United States
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Agency

Development of the Simple Indoor Air Chemistry Simulator (SIACS)

Vito Ilacqua[1], Serena H. Chung[1], Anna Freitheim[2], Sharon Wildberger[3], Jordan Zambrana[4], and Randolph Chapman[5]

[1]National Center for Environmental Research, Office of Research and Development, U.S. EPA; [2]Thurston County Public Health & Social Services Department, Olympia, Washington; [3]Millekn Institute School of Public Health, George Washington University
[3]Association of Schools & Programs of Public Health Fellow at Indoor Environments Division, Office of Radiation and Indoor Air, U.S. EPA; [5]Presidential Management Fellow at Indoor Environments Division, Office of Radiation and Indoor Air, U.S. EPA

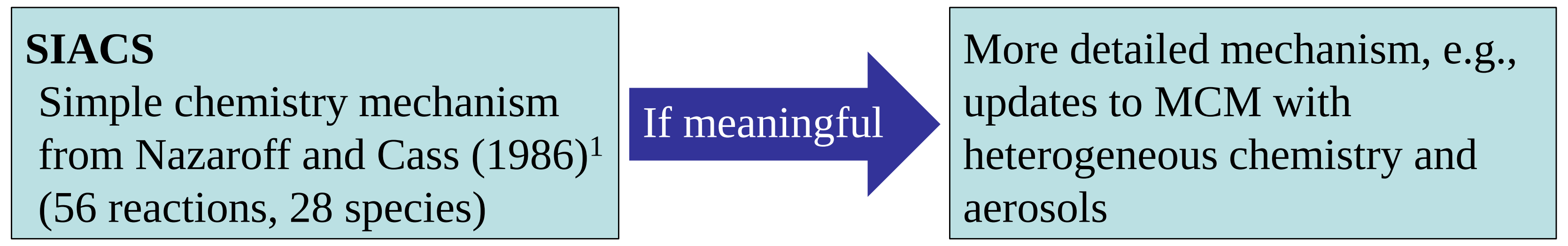
Contacts: chung.serena@epa.gov and ilacqua.vito@epa.gov

Introduction

Exposure to air pollutants occurs mostly indoors, where building characteristics, consumer products, and indoor activities, along with ambient air, all affect indoor air chemistry. Yet, the risk paradigm for ambient air pollution largely omits these factors, and epidemiological analyses leave these sources of heterogeneity uncharacterized as noise. In a changing environment, which will modify indoor-outdoor air exchange rates, the options about how to best manage indoor environments to minimize risk of air pollution become even less clear.

A comprehensive indoor air quality model can be useful to help develop public health guidelines that take into account both ambient air quality and the indoor sources in a particular environment. For example, should people ventilate their houses while cooking if they live near dense traffic? An indoor air quality model can also be useful for developing guidelines and recommendations about adapting building design and use, particularly with respect to measures that attempt to achieve higher energy efficiency by controlling infiltration. Finally, a model may also be useful to indoor air quality practitioners as a diagnostic tool for unexplained indoor sources, using reverse modeling.

A new Simple Indoor Air Chemistry Simulator (SIACS) is being developed with the objective of using it as a screening-level indoor air quality model to identify research questions to be explored with a more complex model with more detailed chemistry.



SIACS
Simple chemistry mechanism from Nazaroff and Cass (1986)[1] (56 reactions, 28 species)

If meaningful

More detailed mechanism, e.g., updates to MCM with heterogeneous chemistry and aerosols

Factors to Consider:

- Locations with different outdoor conditions
- Daytime vs. nighttime
- High outdoor pollution episodes (e.g., wildfires)
- Present vs. projected ambient concentrations
- Present vs. projected meteorological conditions
- Passive infiltration changes, window opening, weatherization

References

[1]Nazaroff WW and Cass GR, Mathematical modeling of chemically reactive pollutants in indoor air, *Environ. Sci. Technol.*, 1986.

[2]Breen et al., A review of air exchange rate models for air pollution exposure assessments, *J. Exp. Sci. Environ. Epid.*, 2014.

[3]Chan et al., Analyzing a database of residential air leakage in the United States, *Atmos., Environ.*, 2005.

[4]Breen et al., Predicting residential air exchange rates from questionnaires and meteorology: Model evaluation in central North Carolina, *Environ. Sci. & Technol.*, 2010.

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Model Formulation and Input

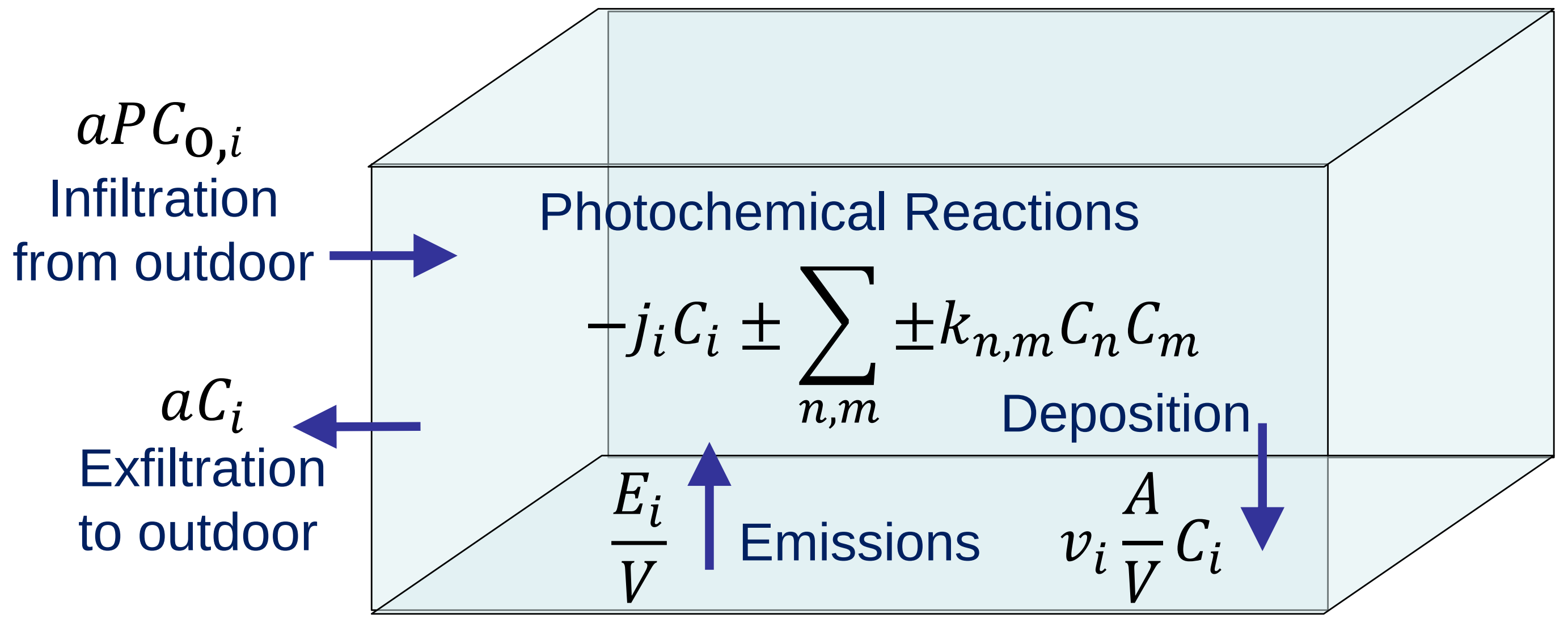

Figure 1. Processes included in the model.

The model assumes the building contains a single well-mixed zone; considers VOC-NOx-ozone chemistry; and accounts for emissions, deposition, ventilation, and filtration. Indoor concentrations of species i, C_i, is solved by mass conservation equation:

$$\frac{dC_i}{dt} = -j_iC_i + \sum_{n,m} \pm k_{n,m}C_nC_m + \frac{E_i}{V} - v_i\frac{A}{V} + C_i aPC_{o,i} - aC_i \qquad (1)$$

- Prescribed input variables for the model are listed in tables 1 and 2.
- For photochemistry, SIACS currently uses the chemical mechanisms from Nazaroff and Cass (1986)[1], where $k_{n,m}$ and j_i represent reaction and photolysis rate constants, respectively.
- The air exchange rate a accounts for air flow due to infiltration and ventilation using the extended Lawrence Berkeley National Laboratory (LBLX) parameterization[2,4]:

$$a = \sqrt{A_{\mathrm{inf}}^2(k_{\mathrm{W}}u^2 + k_{\mathrm{S}}\,|T - T_{\mathrm{o}}|) + Q_{\mathrm{vent}}^2}\;/\;V \qquad (2)$$

Table 1. Input variables with time-dependent values.

Ambient Conditions		Indoor Conditions	
T_o	Outdoor temperature	T	Indoor temperature
u	Wind speed	I_{uv}	Integrated photon flux, 300 – 400 nm
$C_{o,i}$	Outdoor concentrations of species i	I_{vis}	Integrated photon flux, 400 – 760 nm
		E_i	Emission of species i

Table 2. Descriptions of input variables related to building characteristics and values used for preliminary analysis.

Variable	Description	Notes; Values for Preliminary Analysis
V	Volume	350 m^3 (based on 140 m^2 x 2.5 m)
A_{inf}	Effective leakage area for infiltration	0.1 m^2; estimated from Chan et al. (2015)[3]
P	Penetration factor	Assumed to be 1.
Q_{vent}	Ventilation flow rate	Assumed to be 0.
k_w	Stack coefficient	0.000290 $(L/s)^2/(cm^4\ K)$; for a two-story home; Breen et al. (2010)[4]
k_s	Wind coefficient	0.000231 $(L/s)^2/(cm^4\ (m/s)^2)$; for a two-story house with typical sheltering by other houses across the street; Breen et al. (2010)[4]
v_i	Deposition velocity for species i	Depends on surface types.

Preliminary Analysis

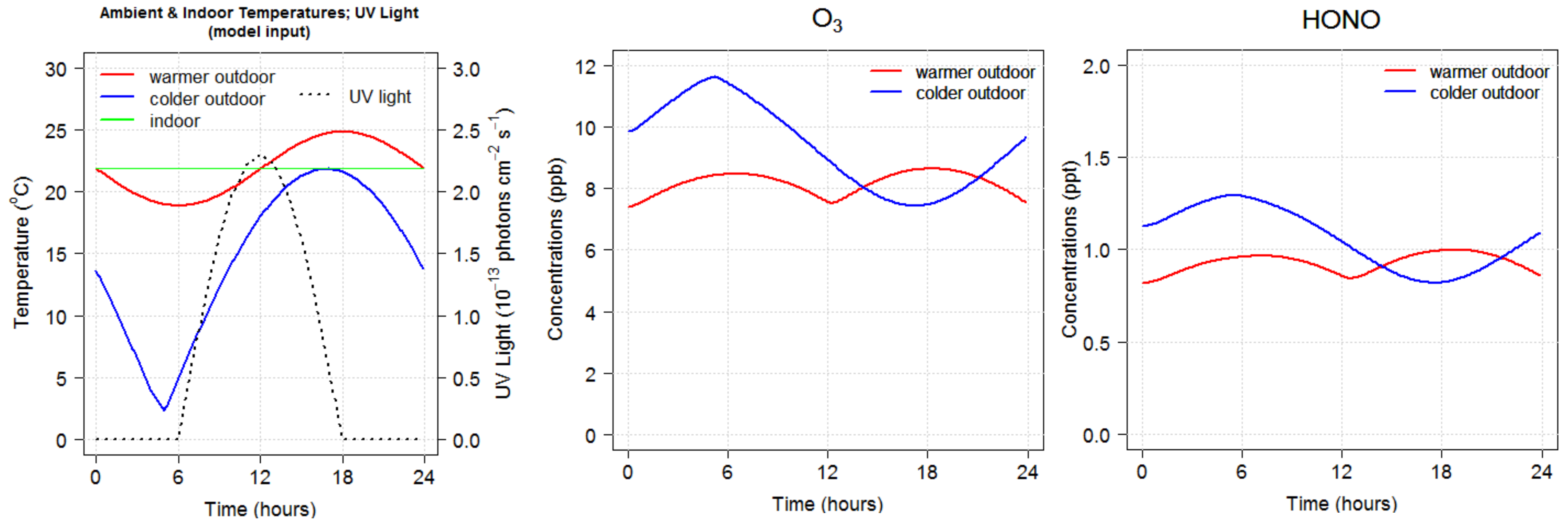

Figure 2. Comparison of modeled indoor concentrations of O_3 (middle) and HONO (right) due to difference in ambient temperature (left). The difference in ambient temperatures represent seasonal differences. The indoor temperature and UV radiation are also shown on the left panel. Results here suggest infiltration seems about as significant as indoor photochemistry on indoor O_3 and HONO levels for the simple cases of zero emissions and constant outdoor concentrations.

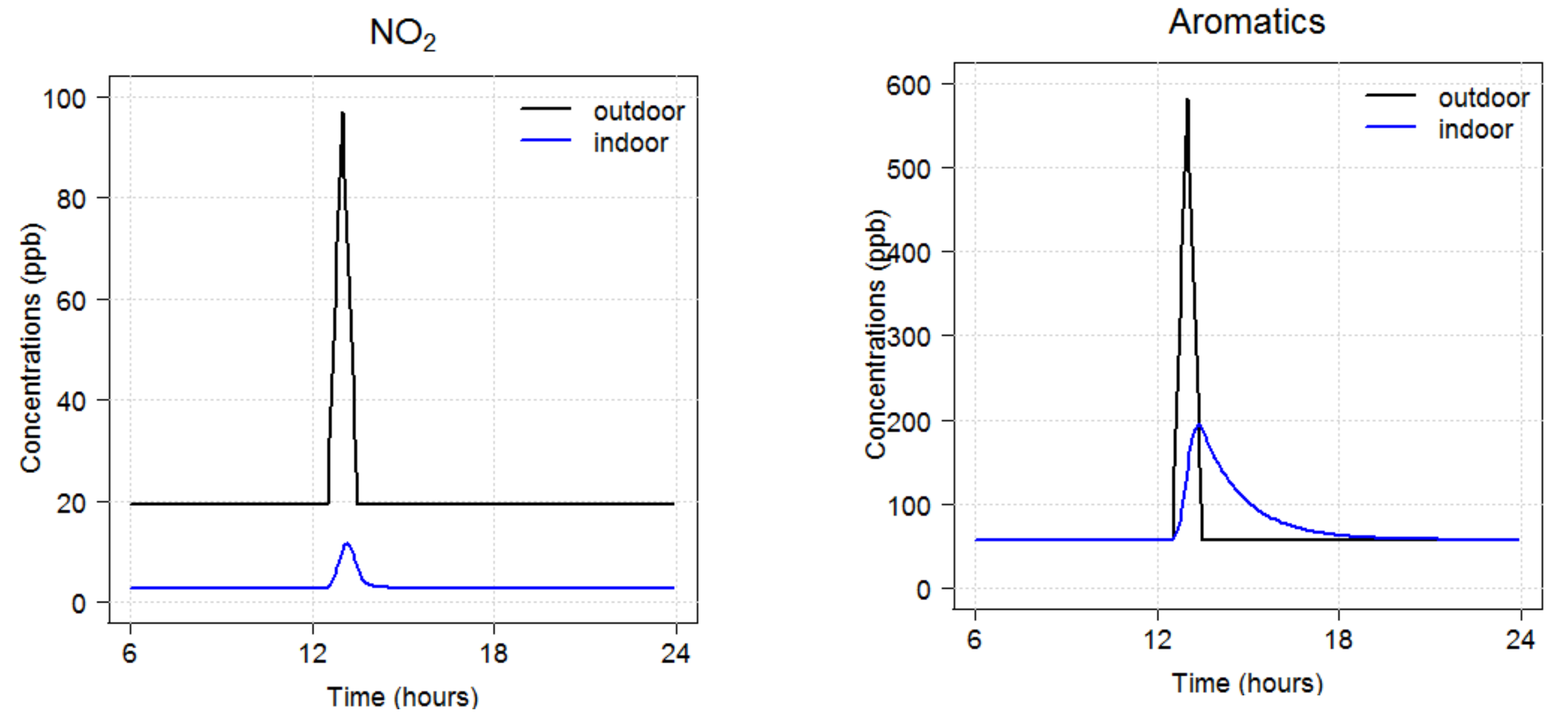

Figure 3. Modeled indoor concentrations of NO_2 (left) and aromatics (right) compared to prescribed outdoor concentrations representing the passing of an outdoor plume. Concentrations indoors, without sources, are lower mainly due to deposition and chemistry.

Summary and Next Steps

- A simple screening-level indoor air quality model is being developed based on chemistry mechanism of Nazaroff and Cass (1986)[1] and Lawrence Berkeley National Laboratory infiltration parameterization[2,4].
- Preliminary analysis suggests:
  - that infiltration due to just seasonal differences seems about as significant as the indoor photochemistry, at low levels of indoor emissions; and
  - significantly reduced exposures indoor compared to outdoors in the absence of indoor sources.
- Future work include:
  - updating the gas-phase mechanism and adding primary aerosols, secondary organic aerosol formation and heterogeneous chemistry; and
  - performing analysis with more realistic ambient conditions (temperature, wind speed, concentrations), emissions rates, indoor light conditions, and ventilation rates.