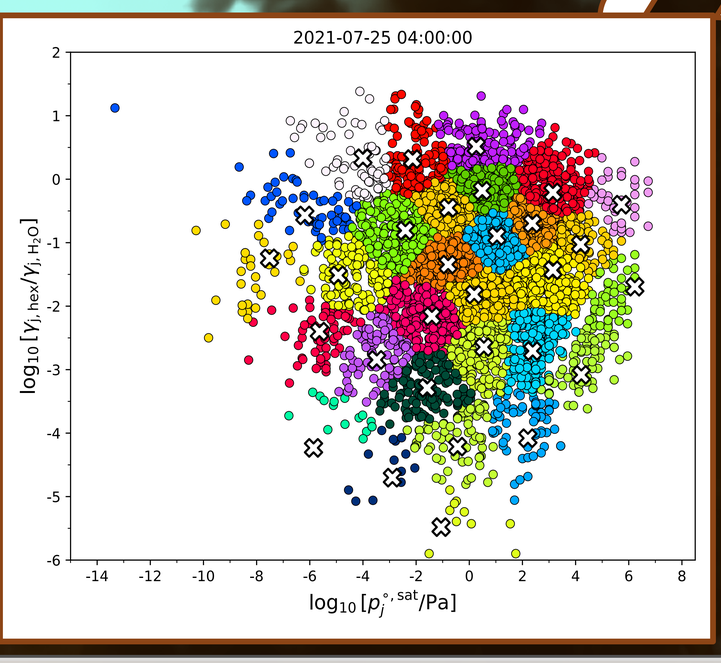

Figure 3: An example of the 2D-Lumping Framework applied on a F0AM-MCM output species case. The colors differentiate between the 30 separate clusters and crosses indicate the surrogates.

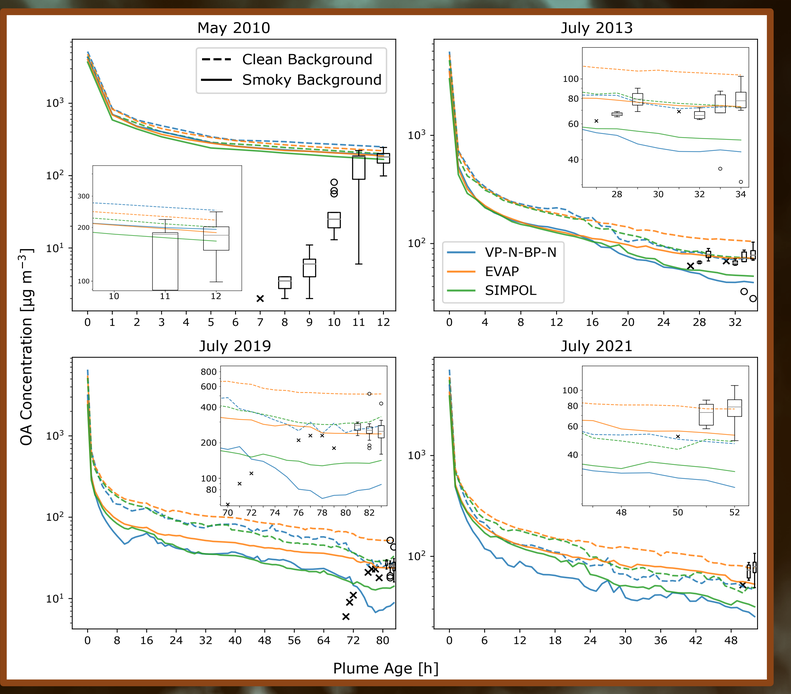

Figure 4: Preliminary predictions of the organic aerosol concentration compared against measurements by the NAPS network station data for $PM_{2.5}$ for four wildfire smoke events that affected the city of Montreal. The insets are zoomed-in views of the final hours before the plume reaches the city.

Step #2: F0AM Box Model

A **volatility distribution** is constructed using the calculated vapor pressures and the reported emission factors. **All non-VOC emission factors are scaled up** by a fixed value for the total to match a reported emission factor for organic aerosol. The emission factors are then converted to emission ratios.

An initial carbon monoxide concentration is chosen, and the emission ratios are scaled accordingly. The **F0AM chemical box model** paired with the **Master Chemical Mechanism** is then used to simulate the evolution of every species' concentration over the life time of a smoke plume.

Trajectories and meteorology from the **HYSPLIT model** are used to constrain the environmental variables.

Step #3: Lump & Partition

The species are then represented on a **2D volatility-polarity grid**. Polarity is determined by calculating the activity coefficient ratio in two distinct solvents (water and hexanediol). The species are then **lumped into a reduced number of surrogate components** to represent the entire aerosol population.

The surrogate components are used as inputs in the thermodynamic multiphase equilibrium **AIOMFAC model.** This predicts the gas-particle partitioning from the mixture of surrogate components while accounting for temperature and relative humidity.

Scan for a FAQ!

Conclusions and Future Work

This framework shows promise as a potential means of predicting total organic aerosol concentrations in wildfire smoke plumes. Work is currently being done to expand the Master Chemical Mechanism to allow for more formation of non-VOC compounds, hopefully removing the need to scale emission factors.

AIOMFAC
Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients