Environment International 94 (2016) 674–686

Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint

Tracking chemicals in products around the world: introduction of a dynamic substance flow analysis model and application to PCBs

Li Li [a,b,*], Frank Wania [b]

[a] College of Environmental Sciences and Engineering, Peking University, 5 Yiheyuan Road, Beijing, 100871, P.R. China
[b] Department of Physical and Environmental Sciences, University of Toronto Scarborough, 1095 Military Trail, Toronto, Ontario M1C 1A4, Canada

ARTICLE INFO

Article history:
Received 15 April 2016
Received in revised form 20 June 2016
Accepted 6 July 2016
Available online 16 July 2016

Keywords:
Chemical in product
PCBs
Substance flow analysis
Anthroposphere
Emission
Flow

ABSTRACT

Dynamically tracking flows and stocks of problematic chemicals in products (CiPs) in the global anthroposphere is essential to understanding their environmental fates and risks. The complex behavior of CiPs during production, use and waste disposal makes this a challenging task. Here we introduce and describe a dynamic substance flow model, named *Chemicals in Products - Comprehensive Anthropospheric Fate Estimation* (CiP-CAFE), which facilitates the quantification of time-variant flows and stocks of CiPs within and between seven interconnected world regions and the generation of global scale emission estimates. We applied CiP-CAFE to polychlorinated biphenyls (PCBs), first to evaluate its ability to reproduce previously reported global-scale atmospheric emission inventories and second to illustrate its potential applications and merits. CiP-CAFE quantifies the pathways of PCBs during production, use and waste disposal stages, thereby deducing the temporal evolution of in-use and waste stocks and identifying their long-term final sinks. Time-variant estimates of PCB emissions into air, water and soil can be attributed to different processes and be fed directly into a global fate and transport model. By capturing the international movement of PCBs as technical chemicals, and in products and waste, CiP-CAFE reveals that the extent of global dispersal caused by humans is larger than that occurring in the natural environment. Sensitivity analysis indicates that the model output is most sensitive to the PCB production volume and the lifetime of PCB-containing products, suggesting that a shortening of that lifetime is key to reducing future PCB emissions.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

Enormous regulatory concerns and research interests surround the issue of problematic high production volume industrial or commercial chemicals that are embedded in consumer products (briefly chemicals in products, or CiPs), such as polychlorinated biphenyls (PCBs), brominated flame retardants (BFRs) and poly- and perfluoroalkyl substances (PFASs) (Fantke et al., 2015; Kogg and Thidell, 2011; Massey et al., 2008). These compounds originate from the *anthroposphere*, i.e., "the part of the environment that is made or modified by humans" (Kuhn and Heckelei, 2010), and migrate into the natural *environment*, which is an aggregate of atmosphere, hydrosphere and pedosphere. Generally, the fate of CiPs within the anthroposphere involves complicated, time-variant flows between multiple stocks, which, together with their complex environmental fluxes and reservoirs, makes it challenging to fully account for their overall global fate over time (Lohmann et al., 2007; Nizzetto et al., 2010). The PCBs are a well-documented example; they remain globally ubiquitous several decades after their production and new uses were prohibited. While the ubiquity of PCBs has been attributed largely to long-range atmospheric transport, international trade in waste electric and electronic equipment (WEEE) has recently been identified as an additional "important" driving force for their global dispersal (Breivik et al., 2016; Breivik et al., 2011). Meanwhile, whereas the continuous presence of PCBs has been ascribed to a large extent to their persistence in the environment, recent evidence indicates that the continuous releases of PCBs from legacy in-use [e.g., PCB-containing joint sealants in service (Diefenbacher et al., 2016; Kohler et al., 2005; Robson et al., 2010)] and waste stocks (Gioia et al., 2011; Hermanson and Johnson, 2007) contribute as well. Therefore, a comprehensive description of flows and stocks of CiPs in the anthroposphere is believed to be an essential prerequisite for appraising their global environmental fate and risk, as well as managing their associated waste in an environmentally sound manner.

To date, certain aspects of anthropospheric flows and stocks have been characterized for selected CiPs using different methodologies. For instance, using a mass balance approach to estimate the global atmospheric emissions of PCBs from 1930 to 2100, Breivik et al. (2002, 2007, 2016) accounted for emissions during product use and waste disposal but ignored those from industrial sources such as production and formulation (Breivik et al., 2010). By contrast, using an emission factor

* Corresponding author at: College of Environmental Sciences and Engineering, Peking University, 5 Yiheyuan Road, Beijing 100871, P.R. China.
E-mail addresses: lili.env@pku.edu.cn, li.environ@gmail.com (L. Li).

http://dx.doi.org/10.1016/j.envint.2016.07.005
0160-4120/© 2016 Elsevier Ltd. All rights reserved.

approach to quantify global emissions of perfluoroalkyl carboxylic acids (PFCAs) from 1951 to 2030, Wang et al. (2014a) concentrated on industrial sources but paid limited attention to emissions of PFCAs and their precursors from end-of-life disposal activities. While it may often be justified to omit less important lifecycle stages for a specific CiP if they do not contribute significantly to overall emissions, incomplete emission inventories, as well as incompatible source divisions therein, hinder a comprehensive, standardized comparison of inventories of the anthropospheric flows and stocks among different CiPs, which would be required for more general, universal conclusions on the anthropospheric behaviors of CiPs.

Meanwhile, a rather limited number of studies have established comprehensive linkages among (i) different anthropospheric in-use and waste stocks, (ii) internal flows within the anthroposphere, and (iii) emissions through the anthroposphere-environment interface, to create a full picture of the anthropospheric fates of CiPs (Abbasi et al., 2015; Earnshaw et al., 2013; Li et al., 2016). For instance, some studies (Tasaki et al., 2004; Vyzinkarova and Brunner, 2013) estimated the stocks of CiPs in commodities or waste but their scope did not include the estimation of emissions. While in some cases (e.g., Morf et al., 2005) such stock analyses can be evaluated on local or regional scales, emission estimates can be fed into environmental fate models to generate estimates of environmental concentrations that can be compared with measurements on a larger global scale. Meanwhile, other studies (Paul et al., 2008; Prevedouros et al., 2006; Sakai et al., 2006) calculated CiP emissions based on rough, static estimates of existing stocks instead of estimating them dynamically from time-dependent input data such as historical production, consumptions and probabilistic lifespan distribution of products. Such an approach cannot characterize the temporal postponement of emissions that can result from temporal "buffer" effects of stocks (van der Voet et al., 2002), thus impeding a further investigation of possible stock management strategies. Furthermore, recent studies have recognized the importance of selected flows in influencing the anthropospheric fate of CiPs, such as (i) chemical flows among different geographic regions that are implicit in the international movement of WEEE (Breivik et al., 2016; Breivik et al., 2011), and (ii) inadvertent recycled chemical flows due to the incomplete destruction of the chemical during material recycling with inadequate identification or separation techniques (Puype et al., 2015; Samsonek and Puype, 2013). These internal flows have often been overlooked in previous anthropospheric fate studies.

In an effort to overcome the limitations in current anthropospheric fate studies, we introduce here a new dynamic substance flow model, named *Chemicals in Products - Comprehensive Anthropospheric Fate Estimation* (CiP-CAFE), as an easy-to-use, standardized, holistic, and verifiable tool to track the global-scale long-term anthropospheric fates for generic CiPs. Provided with basic information for a chemical and its associated products, CiP-CAFE generates temporally- and spatially-explicit estimates of the stocks and flows of CiPs from cradle to grave in the global *anthroposphere*. This information can be further fed into multimedia environmental fate models to investigate the behavior of CiPs in the natural *environment*. For illustration, CiP-CAFE is applied to PCBs and the estimates of stocks and emissions are evaluated by comparisons with those from previous studies; furthermore, the fate of PCBs in the anthroposphere is discussed with the intention to highlight potential applications of this model.

2. Model description

2.1. Basic structure of the CiP-CAFE model

In CiP-CAFE, the world is split into seven regions (Fig. 1a) according to (i) the development of the regional chemical industry, (ii) the status of sound management of chemicals and municipal solid waste (MSW), and (iii) major international trade origins/destinations of chemical-related products (Sigman et al., 2012; UNEP, 2012). Each region is divided into three interconnected *phases* (Fig. 1b), each of which further consists of a set of sequential or parallel *processes* that represent events related to the CiP of interest, e.g., transformation or accumulation (Baccini and Brunner, 2012; Pauliuk et al., 2015). The three phases are the:

(i) *Life Cycle* (LC) of the chemical and its associated products. It encompasses five sequential processes: production (LC1), formulation (LC2), processing (LC3), use (LC4) and in service (LC5); definitions of individual stages are provided in Text S1 in the Supporting Information. This process division is applicable to various CiPs as it is in accordance with the standardized risk assessment framework for chemicals in the EU-Technical Guidance Documents (European Chemicals Bureau, 2003). LC1–LC3 are categorized as *industrial* processes and LC4 and LC5 as *domestic* processes. At process LC2 and continuing to process LC5, a compound is allocated to up to five distinct parallel *applications* (APs) according to region-specific and time-variant distribution ratios; the distribution ratios of all APs sum up to 100% for each single year.

(ii) *Waste Disposal* (WD) of the chemical-related industrial and domestic waste. CiP-CAFE considers five disposal approaches for *general* industrial and end-of-life waste: landfill (WD1), wastewater treatment plant (WWTP, WD2), dumping and simple landfill (WD3), formal MSW incineration (WD4), inadvertent recycling of a CiP along with general MSW recycling/recovery (WD5); and additionally two disposal approaches for *CiP-specific* end-of-life waste: an inappropriate disposal approach that should be avoided (WD6, e.g., rudimentary dismantling and open burning of WEEE) and an environmentally-sound disposal approach (WD7, e.g., best available technique or best environmental practice recommended by the Stockholm or Basel Conventions) (Text S1).

(iii) *Environment* (E) that involves three receiving compartments of the chemical: atmosphere (E1), hydrosphere (E2) and pedosphere (E3).

The movements of a compound between processes are expressed as *flows* (Baccini and Brunner, 2012; Pauliuk et al., 2015), e.g., international trade flows among regions within the anthroposphere (internal flows) or emissions from the anthroposphere to the environment (interphase flows). Inflows and outflows that are associated with a process determine the net accumulation of a compound in the process; this net accumulation is described using as a state variable, *stock* (Fig. 1b). A process is *continuous* if the stock is not always zero, e.g., in-use stock of CiPs in service life (LC5) and waste stock in landfill (WD1); otherwise, the process is *transient* (or *instantaneous*), e.g., generally there being no chemical stockpiles awaiting sale in production (LC1) because most CiPs are manufactured in a build-to-order manner.

2.2. Mass balance equations

CiP-CAFE incorporates two modes (Müller et al., 2014) to calculate flows and stocks of CiPs in the anthroposphere: (i) the *top-down* mode starts the calculation from the production (LC1) process; this mode relates the change of chemical mass within individual LC (Eq. 1) or WD (Eq. 2) processes with the flows that enter and depart from the process using first-order differential equations (the subscripts in the equations are defined in Table 1):

$$\frac{dM(t)_{RE(i),LC(j),AP(k)}}{dt} = INFLOW(t)_{RE(i),LC(j),AP(k)} - OUTFLOW(t)_{RE(i),LC(j),AP(k)} \quad (1)$$

$$\frac{dM(t)_{RE(i),WD(m)}}{dt} = INFLOW(t)_{RE(i),WD(m)} - OUTFLOW(t)_{RE(i),WD(m)} \quad (2)$$

Download English Version:

https://daneshyari.com/en/article/6312917

Download Persian Version:

https://daneshyari.com/article/6312917

Daneshyari.com