Evaluation of Indoor Environmental Concentrations in Buildings with Conditioned and Unconditioned Zones (IECCU) model for predicting TCPP concentrations in a low-energy test house

Dustin Poppendieck[1,*]
Lisa Ng[1]
Stephen Zimmerman[1]

[1] National Institute of Standards and Technology, Gaithersburg, MD 20899
* Presenting author, dustin.poppendieck@nist.gov

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INTRODUCTION

Globally over 100,000 different chemicals are manufactured every year (Levi et al. 2018). It is impossible to measure the fate of all these chemicals in the wide range of indoor environments. The *Indoor Environmental Concentrations in Buildings with Conditioned and Unconditioned Zones (IECCU)* model, developed by the United States Environmental Protection Agency, is one model that can be used to predict potential indoor concentrations. IECCU simulates multiple well-mixed indoor zones using time dependent airflow and temperature inputs. IECCU can model emissions of semi-volatile organic compounds (SVOCs) and other compounds using a mass transfer-based approach.

For this study the IECCU model was evaluated using five years of building operational data (temperature, ventilation, and HVAC system operation) and measured airborne tris(1-chloro-2-propyl) phosphate (TCPP) concentrations from the Net-Zero Energy Residential Test Facility (NZERTF) at the National Institute of Standards and Technology (NIST). TCPP is a flame retardant and is found only in the uncovered open cell spray polyurethane foam (SPF) located in the rim joists between floors in the NZERTF.

The objective of this research was to determine how well the IECCU modeled long-term airborne TCPP concentrations.

METHODS

TCPP concentration in the basement of the NZERTF were measured using thermal desorption gas chromatograph mass spectrometer analysis over five years (Poppendieck et al. 2019). The IECCU model inputs were building and indoor environment parameters (i.e. air zones, temperature and interzonal airflows), sources and sinks of TCPP (mass transfer parameters, areas). Details on the inputs can be found in Poppendieck et al. (2021). The building configuration is shown in Figure 1.

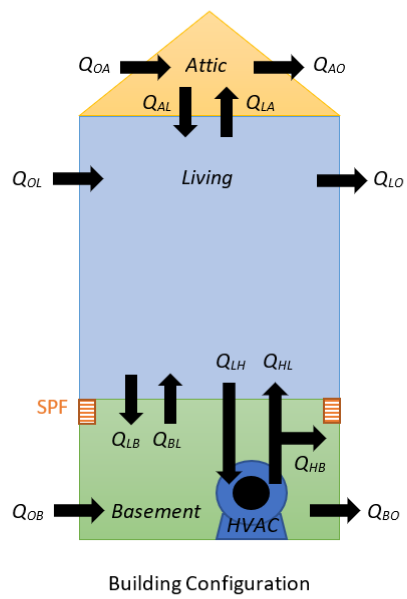

Figure 1. Building configuration used in IECCU simulations. Airflow (Q) subscripts: Outside (O), Attic (A), Living Area (L), Basement (B), HVAC system (H)

Two simulations were performed for a five-year time frame. Simulation and direct concentration measurements started roughly 1.5 years after the SPF application. Simulation 1 used quantified values for the temperature and airflows. For Simulation 1 hourly measured temperatures were averaged for each zone. Measured leakage areas (Ng et al. 2019), hourly indoor and outdoor temperatures, wind speed and direction, HVAC system airflow rates, and HRV airflow rates were used as inputs into CONTAM to determine the quantified airflows. Simulation 2 used the building design values for the temperature and airflows. A sensitivity analysis was performed to determine which of the input parameters had the biggest impact on the IECCU predictions.

RESULTS AND DISCUSSION

Overall, ratios between IECCU predictions and measurements in the basement for Simulation 1 (quantified inputs) increased with time, from 1.6 in 2015 to 4.7 in 2018. Due to diurnal temperature and airflow variations, the daily TCPP concentrations in Simulation 1 varied between 0 μg m^{-3} and 2 μg m^{-3}. Simulation 1 captured the measured concentration changes in July 2014 due to a week of flow and temperature perturbations. The design inputs for Simulation 2 (design values) resulted in predicted concentrations that were 2 μg m^{-3} to 4 μg m^{-3} higher than Simulation 1. The step changes in the Simulation 2 concentration data correspond to increased summer thermostat temperature setpoints.

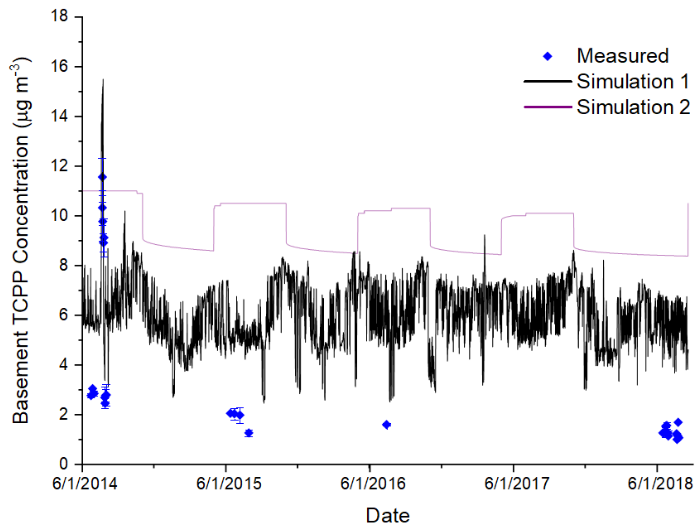

Figure 2. Comparison of TCPP concentrations in the basement simulated using quantified inputs (Simulation 1) and design inputs (Simulation 2). Error bars on triplicate measured samples represent two standard deviations.

Simulation 1 was assessed to determine which of the 20 input parameters had the biggest impact on the model output. These parameters included HVAC distribution ratios, initial TCPP concentration (C_o) along with source and sink partition coefficients (K), diffusion coefficients (D), convective mass transfer coefficient (h_m), along with source and sink depth and areas. Parameters were individually adjusted by ± 0.2, ± 2 and ± 10 based upon the estimated possible error in each parameter. The model was most sensitive to the source mass transfer parameters ($K_{SPF/a}$, $h_{m\ SPF}$, and D_{SPF}) and to the initial TCPP concentration in the SPF (C_o).

CONCLUSIONS

Over a five-year simulation period the IECCU model was able to predict TCPP concentrations within an order of magnitude, although the accuracy decreased with time. To improve the accuracy of the model, more accurate measurements of TCPP mass transfer parameters for SPF are needed, especially source/air partition coefficient ($K_{SPF/a}$) and the initial concentration of the chemical in the source material (C_0).

REFERENCES

Levi, P. G. and J. M. Cullen (2018). "Mapping Global Flows of Chemicals: From Fossil Fuel Feedstocks to Chemical Products." Environ Sci Technol **52**(4): 1725-1734. DOI: https://doi.org/10.1021/acs.est.7b04573.

Ng, L., L. Kinser, S. J. Emmerich and A. Persily (2019). Estimating Interzonal Leakage in a Net-Zero Energy House. Symposium on Whole Building Air Leakage: Testing and Building Performance Impacts**:** 211-229.

Poppendieck, D., M. Gong, L. Ng, B. Dougherty, V. Pham and S. M. Zimmerman (2019). "Applicability of Spray Polyurethane Foam Ventilation Guidelines for Do-It-Yourself Application Events." Building and Environment **157**: 227-234. DOI: https://doi.org/10.1016/j.buildenv.2019.04.033.

Poppendieck, D., M. Gong, S. Zimmerman and L. Ng (2021). "Evaluation of a four-zone indoor exposure model for predicting TCPP concentrations in a low-energy test house." Building and Environment **199**. DOI: 10.1016/j.buildenv.2021.107888.