4FUN

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Deliverable D2.1. List of exposure models to be included in the SWOT analysis

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Dissemination Level		
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1 Introduction

Exposure can be assessed by measuring exposure concentrations, once chemicals are produced, used and emitted. For new chemicals, exposure assessments can only be based on predictions. This involves estimating emissions, pathways and rates of movement of a substance and its transformation or degradation in order to obtain concentrations or doses to which human populations or environmental compartments are or may be exposed. It involves describing the nature and size of the populations or compartments exposed to a substance, and the magnitude and duration of their exposure. The evaluation may concern past or current exposures, or anticipated future exposures. Multimedia exposure models are often used, especially in environmental exposure assessment.

There are many models for assessing exposure to human health and/or the environment. Some of them are multimedia models, which assess the exposure in different environmental matrices, such as soil, water and food chains with different degrees of complexity within each medium. Conversely, others are more specific with regard to a medium or a system (e.g. river or food chain). Other models assess only human health exposure or environmental exposure, while some assess both.

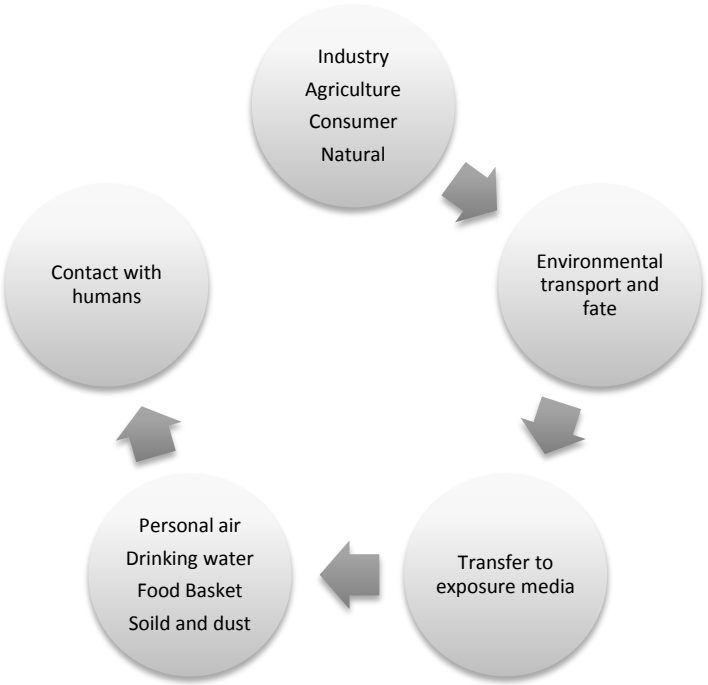

Figure 1: A conceptual illustration of the migration of pollutants from sources, through the multimedia environment and into exposure media, followed by contact with humans (McKone & MacLeod, 2003)

Government programmes used to focus their assessments on single media, such as air, water or food, and specific segments of the population, such as workers, pesticide applicators and consumers. Single-pathway and single-medium assessments are useful to decision-makers because they can provide quantitative risk estimates on which to base risk management decisions. However, such assessments do not provide an estimate of the baseline exposure in the absence of the pathway of concern.

Aggregate exposure assessments estimate total exposure via all pathways and routes and are more complex and costly than single-medium assessments. They require the collection of data and development and implementation of models for the additional pathways and sometimes for additional groups of people to serve as control groups for comparison with the subgroup of interest.

Humans may be exposed to a variety of substances from multiple exposure pathways. A distinction can be made between exposure through environment, exposure from use of consumer products and exposure at the workplace or during professional use. Human exposure to chemicals through multiple environmental pathways is classically estimated by multimedia models, to calculate the distribution of contaminants over environmental matrices and products of interest for human exposure (drinking water, inhaled air, vegetables, meat, fish, milk and other foodstuffs). When combined with data describing human behaviour, such multimedia models provide an estimation of the daily dose inhaled, ingested or dermally adsorbed by the population of interest. Many tools for exposure of humans to chemicals from contaminated air, water and soil have been developed.

Multimedia **environmental** fate models play a significant role in the assessment of the environmental fate of chemicals. Multimedia models have recently been used for the purposes ranging from exposure assessment of industrial chemicals to the long-range transport and persistence potential of chemicals (Mackay, 2001; Cowan et al., 1995; Brandes, 1996; OECD, 2002).

Modelling approaches are used for those assessments because monitoring data are not necessarily sufficient, the future state of the environment cannot be predicted from monitoring data, and mechanistic insights into the fate of chemicals are useful for the strategic assessment of countermeasures.

Existing exposure models can be broadly categorised according to the following types of exposure source: environmental, dietary, consumer product, occupational and aggregate and cumulative (different chemical sources and pathways).

The goal of task 2.1 is to set up an exemplary list with all available exposure modelling tools.. This deliverable is part of WP2 in which the main objective is to identify strengths and weaknesses of the 2-FUN tool using a SWOT analysis. This analysis will be used as an input for the design of the final integrated 2-FUN tool (WP3) that will be in agreement with stakeholders' requirements.

2 Exposure models

2.1 Environmental exposure models

Environmental exposure models have been developed in an effort to quantify human exposure to chemicals via contact with the surrounding environment. A wide range of existing exposure models fall into this category, with individual models tending to focus on human exposures from a limited range of environmental media. Two broad categories of environmental exposure models can be distinguished: (1) environmental concentration models, and (2) human intake models. Environmental concentration models simulate environmental processes in order to generate chemical concentrations in particular media to which humans may come into contact. Environmental concentration models are typically sophisticated mechanistic assessment tools with (or without) a temporal or spatial aspect and involve the use of a series of parameters representing the modelled environment and the chemical in question. Human intake models go one step further by quantifying human chemical intake from contact with the relevant environmental media. Human intake models differ from exposure concentration models in that they require the user to have knowledge of parameters relating to human activities and physiology in addition to parameters representing the chemical and environmental conditions.

Table 1: Examples of environmental concentration models

Model	Description	Author
ADAM	ADAM (Air Force Dispersion Assessment Model) a modified box and Gaussian dispersion model which incorporates thermodynamics, chemistry, heat transfer, aerosol loading, and dense gas effects.	AF Research Laboratory
ADMS-3	Atmospheric Dispersion Modeling System	Cambridge Environmental Research Centre
AFTOX	Gaussian dispersion model that will handle continuous or instantaneous liquid or gas elevated or surface releases from point or area sources.	Kunkel, 1991
Consim	ConSim is designed to provide those concerned with the management of contaminated land with a means of assessing the risk that is posed to groundwater by leaching contaminants.	Golder Associates
HYDRUS	HYDRUS is a software package for simulating water, heat, and solute movement in two- and three-dimensional variably saturated media.	Simunek et al., 2008
MACRO	MACRO is a physically-based one-dimensional numerical model of water flow and reactive solute transport in field soils	Jarvis et al., 1994
PRZM	PRZM is a surface water model that simulates chemical movement in soil within and immediately below the plant root zone.	Carsel et al., 1985
PEARL	Pesticide Emission Assessment at Regional	Tiktak et al., 2000

	and Local scales. It is a one-dimensional numerical model of pesticide behaviour in the soil-plant system.	
PELMO	A one dimensional simulation model simulating the vertical movement of pesticides in soil by chromatographic leaching.	Klein, 1995
EXAMS	EXAMS is a surface water model that evaluates the fate, transport, and exposure concentration of pesticides.	Bruns, 2004
SCI-GROW	SCIGROW is an aquatic model used to estimate pesticide concentrations in ground water.	US EPA, Water Models

Table 2: Examples of human intake models

Model	Description	Author
APEX	Air pollutant exposure model	Graham et al., 2012
HAPEM	Hazardous air pollutant exposure model	Rosenbaum & Huang, 2007
SKINPERM	Estimates the skin permeation coefficient of a chemical from aqueous solutions using physicochemical properties.	Ten Berge, 2006
AirPEx	Air pollution exposure model	Freijer et al., 1997

2.2 Dietary exposure models

Dietary exposure models have been developed to predict human exposure to chemicals resulting from the consumption of contaminated food and water and also for e.g. substances naturally occurring in them.

Model	Description	Author
DEEM	DEEM is a dietary exposure analysis system that may be used to estimate exposure to constituents in foods comprising the diets of the US population, including population subgroups.	Kidwel, et al., 2000
DEPM	The model and database system, correlates extant food information in a format for estimating dietary exposure.	US EPA, 2003
PRIMo	The model is based on national food consumption figures and unit weights provided by Member States and implements internationally agreed risk assessment methodologies to assess the short-term (acute) and long-term (chronic) exposure of consumers.	EFSA
Consumer Exposure Model	Deals with exposure to pesticides via the ingestion of residues in agricultural commodities.	UK Pesticide Safety Directorate
Intake Program	It evaluates exposures via the ingestion of food items and drinking water.	UK Food Standards Agency

Table 3: Examples of dietary exposure models

2.3 Consumer product exposure models

Consumer product exposure models are developed to asses human chemical intake via contact with consumer products.

Table 4: Examples of consumer exposure models

Model	Description	Author
CONSEXPO-3	A range of models for predicting human exposure to chemicals used in consumer products.	Vermeire et al., 1993
PROMISE	A software tool developed for the Solvents Council of the ACC to assist in the exposure assessment of industrial chemicals	American Solvents Council, 2005
MCCEPA	Multi-Chamber Concentration and Exposure Model (MCCEPA)	USEPA/ Office of Research and

		Development
BEAT	Bayesian Exposure Assessment Tool	Health and Safety Laboratory, UK
REx	The residential exposure model evaluates ingestion, inhalation, and dermal contact exposures from a range of residential pesticide products.	Non-dietary Subcommittee of the Organophosphate Case Study Group, USA
MCCEM	Multi-chamber concentration and exposure model (MCCEM). Estimates average and peak indoor air concentrations of chemicals released from products or materials in house.	US EPA Exposure Assessment Tools and Models
CEM	An interactive model, which calculates conservative estimates of potential inhalation exposure and potential and adsorbed dermal exposure to consumer products.	US EPA
PIRAT	The pesticide risk assessment tool (PIRAT) provides screening level estimates of exposure and risk to pesticide inert ingredients that are used in a residential setting, i.e. ingredients other than the active ingredients in pesticide products	US EPA Office of Pesticide Programs (OPP)
WPEM	Wall paints exposure model estimates the potential exposure of consumers and workers to the chemicals emitted from wall paint.	US EPA
SprayExpo	A deterministic model to predict inhalation and dermal exposure during spray application of biocidal products.	BAuA, 2006
ECETOC-TRA	The TRA consists of 3 separate models for estimating exposures to workers, consumers and the environment that arise during a series of events (’exposure scenarios’).	ECETOC, 2012

2.4 Occupational exposure models

Occupation exposure models assess the magnitude of exposure to a variety of substances potentially hazardous to their health in the workplace.

Table 5: Examples of occupational exposure models

Model	Description	Author
EASE	Estimation and assessment of substance exposure	HSE, 2000
POEM	Predictive operator exposure model	PSD, 1992
RISKOFDERM	The RISKOFDERM Dermal Exposure Model is a model for estimating potential dermal exposure, i.e. the total amount of a substance coming into contact with the protective clothing, work clothing and	TNO, 2006

	exposed skin.	
Stoffenmanager	A tool for prioritizing worker health risks to dangerous substances, a quantitative inhalation exposure tool and a REACH Tier one quantitative inhalation exposure tool	Ministry of Social Affairs and Employment, The Netherlands, 2012
EMHG-Expo-Tool	A generic tool that can be used to derive a Tier 1 inhalation exposure value for the workplace	EMKG, BAuA, 2008
ECETOC-TRA	The TRA consists of 3 separate models for estimating exposures to workers, consumers and the environment that arise during a series of events ('exposure scenarios').	ECETOC, 2012

2.5 Aggregate and cumulative exposure models (multimedia models)

In order to quantify total human exposure to a particular chemical it is often necessary to consider exposures from different sources and pathways simultaneously. This requirement has lead to the development of models capable of aggregating different chemical sources and pathways into a single exposure assessment.

Some models listed in Table 6 might also belong in one of the previous listed categories. These models are however defined as aggregated models if they consist of 2 or more compartments.

Table 6: Overview of aggregate exposure models

Model	Description	Author
3MRA	3MRA provides the ability to conduct screening-level risk-based assessment of potential human and ecological health risks resulting from long term (chronic) exposure to HWIR chemicals released from land-based waste management units (WMUs) containing currently listed waste streams.	Johnson et al., 2002
BETR	Modelling the movement of persistent organic pollutants on a continental scale	Toose et al., 2004
BREEZE Risk	Human health and ecological risk assessment modelling system designed to conduct multi-pathway human health risk assessments and food-web based ecological risk assessment modelling.	Breeze
Calendex	Calendar-Based Dietary & Non-Dietary Aggregate and Cumulative Exposure Software System	Petersen et al., 2000
CalTOX	Exposure model for hazardous waste sites	California Department of Toxic Substances Control. Hertwich et al., 2001; McKone, 2001; McKone et al., 2001

CARES	Quantifies risks to human health from exposures to pesticides in drinking water, food and from home-based treatments.	CropLife America, 2002
ChemCan	Human exposure assessment, designed for use in Canada	Canadian Environmental Modelling Centre (CEMC). Webster et al., 2004; Mackay et al., 1991.
ChemFrance	Prediction of persistence and spatial range of organic chemicals	Devillers et al., 1995
CHEMGL	A multimedia compartment model, which predicts fate and transport of chemicals in the Great Lakes region.	Zhang et al., 2003
ChemRange	Prediction of persistence and spatial range of organic chemicals	Scheringer et al.,
ChemSTEER	Estimates occupational inhalation and dermal exposure to a chemical during industrial and commercial manufacturing, processing, and use operations involving the chemical. Estimates releases of a chemical to air, water, and land that are associated with industrial and commercial manufacturing, processing, and use of the chemical.	US EPA
CLEA	Quantifies human exposure to chemicals resulting from direct and indirect contact with contaminated soils	DEFRA, 2002
CREMe	An exposure assessment tool specializing in the areas of population exposure assessment to consumer products, food and environmental concerns.	CREMe Ltd., 2006
CSOIL 2000	CSOIL 2000 calculates the risks that humans are exposed to if they come into contact with soil contamination.	Brand et al., 2007
Ecofate	A computer tool used for assessing chemical emissions from point and non-point source pollution sources for the purpose of developing Ecosystem-based risk assessments and determining potential effect on human health.	Gobas et al., 1998
ECOSENSE	An integrated environmental impact assessment model. Developed to support the assessment of priority impacts resulting from the exposure to airborne pollutants, namely impacts on health, crops, building materials, forests, and ecosystems.	Genon & Brizio, 2005
E-FAST	Provides screening-level estimates of the concentrations of chemicals released to air, surface water, landfills, and from consumer products.	US EPA, 2007
ELPOS	Environmental Long-range Transport and	Beyer & Matthies, 2002

	Persistence of Organic Substances Model	
EN-forc	An environmental food transfer model for organic contaminants	Fierens,et al., 2013
ERDEM	ERDEM is a physiologically-based pharmacokinetic (PBPK) model with a graphical user interface (GUI) front end.	Blancato et al., 2006
EUSES	EUSES is a decision-support instrument which caries out rapid and efficient assessments of the general risks posed by chemical substances	Vermeire et al., 1997
Fug3ONT	A four compartment level II fugacity model for simulating the relative multimedia distribution of non-ionic organic chemicals in a regional environment.	Mackay & Paterson, 1991
G-CIEMS	A spatially resolved and geo-reference dynamic multimedia environmental fate model.	Suzuki et al., 1994
GEMCO	Generic Estuary Model for Contaminants. Designed as an easy-to-use tool to determine the sediment and water concentrations as well as the concentrations and fluxes of contaminants through the different trophic levels in a schematic food web.	Cefic, 2003
GLOBOX	Is a spatially differentiated multimedia fate, exposure and effect model.	Sleeswijk & Heijungs, 2010
GREAT-ER	An advanced environmental exposure model for chemicals in river basins, for use e.g. in the European chemicals risk assessment process (REACH), and in the EU Water Framework Directive (WFD)	Koormann et al., 2006
HAZCHEM	It consists of the following models: estimation of release to the environment, wastewater treatment model, environmental exposure on a regional scale, environmental exposure of water/air/soil on a local scale, characterisation of risk, extrapolation of NOECs	ECETOC, 1994
HESP	Human Exposure to Soil Pollutants (HESP). he model calculates the total exposure of adults and children resulting from pollutants present in soil, via 10 different exposure routes.	Poels & Veerkamp, 1992
Humanex	Combination of EUSES and CSOIL 2000	Bontje, et al., 2005
IMPACT2002+	A LCA method comprising a European multimedia fate and exposure model	Jolliet et al., 2003
INTERA	**INT**egrated **E**xposure for **R**isk **A**ssessment in indoor environments	Asikainen et al., 2012
IRAP-h	RAP-h View is a user-friendly graphical interface for conducting a comprehensive	Lakes Environmental, 2009

	multi-pathway human health risk assessment. It simultaneously calculates risk values for multiple chemicals, from multiple sources, at multiple exposure locations.	
ISMCM	Integrated spatial-multimedia-compartmental model (ISMCM) to assess the multimedia environmental partitioning of volatile and particle-bound pollutants in the environment.	Cohen & Clay, 1994
LIFELINE	Quantifies exposure to and human health risks from pesticides in agricultural crops, drinking water supplies and residences	LifeLine Group, USA
LOTOS-EUROS	LOTOS-EUROS is a regional chemical transport model (CTM) designed for the assessment of gaseous and particulate air pollutants	Segers, 2012
MAFRAM	Multimedia agricultural fate and risk assessment model, for comparing and establishing the general features of new and existing non-volatile organic chemicals (NVOCs) used in agricultural activities, based on simple and readily available properties.	Batiha et al., 2010
MENTOR	A mechanistic source-to-dose Modelling Environment for Total Risk studies. A computational toolbox that provides various modelling and data analysis tools to facilitate assessment of cumulative and aggregate exposure to contaminant mixtures.	Georgopoulos and Lioy, 2003
MEPAS	Hazardous waste site and radioactive waste	Pacific Northwest National Laboratory. Whelan et al., 1992
MMSOILS	The Multimedia Contaminant Fate, Transport, and Exposure Model (MMSOILS) estimates the human exposure and health risk associated with releases of contamination from hazardous waste sites.	USEPA
MODUL'ERS	A modular computational tool for estimating concentrations, exposure and risks levels due to a source of local pollution due to soil pollution or emissions from facilities	Bonnard, 2010
MSCE-POP	For the assessment of the transport and accumulation of POPs in the framework of air quality policies in Europe.	Gusev et al., 2005
MULTIMED	Simulates the movement of contaminants leaching from a waste disposal facility. The model consists of a number of modules which predict concentrations at a receptor due to transport in the subsurface, surface air, or air.	USEPA, 1996

NORMTOX	NORM- TOX models the daily exposure to contaminants from air, soil, drinking and surface water and food products, averaged over a lifetime.	Ragas et al., 2009
OURSON	A dynamic model developed to evaluate radionuclide transfer from surface water to man.	Ciffroy et al., 2006
QWASI	It describes the steady state behaviour of an organic chemical in a lake subject to chemical inputs by direct discharge, inflow in rivers, and deposition from the atmosphere.	Mackay et al., 1983
RAIDAR	RAIDAR is an evaluative, regional-scale, mass balance model for screening level exposure and risk assessment. The model simulates chemical fate and transport in the environment, bioaccumulation in a range of species, food web bioaccumulation, far-field exposures to humans and representative ecological species, and effects (risk).	Arnot et al., 2006
RESRAD	Radionuclide contaminated soil	Yu et al., 1989
RISC	Designed to assess the potential for adverse human health impaxts due to exposure to contaminated soil, water and air, to calculate target clean-up levels for these media, and to estimate the cross-media transport of chemicals in the environment.	Spence & Walden, 1997
SADA	Spatial Analysis and Decision Tools. It incorporates tools from environmental assessment fields into an effective problem solving software.	Stewart & Purucker, 2011
SHEDS	Stochastic human exposure and dose simulation model for multimedia, multiroute/pathway chemicals	Zartarian et al., 2008
SimpleBox	Understanding chemical fate in urban area	Brandes et al., 1996
S-RISK	A mode that allows to calculate human health-based soil remediation values, to perform site-specific human health risk assessment or calculate soil clean-up goals.	Cornelis et al., 2013
SWAT	**SWAT** (**Soil & Water Assessment Tool**) is a river basin scale model developed to quantify the impact of land management practices in large, complex watersheds.	Neitsch et al., 2002
TRIM.FaTE	A spatially explicit, compartmental mass balance model that describes the movement and transformation of pollutants over time, through a user-defined, bounded system that includes both biotic and abiotic compartments.	US EPA, 2005

USES-LCA	The model is based on the European Union system for the evaluation of substances model and is applied for risk assessment purposes in the EU.	RIVM, 1998
USEtox	An environmental model for characterization of human and ecotoxic impacts in Life Cycle Impact Assessment and for comparative assessment and ranking of chemicals according to their inherent hazard characteristics.	Rosenbaum et al., 2008
Vlier-Humaan	A model to determine human exposure caused by soil contamination.	OVAM, 2010
WATSON	Water and soil environmental fate and exposure model of noxious substances at the European scale	Bachman, 2006.
WHATIF	WHATIF is software that integrates a number of calculators, tools, and models for assessing the health of watersheds and streams with an emphasis on fish communities in the Mid-Atlantic Highland region.	Rashleigh et al., 2006
Xtrafood	Model for the impact analysis of contaminants in primary food production	Seuntjes et al., 2006

3 Models to include in the SWOT analysis

Not all models presented in Table 1-6 will be in-depth analysed in the SWOT analysis. The focus will be on the multimedia models from Table 6. Consumer product and occupational exposure models will not be included as the only human pathway in 2-FUN is the exposure of man via environment. Therefore there is no need to include these models in the analysis.

A selection of models will be made in Task 2.3 at the start of the SWOT analysis. In this selection, the following criteria can be considered: a) it should preferably be a multimedia model, b) the model should fit more-or-less in the scope of the identified regulatory frameworks from Task 2.4, c) models, with a focus on a geographical area outside Europe, will be excluded, d) models with a focus only on radionuclides will be excluded, e) older versions of a certain model (e.g. SimpleBox – EUSES) will not be included, f) the scope of the model should be within the scope of the 2-FUN tool.

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