Honeywell RAMBOLL ENVIRONMENT & HEALTH

Memorandum

From: Kun Zhao and Krish Vijayaraghavan, Ramboll
To: Geert Boeije, Mark Boelens, and Dimitrios Papanastasiou, Honeywell
Cc: Ruth Downes, Meera Cush, and Martina Vosteen, Ramboll
Subject: Trifluoroacetic Acid (TFA) Environmental Modelling
Date: May 12, 2023

Ramboll performed on behalf of Honeywell a preliminary modeling study to assess the aquatic effect of atmospheric releases of 2,3,3,3-tetrafluoropropene (HFO-1234yf) due to deposition of trifluoroacetic acid (TFA) and subsequent fate and transport.

- ✓ **A summary of the methods and key findings is provided below.**
- ✓ **The full final report will be submitted to ECHA within the course of the ongoing public consultation.**

In the atmosphere, HFO-1234yf is oxidized to trifluoroacetyl fluoride that hydrolyses in cloud water droplets to TFA which then undergoes gas-phase removal by oxidation, wet deposition through precipitation, and dry deposition under non-precipitating conditions. In this study, it is conservatively assumed that all of the HFO-1234yf emissions are converted to TFA and deposited. The projected annual emissions rate of HFO-1234yf in Europe (7,090 tonnes in 2030) was obtained from the 2023 REACH Dossier Chemical Safety Report (CSR). This total includes releases during service life, leakage, end-of-life recovery, and Mobile Air Conditioner filling and re-fueling, and formulation. The wet and dry deposition rates of TFA resulting from these HFO-1234yf emissions were approximately derived for each sub-basin in the Rhine River watershed by using deposition modeled in a prior atmospheric deposition study (Henne et al., 2012) after scaling to account for the emissions over-estimate in Henne et al. (2012) compared to the current best estimate reported in the REACH Dossier CSR.

Ramboll then conducted fate and transport modeling to simulate the TFA concentrations in the Rhine River, based on the annual average deposition rates provided in the air analysis described above, following the methodology recommended by the United States Environmental Protection Agency (USEPA) Human Health Risk Assessment Protocol (HHRAP) for Hazardous Waste Combustion Facilities.[1]

The following mechanisms were considered in determining the TFA loading of the water column:

- Direct deposition,
- Runoff from surfaces within the watershed,
- Soil erosion over the total watershed,
- Benthic burial, and
- Discharge to ocean.

It is assumed that contributions from other potential mechanisms are negligible compared to the most relevant ones listed above. Moreover, since TFA is persistent in the environment, meaning it does not readily break down or degrade, the model did not account for any chemical or biological transformation of TFA that may occur after its deposition on the ground or water surface. Although TFA is quite volatile

[1] USEPA. 2005. Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities, Final EPA530-R-05-006: Solid Waste and Emergency Response, Washington, D.C.

as a neat solution, once it is in water, it will ionize and should not evaporate; therefore, the loss of TFA through evaporation was not considered in the model.

A series of compartment models that represent the sub-basins of the Rhine River were used to model the transport of TFA in the Rhine River system from the beginning till the end where it discharges into the ocean. The model was simulated for time periods ranging from 0.01 year to 30 years. The TFA concentration for the simulated time period in the water column for each sub-basin was predicted. Based on the simulation results, the TFA concentrations in the river system would reach steady state within an approximately two-month period. The model predicted steady-state TFA concentrations in the Rhine River sub-basins range from 1.7 µg/L for the sub-basin where the Rhine River originates from (i.e., the Alp Rhine/Lake Constance sub-basin) to 5.7 µg/L for the Delta Basin where the Rhine River reaches the North Sea.

These findings reflect the results from a simplified compartment model with assumptions and modeling parameters based on average estimates of each sub-basin or the Rhine River watershed and annual averaged deposition rates. They are aimed to provide rough estimate at the regional level but not accurate high-resolution modeling results for specific areas.