The Journal of Open Source Software

INCHEM-Py: An open source Python box model for indoor air chemistry

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DOI: 10.21105/joss.03224

Software

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Editor: David Hagan

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Submitted: 12 March 2021
Published: 12 July 2021

Summary

In developed countries people spend over 90% of their time indoors where they are exposed to airborne pollutants that are generated indoors or outdoors, some of which are harmful to human health. Occupant activities indoors such as cooking and cleaning can generate numerous chemical compounds and some of these can undergo further reactions to produce a large range of complex chemicals. Current instrumental techniques are unable to measure many of these compounds at present, so models provide the means to try and understand these processes and their impacts. The INdoor CHEMical model in Python (INCHEM-Py) is an open source and accessible box-model that has been re-factored from the indoor detailed chemical model developed by Carslaw (2007) to give researchers deeper insight into the chemical mechanisms behind indoor air chemistry.

Statement of need

Over the last 15 years, the INdoor Detailed Chemical Model (INDCM) has been used to successfully probe the chemistry of indoor air (Carslaw, 2007). However, it relies on proprietary software and requires a high level of chemistry expertise and some Fortran knowledge to edit and use the code. Software tools such as Pybox (Topping et al., 2018), PyCHAM (O'Meara et al., 2020) and AtChem2 (Sommariva et al., 2020) facilitate the use of chemical mechanisms to model atmospheric chemistry, but with a focus on chamber studies or ambient conditions. INCHEM-Py has been designed with a unique set of tools for the specific purpose of modelling indoor air chemistry. As well as a detailed gas-phase chemical mechanism, the new model includes gas-to-particle partitioning for three of the commonly encountered terpenes indoors (limonene and alpha- and beta-pinene), novel indoor photolysis parameterisation, indoor-outdoor air exchange and deposition to internal surfaces. INCHEM-Py is open source, has no black box processes and all inputs can be tracked through the model, allowing for complete understanding of the system. It has been designed to be easy to install for use by academics and students of all abilities, and is sufficiently accessible for further development by the wider indoor air community. The functionality embedded within INCHEM-Py will allow for a wide range of uses including in-depth analysis of experimental measurements, development and testing of new chemical mechanisms and probing numerous indoor scenarios, with the impacts on simulated indoor air pollutant concentrations from variations in parameters such as photolysis, ventilation and deposition rates, outdoor pollutant concentrations, time of year, and building location.

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INCHEM-Py

INCHEM-Py creates and solves a system of coupled Ordinary Differential Equations (ODEs) to progress indoor atmospheric chemical species concentrations through time. It can be used to investigate numerous indoor air chemistry events in world-wide locales providing key insights into the chemical processes involved. INCHEM-Py utilises the Master Chemical Mechanism (MCM) at its core (Jenkin et al., 1997; Saunders et al., 2003), which is near explicit and contains no lumping or use of species surrogates.

ICHEM-Py does not solve for spatial dimensions and assumes a well mixed atmosphere (Carslaw, 2007). Gas-to-particle partitioning is implemented using absorptive partitioning from Pankow (1994) with relevant reactions between particle and gas phase species included within the mechanism (Carslaw et al., 2012). Surface deposition is treated as an irreversible process with rates dependant on the simulated surface area to volume ratio and species deposition velocities (Carslaw et al., 2012). Photolysis rates can be calculated for several indoor lighting sources with different spectral profiles and also for attenuation of sunlight through multiple glass compositions (Zixu Wang, 2021). Daylight hours are derived from latitude and time of year.

The additional chemical mechanisms developed specifically for indoor air scenarios contained within the model have been utilised in a numerous published studies. These include: indoor air chemistry following cleaning with terpene based mixtures (Carslaw et al., 2017, 2012; Carslaw, 2013; Terry et al., 2014); indoor air chemistry following cleaning with chlorine containing bleach (Wong et al., 2017); the impact of outdoor vegetation on indoor air chemistry (Carslaw et al., 2015); the importance of surface interactions for secondary pollutant formation (Kruza et al., 2017); ranking of harmful volatile organic compounds (VOCs) (Carslaw & Shaw, 2019); improved model representation of the formation and composition of aerosols (Kruza et al., 2020); and photolysis of indoor air chemistry following high-concentration hospital/industrial cleaning events (Z. Wang et al., 2020). INCHEM-Py has already been used to determine production rates and reactivity of indoor radical species, to assess the spatial and temporal scales of variability for indoor air constituents (Lakey et al., 2021), and is currently being used to probe the impact of indoor air chemistry on ambient air, as well as to compare the differential secondary pollutant formation potential for different cleaning formulations.

At publication the current stable release of INCHEM-Py is v1.1.

Acknowledgements

The development of this model has been funded by a grant from the Alfred P. Sloan Foundation, grant number 2018-10083. Conclusions reached or positions taken by researchers or other grantees represent the views of the grantees themselves and not those of the Alfred P. Sloan Foundation or its trustees, officers, or staff.

References

Carslaw, N. (2013). A mechanistic study of limonene oxidation products and pathways following cleaning activities. *Atmos. Environ.*, *80*, 507–513. https://doi.org/10.1016/j.atmosenv.2013.08.034

Carslaw, N. (2007). A new detailed chemical model for indoor air pollution. *Atmos. Environ.*, *41*(6), 1164–1179. https://doi.org/10.1016/j.atmosenv.2006.09.038

Carslaw, N., Ashmore, M., Terry, A. C., & Carslaw, D. C. (2015). Crucial Role for Outdoor Chemistry in Ultrafine Particle Formation in Modern Office Buildings. *Environ. Sci. Technol.*, *49*(18), 11011–11018. https://doi.org/10.1021/acs.est.5b02241

Carslaw, N., Fletcher, L., Heard, D., Ingham, T., & Walker, H. (2017). Significant OH production under surface cleaning and air cleaning conditions: Impact on indoor air quality. *Indoor Air*, *27*(6), 1091–1100. https://doi.org/10.1111/ina.12394

Carslaw, N., Mota, T., Jenkin, M. E., Barley, M. H., & McFiggans, G. (2012). A Significant role for nitrate and peroxide groups on indoor secondary organic aerosol. *Environ. Sci. Technol.*, *46*(17), 9290–9298. https://doi.org/10.1021/es301350x

Carslaw, N., & Shaw, D. (2019). Secondary product creation potential (SPCP): A metric for assessing the potential impact of indoor air pollution on human health. *Environ. Sci. Process. Impacts*, *21*(8), 1313–1322. https://doi.org/10.1039/c9em00140a

Jenkin, M. E., Saunders, S. M., & Pilling, M. J. (1997). The tropospheric degradation of volatile organic compounds: A protocol for mechanism development. *Atmos. Environ.*, *31*(1), 81–104. https://doi.org/10.1016/S1352-2310(96)00105-7

Kruza, M., Lewis, A. C., Morrison, G. C., & Carslaw, N. (2017). Impact of surface ozone interactions on indoor air chemistry: A modeling study. *Indoor Air*, *27*(5), 1001–1011. https://doi.org/10.1111/ina.12381

Kruza, M., McFiggans, G., Waring, M. S., Wells, J. R., & Carslaw, N. (2020). Indoor secondary organic aerosols: Towards an improved representation of their formation and composition in models. *Atmos. Environ.*, *240*, 117784. https://doi.org/10.1016/j.atmosenv.2020.117784

Lakey, P., Youngbo, W., Shaw, D., Oesterstroem, F., Mattila, J., Reidy, E., Bottorff, B., Rosales, C. M., Wang, C., Ampollini, L., Zhou, S., Novoselac, A., Kahan, T. F., DeCarlo, P., Abbatt, J. P. D., Stevens, P. S., Farmer, D. K., Carslaw, N., Rim, D., & Shiraiwa, M. (2021). Spatial and Temporal Scales of Variability for Indoor Air Constituents. *Submitted for Publication in Nature Communications Chemistry*.

O'Meara, S., Xu, S., Topping, D., Capes, G., Lowe, D., Alfarra, M., & McFiggans, G. (2020). PyCHAM: CHemistry with Aerosol Microphysics in Python. *J. Open Source Softw.*, *5*(48), 1918. https://doi.org/10.21105/joss.01918

Pankow, J. F. (1994). An absorption model of the gas/aerosol partitioning involved in the formation of secondary organic aerosol. *Atmos. Environ.*, *28*(2), 189–193. https://doi.org/10.1016/1352-2310(94)90094-9

Saunders, S. M., Jenkin, M. E., Derwent, R. G., & Pilling, M. J. (2003). Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds. *Atmos. Chem. Phys.*, *3*(1), 161–180. https://doi.org/10.5194/acp-3-161-2003

Sommariva, R., Cox, S., Martin, C., Boro'nska, K., Young, J., Jimack, P. K., Pilling, M. J., Matthaios, V. N., Nelson, B. S., Newland, M. J., Panagi, M., Bloss, W. J., Monks, P. S., & Rickard, A. R. (2020). AtChem (version 1), an open-source box model for the Master Chemical Mechanism. *Geoscientific Model Development*, *13*(1), 169–183. https://doi.org/10.5194/gmd-13-169-2020

Terry, A. C., Carslaw, N., Ashmore, M., Dimitroulopoulou, S., & Carslaw, D. C. (2014). Occupant exposure to indoor air pollutants in modern European offices: An integrated modelling approach. *Atmos. Environ.*, *82*, 9–16. https://doi.org/10.1016/j.atmosenv.2013.09.042

Topping, D., Connolly, P., & Reid, J. (2018). PyBox: An automated box-model generator for atmospheric chemistry and aerosol simulations. *J. Open Source Softw.*, *3*(28), 755. https://doi.org/10.21105/joss.00755

Wang, Zixu. (2021). *Photolysis of indoor air chemistry* [PhD thesis]. The University of York.

Wang, Z., Kowal, S. F., Carslaw, N., & Kahan, T. F. (2020). Photolysis-driven indoor air chemistry following cleaning of hospital wards. *Indoor Air*, *November 2019*, 1–15. https://doi.org/10.1111/ina.12702

Wong, J. P. S., Carslaw, N., Zhao, R., Zhou, S., & Abbatt, J. P. D. (2017). Observations and impacts of bleach washing on indoor chlorine chemistry. *Indoor Air*, *27*(6), 1082–1090. https://doi.org/10.1111/ina.12402