# Estimating Organophosphate Ester (OPE) Transport, Fate and Emissions in Toronto, Canada using the Multimedia Urban Model (MUM)

T. F. M. Rodgers[1], J.Truong[1, 2], L.M. Jantunen[2,3], P. Helm[4,5], M. L. Diamond,[3,1,5]

[1]Department of Chemical Engineering and Applied Chemistry, University of Toronto, Canada; [2]Centre for Atmospheric Research Experiments, Environment and Climate Change Canada; [3]Department of Earth Sciences, University of Toronto, Canada; [4] Environmental Monitoring and Reporting Branch, Ontario Ministry of Environment and Climate Change; [5] School of the Environment, University of Toronto, Canada.

Key Words: Multimedia Urban Modelling, OPEs, Contaminant Transport & Fate, Fugacity Modelling

OPEs are a group of chemicals found at relatively high levels as environmental contaminants. The usage of OPEs has increased precipitously in recent years following the listing of penta- and octa- BDEs as POPs under the Stockholm Convention.

In this study we used the Multimedia Urban Model of Diamond and co-workers to estimate the transport, fate and emissions of three chlorinated (Cl-OPEs) and three non-chlorinated OPEs (non-Cl-OPEs) in Toronto, Canada. This model has been evaluated for PCBs and PBDEs in Toronto. The three Cl-OPEs modelled were TCPP, TCEP and TDCPP. The three non-Cl-OPEs were EHDPP, TBEP and TPhP. Our goal was to estimate their emissions to Toronto and to evaluate their environmental pathways. Aggregate emissions to the air (0-50 m elevation) were estimated by back-calculating from measured outdoor air concentrations. These results were then evaluated against measured water concentrations in Toronto tributaries.

Based on estimated emissions to air, modelled water concentrations were within an order of magnitude of the measured concentrations, ranging from 78% below for TCPP to 1900% above for TPhP, with an RMSE of 450% of the mean measured water concentration. With the exception of TCPP, the model over-estimated water concentrations. Since the water concentrations were taken independently of the air concentrations, these results gives some credence to the model estimates and showed that the emissions estimates were accurate to approximately an order of magnitude.

The emissions of OPEs ranged from 62 to 250 g/h and were significantly higher than emissions of PCBs and PBDEs calculated using the same model. We found that 40 and 55% of atmospheric loadings Cl-OPEs and non-Cl-OPEs were lost from Toronto by air advection. Twenty-one % of

Cl-OPE loadings were advected from Toronto by surface water in comparison to 5.5% for the non-Cl-OPEs. As expected, transfer from air to water was greater for these highly soluble compounds relative to PCBs and PBDEs. The difference between Cl-OPEs vs non-Cl-OPEs is consistent with their relative differences in water solubility. Degradation of OPEs ranged from 19 to 30 % of atmospheric loadings. The majority of the degradation occurred in the air and the soil phases. These model estimates provide evidence of the relatively high emission rates to air and, by showing OPE mobility in water, lend credence to the hypothesis of long-range transport of Cl-OPEs by rivers.