Science of the Total Environment xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Science of the Total Environment

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

Development of a standard documentation protocol for communicating exposure models

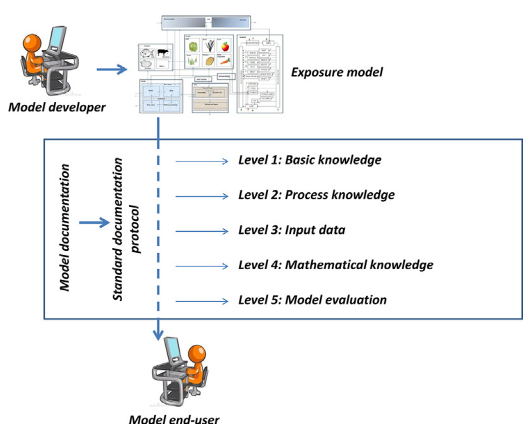
P. Ciffroy [a,*], A. Altenpohl [b], G. Fait [c], W. Fransman [d], A. Paini [e], A. Radovnikovic [e], M. Simon-Cornu [f], N. Suciu [g], F. Verdonck [h]

[a] Electricité de France (EDF) R&D, National Hydraulic and Environment Laboratory, 6 quai Watier, 78400 Chatou, France
[b] Austrian Standards Institute, Heinestr. 38, 1060 Vienna, Austria
[c] AIEFORIA srl, via Gramsci 22, 43036 Fidenza (PR), Italy
[d] TNO, PO Box 360, 3700AJ Zeist, The Netherlands
[e] Institute for Health and Consumer Protection, European Commission, Joint Research Centre, Ispra, Italy
[f] IRSN, Institut de Radioprotection et de Sûreté Nucléaire (IRSN), PRP-ENV, SERIS, LM2E, Cadarache, France
[g] Istituto di Chimica Agraria ed Ambientale, Università Cattolica del Sacro Cuore, via Emilia Parmense 84, 29122 Piacenza, Italy
[h] Arche cvba, Liefkensstraat 35d, 9032 Gent (Wondelgem), Belgium

HIGHLIGHTS

- Improving documentation of exposure models will increase transparency in regulation.
- A standard documentation protocol (SDP) for exposure models will improve transparency.
- The SDP development was based on a wide consultation of interested stakeholders.
- The format and structure of the SDP can facilitate exposure models description.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 20 November 2015
Received in revised form 15 January 2016
Accepted 21 January 2016
Available online xxxx

Editor: Barcelo D.

Keywords:
Standardisation
Exposure model

ABSTRACT

An important step in building a computational model is its documentation; a comprehensive and structured documentation can improve the model applicability and transparency in science/research and for regulatory purposes. This is particularly crucial and challenging for environmental and/or human exposure models that aim to establish quantitative relationships between personal exposure levels and their determinants. Exposure models simulate the transport and fate of a contaminant from the source to the receptor and may involve a large set of entities (e.g. all the media the contaminants may pass though). Such complex models are difficult to be described in a comprehensive, unambiguous and accessible way. Bad communication of assumptions, theory, structure and/or parameterization can lead to lack of confidence by the user and it may be source of errors. The goal of this paper is to propose a standard documentation protocol (SDP) for exposure models, i.e. a generic format and a standard structure by which all exposure models could be documented. For this purpose, a CEN

* Corresponding author.
E-mail address: philippe.ciffroy@edf.fr (P. Ciffroy).

http://dx.doi.org/10.1016/j.scitotenv.2016.01.134

Documentation
Multimedia models
PBPK models

(European Committee for Standardisation) workshop was set up with objective to agree on minimum requirements for the amount and type of information to be provided on exposure models documentation along with guidelines for the structure and presentation of the information. The resulting CEN workshop agreement (CWA) was expected to facilitate a more rigorous formulation of exposure models description and the understanding by users. This paper intends to describe the process followed for defining the SDP, the standardisation approach, as well as the main components of the SDP resulting from a wide consultation of interested stakeholders. The main outcome is a CEN CWA which establishes terms and definitions for exposure models and their elements, specifies minimum requirements for the amount and type of information to be documented, and proposes a structure for communicating the documentation to different users.

1. Introduction

Documenting environmental models has been highlighted as an important step for improving applicability and transparency of models intended for regulatory decision making (US-EPA, 2009). Poor documentation could be acceptable when models are built for initial or exploratory research, where no litigation or regulatory action is expected. However, transparency becomes a key element when models are intended to be used by third parties, e.g. regulators and decision-makers. A standard documentation protocol (SDP), i.e. a generic format and a standard structure for documentation, appears as a convenient way to convey guidelines about how to communicate about models in a comprehensive and transparent way.

In the ecological field, Grimm and Railsback (2005) initially proposed the basic idea of an SDP for documenting models aiming at describing individual organisms (individual-based models, IBM) or agents (agent-based models, ABM). The basic idea was improved by Grimm et al. (2006) and subsequently by Grimm et al. (2010) after having tested the approach on several models. Grimm et al. took this initiative because published descriptions of IBMs models are generally complex in their structures, and then generally hard to read, incomplete and ambiguous. They thus proposed a standard protocol to make reading and understanding IBMs easier for end-users. The proposed SDP was developed and tested by 28 modellers who cover a wide range of fields within ecology. The protocol consisted of three blocks (Overview, Design concepts, and Details), which were subdivided into seven elements: i) Purpose (i.e. explanations of why a complex model is being built and what its purpose; ii) State variables and scales (i.e. the structure of the model by hierarchical levels of entities, the full set of state variables, the temporal and spatial scales); iii) Process overview and scheduling (i.e. a concise verbal and conceptual description of each process and its effects, the scheduling of the model processes by using flow charts); iv) Design concepts (e.g. basic principles, objectives, learning, stochasticity, observation), v) Initialization (i.e. initial conditions assumed), vi) Inputs (i.e. environmental conditions which change over time and space), and vii) Sub-models (detailed explanation of all the sub-models representing the processes including parameterization). These underlying concepts can be widely shared in environmental modelling, but this SDP in its detailed format is not easily transferrable to other fields than the initial scope, IBMs and ABMs. In particular, it contains aspects not relevant for exposure models, while others that would be relevant are missing such as model evaluation.

Regarding another type of model, the quantitative structure–activity relationship (QSAR) model, a Guidance document (OECD, 2007) covers the majority of aspects related to an SDP. It is already an internationally accepted approach and gives stepwise instructions for a very precise way to document the development and verification of a QSAR model. Some OECD principles are generic, stating that a model should be associated with the following information: (1) a defined endpoint, (2) an unambiguous algorithm, (3) a defined domain of applicability, (4) appropriate measures of goodness-of-fit, robustness and predictivity, and (5) a mechanistic interpretation, if possible. Nevertheless, most rules of this Guidance document are specific to QSAR modelling, i.e. briefly speaking, models based on regression analysis between compounds molecular descriptors and a defined endpoint, so that it is not possible to directly apply them for other environmental models. Similarly, the CEN/TR 16364 (2013), provides a concrete standardised modelling procedure relying on a software tool and states the required documentation, but it is an SDP applicable to an even smaller area, the migration of organic substances into water.

Useful recommendations are also given by more generic guidelines, such as Guidance on the development, evaluation and application of environmental models (US-EPA, 2009). It introduced recommendations for the communication of 'Problem identification and specifications' and 'Model development' issues, defined respectively as 'the determination of the right decision-relevant questions and establishment of modelling objectives', and 'the development of the conceptual model that reflects the underlying science of the processes being modelled, and the development of the mathematical representation of that science and the implementation of these mathematical expressions in a computer program'. A WHO report (2005) also contains collective views of an international group of experts and provides clear and structured recommendations for characterizing human exposure models. This WHO report (2005) mostly focused on single-pathway assessments, for specific segments of the population, such as workers in the chemical industry, pesticide applicators and consumers. However, it clearly observed the upcoming trend towards total exposure assessments that include all potential exposure pathways, relying on the so-called 'multimedia models' (MM models).

Human exposure models aim to establish quantitative relationships between personal exposure levels and their determinants. This remains challenging, which is well reflected in the diversity of published exposure models (Tielemans et al., 2008; Bilitewski et al., 2013). As far as occupational exposure is concerned, one approach to help understand the inhalation exposure process has been to use a source–receptor model (Smith et al., 1991) and to describe exposure schematically by deterministic exposure modifiers (Schneider et al., 1991; Woskie et al., 1995; Creely et al., 2005). Mechanistic models based on this approach were developed (e.g. Cherrie et al., 1996; Cherrie and Schneider, 1999). Conceptual models can be based on a stepwise transport of a contaminant from the source to the receptor (Smith et al., 1991; Creely et al., 2005) and are constructed using three types of components, i.e. sources, compartments through which the contaminants may pass from the source to the receptor, and the receptor. As far as exposure through the environment is concerned, MM models were proposed in the 1990s (e.g. McKone, 1993; Maddalena et al., 1995; US EPA, 1999) and have been much more developed since then. These MM models are designed for predicting the distribution of chemicals among environmental compartments such as surface waters, air, soils, sediments, plants, fish, meat, and milk, taking into account the manifold links between all these compartments. Combined with information on human behaviours (dietary patterns, time activity patterns, etc.), such MM models provide an estimation of the daily quantity inhaled or ingested by a target population. Besides the estimation of daily intakes, the determination of internal effective concentrations, i.e., in the target tissues where toxic effects arise, can also be conducted to more comprehensively assess the exposure process, and to more precisely characterize the link between the intakes from the environmental compartments