1. Derivation of Hazard Quotient

Risks were characterized using the HQ approach (Nabholz 1991). HQs can be used to characterize the probability of adverse effects to ecological receptors and often focuses on phylogenetic groups (e.g., algae, invertebrates, and fish). HQs are defined as the quotient of the PECs and PNECs:

$$HQ = \frac{PEC}{PNEC}$$

If a PEC is less than a PNEC the likelihood that an organism will be impacted by the ingredient is low. In contrast, the assumption that an adverse effect will occur if a PEC exceeds a PNEC cannot be made and further evaluation is necessary. The CPIES evaluation represents a concise risk characterization that can be used to initially screen ingredients that are of low concern from ingredients that require further consideration.

Predicted Environmental Concentration

Data regarding concentrations of ingredients in surface water in the US was sourced from reports and peer-reviewed manuscripts identified from Google Scholar searches.

For chemicals that did not have sufficient environmental monitoring data for a risk assessment, PECs were modeled with the Exposure and Fate Assessment Screening Tool (E-FAST) Version 2.0 used by the US Environmental Protection Agency (EPA) (EPA 2013). Modeling is conducted by tracking the mass of the ingredient during the "life-cycle" of the product (Fig.1). Ingredients enter the US by import or manufacture. Ingredients are then used to formulate various products, some of which are not household cleaning products. Then, cleaning products are used in households prior to disposal via drains and landfills (products wiped from surfaces with disposable materials). Once disposed via drains, ingredient concentrations are diluted as a portion of the spent product is mixed with water from bathrooms, kitchens, and other plumbing components and disposed via sanitary sewer systems. Household water is transported to a wastewater treatment facility and treated water is released to receiving water bodies. The calculation for the conservative PEC requires estimates of the ingredient mass, the percent of the ingredient that is removed by wastewater treatment by biological degradation and sorption to sludge as well as estimates of dilution as wastewater effluents are diluted and enter receiving systems.

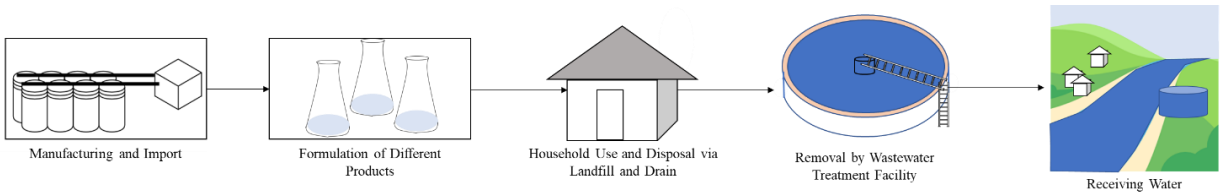

Fig. 1. Conceptual model of ingredient "life-cycle"

The conservative ingredient mass estimate is sourced from data on the total mass of an ingredient imported and manufactured in the US from ChemView (EPA 2020b). Contained in this database is Chemical Data Reporting (CDR) information inclusive of mass ranges of ingredients by year. The maximum mass for the most recently reported year was used for modeling. This information can be limited for some chemicals as manufacturers and importers can specify that the mass of the chemical is considered confidential business information.

For ingredients that did not have a reported mass, a 95th percentile (n=115) of the reported ingredient masses was used as a common value for these ingredients allowing calculation of the PEC. Ten

ingredient masses were three to six orders of magnitude greater than the other ingredients. These ten ingredients were glycerol (56-81-5); 1,2-propanediol (57-55-6); diethanolamine (111-42-2); naphtha, petroleum, light alkylate (64741-66-8); urea (57-13-6); 2-methylpropane (75-28-5); n-butane (106-97-8); propane (74-98-6); distillates, petroleum, hydrotreated middle (64742-46-7); and ethanol (64-17-5). A literature search was performed to identify if a portion of the ingredient masses was utilized for products that were not household cleaners. From this literature search, the percent of the ingredient used for cleaning products or the percent associated with the primary use of the ingredient were identified (e.g., fertilizer for urea, fuel for ethanol). The associated mass from the primary use of the ingredient was then subtracted from the maximum mass. The propellants 2-methylpropane (75-28-5), n-butane (106-97-8), and propane (74-98-6) are used as aerosols in household cleaning products. Of the reported uses available from the CDR database for these ingredients, the majority of the records indicate that they are used as intermediates for the production of other compounds and as fuels and fuel additives. We assumed that the majority of these ingredients would volatilize following use in aerosol sprays and therefore would not be disposed via a drain. These ingredients are therefore not representative of ingredients that may enter surface waters following wastewater treatment and their masses were not included in the calculation of the 95th percentile. The 95th percentile of the remaining ingredient masses was 1 billion pounds.

To refine the PEC calculation further, percent removals of ingredients in wastewater treatment facilities were modeled using the EpiSuite™ 4.11 Sewage Treatment Plant (STP) model (EPA 2020a). The models in EpiSuite™ 4.11 can be used to estimate percent removals based on information contained in internal databases (physical property data), data from chemicals with similar structures, or modeled physical properties. The BIOWIN model of EpiSuite™ 4.11 can be used to estimate biological degradation or the user can enter specific biological degradation rates to be used in EpiSuite™ 4.11. Percent biological degradation was sourced from the Organization for Economic Co-operation and Development's eChemPortal database (OECD 2020) when data from ready and inherent biological degradation test results were available. Percent biological degradation from ready and inherent tests were assigned removal rates for input to EpiSuite™ 4.11 using EPA's interim guidance (EPA 2000).

Final PEC refinement for this initial screen used modeling with E-FAST (EPA 2014) and the Down-the-Drain model. Inputs for this model were maximum masses or the estimated 95th percentile for ingredients and estimated percent removals from wastewater treatment facilities from the aforementioned sources. E-FAST estimated surface water concentrations based on dilution that would occur in a wastewater treatment facility and as treated water mixes with receiving water.

Predicted No Effect Concentration

The Health and Environmental Science Institute's (HESI) EnviroTox Platform (HESI 2019) was used for identification of PNECs for ingredients contained in household cleaning products. The EnviroTox Platform was selected because data are sourced from a comprehensive list of databases containing empirical data. These databases include European Chemicals Agency (ECHA) Registration, Evaluation, Authorization and Restriction of Chemicals (REACH), EPA Ecotoxicology Knowledgebase (ECOTOX), peer-reviewed literature, Japanese Ministry of the Environment (METI), US Geological Survey acute toxicity test results and studies used to develop Quantitative Structure Activity Relationships (QSARs) including Ecological Structure Activity Relationship (ECOSAR) training data sets. The full details of data compilation can be found in the EnviroTox Platform User Guide (HESI 2018). Because information contained in EnviroTox was compiled from a multitude of sources, duplicative data are available for ingredients from sources that cite the same toxicity test. Data sourced from EnviroTox were reviewed to remove duplicative data that could artificially increase or decrease the PNEC. Duplicative effect concentrations were removed that had the same source (source formatting different), different durations

(effects recorded at multiple times for the same test or durations expressed in days and hours), and different response measurements (growth, mortality, and immobilization were equally sensitive response measures for the same test). For duplicative data, results that represented more definitive effects (e.g., mortality is more definitive than intoxication) were retained for derivation of PNECs. For data that were duplicative because 2 durations were presented for the same test (e.g., mortality occurred at day 3 of a 4-day test and data for both durations were reported), data from the shorter duration were retained to derive PNECs.

If there were no empirical data within the EnviroTox Platform, EPA's ECOSAR software was used (EPA 2019). The ECOSAR software uses structure activity relationships to predict lethal concentrations for 50% of organisms (LC_{50}s) and chronic values for different ingredients. Relationships between Kow, alkyl chain lengths, or number of ethoxylates and effect concentrations for specific chemical classes (e.g., neutral organics, aldehydes, cationic surfactants, neutral surfactants) are used for predictions within ECOSAR. The predicted acute LC_{50} or effect concentration for 50% of organisms (EC_{50}) from the most sensitive taxonomic group were used. Assessment factors ranged from 40 (algae) to 50 (fish and daphnids). The assessment factor for the acute to chronic ratio was 4 for algae and 5 for daphnids and fish. The assessment factor to convert from the chronic toxicity value (with acute to chronic ratio) to the concentration of concern used to calculate the HQ was 10 (EPA 2013)

ECOSAR predictions were not used for ingredients that had structures that could not be identified as an existing ECOSAR chemical class and structures that did not meet the structural characteristics of an ECOSAR chemical class based on individual review. PNECs were derived from ECOSAR results using EPA guidance (EPA 2013).