



Modeling the air–soil transport pathway of perfluorooctanoic acid in the mid-Ohio Valley using linked air dispersion and vadose zone models

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ABSTRACT

As part of an extensive modeling effort on the air–soil–groundwater transport pathway of perfluorooctanoic acid (PFOA), this study was designed to compare the performance of different air dispersion modeling systems (AERMOD vs. ISCST3), and different approaches to handling incomplete meteorological data using a data set with substantial soil measurements and a well characterized point source for air emissions. Two of the most commonly used EPA air dispersion models, AERMOD and ISCST3, were linked with the EPA vadose zone model PRZM-3. Predicted deposition rates from the air dispersion model were used as input values for the vadose zone model to estimate soil concentrations of PFOA at different depths. We applied 34 years of meteorological data including hourly surface measurements from Parkersburg Airport and 5 years of onsite wind direction and speed to the air dispersion models. We compared offsite measured soil concentrations to predictions made for the corresponding sampling depths, focusing on soil rather than air measurements because the offsite soil samples were less likely to be influenced by short-term variability in emission rates and meteorological conditions. PFOA concentrations in surface soil (0–30 cm depth) were under-predicted and those in subsurface soil (>30 cm depth) were over-predicted compared to observed concentrations by both linked air and vadose zone model. Overall, the simulated values from the linked modeling system were positively correlated with those observed in surface soil (Spearman's rho, $R_{sp} = 0.59–0.70$) and subsurface soil ($R_{sp} = 0.46–0.48$). This approach provides a useful modeling scheme for similar exposure and risk analyses where the air–soil–groundwater transport is a primary contamination pathway.

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1. Introduction

Ammonium perfluorooctanoate (APFO) is one of the major environmental contaminants of concern in the United States, and its use is growing worldwide. APFO has been used as a surfactant in the manufacture of Teflon[®] and other fluoropolymers by the DuPont Washington Works Facility in Parkersburg, West Virginia, since the early 1950s. There are extensive ongoing efforts to

understand past, present, and future levels of APFO contamination surrounding that specific site (Paustenbach et al., 2007; DuPont, 2008; Shin et al., 2011a). APFO is of recent concern to toxicologists and epidemiologists due to potential liver toxicity, tumorigenicity, dislipidemia, immunotoxicity, and developmental effects (Steenland et al., 2010). Animal studies showed several toxic effects of APFO (Abdellatif et al., 1991; Nilsson et al., 1991; Kennedy et al., 2004; Luebker et al., 2005; Lau et al. 2006, 2007), but little information is available for human health effects of APFO (Steenland et al., 2010). Due to potential adverse health effects, the presence of dissociated APFO in local water supplies has motivated the study of human exposures for residents living near the facility (Emmett et al., 2006; Frisbee et al., 2009; Steenland et al., 2009; Shin et al., 2011b).

APFO is a white solid at ambient temperature, but exists as a vapor when it exits the hot dryer of the facility. When the hot APFO vapor exits through stacks, it tends to condense to form

Abbreviations: AERMOD, American Meteorological Society/EPA Regulatory Model; EPA, Environmental Protection Agency; ISCST3, Industrial Source Complex Short Term version 3; PFOA, perfluorooctanoic acid; PRZM-3, Pesticide Root Zone Model version 3.

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fumes which consist of fine particulates (Seidel et al., 1991; Mendez et al., 2000; Oberdorster et al., 2000). Within several minutes in ambient environments, it coagulates and forms micron-sized particulates ranging from 0.1 to 1 μm in aerodynamic diameter (U.S. EPA, 1990; Seidel et al., 1991; Flagan, 1994; Oberdorster et al., 2000). APFO in a particulate phase is transported to nearby public well fields by wind and is deposited onto the surface of overlying well fields by dry and wet deposition (Davis et al., 2007). When deposited APFO, the undissociated salt form, is in aqueous phase, it dissociates into perfluorooctanoate (PFO^-) and ammonium ion (NH_4^+). In acidic environments, PFO^- is protonated to form perfluorooctanoic acid (PFOA). Thus, the ratio of PFO^-/PFOA is determined based on reported pKa and environmental pH. The reported pKa value of PFOA ranges from 0 to 3.8 (Kissa, 2001; Prevedouros et al., 2006; Burns et al., 2008; Goss, 2008). PFO^- will be dominant in most water bodies and soils since typical environmental pH exceeds 4. PFO^- is also a dominant form both in surface soil and in subsurface soil of this model domain as pH is between 4 and 7 (Collier, 1984). However, the term 'PFOA' is used to describe environmental measurements of the sum of PFO^- and PFOA in the present study to be consistent with other literature.

One of the major reported routes of APFO from the DuPont Washington Works Facility to the local environment is through air emission stacks (Paustenbach et al., 2007). There was a 99% decline in PFOA atmospheric releases from the facility between 2000 and 2006, but high PFOA concentrations have been detected in offsite surface and subsurface soil in 2005 and 2006 (DuPont, 2008), suggesting substantial retardation of vertical transport through the soil. PFOA air–soil transport is considered an important pathway as the highest soil concentrations are measured upstream and downwind of the facility. Davis et al. also supported that PFOA air transport to the surface soils of nearby water supplies located upstream of the facility resulted from wet deposition of air emissions during rain events because groundwater transport was highly unlikely based on the groundwater capture zones (2007).

DuPont conducted an air modeling and monitoring comparison study using AERMOD and ISCST3, two of the most commonly used air dispersion models (DuPont, 2007; US EPA, 1995, 2004). They reported that AERMOD predicts air concentrations better than ISCST3 for both off-site and on-site meteorological data due to improved AERMOD functions for dealing with boundary layer conditions and stability class (DuPont, 2007; Barton et al., 2010). However, there were several limitations to this study. First, sampling dates were randomly chosen within a short period of time, but annual emission rates were used to model short term predictions. Second, 1999 onsite meteorological data were used to predict deposition patterns for September and October 2005, and January 2006. Third, model predictions were compared to concentrations from surface soil/grass samples taken at a depth <2.5 cm although PFOA within this shallow depth could be quickly swept away by runoff in a short period of time or disappear by removal mechanisms that occur in soil such as plant uptake, evaporation, irrigation, and erosion. In contrast, PFOA concentrations in subsurface soil result from fate and transport over longer time scales with more dispersive mixing, and should therefore be less sensitive to short-term variations in source emissions and meteorology.

The present study addresses several limitations of earlier air dispersion modeling efforts. In particular, well-integrated meteorological data is important to use in the prediction of PFOA deposition because wind direction and speed are important parameters of determining the shape and size of dispersion, and precipitation rate accelerates wet deposition near the direct sources of emissions. Therefore, several meteorological data sets were carefully integrated for use in AERMOD and ISCST3 using the nearest airport (i.e., Parkersburg) data. In addition, we also incorporated the

vadose zone model PRZM-3 to simulate the fate and transport of PFOA in surface and subsurface soil, allowing direct comparison with observed soil concentrations.

The objective of our study was to evaluate the linked air–soil model as a predictive tool for the fate and transport of PFOA from the source through atmosphere to the vadose zone by comparing observed and predicted surface and subsurface soil concentrations. We also compared predictions from AERMOD and ISCST3 models and investigated the sensitivity of our results to different approaches for meteorological data processing.

2. Materials and methods

2.1. Sampling data

In this study, we used offsite surface (0–30 cm depth) and subsurface (>30 cm depth) soil samples collected within our air dispersion model domain (Fig. 1) to evaluate the performance of the linked air and vadose zone model by comparing with predicted PFOA concentrations in surface and subsurface soil. A total of 232 surface soil samples were collected previously from 32 locations in August 2002, September and October 2005, and April 2006 (DuPont, 2008). The sample concentrations for each location were averaged for each year. In addition, 242 subsurface soil samples from 10 locations were collected in August 2002 and March and April 2006. There were 12 to 34 subsurface soil samples of varying depth collected at each sampling location. Onsite soil samples that had PFOA concentrations two to four times higher than offsite samples were not included in this analysis because other pathways including the leaching from onsite contaminated anaerobic digestion ponds or landfill may be involved and the large surface area of the facility is covered by pavement. Rationale for selecting sample locations, sampling procedures, and analytical methods for soil samples are described in detail elsewhere (DuPont, 2005; Barton et al., 2010).

2.2. Air dispersion model

2.2.1. Model description

We chose to compare the U.S. EPA Industrial Source Complex Short Term version 3 (ISCST3) model (US EPA, 1995) and the American Meteorological Society/EPA Regulatory Model (AERMOD) (US EPA, 2004) because these models characterize atmospheric dispersion of chemicals well and have been recommended by EPA. Both models are similar in that they use a steady-state Gaussian plume model that predicts the ambient air concentrations and deposition rates at geographical locations defined as receptors, but AERMOD determines the vertical and horizontal dimensions of plumes by type of stability class (US EPA, 2004). A detailed comparison of model features for ISCST3 and AERMOD has been published elsewhere (US EPA, 2003). EPA recommended AERMOD over ISCST3 for regulatory purposes in 2005 (US EPA, 2004). ISC-AERMOD view, graphical interface software, was also used to generate input files for multi-year simulations (Lakes Environmental, Waterloo, Ontario, Canada).

2.2.2. Input parameters

We relied on most of the model input parameters provided by Paustenbach et al. (2007). These parameters include building configuration, stack information, emission rate, and particle size. Building dimension information for the facilities was included in the model to account for the effect of building downwash (U.S. EPA, 1995). Historical stack information such as height, diameter, exit velocity, and temperature was applied to the model by source and year. The procedure of material mass balance to estimate historical air emission rates for the period 1951–2003 is described in detail in

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