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CoZMo-POP 2 – A fugacity-based dynamic multi-compartmental mass balance model of the fate of persistent organic pollutants

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Abstract

CoZMo-POP 2, a dynamic multimedia fate and transport model (MFTM) for describing the long-term fate of persistent organic pollutants (POPs) in a coastal environment or the drainage basin of a large lake is described. The modelled environment, consisting of up to 19 compartments, includes the forest, soils and fresh water bodies of the drainage basin, and a variable number of sequentially arranged marine water units, representing estuarine, coastal, open and deep water environments. Two sediment compartments in each water basin allow to account for the possibility of the simultaneous occurrence of eroding and accumulating bottoms in a water basin. As the movement of POPs in the environment is closely associated with the movement of air, water and organic matter, the model constructs complete steady state mass budgets for air, water and particulate organic carbon (POC) between the model compartments from the environmental parameters supplied by the user. This assures that these input parameters, which can be stored in a database, are all mutually compatible and internally consistent. The CoZMo-POP 2 model takes into account seasonably variable wind speeds, temperatures, canopy developments and OH radical concentrations, and allows for the definition of time-variant emission scenarios. CoZMo-POP 2 is a flexible, dynamic MFTM that can be used for detailed investigation of a particular fate process using a generic environmental scenario, as well as for simulations of the behaviour of a particular POP in a particular environment. All of the model equations, which are expressed in fugacity notation, are provided.
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Keywords: Fugacity; Multimedia model; Persistent organic pollutants; Non-steady state; Level IV

Software availability

Program title: CoZMoPOP2.exe
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Year first available: 2000 (CoZMo-POP 1.0)
Hardware required: IBM compatible PC
Software required: Microsoft Windows 95 or later and WinZip (http://www.winzip.com)
Program language: Microsoft Visual Basic 6.0

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Program size: 2.8 Mb (zipped)/4.5 Mb (unzipped)
Availability and cost: Freely downloadable from http://www.utsc.utoronto.ca/~wania/ upon request by e-mail to frank.wania@utoronto.ca

1. Introduction

Some organic contaminants have the tendency to occur in more than one environmental medium (air, water, and soil) in appreciable amounts. Atmospheric, oceanic and riverine dispersion models alone are thus not suitable for describing comprehensively the transport behaviour of these chemicals. In fact, the exchange of these chemicals between the various environmental media may often be more important for their environmental fate than the advective transport within these environmental media. So-called multimedia fate and transport models (MFTMs) have been developed and used for many years to simulate the fate of such contaminants (Mackay, 2001; Cowan et al., 1995). These models are generally very simple, often lack spatial resolution, and assume steady state, or even equilibrium distribution between the environmental media (Wania and Mackay, 1999). Despite, or maybe because of, their simplicity, they have proven very useful, if not for reproducing or forecasting the real historical fate of a contaminant, then for assessing evaluatively the overall transport and distribution behaviour of organic chemicals. Examples of such use are the estimation of overall persistence and potential for long-range transport (e.g. Scheringer, 1996; Bennett et al., 1999, 2001), or the estimation of multiple exposure pathways (e.g. McKone and MacLeod, 2003; Babendreier and Castleton, 2005).

Most generic MFTMs in common use are steady state models, i.e. they assume that neither chemical emissions, nor environmental parameters change in time, and that the sum of the chemical fluxes in and out of the various model compartments balances each other at any time. Whereas this limitation is justified for many model applications, it is not when the temporal variability of chemical fate and exposure is of interest. The use and emission of chemicals is hardly ever constant on any time scale. For example, pesticide use is higher during the growing season, and the emission of synthetic chemicals increases and declines on longer time scales according to production and use (e.g. Pacyna et al., 2003). Similarly, the environment is undergoing constant change, e.g. on a diurnal, seasonal and a multi-year time scale, and many time-variant environmental factors (e.g. temperature) have an impact on organic chemical behaviour. But even for time-invariant emissions and environments, steady state assumptions may not be valid. This is particularly relevant for chemicals with very slow degradation half lives, which take a very long time for establishing steady state distributions in the environment.

As a result of the limitations of steady state models, several dynamic MFTMs have been developed and used over the years (e.g. Harner et al., 2001; Breivik and Wania, 2002). What has been missing so far, however, is a generic and flexible MFTM that can be adapted to a variety of applications requiring dynamic approaches without the need to change the source code. Here we present such a model, which is called CoZMo-POP 2 (Coastal Zone Model for Persistent Organic Pollutants – Version 2). CoZMo-POP 2 is a non-steady state MFTM for describing the long-term fate of persistent organic pollutants (POPs) in a coastal environment or the drainage basin of a large lake. The design specifications for this model were: (i) The model should be suitable primarily for substances with the partitioning and degradation characteristics of POPs, because it is for these substances that MFTMs are most appropriate (Wania and Mackay, 1999); (ii) The model should be capable of describing the chemical delivery to, and transport within, a wide variety of water bodies and their drainage basin, because it is often aquatic ecosystems that are impacted the most by POPs; (iii) The model should be dynamic and allow for user-defined time-variant emissions, and for seasonally variable environmental parameters, because the seasonal and multi-year time scale is of most interest for POPs.

2. System definition in CoZMo-POP 2

The main rationale for the development of CoZMo-POP 2 was to provide a tool for quantifying environmental pathways, in particular the riverine and atmospheric pathways for delivering POPs to a marine or lake ecosystem, and the transport of POPs within the water body by both water currents and relocating sediments (Fig. 1). The description of the drainage basin is restricted to those aspects that influence the magnitude and the timing of POP delivery to the aquatic system. This implies that the model aims to describe accurately the rates of release (and the seasonal change of this release) of POPs from the main terrestrial storage media for POPs, i.e. soil and vegetation, into the two transport media delivering POPs to the aquatic environment, i.e. atmosphere and fresh water. Vegetation and soil have to be treated separately, if their characteristics of exchange with the atmosphere are different. This is the case for forests, which display much faster uptake for many POPs than grassland and fields planted with agricultural crops (McLachlan and Horstmann, 1998). Key processes are the two-directional exchange, or cycling, of POPs between the atmosphere and aquatic and terrestrial surfaces, and the uni-directional run-off of chemical from soil to fresh water and further to the marine system. Important are further the processes that could lead to loss of chemical during the transport in

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