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Functional Assessment and Statistical Analysis of Nano-Specific Environmental Exposure Tools and Models

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Evaluation of Tools and Models Used for Assessing Environmental Exposure to Manufactured Nanomaterials

Functional Assessment and Statistical Analysis of Nano-Specific Environmental Exposure Tools and Models

INTER-ORGANIZATION PROGRAMME FOR THE SOUND MANAGEMENT OF CHEMICALS

A cooperative agreement among **FAO, ILO, UNDP, UNEP, UNIDO, UNITAR, WHO, World Bank and OECD**

Environment Directorate
ORGANISATION FOR ECONOMIC COOPERATION AND DEVELOPMENT
Paris 2021

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Objective: The objective of this project is to compile available tools and models for the assessment of environmental exposure to manufactured nanomaterials, and to conduct an analysis of their applicability for use in regulatory exposure assessment.

Design: The project assesses the compiled models by providing a functional assessment, statistical analysis, and performance evaluation of each model. The functional assessment assesses the scope (underlying assumptions and foundational algorithms) and use of the tools; the statistical analysis quantifies parametric sensitivity and output uncertainty in models from those tools; the performance evaluation weighs the models against real scenarios (where applicable). Finally, the recommendations provide guidance on the applicability of the tools and models in regulatory assessments.

EXECUTIVE SUMMARY

The work in this report includes the results of two objectives, the first of which is a compilation and prioritization of available tools and models for nanomaterial exposure characterizations. Additionally, the work in this report contains the results of the second objective that is a functional assessment and statistical analysis of a prioritized selection of the models compiled from the first objective. The compilation of models was completed as an Excel spreadsheetcontaining summary details on a list of 24 models and tools including Material Flow Analysis (MFA) models, Environmental Fate Models (EFM), and spatially explicit river models. Models were prioritized and selected for further evaluation using a set of prioritization criteria. The prioritized models were then subjected to a functional assessment and statistical analysis. The functional assessment presents details of the models and tools that include installation, user requirements, data requirements, input parameters, model outputs, assumptions made, and algorithms used. The statistical analysis contains two types of analyses: an uncertainty analysis conducted using Monte Carlo Simulations (MCS) and a systematic sensitivity analysis using a standard sensitivity score. Default scenarios were chosen for each model or tool, and a set of input parameters were chosen for uncertainty and sensitivity analysis.

Ten models were selected for analysis out of the 24 in the inventory from the first objective. These models are: DPMFA, nanoRelease, nanoFate, SimpleBox4nano, nanoDUFLOW, WASP8, LearNano, Mendnano, Rhone/Rhine river model, and WASP7. The Rhone/Rhine model was omitted from the second objective due to inaccessibility. Additionally, WASP7 was omitted due to recommendations from the developers to use WASP8 instead. Both LearNano and MendNano were functionally assed, but not statistically analyzed due to unresolvable error messages. Thus, six models out of the 10 prioritized were fully analyzed. The results of the analysis for these models are included in this report, as well as the results of the functional assessment for LearNano and MendNano. The uncertainty analysis revealed that some models to display larger variance in the model output, while some models display very little or no variance at all in the model output. The sensitivity analysis revealed that the model outputs respond predictably to systematic changes to a majority of the input parameters tested. Though it was not intended, it was discovered that a benefit of the sensitivity analysis conducted in this study is the utility to probe for bugs and unexpected behaviour in the model output. Specifically, the sensitivity analysis on SimpleBox4nano revealed a bug in the version of the model provided. The author fixed the bug and provided a new version of this model for re-analysis. The new results were able to test and reveal that the bug was indeed fixed. This report also contains recommendations for model suitability based on the functional assessment, the uncertainty analysis, and the sensitivity analysis. Additionally, this report specifically recommends further analysis to be conducted if there is a need to explore these models in more detail.

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ABBREVIATIONS

CNT	Carbon Nano Tubes
DPMFA	Dynamic Probabilistic Material Flow Analysis
EFM	Environmental Fate Model
ENP	Engineered Nanoparticle
GMP	Good Modeling Practices
GUI	Graphical User Interface
JCGM	Joint Committee for Guides in Metrology
LCIA	Life-Cycle Inventory Assessment
MCS	Monte Carlo Simulations
MFA	Material Flow Analysis
MWCNT	Multi-Walled Carbon Nano Tubes
NM, MNM	Manufactured Nanomaterial
OAT	One-at-a-time
ODE	Ordinary Differential Equation
OECD	Organization for Economic Co-operation and Development
PDBM	Parameter database and database manager
PDF	probability density function
POM	Particulate Organic Matter
SB4N	SimpleBox4Nano
STP	Sewage Treatment Plant
WASP	Water Quality Analysis Simulation Program
WIP	Waste Incineration Plant
WPMN	Working Party on Manufactured Nanomaterials
WSM	Watershed Model
WWTP	Waste Water Treatment Plant

1 BACKGROUND AND PURPOSE

1. In 2015, the OECD WPMN was tasked with identifying the available data on consumer and environmental exposure and mitigation measures, with the aim of prioritizing future work and research needs. A survey on Consumer and Environmental Exposures to MNMs collected data on the importance and availability of information related to exposure assessment (OECD, 2016[1]). The analysis of the responses to the survey identified exposure models for use in characterizing or estimating consumer and/or environmental exposure to MNMs to be of high importance, requiring further investigation. As such, in the spring of 2017, Canada submitted a proposal to the OECD WPMN to lead a project entitled "Compilation of Available Tools and Models Used for Assessing Environmental and Consumer Exposure to Manufactured Nanomaterials and Evaluation of their Applicability in Exposure Assessments" (OECD, 2017[2]). The project aimed to (1) Compile the available tools and models for assessing environmental and consumer exposure to MNMs (Manufactured Nanomaterials), and (2) Evaluate their applicability to regulatory NM exposure assessment. The outcomes of consumer and environmental parts of the project are provided separately. This report includes the environmental portion of the project.

2. Under the first objective, an inventory of available models and tools for assessing environmental exposure to MNM was created through an extensive literature review of peer-reviewed publications, the outcomes from recent international projects and inventories, and consultation with the WPMN member countries. The inventory is provided in an Excel file, Inventory of Environmental Exposure Tools for Nanomaterials.xlsx. The inventory contains both nano-specific models/tools and models/tools developed for chemicals that have been applied to the exposure assessment of nanomaterials. If available, the inventory provides information on the model/tools' name and version, country of origin, description, accessibility, input parameters, applicability domain, environmental and technical compartments (e.g., landfill, waste incineration plant, waste water treatment plant) considered by the model/tool, user friendliness, output, validation, limitations and assumptions made. The inventory includes 24 models/tools and can be divided into three categories: nano-specific mass flow analysis models/tools (10), nano-specific environmental fate models/tools (13), and models/tools developed for chemicals that have been applied to the exposure assessment of nanomaterials (1).

3. Under the second objective, an evaluation of the applicability of the listed models/tools was conducted in consultations with WPMN experts and collaborators. The evaluation process includes a functional assessment, uncertainty analysis, and sensitivity analysis. The functional assessment contains two categories of information: the mechanistic assessment and the theoretical assessment. The mechanistic assessment presents information on version, dependencies, installation, usage, modeling features. The theoretical assessment presents information on assumptions, algorithms, input parameters, and model output. The uncertainty analysis uses Monte Carlo Simulations (MCS) to propagate input parameter probability distribution, and quantifies the uncertainty in the output using defined metrics. The sensitivity analysis uses a systematic one-at-a-time (OAT) method to produce sensitivity response graphs

and overall sensitivity tables that highlight the most and least sensitivity input parameters in the model.

4. Nanomaterial exposure models are an application of traditional chemical exposure models (e.g. Environmental Fate Models (EFM), Material Flow Models (MFA), and Hydrology models coupled with chemical processes) that extends the scope of exposure models to include nano-specific chemical and physical processes. The extension of chemical exposure models to include nanomaterial exposure scenarios has been conceptually building on exposure models for bulk chemicals over the last 25 years (Di Guardo et al., 2018[3]). The development of nanomaterial exposure models is conceptually building on exposure models for bulk chemicals (Di Guardo et al., 2018[3]). A challenge in the development of exposure models for nanomaterials is to adapt models and tools to a suitable level for regulatory assessment, as well as to improve the availability of chemical property data, and emission data required to run the models in question. Additional developments also include efforts to define metrics for human- or environmental exposure hazards that can be solved using fate and exposure modeling. Moreover, it was identified that exposure models and tools need to be clearly understood by users, credible, and reliable, to be used in regulatory risk assessment (Di Guardo et al., 2018[3]). As exposure models become more readily acceptable as decision-making tools in risk assessment, Good Modeling Practices (GMP) were developed, containing principles intended to enhance the transparency and the quality of risk assessments that rely on exposure models (Buser et al., 2012[4]). A major factor identified in Busser et al. 2012 to increase the reliability of exposure models is to perform uncertainty analysis, as well as to perform sensitivity analysis to understand the relationship between the input parameters and the model output. A recent review on available input data to supply MFA type exposure modeling tools claims that there is a lack of available input data, and that current MFA rely on extrapolated information, assumptions, or expert opinions in a semi-quantitative fashion (Caballero-Guzman and Nowack, 2016[5]).

5. Despite the large contributions from groups internationally to bring chemical exposure models to a suitable level for risk assessment, there remains a lot of work to be done for nanomaterial exposure models. Since nanomaterial exposure models are an extension of chemical exposure models, they introduce new mechanics and processes to represent the unique behaviour of nanomaterials in the environment. These newly included processes and mechanics still require examination and scrutiny, and thus nanomaterial exposure models need to be tested and evaluated to enhance their transparency, understandability, and reliability. Moreover, to bring these tools and models to a suitable level for risk assessment, uncertainty and sensitivity analysis need to be performed in order provide a minimum level of confidence for their application within an environmental assessment of a MNM. Lastly, there exists a lack of available input data for these nanomaterial exposure models. This lack of input data may restrict the applicability of the tools and models to specific scenarios. Thus, here we are motivated to collect and organize input data from a variety of sources to identify areas where input data are lacking, but also to find opportunities for these data to be shared among the tools to open up their applicability to more scenarios.

6. The goal of this project is to compile and evaluate available nanomaterial environmental exposure tools and models with the aim to address the issues discussed with respect to transparency, understandability, reliability, and availability of input parameter data.

2 INVENTORY AND PRIORITIZATION OF TOOLS AND MODELS

2.1 Inventory of tools and models

7. The compilation of available tools is the first objective of this project and is presented here. The work of compiling and creating an inventory of tools and models took place during the year of 2018.

8. The inventory of tools & models was constructed by consultation within the WPMN member countries, and by searching the following resources:

- Analysis of the Survey on Available Methods and Models for Assessing Exposure to Manufactured Nanomaterials (OECD, 2015[6])
- Investigating the Different Types of Risk Assessments, Tools Available for Risk Management Measures, and Uncertainties Which Guide Additional Nanospecific Data Needs in Member Countries (OECD, 2016[7])
- Information and Data Used for Assessing Consumer and Environmental Exposure to Manufactured Nanomaterials (OECD, 2016[1])
- Consumer and Environmental Exposure to Manufactured Nanomaterials - Information used to characterize exposures: Analysis of a Survey (OECD, 2017[8])
- Evaluation of environmental exposure models for engineered nanomaterials in a regulatory context (Nowack, 2017[9])
- Evaluation of the availability and applicability of computational approaches in the safety assessment of nanomaterials (Worth et al., 2017[10])
- NANoREG Toolbox for the safety assessment of nanomaterials (Jantunen et al., 2018[11])
- Google Scholar – peer-reviewed online academic journals and books, conference papers, thesis and dissertations, preprints, abstracts, and technical reports

9. Information collected for the inventory included models/tools' name and version, country of origin, description, accessibility, input parameters, applicability domain, environmental and technical compartments considered by the model/tool, user friendliness, output, validation, limitations and assumptions made, if available.

2.1.1 Summary of model types in the inventory

2.1.1.1 Material Flow Analysis (MFA)

10. MFA type models, in general, are models used to quantify flows of materials in systems containing nodes and connections between nodes. In an environmental chemical and physical

context, the nodes consist of environmental compartments (such as air, water, soil) as well as other compartments that represent the industrial sector including waste and treatment (often referred to as the technosphere). Additionally, in the environmental context, the connections between the nodes consist of pathways between environmental compartments where it is possible for material to flow (e.g. there may exist a pathway for material to flow from a waste water treatment plant to environmental waters). MFA type models typically summarize the flow of material using an initial or recurring inflow material volume, and a set of parameters called transfer coefficients that describe proportions of materials that flow between each compartment according to a variety of algorithms (that depends on the specific model). Thus, in an environmental context, MFA models simplify physical and chemical processes that are responsible for material flow through a set of coefficients and production volumes. As such, physical and chemical processes are not explicitly modelled in MFA type models. As a result of the simplification of processes to a set of coefficients, there are no nano-specific parameters for MFA models. What makes a MFA model nano-specific is that a system is designed to include nanomaterial production volumes and possible compartments to which these volumes flow.

2.1.1.2 Environmental Fate Model (EFM)

11. Environmental fate models explicitly take into consideration physical and chemical processes assumed to be responsible for the transfer of chemicals between different environmental media (such as air, water, soil, and sediment). Additionally, environmental fate models explicitly account for physical and chemical processes responsible for the transformation or degradation of chemicals into other species. A widely acceptable modeling practice for fate models is to assume pseudo-first order kinetics for transfer and transformation processes. As a result, kinetic equations are derived for these processes, and put together in a system of mass balance equations that can be solved using standard differential equation solvers. Fate models that explicitly describe transformation and transfer of chemicals within a system of multiple connected environmental compartments are widely acceptable, and commonly referred to as multimedia mass-balance models. More complicated versions of multimedia mass balance models include an iterative time step, where the mass balance equations are solved at every time step. In such iterative models, if the input parameters of the mass balance equations are updated at every step, these models are considered to be dynamic. Dynamic models reflect the changes that occur in the environment as a function of time. For example, nanoFate uses real daily temperature, precipitation, and wind speed values that occur over a number of years in mass balance calculations on a daily time step. What makes an environmental fate model specific to nanomaterials is the inclusion of kinetic processes believed to describe the behaviour of nanomaterials in the environment. Such processes include for example aggregation and agglomeration kinetics.

2.1.1.3 Spatially explicit river models

12. Spatially explicit river models estimate concentrations of nanomaterials in a well resolved model of a particular river system. For example, the nanoDUFLOW model presented in this study divides the river Dommel (in the Netherlands) into 477 individual spatially defined connected sections. River models typically only include environmental compartments such as water, sediment, and deeper sediment. River models use complex algorithms to solve water flow dynamically in each river section. These models can estimate concentrations of nanomaterials as a function of time and distance in the river system by integrating specific processes like advection, aggregation, sedimentation and resuspension among others. For example the nanoDUFLOW model provides a shear rate (derived from the DUFLOW hydrology calculations of flow rate) as an input to the well known Stokes equation that here models

aggregation and sedimentation. Spatially explicit river models require a large number of specific spatial parameters to adequately define the river system. Other parameters are dependent on which processes are modeled (e.g. attachment efficiency parameters are required for aggregation).

2.1.1.4 Compilation of tools and models

13. The inventory of the tools and models was compiled in an Excel file by reviewing existing tools and models. The inventory contains select information on identified nano-specific tools and models, and chemical tools and models that may be applicable to exposure assessment of nanomaterials, including information on the tools and models' names and versions, country of origin, description, accessibility, input parameters, applicability domain, environmental and technical compartments considered by the tool or model, user friendliness, output, validation, limitations and assumptions made, if available. The inventory includes 24 tools and models and can be divided into three categories: nano-specific MFA tools and models (10), nano-specific EFM tools and models (9), and spatially explicit river models (5). The list of models included in the inventory is summarized in table 1 below.

Table 1. List of models and tools included in the inventory

Name	Reference	Model Type	Retained for Evaluation
DPMFA	(Bornhöft, 2017[12])	MFA	Yes
LearNano	(Liu et al., 2015[13])	MFA	Yes
nanoRelease	(Song et al., 2017[14])	MFA	Yes
No name	(Arvidsson, Molander and Sandén, 2011[15])	MFA	No
No name	(Boxall et al., 2007[16])	MFA	No
No name	(Caballero-Guzman, Sun and Nowack, 2015[17])	MFA	No
No name	(Gottschalk, Scholz and Nowack, 2010[18])	MFA	No
No name	(Mueller et al., 2013[19])	MFA	No
No name	(O'Brien and Cummins, 2010[20])	MFA	No
No name	(Walser and Gottschalk, 2014[21])	MFA	No
SimpleBox4Nano	(Meesters et al., 2014[22])	EFM	Yes
nanoFate	(Garner, Suh and Keller, 2017[23])	EFM	Yes
MendNano	(Liu and Cohen, 2014[24])	EFM	Yes
GWAVA	(Dumont et al., 2012[25])	EFM	No
E-FAST2	(U.S. EPA, 2010[26])	EFM	No
NanoFASE	http://www.nanofase.eu/	EFM	No
FINE	(Money, Reckhow and Wiesner, 2012[27])	EFM	No
No name	(Barton et al., 2015[28])	EFM	No
GUIDEnano	https://www.guidenano.eu/	EFM	No
No name	(Sani-Kast et al., 2015[29])	River	Yes
nanoDUFLOW	(Dale et al., 2015[30])	River	Yes
WASP8	(Bouchard et al., 2017[31])	River	Yes
WSM/WASP7	(Dale et al., 2015[30])	River	Yes
No name	(Praetorius, Scheringer and Hungerbühler, 2012[32])	River	No

2.1.1.5 Input Parameter Types

14. The parameter types defined in table 2 below are designed here in this study as categories under which the input parameters of the modeling tools can be placed for comparison. The classification of parameters into their respective types for each modeling tool can be found under the **Input Parameters** sub-heading for each assessment. The parameter

type classification is also used as a means to classify parameters in the database that was created for this project for the purpose of comparison and analysis.

Table 2. Input parameter types used for classification and comparison

Parameter type	Description	Examples
Compartment	Nominal existence of a physical space or medium	Air, water, soil, waste water treatment plant
Compartment Property	A quantitative or qualitative property belonging to the physical space or medium	Area, volume, density, wind speed, water flow rate, pH
Substance	A physical material	Organic or inorganic chemicals, nanomaterials, particulate matter, natural colloids
Substance Property	A quantitative or qualitative property belonging to the physical material	Density, radius, size, molecular weight, attachment efficiency
Transfer	The nominal existence of a transfer of material from one compartment to another	Vaporization, deposition, a connection between a waste water treatment plant and environmental waters
Transfer Property	A quantitative or qualitative property belonging to the transfer	A transfer coefficient, a rate of exchange, a rate constant
Transformation	The nominal existence of a transformation of one material into another	Dissolution, reactions (product formation), aggregation, agglomeration
Transformation Property	A quantitative or qualitative property belonging to a transformation	A reaction rate, a rate constant, an equation defining the transformation
Release	The nominal existence of introduction of material to a system	Emission of nanomaterial to an environmental compartment, production of material at a facility, import of material into a country
Release Property	A quantitative or qualitative property belonging to the release	A production volume, an emission rate, a function defining a release pattern, a lifetime
Temporal	The nominal existence of time in a system	Long-term average, a day, a year, a duration of a process
Temporal Property	A quantitative or qualitative property belonging to a temporal parameter	A time-step resolution (daily, yearly, etc.), steady-state calculation, time-dynamic calculation, A function defining a time dependent process
Meta	The nominal existence of instructions on how the tool can be customized for modeling	A choice of algorithms, a choice of materials, a choice of dynamic or steady-state calculations
Meta Property	A specific configuration of a meta parameter	Euler or COSMIC algorithms

2.2 Prioritization of tools and models

15. The first objective encompasses the prioritization of the models and tools, accordingly to a set of prioritizing criteria (2.2.1). The prioritization step narrowed the list of tools and models to be evaluated within the second objective.

2.2.1 Criteria used for prioritization

1) The **domain** of the model should address one or more of the following environmental media: soil, sediment, air, water, or other applications.

2) The model **scope** should be broad enough to be applied across a variety of emission and exposure scenarios.

3) The model should have **supporting documentation** that are easily available to users and are transparent with respect to model principles and algorithms.

4) **Dynamic models** should account for changes in exposure over the **long-term (at least 5 years)**.

5) The model contains appropriate **default values** for input parameters and allows for **user-overrides**.

2.2.2 Summary of models prioritized for further evaluation

2.2.2.1 DPMFA (Bornhöft, 2017[12])

16. DPMFA is a modeling tool that is a modified version of Gottschalk, Scholz and Nowack. (2010[18]). The tool uses a dynamic probabilistic material flow analysis approach. It estimates nanomaterial flows from production, manufacturing and consumption to the environment (air, surface water, ground water, sediment, and soil), waste incineration plants (WIPs), landfills, and waste water treatment plants (WWTPs), and recycling processes. In addition to the uncertainty assessment performed in Gottschalk, Scholz and Nowack (2010[18]), this approach considers the dynamic behaviour of the system over time. The output of the model provides the probability distributions of nanomaterial volumes for a number of specified compartments over time.

2.2.2.2 nanoRelease (Song et al., 2017[14])

17. NanoRelease is a dynamic, stochastic material flow analysis model developed by Song et al. (2017[14]). It estimates manufacturing, in-use and end-of-life releases to the environment (air, water, and soil) and landfill over time on a global scale. The model applies uncertainty analysis to specific model parameters (use release rate, average product lifetime, and annual production volume). The output of the model provides the total annual release of NMs in tonnes with uncertainty ranges.

2.2.2.3 nanoFate (Garner, Suh and Keller, 2017[23])

18. NanoFate is a dynamic, multimedia mass balance model developed by Garner et al. (Garner, Suh and Keller, 2017[23]). It estimates NM transport and concentrations in the atmosphere (including air and aerosols), soil (including surface soil solids, pore water and deep soil compartments), fresh and coastal water (including suspended sediments), and freshwater and coastal water sediments on a regional scale. It assumes that each environmental compartment is well mixed. The output of this model provides the concentration and mass fraction of NMs in each compartment over time in three different physical-chemical forms: (i) free particles and small homoaggregates, (ii) heteroaggregated and (iii) dissolved.

2.2.2.4 SimpleBox4nano (Meesters et al., 2014[22])

19. SimpleBox4nano is a modified version of the SimpleBox tool. It is a multimedia mass balance model suitable for screening assessment. It estimates NM transport and concentrations in air, rain, surface water, sediment and soil on regional, continental and global spatial scales. It assumes that each environmental compartment is well mixed. The output of this tool provides the mass concentrations of NMs in each compartment at steady-state in three different physical-chemical forms: (i) freely dispersed, (ii) heteroaggregated with natural colloids (450 nm), (iii) heteroaggregated with coarse natural particles (>450 nm). In addition to the steady-state analysis, the model also provides a time-dynamic analysis option.

2.2.2.5 nanoDUFLOW (Quik, de Klein and Koelmans, 2015[33])

20. NanoDUFLOW is a nanomaterial water quality model implemented in the DUFLOW Modelling Studio (v3.8.7) developed by Quik, de Klein and Koelmans (2015[33]). It is a dynamic, spatially-resolved model that simulates one-dimensional unsteady flow in open-channels. The model runs using particle number concentrations and converts the output to total mass concentrations of manufactured NMs in the water column and sediments with respect to river distance and time. It also considers the concentration of manufactured NM homo- and hetero-

aggregates separately, as a function of manufactured NM and natural suspended solid size classes.

2.2.2.6 WASP8 (Bouchard et al., 2017[31])

21. The Water Quality Analysis Simulation Program (WASP) is a dynamic, spatially resolved tool. It estimates the fate and transport of environmental contaminants in surface waters and sediments. WASP allows users to investigate 1, 2, and 3 dimensional systems. The update from WASP7 contains an Advanced Toxicant module, which includes a new state variable class for nanomaterials. The output of this tool provides the total steady-state mass concentration of manufactured NMs in the water column and surface sediments with respect to river distance and time. It also considers the concentrations of manufactured NM bound to sand, silt, clay and particulate organic matter within the water column and sediments.

2.2.2.7 LearNano (Liu et al., 2015[13])

22. LearNano uses a life cycle inventory assessment modelling approach to estimate nanoparticle flows from production and use to the environment (air, water, and soil), WIPs, landfills, WWTPs on a regional scale. Manufactured NM production rates and transfer coefficients are obtained from a parameter database by specifying the manufactured NM(s), application(s), and region(s) of interest. The output of the tool provides manufactured NM mass flows amongst compartments, which is visually represented using Sankey diagrams. Distribution of release rates may also be modelled on a country or global scale.

2.2.2.8 MendNano (Liu and Cohen, 2014[24])

23. MendNano is a web-based environmental fate modeling tool from the same developers as LearNano, and is hosted on the same website. The model is a dynamic fate modeling tool that iteratively solves as system of differential equations that describes the kinetic behaviour of nanomaterial transfers between compartments such as sediment, air, water, and soil. Mendnano considers nanomaterial particle size distribution. The tool provides a graphical user interface that allows users to customize exposure scenarios from a number of pre-organized input parameters that are supplied by several databases. Documentation and user-guide is provided.

2.2.2.9 Rhone/Rhine (Sani-Kast et al., 2015[29])

24. This model was based on established multimedia fate models for organic chemicals, but process descriptions were adjusted to account for nanoparticle-specific properties and behaviour in the environment. It assumes that each environmental compartment is well mixed. The output of this model provides the steady-state mass concentrations and particle concentrations of NMs in the water column and sediments, with respect to river distance. It also considers the concentrations of NM bound to suspended particulate matter in the water column. Sani-Kast et al. (2015[29]) presents a model that is a modified version of Praetorius et al. (Praetorius, Scheringer and Hungerbühler, 2012[32]). It considers the impact of spatial and temporal variability in environmental conditions on the fate of manufactured NMs. The output of this model provides the mass concentrations of NMs in the water column and sediments in two dimensions, with respect to river distance and time. The Rhone/Rhine model was not retained for further evaluation due to inaccessibility of the model code from the developers.

2.2.2.10 WASP7 (Dale et al., 2015[30])

25. Dale et al. (2015[30]) coupled the James River Basin portion of the Phase 5.3.2 Chesapeake Bay Watershed Model (WSM) with WASP7. WSM was designed to facilitate sediment and nutrient management planning in the Chesapeake Bay. In this adaptation, WSM was used to model manufactured NM runoff loads, effluent loads and stream hydrology that are then read into WASP7. WASP7 is a dynamic, spatially-resolved model that evaluates the fate and transport of environmental contaminants in surface waters and sediments. It assumes that each environmental compartment is well mixed. Both models were configured to model nanoparticle fate. WSM provides the nanoparticle load to river from effluent and agricultural runoff over time. WASP7 then calculates the mass percent of nanoparticles in the water column, oxic surface sediments and anoxic deep sediments with respect to time and space. The WASP7 model was not retained for further evaluation due to inaccessibility of the model code. The developers instead pointed us to WASP8 (see section 2.2.2.6) as an updated replacement for WASP7.

3 METHODOLOGY

26. The project contains a functional assessment, a statistical analysis, an evaluation, and provides recommendations on the applicability and suitability for these tools to be used in regulatory risk assessment. The functional assessment assesses the user-friendliness, the scope, the underlying assumptions, algorithms, and describes the input parameters and model output for transparency and understandability. The statistical analysis contains an uncertainty and sensitivity analysis that quantifies the uncertainty in the model output, and quantifies the sensitivity in the model input parameters respectively. The statistical analysis aims to enhance the reliability and decision-making power of these tools. Using the findings from the functional assessment, the results of the analysis, and real data where possible, this project evaluates the tools based on their depth and realism. Finally, this project relies on the completed work herein to provide recommendations on the applicability, usability, and suitability for these tools to be used in regulatory risk assessment.

3.1. Test system information

27. Details about the computer system on which the functional assessments were performed are summarized in table 3 below:

Table 3: Summary of test system information.

Processor:	Intel® Core™ i5-6300U CPU @ 2.40GHz
RAM:	32.0 GB
OS:	64-bit Windows 10 Enterprise, x64-based processor

3.2 Functional assessment

28. The functional assessment section of this report has three goals: (1) Allow users to compare modeling tools based on applicability criteria, usage, and features. (2) Assure users that models have been independently installed and run. (3) Summarize assumptions, algorithms, input parameters, and outputs of the models. The functional assessment contains two metrics that were developed to help objectively rank models according to their scope, and according to their user-friendliness. These metrics, the applicability criteria score, and the difficulty scale, are described below.

3.2.1 Applicability criteria score

29. The criteria that were used to prioritize the modeling tools in the compilation part of the project are reiterated below in this applicability score. They are used here for the functional assessment in a criteria score that can be found under the **Features** sub-heading for each modeling tool's assessment. The goal of the applicability criteria score is to summarize the

features of each modeling tool into a number, thereby allowing the user to compare modeling tools using a single metric. The interpretation and definition of the score are described explicitly below. For details about the scoring parameters such as weights (α), individual scoring features within the five applicability criteria, or to see details about each modeling tool's individual score, review the spreadsheet entitled applicability_criteria_score.xlsx

3.2.1.1 Applicability Criteria:

1) The **domain** of the model should address one or more of the following environmental media: soil, sediment, air, water, or other applications.

2) The model **scope** should be broad enough to be applied across a variety of emission and exposure scenarios.

3) The model should have **supporting documentation** that are easily available to users and are transparent with respect to model principles and algorithms.

4) **Dynamic models** should account for changes in exposure over the **long-term**.

5) The model contains appropriate **default values** for input parameters and allows for **user-overrides**.

3.2.1.2 Score Definition:

30. Each criteria has a weight (α) between 0 and 1 representing the importance of the criteria.

31. For a given model to be scored, each criteria is given a presence value (P);

P = 0 where the model does not meet the criteria

P = 1 where the model does meet the criteria

32. The score (S_c) is the sum-product of the weights and presence values.

$$S_c = \sum_i \alpha_i P_i \qquad [1]$$

33. The score is normalized as a value between 0 and 1, relative to the highest possible score.

3.2.1.3 Score Interpretation:

1) The score is a value between 0 and 1.

2) A score of 0 means the model does not meet any of the applicability criteria.

3) A score of 1 means the model perfectly meets the applicability criteria.

4) A score between 0 and 1 means the model matches some of the applicability criteria.

5) The closer the score is to 1, the better it matches the applicability criteria.

3.2.2 Difficulty scale

34. The difficulty scale places models on a scale that allows users to compare the user-friendliness of each tool relative to each other based on clearly defined criteria. There are four criteria; (1) the first criteria pertains to the use (or lack) of a graphical user interface (GUI). (2)

The second criteria pertains to the computer storage and manipulation of the input parameters. (3) The third criteria pertains to the computer storage and retrieval of the model output. Finally, (4) the fourth criteria pertains to the presence and quality of the user-guides or documentation that support the tools. The difficulty scale is arbitrarily defined from 1 to 5; 1 being easiest to use to 5 being the most difficult. A model is scored on the scale according to the difficulty of its usage. Individual details about how each tool places on the scale according to the criteria are provided under the tool's respective **Usage** sub-heading. General descriptions for the criteria are provided in table 4:

Table 4: Model characteristics considered and their placement on the difficulty scale.

Difficulty Scale	Example Model Characteristics
1 (Easiest to use)	1. **Intuitive** graphical interface. (GUI) 2. Input parameters are **specified in the GUI** 3. Results are stored in **.csv or .xlsx** 4. User guide is **well written**
2	1. **Intuitive** graphical interface. 2. Input parameters are **specified in .xslx** 3. Results are stored in **.csv or .xlsx** 4. User guide is **well written**
3	1. Graphical interface **provided**. 2. Input parameters are **specified in one or more formats.** 3. Results are stored in **.csv or .xlsx** 4. User guide is **provided.**
4	1. Graphical interface **missing, limited, or complicated.** 2. Input parameters are **specified using scripts.** 3. Results are available in **binary.** 4. User guide is **missing, limited, or complicated.**
5 (Most difficult to use)	1. Graphical interface **missing.** 2. Input parameters are **specified using scripts.** 3. Results are available in **binary.** 4. User guide is **missing.**

3.3 Statistical analysis

3.3.1 Selection of tested parameters

35. The parameters for the sensitivity and uncertainty analysis were chosen using the functionality of PDBM (see appendix 8.2). The chosen parameters are all numeric parameters where it is sensible to devise a range of values for testing. For the Monte Carlo simulations, all numeric parameters were chosen for random sampling, with the exception of some constants like pi or gravitational acceleration. For the sensitivity testing, as many parameters were chosen as it was practical for the time-period in which the testing took place (which differed for each tool depending on the run time of the tool). Tools that took longer to run were tested on fewer parameters. Where it was not practical to test all parameters, priority was given to parameters that described the physical or chemical properties specific to the nanomaterial being modelled (e.g. hetero- or homo-aggregation rates, particle size, or radius.)

3.3.2 Description of scenarios tested for each modeling tool

3.3.2.1 DPMFA

36. The default DPMFA scenario chosen for analysis is from the Bornhöft (2017[12]) publication (whose input parameters can be found in the Bornhöft (2017[12]) supplemental

information). The scenario represents a dynamic Carbon Nano Tubes (CNT) simulation in Switzerland with varying production volumes in each year from 2003 to 2020. The model offers no spatial resolution, but uses market data on the production, manufacturing, consumption and distribution of CNT in the market in Switzerland. These market data are translated as transfer coefficients in the coefficients matrix of the Leontief input-output model (Leontief, 1986[34]). The model describes Switzerland's market as connected compartments each having (either during or at the end of the simulation) a single value of CNT volume per time step of the simulation. These compartments include CNT production, manufacturing, consumption, paint, textiles, energy, sensors, aerospace, Waste Incineration Plants (WIP), Sewage Treatment Plants (STP), surface and waste waters, and air. Output compartments wherein CNT volume estimations are made at the end of the simulation include elimination (removal from the system), recycling, export, cement plant, landfill, sediment and soil. Nanomaterial volumes are input as yearly inflow volumes (in tonnes) into the production compartment. Nanomaterial volumes are output as yearly outflow volumes (in tonnes) in each of the output compartments (as mentioned above). The uncertainty metrics (described in section 3.3.3) are calculated on the output for each time step, for the output compartments soil, sediment, recycling, landfill and export. The sensitivity (described in section 3.3.4) is calculated for each output compartment for each time step. There are no nano-specific processes or parameters involved with this model.

3.3.2.2 nanoRelease

37. The default nanoRelease scenario chosen for analysis is from the Song et al. (2017[14]) publication (wherein the relevant input parameters can be found). The scenario represents a dynamic TiO_2 nanoparticle simulation in the United Sates using stochastic lifetimes of the nanomaterial in each compartment in each year from 2000 to 2020. The model offers no spatial resolution, but uses market data on the production, manufacturing, consumption and distribution of TiO_2 nanoparticles in the paint market in the United States. These market data are translated as percentages of nanoparticles being transferred from one compartment to other compartments, as well as average lifetimes of nanoparticles in each compartment. The model describes the lifecycle of TiO_2 nanoparticles in the United States paint market as connected compartments that either represent different stages of the life cycle (e.g. production, manufacturing, consumer use, or end-of-life) or represent sectors of the paint market (e.g. construction and building, household and furniture, medical, packaging, electronics, automotive). The model predicts output volumes of TiO_2 nanoparticles in tonnes in the following environmental compartments; air, water, soil, and landfill. Nanomaterial volumes are input as stochastic yearly production volumes of TiO_2 nanoparticles in tonnes. Nanomaterial volumes are output as volumes of TiO_2 nanoparticles in tonnes in each of the output environmental compartments for each time step (year) of the simulation. The uncertainty mertrics (described in section 3.3.3) are calculated on the output for each time step and for each output environmental compartment. The sensitivity (described in section 3.3.4) is calculated for each time step and for each output environmental compartment. There are no nano-specific processes or parameters involved with this model.

3.3.2.3 nanoFate

38. The default nanoFate scenario chosen for analysis is from the Garner et al. (Garner, Suh and Keller, 2017[23]) publication (whose input parameters can be found in the Garner et al. 2017 supplemental information). The scenario represents a dynamic TiO_2 nanoparticle simulation in the San Francisco Bay area in California, United States. The scenario simulates the fate of TiO_2 nanoparticles in environmental compartments by taking into account nano-specific kinetic processes like homo- and hetero-aggregation, first-order mass transport

processes, and dynamic environmental conditions like temperature, wind speed, and precipitation for every day from 2010 through 2014 (5 years in total). The model offers spatial resolution on environmental compartments such as air, marine and fresh water, marine and fresh sediment, and four types of soil (urban, agricultural, undeveloped, and bio-solids). The model includes substance chemical and physical parameters like particle size, aggregate radius, density, dissolution rates, sedimentation rates, heteroaggregation rates, and soil partition rates. The model also includes environmental parameters including the density and spatial properties of the environmental media, the temperature, wind-speed, and precipitation among other parameters. Nanomaterial volumes are input as kg of TiO_2 per day. Nanomaterial volumes are output as concentrations of TiO_2 in each of the environmental compartments in kg/m^3 for each time step of the simulation. The uncertainty mertrics (described in section 3.3.3) are calculated on the output for each time step and for each output environmental compartment (where all soil type concentrations are summed.) The sensitivity (described in section 3.3.4) is calculated for each time step and for each output environmental compartment. Nano-specific processes for this scenario are homo- and hetero-aggregation of nanoparticles.

3.3.2.4 SimpleBox4nano

39. The default SimpleBox4nano scenario chosen for analysis is from the Meesters et al. (2014[22]) publication (whose input parameters can be found in the SimpleBox4nano spreadsheet). The scenario represents a steady state TiO_2 nanoparticle simulation in Switzerland. The model simulates the fate of TiO_2 nanoparticles in environmental compartments at steady state using nano-specific processes like hetero- and homoaggregation, and dissolution as a removal process. The model offers limited spatial resolution on environmental compartments such as air, water, soil and sediment. Volumes, areas, depths among other environmental parameters are provided on a regional, continental or global scale. The model includes substance specific parameters like the radius of the nanoparticle, the density of the nanoparticle, attachment efficiencies, and dissolution rates among other parameters. Nanomaterial volumes are input as emission rates in metric tons per year that are converted to mol/s in any of the environmental compartments. Nanomaterial volumes are output in g/L, g/m^3 or g/kg for free nanoparticles, and for hetero-agglomerates of two different size categories in each environmental compartment. The uncertainty metrics (as described in section 3.3.3) are calculated for the sum of all three species of nanomaterial in all environmental compartments. That is, the uncertainty metrics are calculated from the individual outputs from the “nano micro output” page of the excel file. More specifically, the uncertainty is calculated from the “Concentration ENPs (S+A+P)” box. Moreover, all media of different kinds are summed together to form a single output for that media (e.g. all soil types, “Natural soil”, “Agricultural Soil”, and “Other Soil” are summed together to simplify to one soil output representing all three types). The same simplification is done for all media such that the uncertainty for each media can be represented unitarily for each media type (i.e. one fresh water output, one marine water output, one soil output, one sediment output.) This simplification of the output is for the purpose of summarizing the results in a coarse fashion that makes it easy to present the results in this report. The sensitivity (described in section 3.3.4) is calculated on each species individually and for each environmental compartment.

3.3.2.5 nanoDUFLOW

40. The default nanoDUFLOW scenario chosen for analysis is from the Quik et al. (Quik, de Klein and Koelmans, 2015[33]) publication (whose input parameters can be found in the supplemental information). The scenario represent a dynamic CeO_2 nanoparticle simulation in a section of the Dommel river system in the Netherlands for 5 days using a time step of 5

minutes with hydrological conditions being constant in time. The model simulates the fate of five size classes of CeO_2 nanoparticles in the waters and sediments of the river system using vetted hydrological processes from DUFLOW in combination with nano-specific processes like hetero- and homoaggregation, dissolution, degradation, sedimentation and resuspension. The model offers a high degree of spatial resolution by representing a roughly 40 km stretch of the Dommel in 477 water and sediment compartments each with their own spatial and flow parameters. Nanomaterial volumes are input as initial concentrations of nanomaterial in g/L, as well as boundary conditions determining the inflow of nanomaterial in g/L. Nanomaterial volumes are output as concentrations in g/L in each sediment and water compartment, for each species of nanomaterial and for each time step of the simulation. The uncertainty metrics (described in section 3.3.3) are calculated for the sum of concentrations for all five size classes in each compartment during the last time step of the simulation. The sensitivity (described in section 3.3.4) is calculated for each species individually in each compartment and for each time step.

3.3.2.6 WASP8

41. The default WASP8 scenario chosen for analysis is from the Bouchard et al. (2017[31]) publication (whose input parameters can be found in the supplemental information). The scenario represents a dynamic Multi-Walled Carbon Nano Tubes (MWNCT) nanoparticle simulation in a section of the Brier Creek river system in central eastern Georgia USA for 10 years using a daily time step. The model simulates the fate of four species of MWCNT (free, MWCNT-silt, MWCNT-clay, MWCNT-POM (Particulate Organic Matter)) in the Brier Creek river system using nano-specific processes including hetero-aggregation, settling and resuspension. The model offers a high degree of spatial resolution that divides the river section of over 100 km into 12 sections that include water, sediment, and deeper sediment. Nanomaterial volumes are input as load quantities of free MWNCT at a default of 0.1 kg/day in the most upstream part of the river system. Nanomaterial volumes are output as concentrations in mg/L in each of the environmental compartments for each section of the river system for each time step of the simulation. The uncertainty metrics (described in section 3.3.3) are calculated as the sum of all concentrations for all species in each compartment during the last time step of the simulation. The sensitivity (described in section 3.3.4) is calculated for each species individually, in each compartment and for each time step of the simulation.

3.3.3 Uncertainty analysis

42. The uncertainty analysis follows a Monte Carlo simulation method that follows the guidance from JCGM's guidance document on the propagation of distributions (JCGM, 2008[35]) Probability distributions are estimated for each parameter. The distribution type, associated estimated error, and number of samples are described in table 9. All parameter values are randomly sampled simultaneously according to their respective probability distributions (approximated using NumPy's numpy.random module.)

43. Table 5 below, presents a summary of the conditions used for the uncertainty and sensitivity analysis. The tool column identifies the name of the tool. The uncertainty conditions column shows sub tables for each tool identifying probability distribution types, error ranges, and number of samples used in the Monte Carlo Simulations. The sensitivity conditions column shows sub tables for each tool identifying ranges of parameter values and size of range (number of values in the range) used for the sensitivity testing. If error ranges are provided by the author (like for DPMFA for example,) then those error ranges are used. Otherwise, error ranges are estimated to be +/- 50% of the default values. In the case of nanoFate, error ranges of +/- 10% of the default values are used because using error ranges of 50% caused the program to crash. Thus for lack of available trouble-shooting time, smaller error ranges were used to produce

values closer to the default in order to prevent the program from crashing. LearNano and MendNano are not included in table 9 since the analysis was not performed (due to unresolved error messages).

Table 5: Summary of conditions for uncertainty and sensitivity analysis.

Tool	Uncertainty Conditions		Sensitivity Conditions	
DPMFA	Distribution types	Triangular, Normal, Uniform	Value range	Production Volumes: Range from publication [5] Transfer Coefficients: (0,1)
	Error range	Values from publication [5]		
	Number of samples	100 000	Range size	1 000
nanoRelease	Distribution types	Triangular, Normal	Value range	For factors and coefficients: (0,1) For all other parameters: +/- 0.5x Default value
	Error range	0.5x Default value		
	Number of samples	100 000	Range size	1 000
nanoFate	Distribution types	Normal	Value range	For factors and coefficients: (0.1,0.99) For all other parameters: +/- 0.1x Default value
	Error range	0.1x Default value		
	Number of samples	220	Range size	5
SimpleBox4nano	Distribution types	Normal	Value range	+/- 0.5x Default value
	Error range	0.5x Default value	Range size	100
	Number of samples	3 000		
nanoDUFLOW	Distribution types	Normal, Uniform	Value range	+/- 0.5x Default value
	Error range	0.5x Default value	Range size	10
	Number of samples	200		
WASP8	Distribution types	Normal, Uniform	Value range	+/- 0.5x Default value
	Error range	0.5x Default value	Range size	5
	Number of samples	200		

44. The metrics used to quantify the uncertainty in the output are described below:

Expectation for the random output variable X:

$$E(X) = \int_{-\infty}^{\infty} \varepsilon g_x(\varepsilon)\, d\varepsilon \qquad [2]$$

Variance for the random output variable X:

$$V(X) = \int_{-\infty}^{\infty} [\varepsilon - E(X)]^2 g_x(\varepsilon) d\varepsilon \qquad [3]$$

Standard Deviation for the random output variable X:

$$Stdev(X) = [V(X)]^{1/2} \qquad [4]$$

Stipulated Coverage Interval:

45. Symmetric or shortest 95 % probability coverage interval centralized around the expectation.

Lower bound of coverage interval:

46. The lower bound (smallest positive value) of the stipulated 95 % probability coverage interval.

Upper Bound of Coverage Interval:

47. The upper bound (highest positive value) of the stipulated 95 % probability coverage interval.

48. Where $g_x(\varepsilon)$ is the probability density function (PDF) describing the output variable for values ε of the output variable X within the interval between the lowest and highest values in the distribution of output values. PDFs were approximated by histograms bound by the lowest and highest values in the distribution of output values using a number of bins equal to 301, and normalized such that the integral of the PDF sums to 1.

49. In the uncertainty analysis results section (4.x.2), if the output is a time series, then the metrics are calculated for each time step and presented graphically in a time-series plot. The metrics for the last time step are also summarized in a table. If the output is a single value, then the metrics are presented graphically in a histogram approximating the PDF, as well as summarized in a table.

50. The output of the uncertainty analysis is a set of metrics as described above (expectation, variance, standard deviation, and confidence interval). How these metrics should be interpreted is described in this paragraph. The expectation is the expected value of the output. That is we expect the value of the output to be the value that is calculated by the expectation integral. The variance and standard deviation describe the spread of possible values around the expectation. The standard deviation is the square root of the variance, and thus we can simply refer to the standard deviation to describe the spread of possible values around the expectation. The larger the standard deviation, the larger the spread. In other words, the standard deviation in the output is a single value that summarizes the uncertainty surrounding the expected value that is caused by uncertainty in the input parameters. The confidence interval is defined by a percentage or proportion, an upper bound, and a lower bound. The upper and lower bound defines the area of the probability density where a given percentage of the density can be found. For example, a 95% confidence interval provides the boundary in the density histogram within which 95% of the probability density can be found. For the following interpretation we will use 95% as an example value (however, the confidence interval can be defined for any percentage of the probability density). The confidence interval then should be interpreted as the interval within which you can find the output value with a 95% probability. That is, the probability that the output takes on any value within the interval is 95%. In other words, there is a 5% chance that the output takes on a value outside of this interval.

51. Thus, as the metrics are interpreted in a rather general way above, the user has freedom to define a confidence interval, or a qualitative value (such as low or high uncertainty) to a standard deviation depending on the needs of the user. If the output is normally distributed, then it is possible to normalize the distribution such that standard deviations can be compared across different scenarios.

3.3.4 Sensitivity analysis

52. The sensitivity analysis in this report is performed on each model individually. The sensitivity analysis quantifies the sensitivity of a parameter with respect to the model using a conventional sensitivity score described in MacLeod et al. (MacLeod, Fraser and Mackay, 2002[36]), reiterated here in the formula below:

$$S = \frac{\Delta O / O_1}{\Delta I / I_1} \quad [5]$$

$$\Delta O = O_2 - O_1 \quad [6]$$

$$\Delta I = I_2 - I_1 \quad [7]$$

53. Where:

- S is the sensitivity of a given parameter.
- O_1 is the original output value.
- O_2 is the output value that results from the incremented input value.
- I_1 is the original input value.
- I_2 is the incremented input value.

54. As it is described in MacLeod et al. 2002, $\Delta I/I_1$ is chosen such that the increment by which we are altering the input parameter value is 0.1%.

55. Thus, $\Delta I/I_1$ always equals 0.001. The process of quantifying the sensitivity for a set of parameters is essentially the same for each model. Each analysis was performed in a slightly different way, to accommodate differences in how each program runs on a computer. However, these differences do not affect the general methodology of quantifying sensitivity in such a way that the results are no longer comparable.

56. The general steps of the sensitivity analysis algorithm performed on each model are summarized below:

1) Chose a set of parameters.
2) Estimate the range of parameter values to quantify the sensitivity:
    - If any measure of error σ is provided for a value μ, then this error is used to estimate the range as such: [μ - σ, μ + σ].
    - For any factor whose value is always between 0 and 1, the range is [0, 1].
    - If a range is explicitly given by the author, then this range is used.
    - If none of the above occur, then the range for a given parameter value μ is +/- 50% of its value: [(μ - 0.5*μ), (μ + 0.5* μ)], unless otherwise specified due to practical limitations.
3) Sample a linear range of parameter values using the parameter range defined in 2).
4) The number of values within the linear range depends on the practical reason of how quickly the model can produce an output. For example, it was possible to quantify the sensitivity for 1000 parameter values within the specified range for DPMFA, whereas for SB4N it was only possible to quantify the sensitivity for 100 parameter values within the specified range.
5) For each parameter, and for each value in the sampled range of that parameter, one at a time, the value is set as the input (I_1) , while the other parameters are default.
6) The output (O_1) is collected for each of the iterations described in 4).
7) For each parameter, and for each value in the sampled range of that parameter, one at a time, the value is set as the input plus the 0.1% increment (I_2), while the other parameters are default.
8) The output (O_2) is collected for each of the iterations described in 6).
9) For each output in O_1 and O_2, ΔO is calculated as described in equation [2]
10) The sensitivity of the parameter for each parameter value tested is calculated as described in equation [1] where the denominator is set at 0.001.

57. The number of sensitivity score values, and their meaning depends on the shape and size of the output. In general the sensitivity score can be interpreted as follows:

- A sensitivity score of 1 means changing input by 0.01 percent changes the output by 0.01 percent
- A sensitivity score of greater than 1 means changing the input by 0.01 percent changes the output by more than 0.01 percent
- A sensitivity score of less than 1 means changing the input by 0.01 percent changes the output by less than 0.01 percent
- A sensitivity score of zero means that changing the input has no effect on the output

58. The overall sensitivity of each parameter is the average sensitivity calculated for the output in each compartment, for each time step of the model, for each parameter value.

59. The parameter vs sensitivity plots show the average sensitivity of all tested parameter values for the output in each compartment, for each time step.

4 ASSESSMENTS AND ANALYSES

60. Section 4 Assessments and Analyses presents the results of the functional assessments and statistical analyses for each of the tools and models evaluated. An exact description of what information is presented can be found in the appendix (section 8.1; Assessment Overview). Section 4 is divided into subsections that present the results for each of the tools and models individually. Thus each tool or model has been assessed and analyzed individually, and their assessment and analysis can be found in a section that can be read independently from the other tools or models. First, the assessment is presented and summarizes the functionality, user-friendliness and scope of the model. Second, the results of the statistical analysis are presented, which summarize the uncertainty and sensitivity analysis. Then a high level discussion is presented whose purpose is to summarize in text the results of the assessment and analysis, including interpretation.

4.1 DPMFA

4.1.1 Functional assessment

4.1.1.1 MECHANISTIC ASSESSMENT

4.1.1.1.1 AUTHOR: Nikolaus Bornhöft

4.1.1.1.2 VERSION: 0.921

4.1.1.1.3 ACCESSIBILITY:

Table 6: Accessibility information for DPMFA.

COST	Free
MODEL ACCESS SOURCE	https://pypi.org/project/dpmfa-simulator/
DOCUMENTATION SOURCE	https://www.zora.uzh.ch/id/eprint/152424/1/152424.pdf

4.1.1.1.4 DEPENDENCIES:

1. Python 2.7

   Python dependencies:

   - NumPy
   - Matplotlib

4.1.1.1.5 INSTALLATION:

1) Install Python 2.7, NumPy, and Matplotlib

2) Use executable file (dpmfa-simulator-0.921.win32.exe) to install the model software.
3) Requires administrative rights on Windows 10
4) Alternatively, the model software can be installed from the command-line terminal using:

```
>pip install dpmfa-simulator
```

4) Lastly, the model software can be installed from the command-line terminal using:

```
>cd Documents\Project_Exposure_Models_NM\Models\DPMFA\dpmfa-simulator-0.921
>python setup
```

4.1.1.1.6 FOLDER AND FILE STRUCTURE

N/A

4.1.1.1.7 USAGE:

Summary:

1) Graphical interface missing.
2) Input parameters are specified using programming scripts.
3) Results are available in binary, scripting is required to re-format results.
4) User guide is comprehensive.

Difficulty Rating:

Table 7: Difficulty rating for DPMFA.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.1.1.1.8 FEATURES:

1) MFA
2) **Domain:** Soil, Sediment, Air, Water
3) **Scope:**
   - Any number of compartments and connectivities.
   - No spatial resolution.
   - Time-series
4) **Supporting documentation:** includes user-guide and publication.
5) The model is **dynamic**, probabilistic, and accounts for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.73

4.1.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):

- Flow of carbon nanotubes (CNT) in Switzerland

- 31 compartments and sinks, 80 transfers
- Air, Soil, Water, Sediment, WIP, STP, Landfill, Production, Manufacture, Consumption
- 2003-2014

2) **Results**:

- Consistent with previous modeling studies

4.1.1.2 THEORETICAL ASSESSMENT

4.1.1.2.1 ASSUMPTIONS:

Table 8: Summary of assumptions made by DPMFA.

Model Feature	Assumption
Compartment	- Non-spatial blocks - Sink: no material flow out of sink - Stock: material released out of stock
Transfer	- Transfer coefficients - Leontief Model - Mass Balance
Transformation	- Transformations are not present in the model
Substance	- Substance properties are not present in the model
Time	- Time-series - Yearly resolution - Dynamic: re-evaluation of parameters at each time step - Flow of material simultaneous and instantaneous at each time-step - Stochastic evolution of simulation

4.1.1.2.2 ALGORITHMS:

1) Monte-Carlo Simulation – random sampling of parameter values
2) Iterative time step – to update stocks and sinks with flow quantities
3) Leontief model – To calculate absolute material flow quantities (Leontief, 1986[34])

4.1.1.2.3 INPUT PARAMETERS:

Table 9: Summary of input parameters for DPMFA.

Parameter Type	Summary Note	Parameter Format
Compartment	Defined by name	Script
Compartment Property	Sink or stock	Script
Transfer	Coefficient	Script
Transfer Property	Position in matrix	Script
Transformation	None	None
Transformation Property	None	None
Release	Rate	Script
Release Property	Release delay/ Amount in tonnes	Script
Substance	None	None
Substance Property	None	None
Temporal	Duration of simulation	Script
Temporal Property	Time resolution	Script

4.1.1.2.4 MODEL OUPUT:

Table 10: Summary of model output for DPMFA.

Output Type	Output unit	Summary Note	Output Format
Single value	None	None	None
Time-Series	Same as input unit	Absolute quantity	Script

4.1.1.2.5 NANOMATERIAL APPLICATIONS:

[TiO_2, ZnO, Ag, CNT]

4.1.2 Uncertainty analysis

61. The table 11 below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the DPMFA model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics in the last time step (year) of the model output in the unit of tonnes for each of the endpoint compartments wherein CNT resides at the end of the simulation.

Table 11: Summary of quantified uncertainty metrics for DPMFA.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Soil	1271.72	67745.26	260.28	1013.29	761.63	1774.92
Sediment	851.73	77458.47	278.31	1071.10	318.44	1389.53
Landfill	26213.30	1.69e7	4112.69	16225.91	18084.72	34310.63
Recycling	36579.60	1.70e8	13051.75	49167.44	12045.02	61212.46
Export	10632.04	1.60e7	3994.51	15077.74	3126.91	18204.665

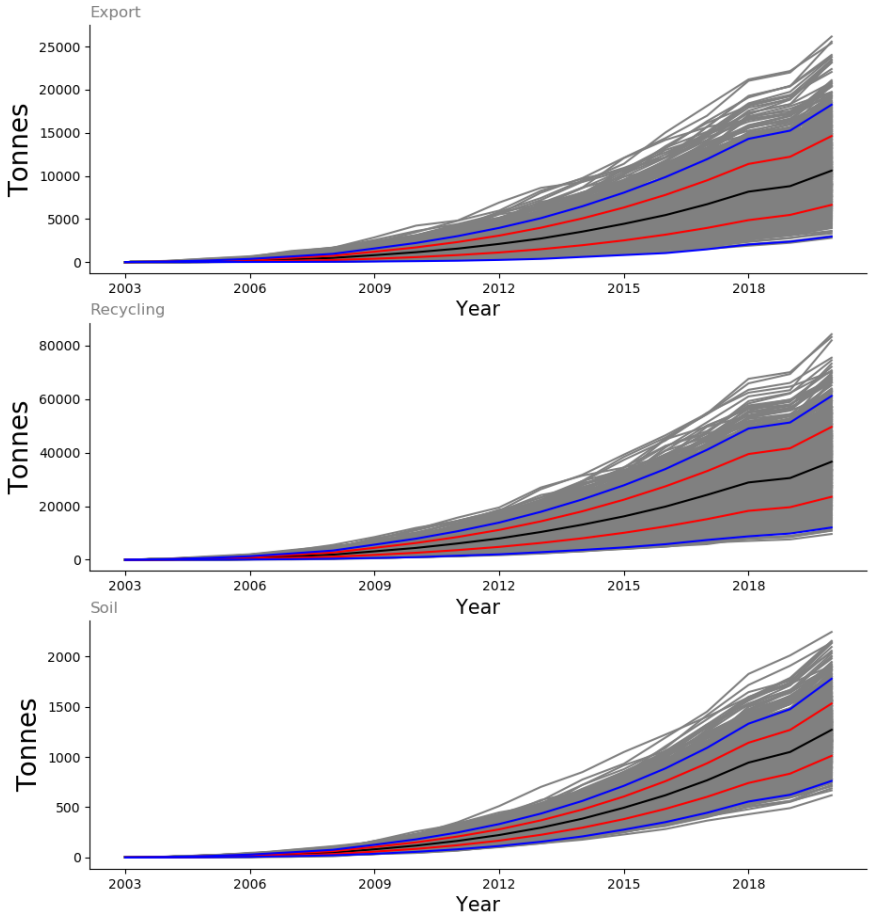
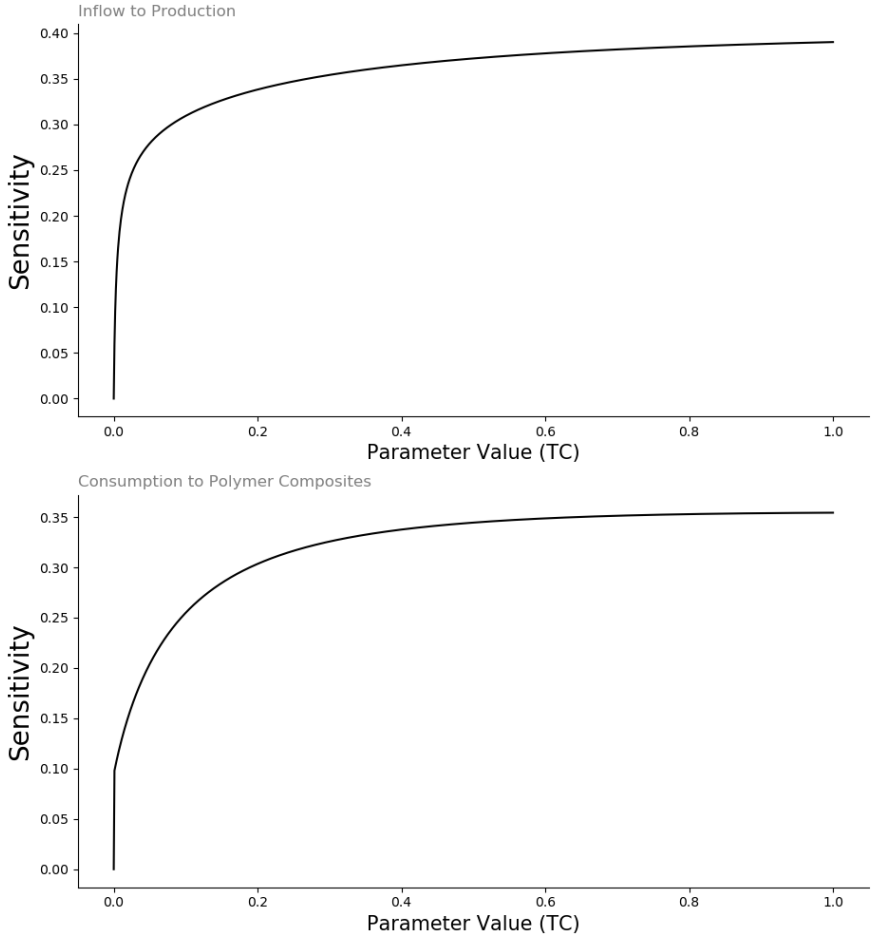


Figure 1. Output uncertainty for CNT volume in some output compartments for DPMFA.

Note: Figure 1 shows the output uncertainty for CNT volume in some of the output compartments of the tested scenario for DPMFA. The x-axis shows time-step in years, and the y-axis shows CNT volume in metric tonnes. Grey lines show first 1000 samples of the output from the MCS. Black lines show the expectations for each year. Red lines show +/- the standard deviation for each year. Blue lines show the boundaries of the 95% coverage interval. Names of the output compartments are labelled in grey in the top left of each plot: export, landfill, recycling, sediment, and soil.

4.1.3 Sensitivity Analysis



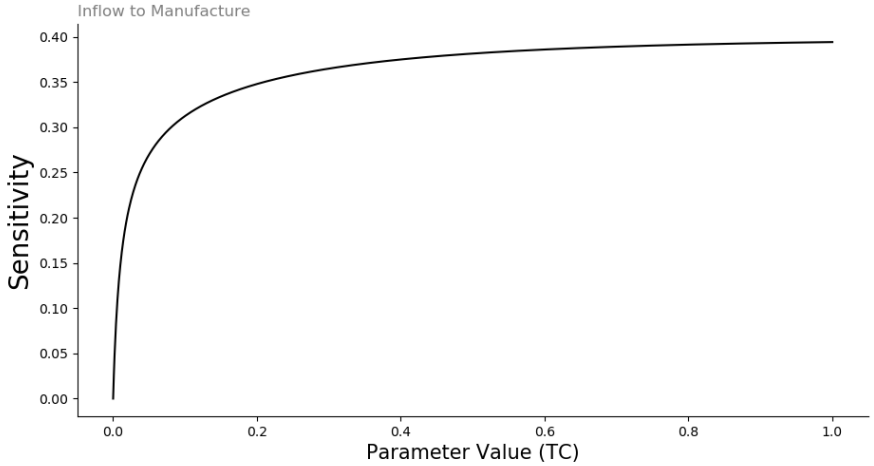


Figure 2. Sensitivity for the most sensitive parameters for DPMFA.

Note: Figure 2 shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for DPMFA. The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the TC for inflow to production, inflow to manufacture, and consumption to polymer composites.

62. In Table 12 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity for all time-steps, in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing (same as in publication [5]). The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 12: Overall sensitivity for each parameter for DPMFA.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Inflow volume	0.94444	10871.3	246	90216	tonnes
TC: Inflow to Manufacture	0.36314	0.00500	0	1	-
TC: Inflow to Production	0.35755	0.00500	0	1	-
TC: Consumption to Polymer Composites	0.32217	0.84000	0	1	-
TC: Consumption to Paint	0.30545	0.01400	0	1	-
TC: Consumption to Textiles	0.29080	0.00020	0	1	-
TC: Inflow to Consumption	0.28257	0.99000	0	1	-
TC: Consumption to Energy	0.24149	0.09100	0	1	-
TC: Consumption to Automotive	0.21660	0.01300	0	1	-
TC: Consumption to Aerospace	0.20920	0.00600	0	1	-
TC: Consumption to Consumer Electronics	0.20911	0.03100	0	1	-
TC: Consumption to Sensors	0.20481	0.00400	0	1	-
TC: Polymer Composites to Air	0.10785	0.01200	0	1	-
TC: WIP to Elimination	0.09548	0.98000	0	1	-
TC: Treated Water to Sewage Sludge 3	0.09219	0.95000	0	1	-
TC: Energy to Recycling	0.08076	0.75000	0	1	-
TC: Energy to Export	0.07596	0.20000	0	1	-
TC: Energy to WIP	0.06793	0.05000	0	1	-
TC: Sewage Sludge to Cement Plant	0.06212	0.22000	0	1	-
TC: Sewage Sludge to WIP	0.06017	0.78000	0	1	-
TC: Production to Air	0.05801	0.24000	0	1	-
TC: Production to Waste Water	0.05655	0.74000	0	1	-
TC: Paints to Waste Water	0.05507	0.01000	0	1	-
TC: Polymer Composites to WIP	0.04947	0.98800	0	1	-
TC: Soil to Surface Water	0.04614	0.00549	0	1	-
TC: Air to Surface Water	0.04563	0.03000	0	1	-
TC: Manufacture to Waste Water	0.04380	0.33000	0	1	-
TC: STP to Surface Water	0.04184	0.03200	0	1	-
TC: Waste Water to Surface Water	0.04160	0.01800	0	1	-
TC: Paints to Surface Water	0.03945	0.01000	0	1	-
TC: Manufacture to Air	0.03927	0.35000	0	1	-

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
TC: Wet Scrubber to Air	0.03509	0.00100	0	1	-
TC: Paints to Air	0.03464	0.01000	0	1	-
TC: Paints to Soil	0.03443	0.01000	0	1	-
TC: Manufacture to WIP	0.03241	0.33000	0	1	-
TC: Aerospace to Air	0.01982	0.01000	0	1	-
TC: Air to Soil	0.01791	0.97000	0	1	-
TC: Solid Ash to Export	0.01658	0.22000	0	1	-
TC: Paints to Landfill	0.01629	0.50000	0	1	-
TC: Solid Ash to Landfill	0.01611	0.78000	0	1	-
TC: Paints to Recycling	0.01557	0.46000	0	1	-
TC: WIP Filter to Solid Ash	0.00795	0.99700	0	1	-
TC: Ashes to Landfill	0.00675	0.81000	0	1	-
TC: Aerospace to Recycling	0.00549	0.60000	0	1	-
TC: Aerospace to WIP	0.00525	0.39000	0	1	-
TC: Sensors to Export	0.00417	0.20000	0	1	-
TC: Consumer Electronics to Export	0.00415	0.20000	0	1	-
TC: Sensors to Recycling	0.00389	0.75000	0	1	-
TC: Consumer Electronics to Recycling	0.00377	0.75000	0	1	-
TC: Sensors to WIP	0.00321	0.05000	0	1	-
TC: Consumer Electronics to WIP	0.00244	0.05000	0	1	-
TC: Automotive to Air	0.00189	0.01000	0	1	-
TC: Textiles to Waste Water	0.00131	0.02000	0	1	-
TC: Textiles to Air	0.00094	0.02000	0	1	-
TC: Textiles to WIP	0.00053	0.96000	0	1	-
TC: Automotive to Export	0.00051	0.20000	0	1	-
TC: Automotive to Recycling	0.00037	0.40000	0	1	-
TC: Automotive to WIP	0.00036	0.39000	0	1	-
TC: Treated Water to Sewage Sludge 4	0.00000	0.50000	0	1	-
TC: Treated Water to Sewage Sludge 2	0.00000	0.93000	0	1	-
TC: Treated Water to Sewage Sludge 1	0.00000	0.88000	0	1	-

4.1.4 Discussion

63. Dynamic Probabilistic Material Flow Analysis (DPMFA) is a material flow analysis (MFA) modeling tool that simulates the dynamic flow of material through a variety of processes including periodic updating of stocks and sinks, scheduled releases, and random sampling of transfer coefficients. DPMFA provides no graphical user interface, as it is accessed entirely through Python scripting and the command-line terminal. DPMFA is well documented, and a detailed user-guide is provided, making it relatively easy to use and access its features. Because DPMFA does not provide a graphical interface, it is used entirely through Python scripting, and the output requires coding knowledge to obtain, DPMFA scores a 4/5 on the difficulty rating. DPMFA's features includes domains such as soil, sediment, air, and water (among many other market-related domains). DPMFA is highly modular as the user of the tool can design the model scenario from the begining and can implement any number of compartments

and connectivity between compartments. DPMFA does not require the use of spatial data, and yields a time-series output containing absolute quantities of material in desired end-point compartments. DPMFA is dynamic, probabilistic, and accounts for long term changes. Because of its many features, DPMFA scores a 0.73 on the applicability criteria score. DPMFA uses the Leontief model to calculate absolute flow quantities, while using a built-in Monte-Carlo simulator that randomly samples transfer coefficients that are used to determine flows of material in a matrix. Required input parameters are minimal, and are limited by the number of connections between compartments. Input parameters include initial volumes of material, estimated releases for each time-step, transfer coefficients, and parameters that define delays and functional release of material from stocks. The uncertainty analysis reveals that DPMFA performs as expected, with the uncertainty becoming larger as the simulation progresses through time. The sensitivity analysis reveals that DPMFA performs in a predictable and explicable manner. The most sensitive parameters are the initial inflow volume of material, and transfer coefficients whose value is above 0.25. Some parameters where revealed to be completely insensitive with respect to the output of the model.

4.2 nanoRelease

4.2.1 Functional assessment

4.2.1.1 MECHANISTIC ASSESSMENT

4.2.1.1.1 AUTHOR: Anastasia Lazareva, Arturo A. Keller

4.2.1.1.2 VERSION: 2019-06-17

4.2.1.1.3 ACCESSIBILITY:

Table 13: Accessibility information for nanoRelease.

COST	Free
MODEL ACCESS SOURCE	https://github.com/RunshengSong/vintage_model
DOCUMENTATION SOURCE	https://pubs.acs.org/doi/pdf/10.1021/acs.est.7b01907

4.2.1.1.4 DEPENDENCIES:

Python 3.x

Python dependencies:

- Numpy
- Pandas
- SciPy
- matplotlib

Jupyter Notebook

4.2.1.1.5 INSTALLATION:

1) Download the repository from the source.
2) Fill out template scripts, and then run the scripts in the command line.

3) Run default scenario in Jupyter Notebook.

4.2.1.1.6 Folder and File Structure:

64. Folders for input parameter data, and output results need to be specified in Python scripts. Developer provides folder structure.

4.2.1.1.7 USAGE:

Summary:

1) Graphical interface is **missing**.
2) Input parameters are **speficied in a spreadsheet, and in a script**.
3) Results are available in **binary, scripting is required to re-format results**.
4) User guide is missing.

Difficulty Rating:

Table 14: Difficulty rating for nanoRelease.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.2.1.1.8 FEATURES:

1) MFA
2) **Domain:** Air, Water, Soil, Sediment
3) **Scope:** High modularity.
4) **Supporting documentation:** one publication. User-guide missing entirely.
5) The model is **dynamic**, and steady-state, probabilistic, and accounts for **long-term** changes.
6) **Default parameters** are provided for some scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.65

4.2.1.1.9 PROVIDED EXAMPLE:

(1) Scenario(s):

- Release and flow of nanomaterial in the US.
- 2000-2020
- TiO_2, SiO_2, FeO_x
- Use in paints and coatings by seven product applications
- Using production volume and market projection information

(2) Results:

- Claim that compared to 2016, in 2020:
- Annual release of nanomaterial will increase by 30-40%

- Stock will increase by 28-34%

4.2.1.2 THEORETICAL ASSESSMENT

4.2.1.2.1 ASSUMPTIONS:

Table 15: Summary of assumptions made by nanoRelease

Model Feature	Assumption
Compartment	- Non-spatial blocks - Sources, stocks, and sinks
Transfer	- Source releases as function of annual production volume - In-use release as amount of nanomaterial released immediately at use - End-of-life release as amount of disposed nanomaterial - Total release as sum of all release type
Transformation	- No transformations are assumed in the model
Substance	- Substances have lifetimes in each compartment
Time	- Re-evaluation of model parameters at each time step for dynamics - Annual time-step that can span many years - Stochastic evolution of simulation

4.2.1.2.3 ALGORITHMS:

1) Monte Carlo Simulation – for uncertainty, and stochastic evolution of simulation
   - Potential flaw in normal_generator function in monte_carlo_lifetime.py
   - Upper and lower bounds on normal random sampling creaters an abundance of events with the values equal to the upper and lower bounds
2) Direct Calculations of lifetime probability distributions using Weibull function
   - Weibull gives probability of lifetime for a nanomaterial in a compartment
3) Mersenne Twister (Numpy.random.normal) – for pseudo-randomness

4.2.1.2.4 INPUT PARAMETERS:

Table 16: Summary of input parameters for nanoRelease.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name	Spreadsheet
Compartment Property	- Source, stock, sink	Spreadsheet
Transfer	- Proportions	Script
Transfer Property	- Fractional distribution - Weibull probability distribution	Spreadsheet, Script
Transformation	None	None
Transformation Property	None	None
Release	Annual production volume (Rate)	Spreadsheet
Release Property	- Yearly release - Release function (dependent on compartment type)	Script
Substance	- Defined by name	Spreadsheet
Substance Property	- Average lifetime, with error (Weibull parameters)	Spreadsheet
Temporal	Years, duration of simulation	Script
Temporal Property	- Yearly time step - Re-evaluation of model parameters at each time step	Spreadsheet, Script

4.2.1.2.5 MODEL OUTPUT:

Table 17: Summary of model output for nanoRelease.

Output Type	Output unit	Summary Note	Output Format
Single value	Tons	Amount released for the year	Script
Series	Amount vs Year	Amount over time, Multivariate	Script
Diagram	Sankey Diagram	Shows total flows for all compartments	Script

4.2.1.2.6 NANOMATERIAL APPLICATIONS:

[TiO_2, SiO_2, FeO_x]

4.2.2 Uncertainty analysis

65. The table 18 below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the nanoRelease model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics in the last time step (year) of the model output in the unit of tonnes for a selection of the endpoint compartments wherein TiO_2 resides at the end of the simulation.

Table 18: Summary of quantified uncertainty metrics for nanoRelease.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Air	3082.77	3.83e6	1956.80	6775.41	34.22	6809.63
Water	44.62	708.93	26.63	94.68	0.42	95.10
Soil	386.97	84041.90	289.90	950.17	7.31	957.48
Landfill	28566.45	3.2e8	17981.31	62680.40	310.30	62990.70

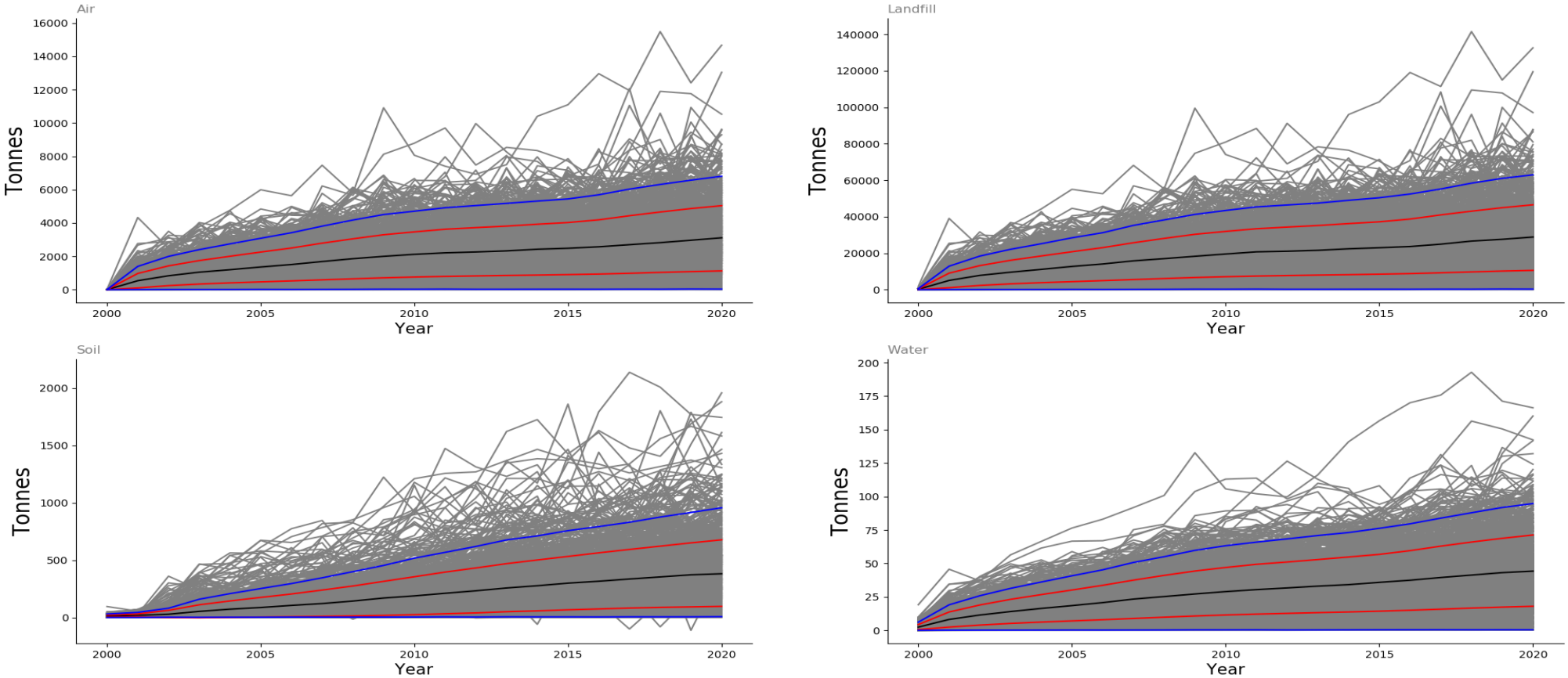
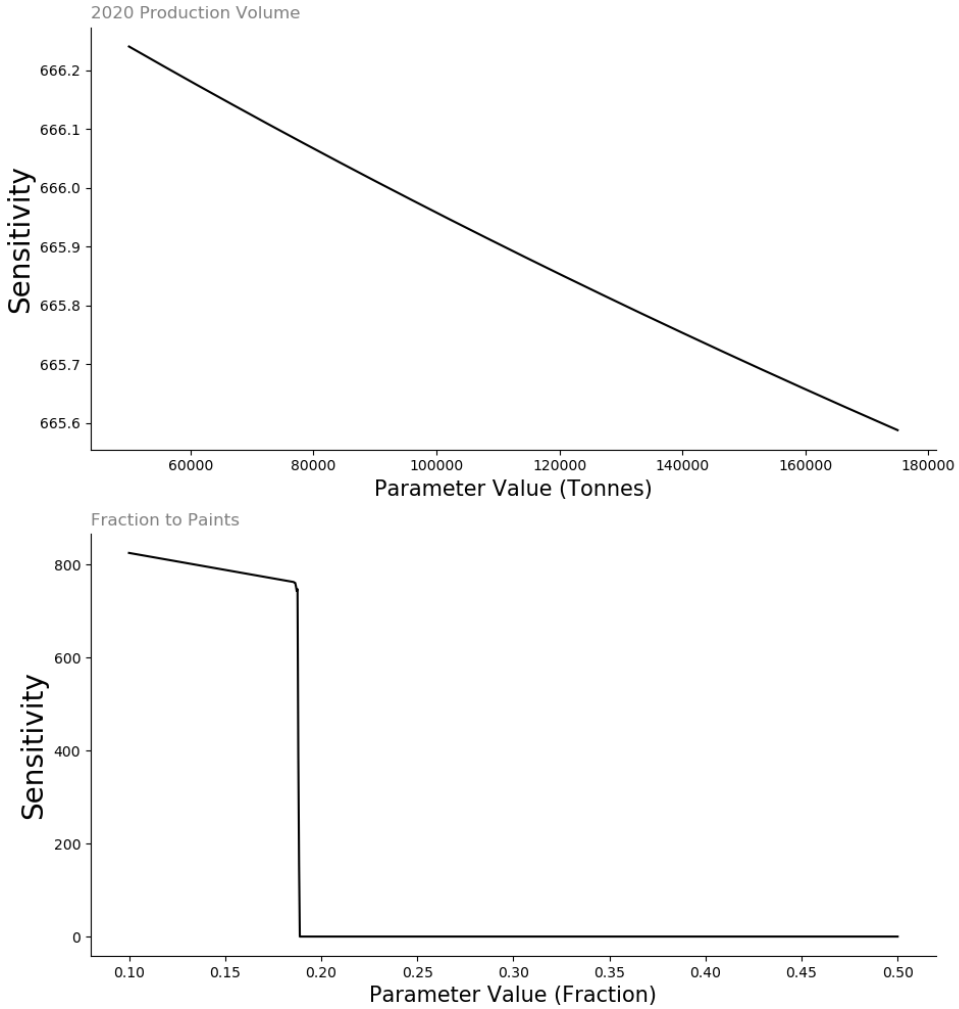


Figure 3. Output uncertainty for TiO2 volume in the output compartments for NanoRelease.

Note: Figure 3 shows the output uncertainty for TiO2 volume in the output compartments of the tested scenario for NanoRelease. The x-axis shows time-step in years, and the y-axis shows TiO2 volume in metric tonnes. Grey lines show first 1000 samples of the output from the MCS. Black lines show the expectations for each year. Red lines show +/- the standard deviation for each year. Blue lines show the boundaries of the 95% coverage interval. Names of the output compartments are labelled in grey in the top left of each plot: air, landfill, soil, and water.

4.2.3 Sensitivity analysis



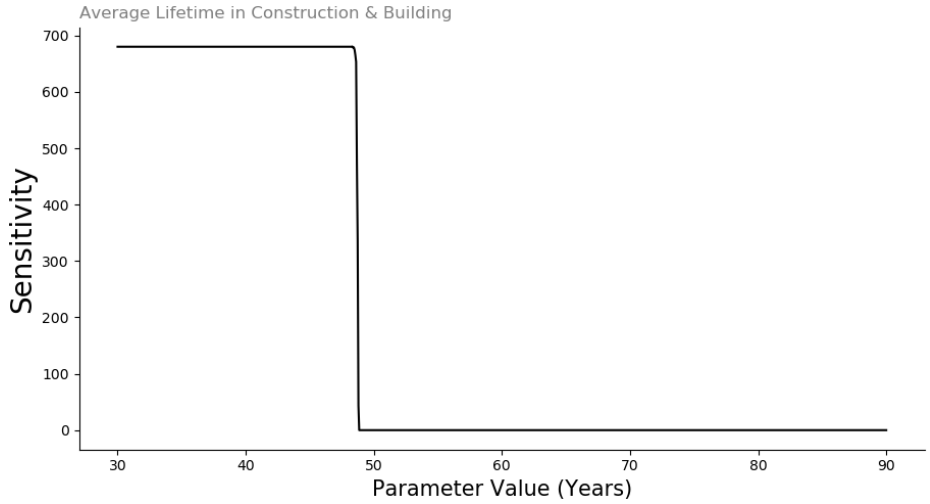


Figure 4. Sensitivity for the most sensitive parameters of NanoRelease.

Note: Figure 4 shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for NanoRelease. The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the 2020 production volume, the average lifetime in construction and building, and the fraction of TiO2 going to the paints industry

66. In Table 19 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity for all time-steps, in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing (same as in publication [5]). The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 19: Overall sensitivity for each parameter for nanoRelease.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
2020 Production Volume	665.8997145	115850.3	57925.14	173775.4	Tonnes
2019 Production Volume	664.3968391	112476	56238	168714	Tonnes
2018 Production Volume	662.8154340	109200	54600	163800	Tonnes
2017 Production Volume	660.7282859	105000	52500	157500	Tonnes
2016 Production Volume	659.6001730	100000	50000	150000	Tonnes
2015 Production Volume	658.5110305	93500	46750	140250	Tonnes
2014 Production Volume	657.3293643	89000	44500	133500	Tonnes
2013 Production Volume	656.0979368	87000	43500	130500	Tonnes
2012 Production Volume	654.9430842	85000	42500	127500	Tonnes
2011 Production Volume	653.6348015	83500	41750	125250	Tonnes
2010 Production Volume	652.0118518	82800	41400	124200	Tonnes
2009 Production Volume	650.4962534	80000	40000	120000	Tonnes
2008 Production Volume	648.5372215	78000	39000	117000	Tonnes
2007 Production Volume	646.9474794	73000	36500	109500	Tonnes
2006 Production Volume	645.1039631	68000	34000	102000	Tonnes
2005 Production Volume	643.6526818	61000	30500	91500	Tonnes
2004 Production Volume	641.1404884	56000	28000	84000	Tonnes
2003 Production Volume	637.8161474	51000	25500	76500	Tonnes
2002 Production Volume	632.1821463	47000	23500	70500	Tonnes
2001 Production Volume	621.9741966	42727.27	21363.64	64090.91	Tonnes
2000 Production Volume	589.3088343	38842.98	19421.49	58264.47	Tonnes
Average Lifetime: Construction & Building	212.2947279	60	30	90	Years
Average Lifetime: Other Industries	212.2922627	20	10	30	Years
In-Use Release Rate: Other Industries	212.2868952	0.01	0	1	1/Year
In-Use Release Rate: Packaging	212.2830400	0.01	0	1	1/Year
Average Lifetime: Household & Furniture	212.2824210	15	7.5	22.5	Years
Average Lifetime: Medical	212.2821061	15	7.5	22.5	Years
In-Use Release Rate: Household & Furniture	212.2802914	0.01	0	1	1/Year
Average Lifetime: Automotive	212.2797497	13	6.5	19.5	Years
Repainting Frequency: Construction & Building	212.2745886	10	5	15	Years
Repainting Frequency: Household & Furniture	212.2745513	8	4	12	Years
Repainting Frequency: Packaging	212.2745385	0	0	0	Years
Repainting Frequency: Medical	212.2745385	0	0	0	Years
Repainting Frequency: Electronics	212.2745385	0	0	0	Years

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Repainting Frequency: Other Industries	212.2744867	2	1	3	Years
Repainting Frequency: Automotive	212.2741682	8	4	12	Years
Average Lifetime: Electronics	212.2734737	5	2.5	7.5	Years
Market Share: Packaging	212.2729662	0.06	0.03	0.09	-
In-Use Release Rate: Medical	212.2713331	0.01	0	1	1/Year
Average Lifetime: Packaging	212.2697638	2	1	3	Years
In-Use Release Rate: Automotive	212.2684354	0.01	0	1	1/Year
In-Use Release Rate: Electronics	212.2677205	0.01	0	1	1/Year
Market Share: Automotive	212.2670464	0.06	0.03	0.09	-
Market Share: Medical	212.2661518	0.13	0.065	0.195	-
Market Share: Household & Furniture	212.2634567	0.14	0.07	0.21	-
Market Share: Construction & Building	212.2596493	0.45	0.225	0.675	-
Market Share: Electronics	212.2581143	0.06	0.03	0.09	-
Market Share: Other Industries	212.2547636	0.1	0.05	0.15	-
In-Use Release Rate: Construction & Building	212.2462354	0.01	0	1	-
To Paints Fraction	175.0925373	0.3	0.15	0.45	-

4.2.4 Discussion

67. nanoRelease is a dynamic and probabilistic MFA tool that simulates the dynamic flow of material through a variety of processes including manufacturing release, in-use release, and end-of-life release of material while implementing a stochastic evolution of material flow through time using probability distributions. nanoRelease does not provide a graphical user interface. Its features are used entirely through Python scripting, and the command-line terminal. nanoRelease is well documented. However, the lack of a user-guide makes implementing nanoRelease time-consuming and difficult. Due to the difficulty of implementing nanoRelease, lack of graphical interface and lack of user-guide; nanoRelease scores a 5/5 on the difficulty rating. nanoRelease's features include a domain that includes air, water, soil and sediment (among other market-related compartments). nanoRelease is modular and allows users to implement a model from scratch and define any number of compartments and connectivity between compartments. nanoRelease is dynamic, probabilistic, and accounts for long-term changes. Because of its features, nanoRelease scores a applicability criteria score of 0.65. Flows of material are determined using a linear combination of equations that factor in the stochastic behaviour of the system using probability distributions that describe the lifetime of a material in a given compartment. Input parameters include the parameters that describe lifetime probability distributions, initial volumes of materials, and fractions that divide the material into different compartments. The uncertainty analysis reveals that nanoRelease performs as expected with the uncertainty becoming larger as the simulation progresses through time. The sensitivity analysis reveals unexpected behaviour, as the sensitivity of some parameters does not behave predictably, and cannot be explained given the information that is available. For example, the sensitivity of the average lifetime of the material in construction and building is constant up until around 50 years, then drops off to zero. We would expect the sensitivity to be constant for any value of average lifetime, yet the output is completely insensitive to average lifetimes above approximately 50 years. What is concerning is that the average lifetime that is used in a publication using nanoRelease is 60 years (which is above the value where this parameter becomes insensitive to the output). The sensitivity of the fraction to paints reveals a similar pattern of sensitivity as the average lifetime in construction and building, by dropping off to zero after a certain value. Other parameters are not yet explored, but it is possible (and likely) that this pattern will emerge for those parameters as well. The most sensitive parameters are the production volumes

of material, the lifetimes of material in particular compartments, followed by repainting frequencies and market-shares. No parameters were revealed to have a net zero sensitivity for the range of values that were tested.

4.3 nanoFATE

4.3.1 Functional assessment

4.3.1.1 MECHANISTIC ASSESSMENT

4.3.1.1.1 AUTHOR: Kendra L. Garner, Arturo A. Keller

4.3.1.1.2 VERSION: 3.0

4.3.1.1.3 ACCESSIBILITY:

Table 20: Accessibility information for nanoFate.

COST	Free
MODEL ACCESS SOURCE	keller@bren.uscsb.edu
DOCUMENTATION SOURCE	Garner et al. 2017

4.3.1.1.4 DEPENDENCIES:

N/A

4.3.1.1.5 INSTALLATION:

1. Ensure correct file and folder structure (described below). The user will need to extract the program files from a number of zip files, then place them in the correct folder structure described in 4.3.1.1.6.

2. Specify input parameters in spreadsheet

ENSURE THAT Output folder is EMPTY!

3. Run GUI

4.3.1.1.6 FOLDER AND FILE STRUCTURE:

68. In Table 25 below, each column represents a tier in the folder structure. Dark-grey rectangles represent folders with their folder name included. Light-grey rectangles represent files. Files or folders are located in the folder rectangles directly to the left of the respective file or folder.

Table 21: Folder and file structure for nanoFate.

Tier 1	Tier 2	Tier 3
nanoFate/	Default Data/	Default Chemicals/
		Default Regions/
	Input/	ChemParam.xlsx
		ChemRelease.xlsx
	Output/	
	Tool/	Ag_eq_dis.mat
		CeO2_eq_dis.mat
		CuO_eq_dis.mat
		nanoFate.exe
		SiO2_eq_dis.mat
		TiO2_eq_dis.mat
		ZnO_eq_dis.mat

4.3.1.1.7 USAGE:

Summary:

1) Graphical interface limited.
2) Input parameters are specified using spreadsheets.
3) Results are available in spreadsheets.
4) User guide is well written.

Difficulty Rating:

Table 22: Difficulty rating for nanoFate.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.3.1.1.8 FEATURES:

1) EFM
2) **Domain:** Soil, Sediment, Air, Water
3) **Scope:** Medium-high modularity.
   - Limited number of compartments.
   - Sub-compartments included.
   - Spatial resolution
   - Daily time resolution
4) **Supporting documentation:** includes user-guide and publication.
5) The model is **dynamic,** deterministic, and accounts for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.89

4.3.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):
   - Fate and transport of CeO_2, CuO, TiO_2, ZnO in San Fransico Bay area
   - Ten years of simulation; 2005-2014.
   - Plethora of chemical processes in Soil, Water, Air, and Sediment.
   - Use of meteorological data.
2) Results:
   - Even soluble metal oxides may accumulate as nanoparticles in the environment.
   - Exceed minimum toxic threshold (USA).

4.3.1.2 THEORETICAL ASSESSMENT

4.3.1.2.1 ASSUMPTIONS:

Table 23: Summary of assumptions made by nanoFate.

Model Feature	Assumption
Compartment	- Spatial resolution (pseudo- 2D and 3D) - Flow dependent on transfer type - Based on real region - Physical medium (air, water, soil) - Homogeneous distribution of nanomaterial within compartment
Transfer	- Instantaneous (at time step) - Rate-limiting mass transfer - Pseudo-first order rate processes - Mass Balance
Transformation	- Instantaneous (at time step) - Pseudo-first order rate processes - All transformations (dissolution, aggregation, adsorption) irreversible
Substance	- Nanomaterials, aerosols, particulate matter - Radius and density as single value
Time	- Time-series - Daily time step - Re-evaluation of model parameters at each time step - Deterministic evolution of simulation

4.3.1.2.2 ALGORITHMS:

1) Ordinary differential equation solver – to solve mass transfers at each time step.
   - MATLAB's **ode15** package (Included in the executable file).
2) Iterative re-evaluation of model parameters at each time step – dynamic behaviour

4.3.1.2.3 INPUT PARAMETERS:

Table 24: Summary of input parameters for nanoFate.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name	Spreadsheet
Compartment Property	- Spatial properties (e.g. height) - Medium properties (e.g. density, flow) - Meteorological properties (e.g. temperature, rainfall)	Spreadsheet
Transfer	- Rate	Spreadsheet
Transfer Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	Spreadsheet
Transformation	- Rate (irreversible)	Spreadsheet
Transformation Property	- Pseudo first order rate processes - Chemical processes - Physical processes (e.g. Stoke's Law)	Spreadsheet
Release	- Rate	Spreadsheet
Release Property	- Every time step	Spreadsheet
Substance	- Defined by name	Spreadsheet
Substance Property	- Density - Radius - Mass	Spreadsheet
Temporal	- Duration - Temporal Resolution	Spreadsheet
Temporal Property	- Yearly to daily resolution	Spreadsheet

4.3.1.2.4 MODEL OUTPUT:

Table 25: Summary of model output for nanoFate.

Output Type	Output unit	Summary Note	Output Format
Single value	Kg/m^3	Long term average	Spreadsheet
Time-Series	Kg/m^3	Daily concentration	Spreadsheet

4.3.1.2.5 NANOMATERIAL APPLICATIONS:

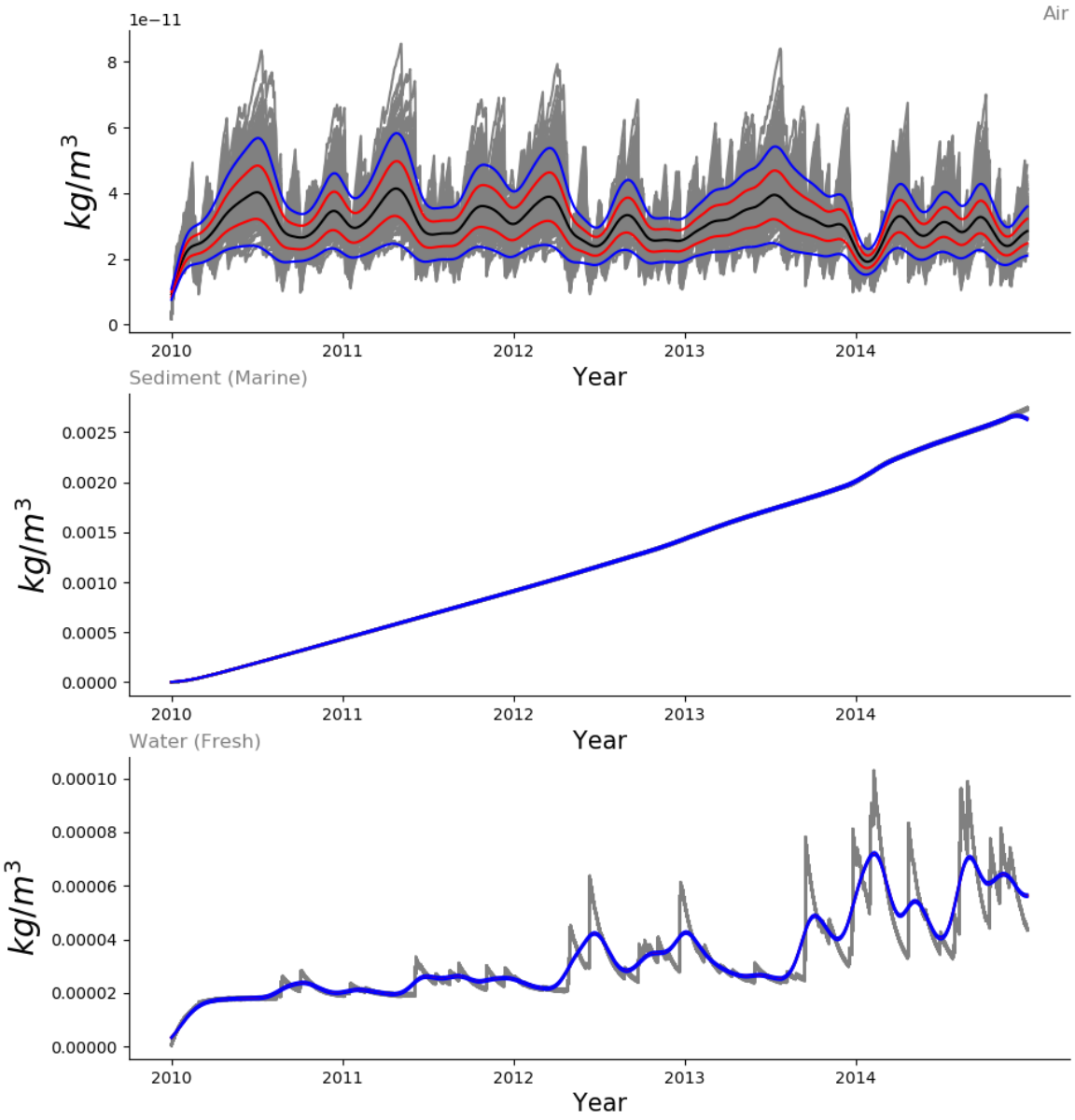
[CeO_2, CuO, TiO_2, ZnO]

4.3.2 Uncertainty analysis

69. The table 26 below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the nanoFate model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics in the last time step (day) of the model output in the unit of kg/m^3 for a selection of the endpoint compartments wherein TiO_2 resides at the end of the simulation.

Table 26: Summary of quantified uncertainty metrics for nanoFate.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Air	3.30e-11	2.12e-23	4.61e-12	1.83e-11	2.39e-11	4.22e-11
Water (Marine)	4.09e-6	1.63e-15	4.04e-8	1.72e-7	4.00e-6	4.18e-6
Water (Fresh)	4.38e-5	3.99e-14	2.00e-7	7.84e-7	4.34e-5	4.42e-5
Sediment (Marine)	0.00274	2.95e-11	5.43e-6	2.09e-5	0.00273	0.00275
Sediment (Fresh)	0.09997	2.18e-7	0.00015	0.00058	0.09968	0.10027
Soil (All)	0.01545	1.16e-9	3.40e-5	0.00012	0.01539	0.01551


Air
1e−11
kg/m3
Year
Sediment (Marine)
kg/m3
Year
Water (Fresh)
kg/m3
Year

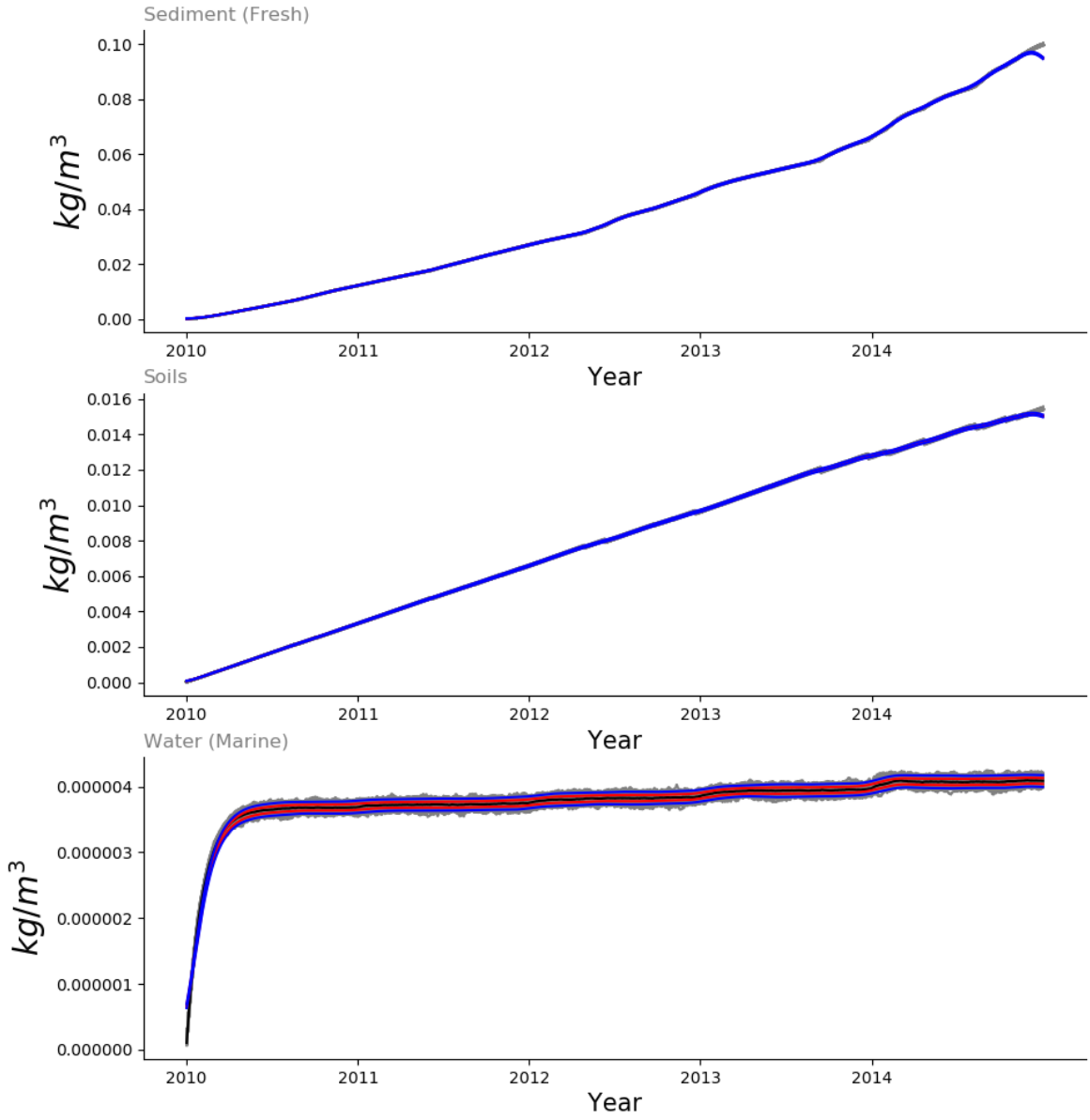


Figure 5. Output uncertainty for TiO2 concentration in the output compartments of nanoFate.

Note: Figure 5 shows the output uncertainty for TiO2 concentration in the output compartments of the tested scenario for nanoFate. The x-axis shows time-step in years, and the y-axis shows TiO2 concentration in kg/m3. Grey lines show the entire 220 samples of the output from the MCS. Black lines show the expectations for each year. Red lines show +/- the standard deviation for each year. Blue lines show the boundaries of the 95% coverage interval. Names of the output compartments are labelled in grey in the top left of each plot: air, sediments, soil, and waters. Expectation, standard deviation, and coverage interval lines are filtered using a Gaussian convolution filter with a window size of 100 days and a standard deviation of 20 days. Note: Expectation and standard deviation lines are hindered by the blue coverage interval lines due to the large range of values shown on the y-axis relative to the small range of values covered by the 95% probability coverage interval.

4.3.3 Sensitivity analysis

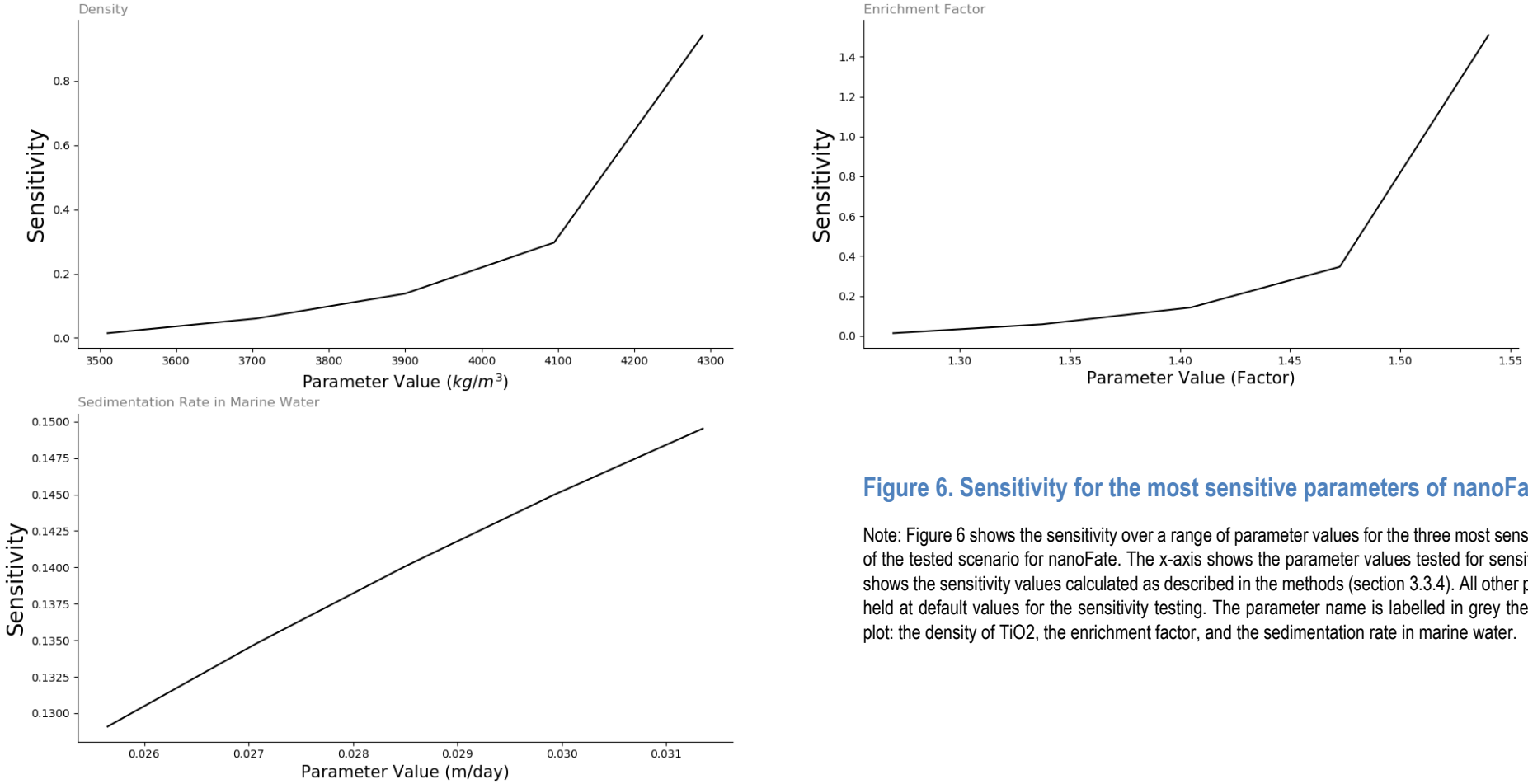


Figure 6. Sensitivity for the most sensitive parameters of nanoFate.

Note: Figure 6 shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for nanoFate. The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the density of TiO2, the enrichment factor, and the sedimentation rate in marine water.

70. In Table 27 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity for all time-steps, in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing. The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 27: Overall sensitivity for each parameter for nanoFate.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Enrichment Factor	0.413765	1.4	1.26	1.54	--
Density	0.290641	3900	3510	4290	kg/m^3
Sedimentation Rate Marine	0.139688	0.0285	0.02565	0.03135	m/day
Heteroaggregation in air	0.069986	19.4323	17.48907	21.37553	m^3/kg*day
Soil Partition Rate for Soil Type 4 (%)	0.057429	0.95	0.1	0.99	--
Average Aggregate Radius	0.055279	500	450	550	nm
Soil Partition Rate for Soil Type 2 (%)	6.75E-05	0.98	0.1	0.99	--
Soil Partition Rate for Soil Type 3 (%)	1.25E-06	0.95	0.1	0.99	--
Heteroaggregation in marine	6.36E-07	19432.3	17489.07	21375.53	m^3/kg*day
Soil Partition Rate for Soil Type 1 (%)	5.11E-07	0.99	0.1	0.99	--
Heteroaggregation in freshwater	7.39E-08	1044.1	939.69	1148.51	m^3/kg*day
Size	0	60	54	66	nm
Sedimentation Rate Freshwater	0	0.0001	0.00009	0.00011	m/day

4.3.4 Discussion

71. nanoFate is a dynamic deterministic environmental fate modeling tool that takes explicit account of nano-specific chemical and physical parameters such as particle size, average aggregate radius, and a set of rate constants that define the transfer of nanoparticles between compartments including soil, air, sediment, and water. nanoFate provides a simple graphical user interface, and users are allowed to select and modify pre-organized spreadsheets containing parameters for a number of different nanoparticles and a number of different regions. No coding knowledge is required, and a user-guide is provided and well written, making nanoFate relatively easy to install and use. Because of its ease of use, nanoFate scores a 2/5 for a difficulty rating. However, nanoFate's ease of use comes at a cost of modularity, providing limited ability to define compartments and connectivity. nanoFate's domain includes soil, sediment, air, and water (among other sub-compartments). nanoFate provides a high time resolution (daily resolution) but at a cost of computational time due to the dynamic re-evaluation of model parameters at each time-step. The model is dynamic, deterministic and accounts for long-term changes. Because of its depth of modeling features, and inclusion of many kinetic processes, nanoFate scores a 0.89 for the applicability criteria score. The model determines the transfer of nanomaterial between compartments dynamically by re-evaluating kinetic parameters at each time step and by solving the system of differential kinetic equations using a standard ordinary differential equation solver. The model requires a large number of parameters, including parameters that describe the nanomaterial, parameters that describe the physical properties of the compartments, and meteorological parameters such as wind speed, precipitation, and temperature. The uncertainty analysis reveals peculiar behaviour, as the uncertainty in the model remains constant throughout the model. The constant uncertainty is most likely attributable to the deterministic structure of the model. The sensitivity analysis reveals that the model behaves as expected for the parameters that display sensitivity, the sensitivity for the given parameters is predictable and explainable. The most sensitive parameters are soil partition

rates, and average aggregate radius of the nanomaterial. Unusually, the output of the model is completely insensitive to the size of the nanoparticle for the range of values that were tested. As the overall output for the sensitivity is calculated using the output values in each environmental compartment, a sensitivity of zero means that the output in any of the compartments is completely insensitive to changes in the input parameter. Note that the small range of values chosen for testing sensitivity and uncertainty is small because the default 50% range caused the program to crash. Thus, in the interest of time, a range of 10% was chosen and was found to cause no errors in the program.

4.4 SimpleBox4nano

4.4.1 Functional assessment

4.4.1.1 MECHANISTIC ASSESSMENT

4.4.1.1.1 AUTHOR: Johannes A. J. Meesters, Joris Quik

4.4.1.1.2 VERSION: 4.01, 2019-09-30

4.4.1.1.3 ACCESSIBILITY:

Table 28: Accessibility information for SimpleBox4nano.

COST	Free
MODEL ACCESS SOURCE	rivm.nl/simplebox4nano
DOCUMENTATION SOURCE	https://pubs.acs.org/doi/pdf/10.1021/es500548h

4.4.1.1.4 DEPENDENCIES:

72. The R dependencies are used for the time-dynamic option of SB4N. Otherwise, steady-state calculations are performed in the main excel spreadsheet.

(1) R 3.x

R dependencies:

- openxlsx
- ggplot2
- deSolve
- reshape2

4.4.1.1.5 INSTALLATION:

1) Install R
2) Download SB4N spreadsheet and R scripts
3) Customize, and add path to R script

4.4.1.1.6 FOLDER AND FILE STRUCTURE:

N/A

4.4.1.1.7 USAGE:

Summary:

1) Graphical interface is missing.
2) Input parameters are specified in a spreadsheet.
3) Results are available in excel.
4) User guide is well written.

Difficulty Rating:

Table 29: Difficulty rating for SimpleBox4nano.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.4.1.1.8 FEATURES:

1) EFM
2) **Domain:** Soil, Sediment, Air, Water
3) **Scope:** Medium-high modularity. Limited in number of compartments.
4) **Supporting documentation:** user-guide and publication provided.
5) The model offers **steady-state or time-dynamic calculations**, deterministic, and accounts for **long-term** changes.
6) **Default parameters** are provided for some scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.92

4.4.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):
   - nano-TiO_2 emissions in Switzerland
   - Soil, Sediment, Air, Water
2) Results:
   - Comparable to a previous study

4.4.1.2 THEORETICAL ASSESSMENT

4.4.1.2.1 ASSUMPTIONS:

Table 30: Summary of assumptions made by SimpleBox4nano.

Model Feature	Assumption
Compartment	- Spatial resolution (pseudo- 3D, conjoined cubic compartments) - Physical media (Water, Air, Soil, Sediment) - Homogeneous distribution of nanomaterial - Well mixed
Transfer	- Pseudo-first order rate processes - Mass Balance
Transformation	- Pseudo-first order rate processes - Stoke's Law - Brownian motion
Substance	- Nanomaterials, particulate matter - Particle size determines physical behaviour
Time	- Steady-state solution of mass balance equation (LTA) - Re-evaluation of model parameters at each time step for dynamics - Variable time-step that can span years

4.4.1.2.2 ALGORITHMS:

1) R's deSolve ODE solver – solution to mass balance equations
2) Deterministic functions – time series modeling of dynamic behaviour

4.4.1.2.3 INPUT PARAMETERS:

Table 31: Summary of input parameters for SimpleBox4nano.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name	Spreadsheet
Compartment Property	- Spatial properties (e.g. volume) - Medium properties (e.g. density, flow rate) - Sediment, Water, Air, Soil	Spreadsheet
Transfer	- Rate	Spreadsheet
Transfer Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	Spreadsheet
Transformation	- Rate	Spreadsheet
Transformation Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	Spreadsheet
Release	- Rate	Spreadsheet
Release Property	- Initial - Regular	Spreadsheet
Substance	- Defined by name	Spreadsheet
Substance Property	- Density - Size - Mass	Spreadsheet
Temporal	- Dynamic - Steady-state	Script Spreadsheet

Parameter Type	Summary Note	Parameter Format
Temporal Property	- Deterministic time-series - Deterministic long-term average (steady-state)	Script Spreadsheet

4.4.1.2.4 MODEL OUTPUT:

Table 32: Summary of model output for SimpleBox4nano.

Output Type	Output unit	Summary Note	Output Format
Single value	g/m³ (Soil), g/kg (Sediment), g/L (Water)	PEC at Steady-state, Output unit depends on species and environmental compartment (155 single outputs in total)	Spreadsheet
Series	Conc vs time-step	Concentration over time	Script

4.4.1.2.5 NANOMATERIAL APPLICATIONS:

[CeO_2, TiO_2, ZnO]

4.4.2 Uncertainty analysis

73. The tables (33 and 34) below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the SimpleBox4nano model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics of the model output in the unit of kg/m³ in the air compartment, in kg/L in the water compartments, and g/kg in the sediment and soil compartments for a selection of the endpoint compartments wherein TiO_2 resides at the end of the simulation.

Table 33: Summary of quantified uncertainty metrics for SB4N v4.01 2019-09-30.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Air	1.46E-07	5.11E-15	7.15E-08	2.74E-07	8.93E-09	2.83E-07
Water (Marine)	6.51E-05	4.22E-10	2.05E-05	7.99E-05	2.49E-05	1.05E-04
Water (Fresh)	4.83E-04	2.60E-08	1.61E-04	6.39E-04	1.63E-04	8.02E-04
Sediment (Marine)	5.97E-03	7.05E-06	2.65E-03	0.01027923	8.16E-04	0.011096
Sediment (Fresh)	1.72E-02	6.44E-05	8.03E-03	3.10E-02	1.73E-03	3.27E-02
Soil (All)	0.084606	1.57E-03	0.039565	0.15174231	8.75E-03	0.16049

Table 34. Summary of quantified uncertainty metrics for SB4N v4.01 2020-11-04.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Air	1.48E-07	5.08E-15	7.13E-08	2.76E-07	1.06E-08	2.86E-07
Water (Marine)	6.56E-05	3.84E-10	1.96E-05	7.56E-05	2.78E-05	1.03E-04
Water (Fresh)	4.86E-04	2.40E-08	1.55E-04	6.01E-04	1.84E-04	7.85E-04
Sediment arine)	6.42E-03	6.91E-06	2.63E-03	0.01004926	1.37E-03	0.01142
Sediment (Fresh)	1.88E-02	6.49E-05	8.06E-03	3.06E-02	3.44E-03	3.41E-02
Soil (All)	0.099741	1.85E-03	0.043021	0.16435716	1.78E-02	0.182167

Figures 7 and 8 below show the output uncertainty for TiO_2 concentration in some of the output compartments of SB4N v4.01 2019-09-30 (Figure 7) and SB4N v4.01 2020-11-04 (Figure 8). The individual plots are probability density histograms with 301 bins. The x-axis shows bins representing concentration values in their respective units depending on the medium of the compartment. Y-axis shows likelihood of respective concentration value. The black line shows the expectation for the sample set. The red regions show +/- the standard deviation. The blue regions show the 95% probability coverage interval. The compartment names are labelled in grey in the top left of each plot: air, waters, sediments and soils.

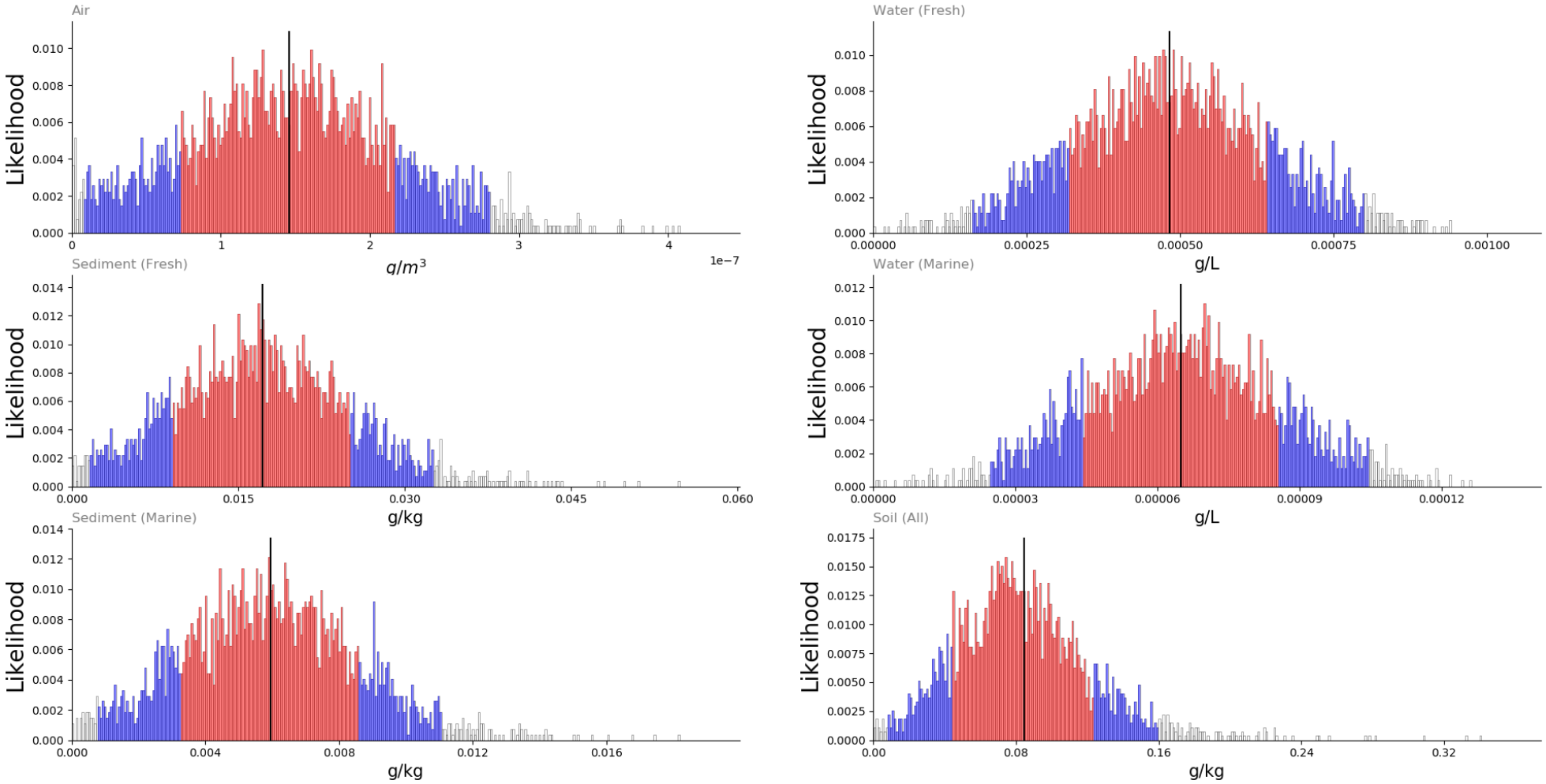


Figure 7. Output uncertainty for TiO2 concentration in some output compartments of SB4N (v4.01 2019-09-30)

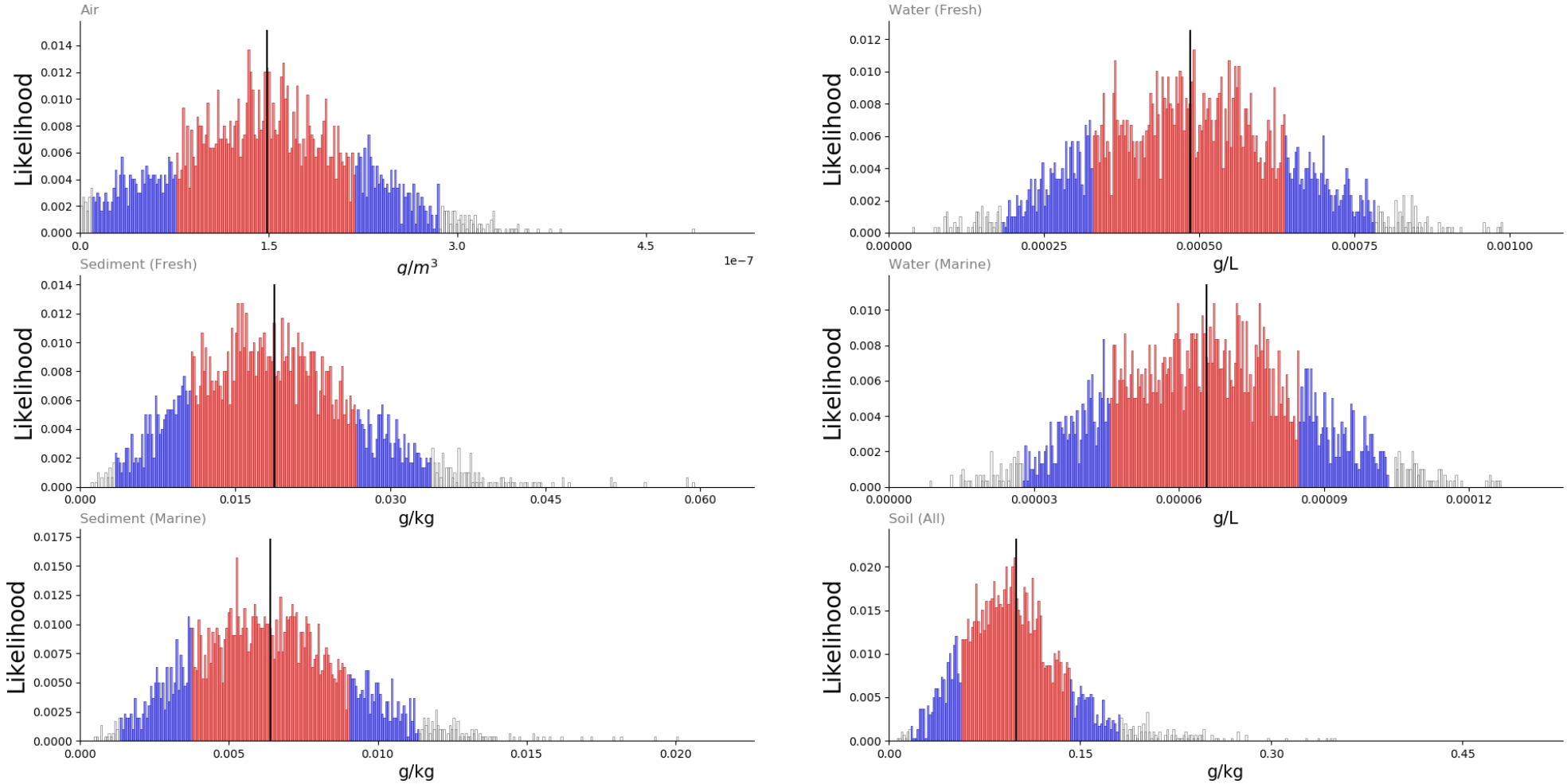


Figure 8. Output uncertainty for TiO2 concentration in some output compartments for SB4N (v4.01 2020-11-04)

4.4.3 Sensitivity analysis

74. Figures 9 and 10 below shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for SB4N v4.01 2019-09-30 (Figure 9) and SB4N v4.01 2020-11-04 (Figure 10). The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the emission of TiO_2 to air, the thermal velocity of TiO_2, and the radius of TiO_2.

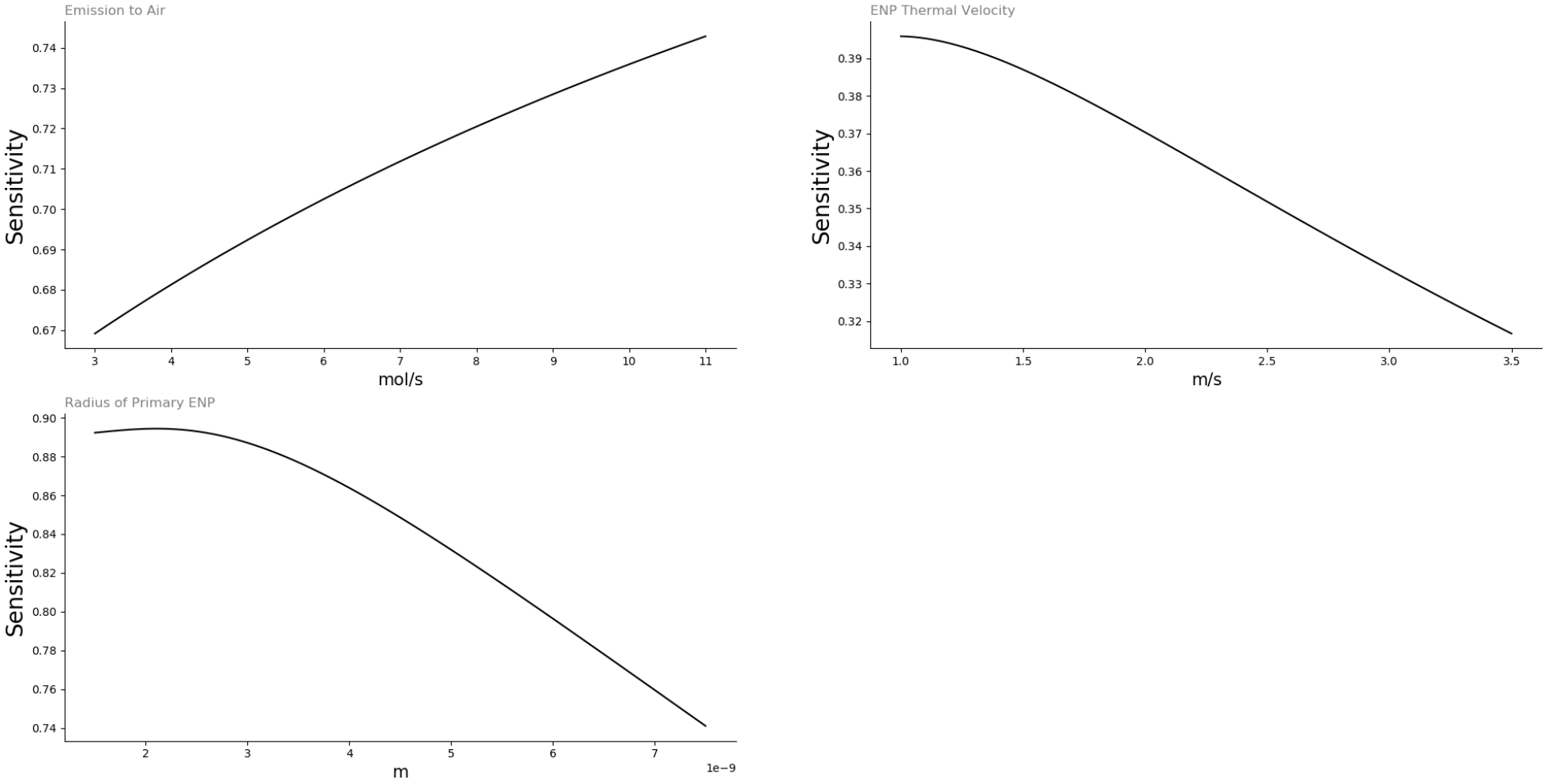


Figure 9. Sensitivity for the most sensitive parameters of SB4N (v4.01 2019-09-30)

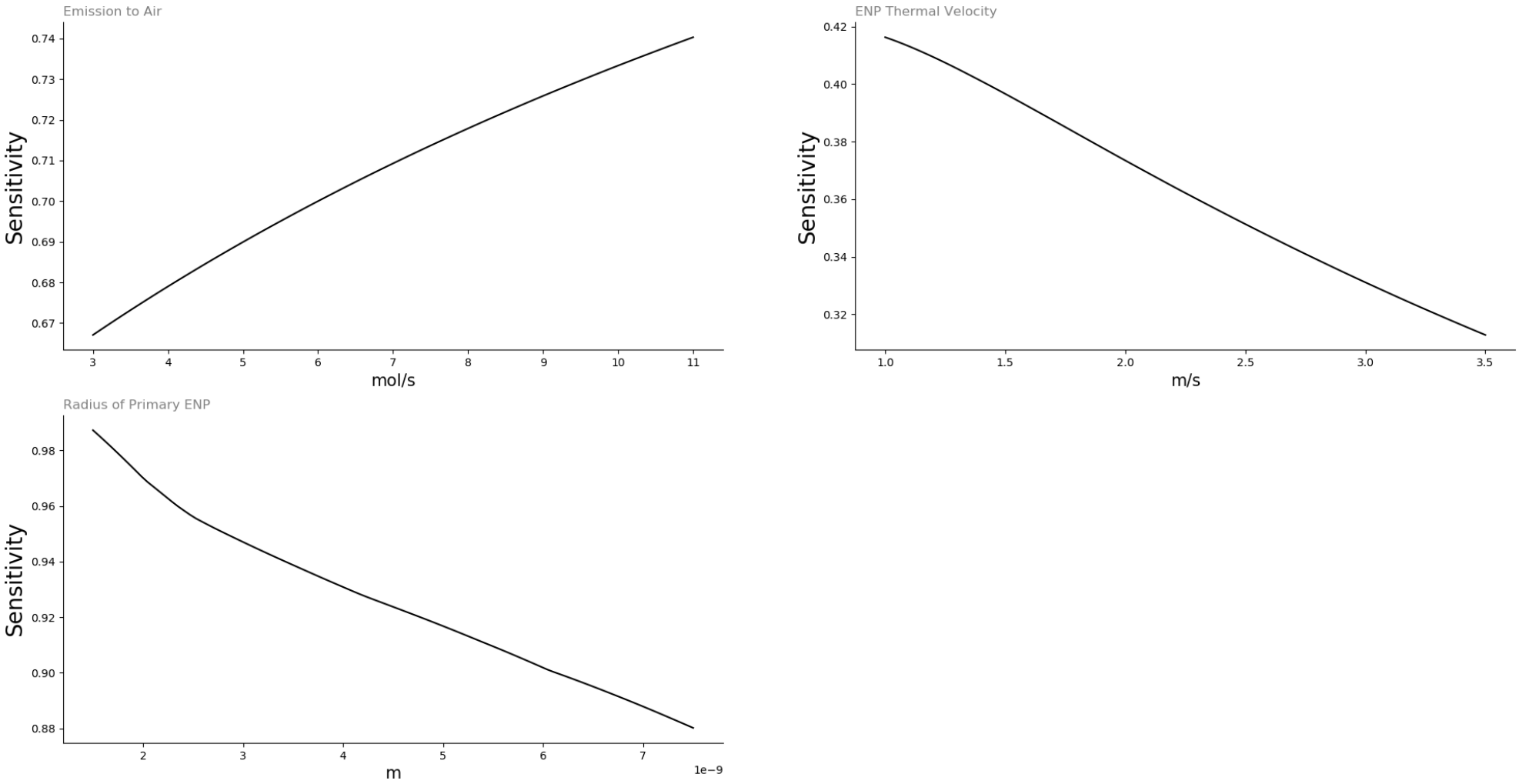


Figure 10. Sensitivity for the most sensitive parameters of SB4N (v4.01 2020-11-04).

75. In Table 35 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing. The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 35. Overall sensitivity for each parameter for sb4n v4.01 2019-09-30.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Radius primary ENP	0.838334	5E-09	2.5E-09	7.5E-09	m
EMISSION to air	0.709861	6.69449	3.347245	10.04174	mol/s
ENP thermal velocity	0.360035	2.126986	1.063493	3.190479	m/s
ENTHALPY of vaporization	0.253365	380935.1	190467.5	571402.6	J/mol
MASS of a single ENP	0.17911	2.21E-21	1.11E-21	3.32E-21	kg
EMISSION to agricultural soil	0.172622	6.69449	3.347245	10.04174	mol/s
Gravitational settling velocity A in water	0.115504	6.2E-10	3.1E-10	9.3E-10	m/s
EMISSION to fresh water	0.11041	6.69449	3.347245	10.04174	mol/s
Octanol/water PARTITION COEFFICIENT of the dissolved species	0.049274	2750	1375	4125	-
Gravitational settling velocity P in water	0.046788	4.36E-07	2.18E-07	6.54E-07	m/s
ENP Knudsen Number	0.040136	13.2	6.6	19.8	-
ENTHALPY of dissolution	0.009102	10000	5000	15000	J/mol
Hamaker constant heteroagglomerate (ENP, water, SiO2)	0.004312	6.9E-21	3.45E-21	1.04E-20	J
VAPOR PRESSURE of pure chemical at 25 oC	0.003485	2.41E-36	1.2E-36	3.61E-36	Pa
VOLUME of a single ENP	9.95E-06	5.24E-25	2.62E-25	7.85E-25	m^3
pH other soil	0	7	3.5	10.5	-
pH aerosol	0	3	1.5	4.5	-
pH agricultural soil	0	7	3.5	10.5	-
pH natural soil	0	5	2.5	7.5	-
pH in sea water	0	8	4	12	-
pH fresh water	0	7	3.5	10.5	-
pH cloud water	0	5.6	2.8	8.4	-
Melting point of pure chemical	0	325.1	162.55	487.65	K
Water SOLUBILITY of pure chemical at 25 oC	0	0.47277	0.236385	0.709155	mol/m^3
Gravitational settling velocity P in air	0	0.000169	8.45E-05	0.000254	m/s

Table 36. Overall sensitivity for each parameter for SB4N v4.01 2020-11-04.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Radius primary ENP	0.925993	5E-09	2.5E-09	7.5E-09	m
EMISSION to air	0.707402	6.69449	3.347245	10.04174	mol.s-1
ENP thermal velocity	0.36346	2.126986	1.063493	3.190479	m.s-1
ENP Knudsen Number	0.194764	13.2	6.6	19.8	-
MASS of a single ENP	0.179625	2.21E-21	1.11E-21	3.32E-21	kg
EMISSION to agricultural soil	0.174776	6.69449	3.347245	10.04174	mol.s-1
Gravitational settling velocity A in water	0.119353	6.2E-10	3.1E-10	9.3E-10	[m.s-1]
EMISSION to fresh water	0.110718	6.69449	3.347245	10.04174	mol.s-1
Gravitational settling velocity P in water	0.108795	4.36E-07	2.18E-07	6.54E-07	[m.s-1]
Hamaker constant heteroagglomerate (ENP, water, SiO2)	0.005427	6.9E-21	3.45E-21	1.04E-20	[J]
VOLUME of a single ENP	4.11E-05	5.24E-25	2.62E-25	7.85E-25	m3
pH natural soil	0	5	2.5	7.5	-
pH other soil	0	7	3.5	10.5	-
pH agricultural soil	0	7	3.5	10.5	-
pH aerosol	0	3	1.5	4.5	-
pH in sea water	0	8	4	12	-
pH fresh water	0	7	3.5	10.5	-
pH cloud water	0	5.6	2.8	8.4	-
Melting point of pure chemical	0	325.1	162.55	487.65	K
ENTHALPY of dissolution	0	10000	5000	15000	J.mol-1
Water SOLUBILITY of pure chemical at 25 oC	0	0.47277	0.236385	0.709155	mol.m-3
ENTHALPY of vaporization	0	380935.1	190467.5	571402.6	J.mol-1
VAPOR PRESSURE of pure chemical at 25 oC	0	2.41E-36	1.2E-36	3.61E-36	Pa
Octanol/water PARTITION COEFFICIENT of the dissolved species	0	2750	1375	4125	-
Gravitational settling velocity P in air	0	0.000169	8.45E-05	0.000254	[m.s-1]

Table 37. Comparison of the two versions of SB4N.

Parameter	2019-09-30 Sensitivity	2020-11-04 Sensitivity
Radius primary ENP	0.838333752	0.925992799
EMISSION to air	0.709860812	0.707402196
ENP thermal velocity	0.36003477	0.363459594
ENTHALPY of vaporization	0.253364851	0
MASS of a single ENP	0.179109705	0.179625076
EMISSION to agricultural soil	0.172622404	0.174775641
Gravitational settling velocity A in water	0.115504316	0.119352863
EMISSION to fresh water	0.110410215	0.110718491
Octanol/water PARTITION COEFFICIENT of the dissolved species	0.049273652	0
Gravitational settling velocity P in water	0.046788361	0.108794984
ENP Knudsen Number	0.040135632	0.194764182
ENTHALPY of dissolution	0.009101734	0
Hamaker constant heteroagglomerate (ENP, water, SiO2)	0.004312282	0.005426807
VAPOR PRESSURE of pure chemical at 25 oC	0.003484832	0
VOLUME of a single ENP	9.95042E-06	4.1082E-05
pH other soil	0	0
pH aerosol	0	0
pH agricultural soil	0	0
pH natural soil	0	0
pH in sea water	0	0
pH fresh water	0	0
pH cloud water	0	0
Melting point of pure chemical	0	0
Water SOLUBILITY of pure chemical at 25 oC	0	0
Gravitational settling velocity P in air	0	0

4.4.4 Discussion

76. SimpleBox4nano (SB4N) is a deterministic nanomaterial environmental fate modeling tool better known for its steady-state functionality, but also includes some dynamic functionality. SimpleBox4nano is a multimedia mass balance model (so called Mackay type). The steady-state functionality of SB4N is run entirely in a well-designed spreadsheet that provides default input parameters for a number of scenarios. The dynamic functionality of SB4N requires some knowledge of R scripting, and may be difficult for some users to access. SB4N provides a clearly written user-guide, and calculation of the output is nearly instant once input parameters are set. The output is collected in the same spreadsheet, and is easy to extract. Since the dynamic functionality of the modeling tool requires some coding knowledge, the modeling tool scores a 4/5 for difficulty rating. However, since SB4N is most popularly known for its steady-state functionality that is quite easy to use, it may be relatively more convenient than other modeling tools that exclusively require coding knowledge. SB4N's features includes domains such as soil, sediment, air and water (among other distinctions within these compartments). The model includes dynamic functionality, and accounts for long-term changes. Because of its depth of modeling features, SB4N scores a very high applicability criteria score of 0.92. SB4N determines flows of material by solving a system of differential equations representing the kinetic processes of the system using a standard ordinary differential equation solver. SB4N's input parameters include a plethora of rate constants, parameters that describe the physical chemistry of the system such as melting points and vapor pressure, as well as parameters that describe the physical properties of the environmental compartments. Nano-specific parameters include dissolution rate constants and attachment efficiencies. SB4N outputs a steady-state concentration of nanomaterial in these compartments under such parameters. The uncertainty analysis reveals that SB4N performs as

expected, producing steady state output with roughly normal shape. The sensitivity analysis revealed that the octanol/water partition coefficient of dissolved species showed sensitivity to the output where it shouldn't be sensitive. Thus a new version of SB4N was provided with the bug fixed. This new version was re-analyzed for uncertainty and sensitivity. The results of the new analysis show that the new version of SB4N correctly displays zero sensitivity to the octanol/water partition coefficient of dissolved species. The results of the uncertainty and sensitivity analysis for both versions are shown in the tables and figures above (the older version labelled as 2019-09-30 and the newer version labelled as 2020-04-11). Table 37 compares the overall sensitivity from the parameters of the two versions. In this table, it is shown that some other input parameters no longer display sensitivity to the output. Additionally, the three most sensitive parameters remain the same for both versions.

4.5 nanoDUFLOW

4.5.1 Functional assessment

4.5.1.1 MECHANISTIC ASSESSMENT

4.5.1.1.1 AUTHOR: Joris T.K. Quik

4.5.1.1.2 VERSION: v3.8.7

4.5.1.1.3 ACCESSIBILITY:

Table 38. Accessibility information for nanoDUFLOW.

COST	Free
MODEL ACCESS SOURCE	Email author: joris.quik@rivm.nl
DOCUMENTATION SOURCE	https://pubs.rsc.org/en/content/articlelanding/2016/en/c5en00270b#!divAbstract

4.5.1.1.4 DEPENDENCIES:

1) R 3.x

   R dependencies:

   - timeDate
   - RColorBrewer
   - plotrix
   - reshape2

2) DUFLOW Modelling Studio (DMS v3.8.7)

   - Note: nanoDUFLOW is a model implemented in the DUFLOW software.

4.5.1.1.5 INSTALLATION:

1) Install R.
2) Use executable file (DMS387Release.exe) to install the program (by following the instructions)
3) Customize, and add path to Rshell script.

4) Open DMS, open the provided model file (provided by model source), run the model by pressing F5, then save and close.

5) Now you ca use R scripts to manipulate input parameters, boundary, and initial conditions.

4.5.1.1.6 FOLDER AND FILE STRUCTURE:

N/A

4.5.1.1.7 USAGE:

Summary:

1) Graphical interface is **provided, but complicated**.
2) Input parameters are **specified using programming scripts, and graphical interface**.
3) Results are available in the **GUI, but scripting is preferred to re-format results**.
4) User guide is **provided, but complicated**.

Difficulty Rating:

Table 39. Difficulty rating for nanoDUFLOW.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.5.1.1.8 FEATURES:

1) Hydrology, EFM
2) **Domain:** Sediment, Water
3) **Scope:** Medium modularity. Applicability to a variety of river systems.
4) **Supporting documentation:** user-guides and publications provided.
5) The model is **dynamic**, spatially explicit, deterministic, but **does not** account for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.81

4.5.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):
   - Flow of nanomaterial in the river Dommel (The Netherlands).
   - Spatially explicit using DUFLOW
   - Ag and CeO_2 nanoparticles
2) Results:
   - Spatially explicit fate modeling

- Simplifying nanomaterial size distributions
   - Effect of varying emission input on the output

- Use of measured heteroaggregation rate constants

4.5.1.2 THEORETICAL ASSESSMENT

4.5.1.2.1 ASSUMPTIONS:

Table 40. Summary of assumptions made by nanoDUFLOW.

Model Feature	Assumption
Compartment	- Spatial resolution (pseudo- 2D, conjoined rectangular compartments) - Water flow modeled by St. Venant equations in concordance with Preissman scheme. - Compartments composed of water and sediment - Heterogenous or uniform distribution of material
Transfer	- Advection-diffusion equation solved simultaneously with hydrology for all compartments. - Pseudo-first order rate processes - Mass Balance
Transformation	- Pseudo-first order rate processes - Smoluchowski equation for aggregation - Stoke's Law for sedimentation
Substance	- Nanomaterials, particulate matter - Five size classes of PSD.
Time	- Re-evaluation of model parameters at each time step - Probabilistic evolution of model simulation by Monte Carlo simulation

4.5.1.2.2 ALGORITHMS:

1) Monte-Carlo Simulation – random sampling of parameter values
2) Iterative time step – for dynamic re-evaluation of model parameters
3) ODE Solver – to solve mass balance equations.

4.5.1.2.3 INPUT PARAMETERS:

Table 41: Summary of input parameters for nanoDUFLOW.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by boundaries in DUFLOW GUI	Binary for GUI
Compartment Property	- Spatial properties (e.g. length, width) - Medium properties (e.g. density, flow rate) - Sediment or Water	Binary for GUI
Transfer	- Various rate constants	Spreadsheet
Transfer Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	Spreadsheet
Transformation	- Various rate constants	Spreadsheet
Transformation Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	Spreadsheet
Release	- Quantity	Spreadsheet
Release Property	- Initial	Spreadsheet
Substance	- Defined by name	Spreadsheet
Substance Property	- Density - Radius - Mass	Spreadsheet
Temporal	- Monte Carlo Simulation parameters - Duration of simulation	Script
Temporal Property	- Temporal resolution (virtually any)	Script

4.5.1.2.4 MODEL OUTPUT:

Table 42. Summary of model output for nanoDUFLOW.

Output Type	Output unit	Summary Note	Output Format
Single value	ng/L	Downstream retention	Script
Series	Conc vs m	Concentration over distance	Script
Series	Conc vs time	Concentration over time	Script

4.5.1.2.4 NANOMATERIAL APPLICATIONS

[CeO_2, Ag]

4.5.2 Uncertainty analysis

77. The table 43 below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the nanoDUFLOW model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics in the most downstream compartment of the river system of the model output in the unit of g/L in water, or g/m^2 in sediment in the last time step wherein CeO_2 resides at the end of the simulation.

Table 43. Summary of quantified uncertainty metrics for nanoDUFLOW.

Compartment Name	expectation	variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Water	0.0296	0.000982	0.0313	0.101	0.000204	0.1011
Sediment	0.00229	6.14e-5	0.00783	0.0161	0.000133	0.0163

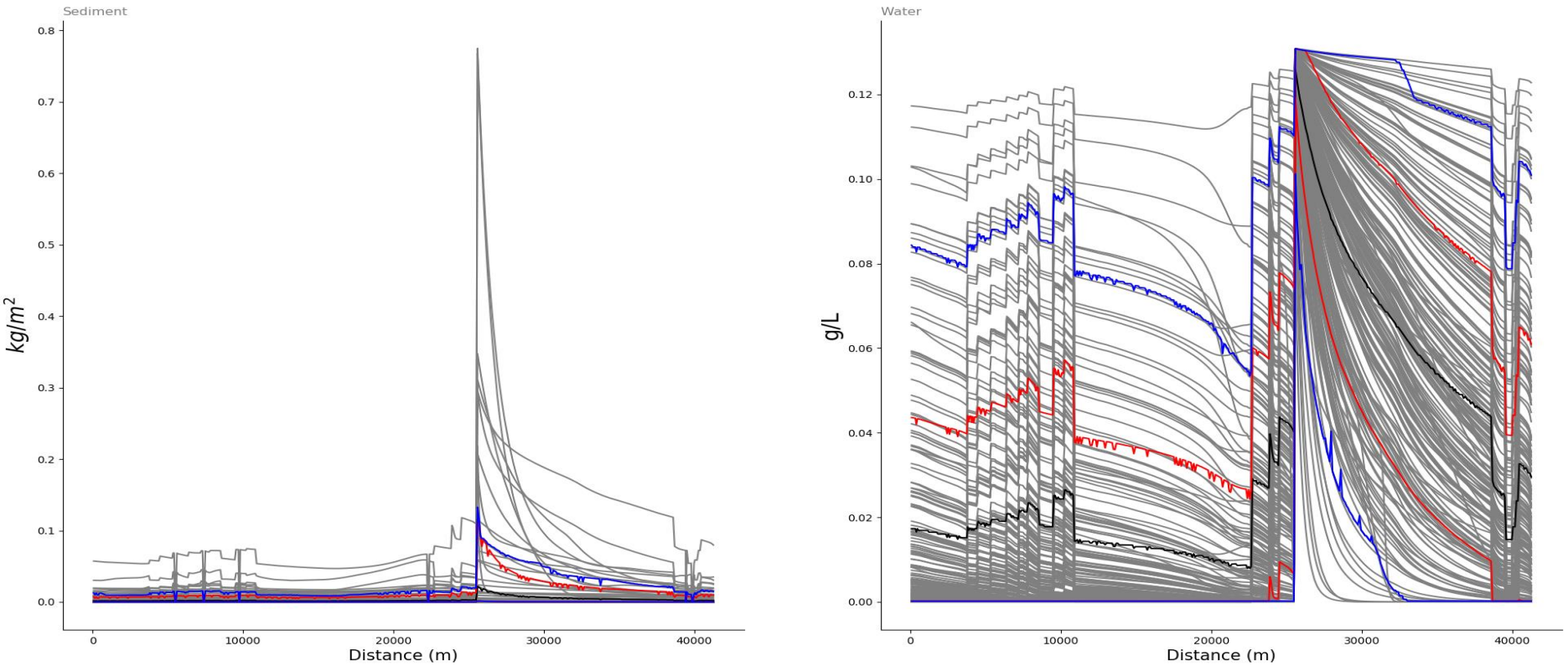


Figure 11. Output uncertainty for CeO2 concentration in the output compartments for nanoDUFLOW.

Note: Figure 11 shows the output uncertainty for CeO2 concentration in the output compartments of the tested scenario for nanoDUFLOW. The x-axis shows river distance in meters, and the y-axis shows CeO2 concentration in the respective unit for the compartment. Grey lines show all 199 samples of the output from the MCS. Black lines show the expectations for each year. Red lines show +/- the standard deviation for each year. Blue lines show the boundaries of the 95% coverage interval. Names of the output compartments are labelled in grey in the top left of each plot: sediment and water.

4.5.3 Sensitivity analysis

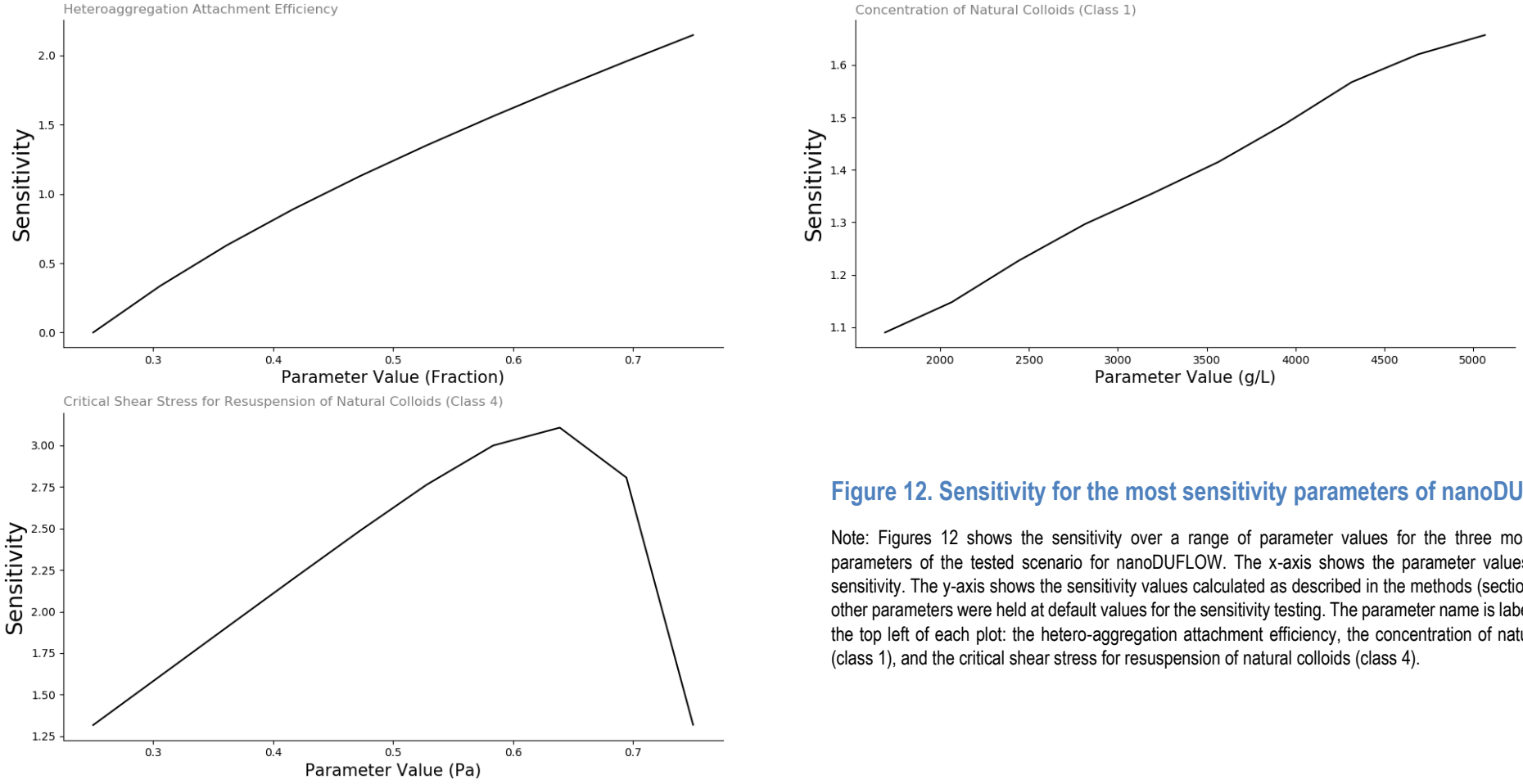


Figure 12. Sensitivity for the most sensitivity parameters of nanoDUFLOW.

Note: Figures 12 shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for nanoDUFLOW. The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the hetero-aggregation attachment efficiency, the concentration of natural colloids (class 1), and the critical shear stress for resuspension of natural colloids (class 4).

78. In Table 44 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity for each time step, in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing. The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 44. Overall sensitivity for each parameter for nanoDUFLOW.

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Critical shear stress for resuspension NCs 4	2.250234	0.5	0.25	0.75	Pa
concentration natural colloids class 1	1.386222	3378	1689	5067	g/L
Attachment efficiency hetero aggregation	1.175939	0.5	0.25	0.75	-
Critical shear stress for resuspension NCs 1	0.94978	0.5	0.25	0.75	Pa
Resuspension constant NCs4	0.463228	100	50	150	g/m^2/day
Density water	0.364078	999	499.5	1498.5	kg/m^3
Viscosity water	0.358366	0.00114	0.00057	0.00171	kg/s*m
Radius natural colloid class 1	0.208716	1.5E-07	7.5E-08	2.25E-07	m
Density natural colloids	0.206013	2120	1060	3180	kg/m^3
Radius nanoparticle aggregate class 1	0.196699	3E-08	1.5E-08	4.5E-08	m
concentration natural colloids class 3	0.146653	3.38	1.69	5.07	g/L
Radius natural colloid class 2	0.128541	6.28E-07	3.14E-07	9.42E-07	m
Radius natural colloid class 5	0.110607	0.00004	0.00002	0.00006	m
sediment stock natural colloids in sediment class 2	0.103835	24936.43	12468.22	37404.65	g/m^2
concentration nanoparticles class 2	0.103495	0.0379	0.01895	0.05685	g/L
sediment stock natural colloids in sediment class 3	0.100195	2244.279	1122.14	3366.419	g/m^2
sediment stock natural colloids in sediment class 5	0.100082	22.44279	11.2214	33.66419	g/m^2
sediment stock natural colloids in sediment class 4	0.098729	249.3643	124.6822	374.0465	g/m^2
Density natural colloids	0.067769	2120	1060	3180	Kg/m^3
Density natural colloids	0.064837	2120	1060	3180	Kg/m^3
Radius natural colloid class 3	0.05184	2.5E-06	1.25E-06	3.75E-06	m
concentration nanoparticles class 4	0.040557	0.023	0.0115	0.0345	g/L
Density natural colloids	0.018416	2120	1060	3180	kg/m^3
concentration nanoparticles class 1	0.010384	0.000547	0.000274	0.000821	g/L
Density natural colloids	0.007052	2120	1060	3180	kg/m^3
Resuspension constant NCs2	0.006112	100	50	150	g/m^2/day
Resuspension constant NCs1	0.001982	100	50	150	g/m^2/day
maximum flow velocity	0.001193	1	0.5	1.5	m/s
Burrial rate NCs in sediment	0.001016	3.17E-09	1.59E-09	4.76E-09	t/m^{2}s
extra factor for sedimentation	6.24E-08	1	0.5	1.5	-
Radius natural colloid class 4	0	0.00001	0.000005	0.000015	m
Critical shear stress for resuspension NCs 5	0	0.5	0.25	0.75	Pa
concentration natural colloids class 2	0	125.1	62.55	187.65	g/L

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
Critical shear stress for resuspension NCs 3	0	0.5	0.25	0.75	Pa
Critical shear stress for resuspension NCs 2	0	0.5	0.25	0.75	Pa
concentration nanoparticles class 3	0	0.0629	0.03145	0.09435	g/L
Radius primary nanoparticle	0	1E-08	5E-09	1.5E-08	m
Radius nanoparticle aggregate class 5	0	6E-07	3E-07	9E-07	m
Radius nanoparticle aggregate class 4	0	3E-07	1.5E-07	4.5E-07	m
Radius nanoparticle aggregate class 3	0	1.5E-07	7.5E-08	2.25E-07	m
Radius nanoparticle aggregate class 2	0	7.5E-08	3.75E-08	1.13E-07	m
Fractal dimenstion nP aggregate	0	2.5	1.25	3.75	-
concentration nanoparticles class 5	0	0.000956	0.000478	0.001434	g/L
concentration natural colloids class 4	0	0.125	0.0625	0.1875	g/L
Fraction water in sediment	0	0.7	0.35	1.05	-
Attachment efficiency homo aggregation	0	0.5	0.25	0.75	-
extra test factor for correction CORnc1	0	1	0.5	1.5	-
Density primary nanoparticles	0	7650	3825	11475	kg/m^3
extra test factor for correction CORnc5	0	1	0.5	1.5	-
Burrial rate NCs in sediment	0	3.17E-09	1.59E-09	4.76E-09	t/m^2s
extra test factor for correction CORnc2	0	1	0.5	1.5	-
Burrial rate NCs in sediment	0	3.17E-09	1.59E-09	4.76E-09	t/m^2s
Resuspension constant NCs5	0	100	50	150	$g/m^2/day$
Burrial rate NCs in sediment	0	3.17E-09	1.59E-09	4.76E-09	t/m^2s
Resuspension constant NCs3	0	100	50	150	$g/m^2/day$
Burrial rate NCs in sediment	0	3.17E-09	1.59E-09	4.76E-09	t/m^2s
extra test factor for correction CORnc3	0	1	0.5	1.5	-
extra test factor for correction CORnc4	0	1	0.5	1.5	-

4.5.4 Discussion

79. nanoDUFLOW is a probabilistic and dynamic modeling tool that couples the water flow and quality functionality of DUFLOW with nanomaterial transformation processes such as homo- and heteroaggregation, dissolution and degradation. nanoDUFLOW is run using R scripts that need to be modified to work on the user's computer, and thus requires experience with R scripting. Because of its large number of parameters, and level of skill required to manipulate input parameters and collect the output, nanoDUFLOW scores a 5/5 on the difficulty rating. nanoDUFLOW's features include a high level of modularity that comes with a large number of parameters. The modeling tool is spatially explicit, and requires a large number of physical or spatial parameters on the water system that it models including water flow rates, and other physical properties of the sediment in the water system. The modeling tool uses vetted hydrological computation methods, and computes the quality and flow in the water system dynamically by re-evaluating model parameters at each time-step. Because of its depth of modeling features, but also lack of environmental compartments such as soil and air, the model scores a 0.81 for its applicability criteria score. The uncertainty analysis reveals that nanoDUFLOW produces output with a variance that is large for some locations within the river system. The output of the uncertainty analysis contains several values that are potential outliers. The source of the large variance is unknown as far as the current analysis can tell, thus more analysis would be required to reveal parameters contributing

to the large variance in the output. The sensitivity analysis reveals input parameter behaviour that produces a predictable sensitivity response that can be explained.

4.6 WASP8

4.6.1 Functional assessment

4.6.1.1 MECHANISTIC ASSESSMENT:

4.6.1.1.1 AUTHOR: Brian Avant

4.6.1.1.2 VERSION: v8.32

4.6.1.1.3 ACCESSIBILITY:

Table 45. Accessibility information for WASP8.

COST	Free
MODEL ACCESS SOURCE	https://www.epa.gov/ceam/wasp8-download#text
DOCUMENTATION SOURCE	https://www.epa.gov/ceam/wasp-model-documentation

4.6.1.1.4 DEPENDENCIES:

WRDB (https://www.wrdb.com)

Optional programs:

BASINS with plugins: HSPF, WASP, SWAT, SWMM, GWLF

4.6.1.1.5 INSTALLATION:

1) Download and run executable installer (wasp-version-8.32-install-64-bit-04-02-2019.exe)

2) Install WRDB (Setup WRDB 6_1_0_61.exe)

3) Optionally, install BASINS for input data support (BASINS4.5ModelPlugins.2019.03.exe)

4.6.1.1.6 FOLDER AND FILE STRUCTURE

N/A

4.6.1.1.7 USAGE:

Summary:

1. Graphical interface is **provided, but complicated.**
2. Input parameters are **specified in a spreadsheet, and in graphical interface**.
3. Results are available in **graphical interface, exportable to csv or spreadsheet**.
4. User guide is **well written.**

Difficulty Rating:

Table 46. Difficulty rating for WASP8.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.6.1.1.8 FEATURES:

1) EFM
2) **Domain**: Sediment, Water
3) **Scope**: High modularity. Unlimited number of compartments. Spatially explicit.
4) **Supporting documentation**: includes user-guides, tutorial videos, and publication.
5) The model is **dynamic** or steady-state, deterministic, spatially explicit, and accounts for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.88

4.6.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):

- Flow of nanomaterial in Brier Creek watershed (Brier Creek at Millhaven, GA, USA)
- Spatially explicit modeling using 42 segments including surface-, and deep sediments
- Carbon Nanotubes (CNT)
- CNT flow vs distance
- CNT flow vs time (many years)

2) Results:

- Shows modeling of CNT flow with kinetic sorption process

4.6.1.2 THEORETICAL ASSESSMENT

4.6.1.2.1 ASSUMPTIONS:

Table 47. Summary of assumptions made by WASP8.

Model Feature	Assumption
Compartment	- 2D or 3D spatial blocks (rectangular approximations) - Volume (cubic) - Real river sections broken up into compartment blocks - Water, or sediment
Transfer	- Differential mass balance - Kinematic wave equation (free-flowing reaches) - Weir overflow equation (ponded reaches) - Dynamic flow equations (backwater reaches) - Internal transfer flows (e.g., dam withdrawals)
Transformation	- Heteroaggregation - Stoke's Law for rate of collision
Substance	- Nanomaterial and other particulate matter - Physical and chemical properties (density, porosity, etc.)
Time	- Re-evaluation of model parameters at each time step for dynamics - Annual time-step that can span many years - Deterministic evolution of simulation

4.6.1.2.2 ALGORITHMS:

1) ODE solver for mass balance equations (three options):

   Three solution techniques (choice):

   Euler – Simple/Quick –Source checked

   COSMIC – Complex/Flux Limiting – Source missing

   Runge-Kutta – Intermediate – Source checked

2) Iterative time step – for time-series calculation of nanomaterial concentration.

4.6.1.2.3 INPUT PARAMETERS:

Table 48. Summary of input parameters for WASP8.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name and section	GUI, DB
Compartment Property	- Spatial properties (e.g. volume) - Medium properties (e.g. density, flow rate) - Sediment, Water - Meteorological data	GUI,DB
Transfer	- Rate	GUI, DB
Transfer Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	GUI, DB
Transformation	- Rate	GUI, DB
Transformation Property	- Pseudo first order rate processes - Rate constants - Chemical processes - Physical processes	GUI, DB
Release	- Rate	GUI, DB
Release Property	- Initial - Regular	GUI, DB
Substance	- Defined by name	GUI, DB
Substance Property	- Density - Size - Molecular weight - Atmospheric deposition	GUI, DB
Temporal	- Dynamic - Steady-state	GUI, DB
Temporal Property	- Deterministic time-series - Deterministic long-term average (steady-state)	GUI, DB

4.6.1.2.4 MODEL OUTPUT:

Table 49. Summary of model output for WASP8.

Output Type	Output unit	Summary Note	Output Format
Single value	Conc: ng/L	Nanomaterial steady-state concentration	GUI, csv, spreadsheet
Series	Conc vs Year	Conc over time, multivariate	GUI, csv, spreadsheet
Series	Conv vs Km	Conc over distance in watershed	GUI, csv, spreadsheet

4.6.1.2.5 NANOMATERIAL APPLICATIONS:

[CNT]

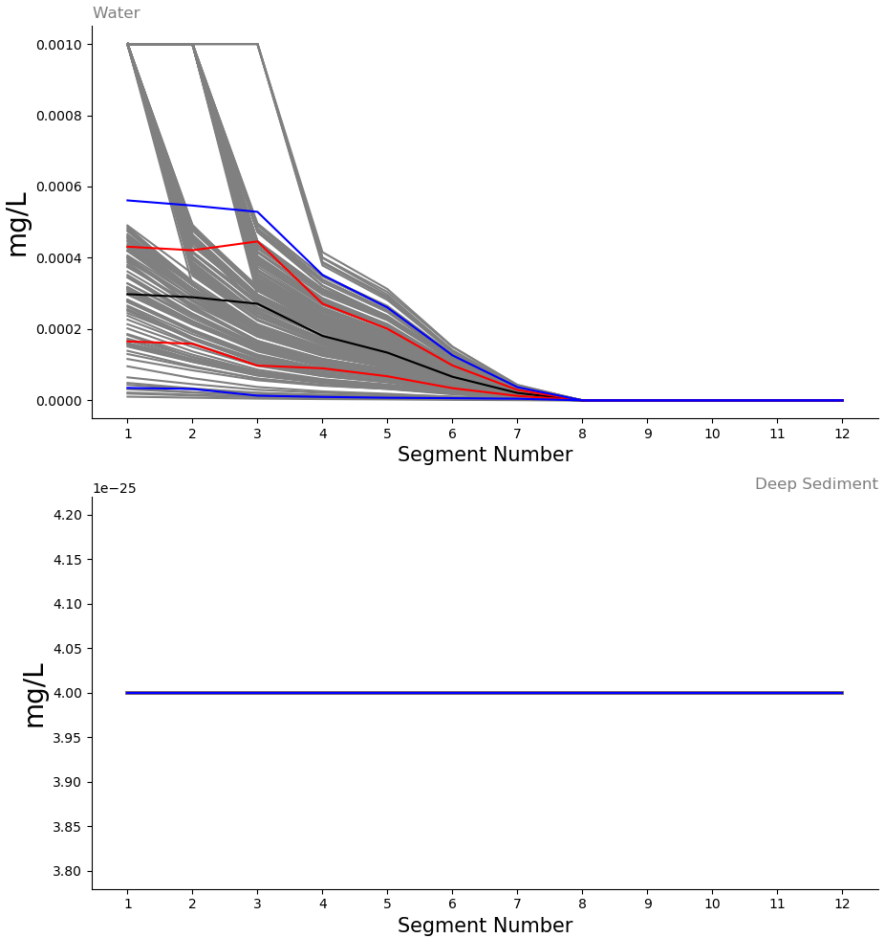
4.6.2 Uncertainty analysis

80. The table below summarizes quantified metrics calculated from the output of Monte Carlo Simulations on the WASP8 model according to the methods described for the uncertainty analysis. The table shows the quantity for the metrics in the middle compartment of the river system of the model

output in the unit of kg/L in water, or kg/kg in sediment in the last time step wherein MWCNT resides at the end of the simulation.

Table 50. Summary of quantified uncertainty metrics for WASP8.

Compartment Name	Expectation	Variance	Standard deviation	Stipulated coverage	Lower coverage interval	Upper coverage interval
Water	0.000134171386 27560323	4.429422977642 353e-09	6.655391031068 237e-05	0.000253002407 01844185	7.360092795775 1235e-06	0.000260362499 81421696
Sediment	4.000000078165 9255e-25	0.0	0.0	0.0	4.000000078165 9255e-25	4.000000078165 9255e-25
Deep Sediment	4.000000078165 9255e-25	0.0	0.0	0.0	4.000000078165 9255e-25	4.000000078165 9255e-25



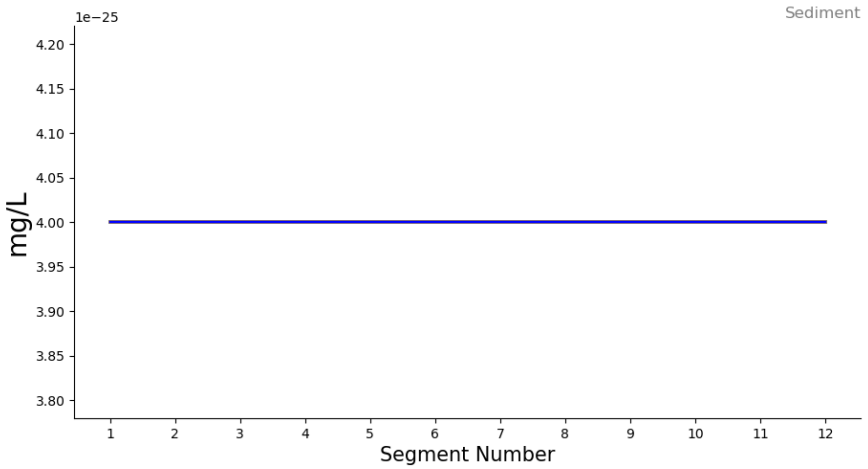


Figure 13. Output uncertainty for MWCNT concentration in the output compartments of WASP8.

Note: Figure 13 shows the output uncertainty for MWCNT concentration in the output compartments of the tested scenario for WASP8. The x-axis shows the river segment number, and the y-axis shows MWCNT concentration in the respective unit for the compartment. Grey lines show all 200 samples of the output from the MCS. Black lines show the expectations for each year. Red lines show +/- the standard deviation for each year. Blue lines show the boundaries of the 95% coverage interval. Names of the output compartments are labelled in grey in the top left of each plot: deep sediment, sediment, and water.

4.6.3 Sensitivity analysis

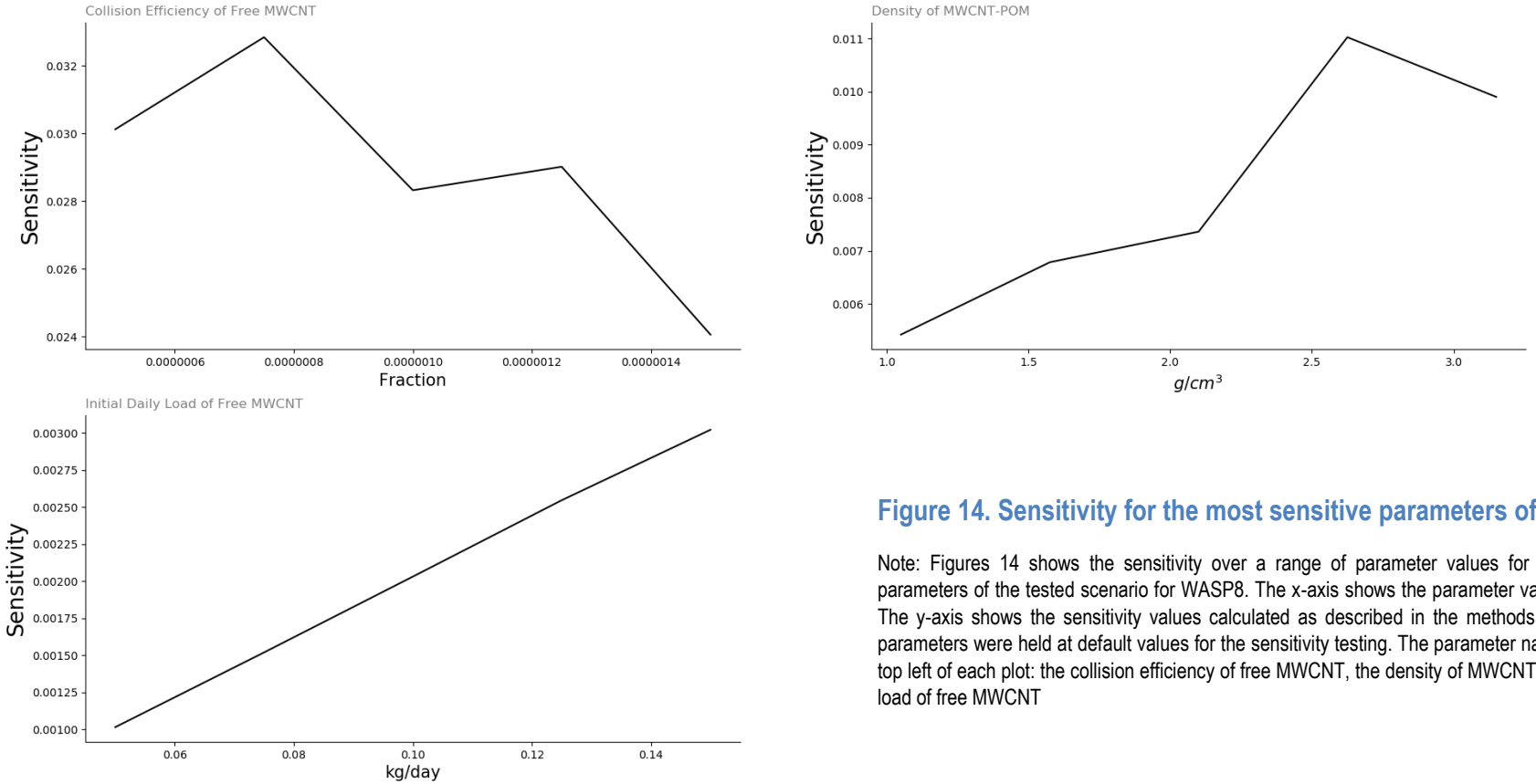


Figure 14. Sensitivity for the most sensitive parameters of WASP8.

Note: Figures 14 shows the sensitivity over a range of parameter values for the three most sensitive parameters of the tested scenario for WASP8. The x-axis shows the parameter values tested for sensitivity. The y-axis shows the sensitivity values calculated as described in the methods (section 3.3.4). All other parameters were held at default values for the sensitivity testing. The parameter name is labelled in grey the top left of each plot: the collision efficiency of free MWCNT, the density of MWCNT-POM, and the initial daily load of free MWCNT

81. In Table 51 below, the parameter column shows the name of the parameter. The sensitivity column shows the overall sensitivity for each time step, in each compartment for a parameter calculated as described in the methods for the sensitivity analysis. The default value column shows the default value of the parameter used for sensitivity testing. The lower and upper bound columns respectively show the lower and upper bounds for the range of values tested for each parameter. The unit column shows the unit value of the parameter ('-' means the parameter has no unit). The rows highlighted in green show the top most sensitive parameters, and the rows highlighted in orange show parameters with the lowest sensitivity.

Table 51.Overall sensitivity for each tested parameter for WASP8

Parameter	Sensitivity	Default Value	Lower Bound	Upper Bound	Unit
free MWCNT collision efficiency	0.028876	0.000001	5E-07	1.5E-06	fraction
MWCNT-POM density	0.008098	2.1	1.05	3.15	g/cm^3
free MWCNT initial time load	0.002025	0.1	0.05	0.15	kg/day
MWCNT-clay collision efficiency	0.001923	0.000001	5E-07	1.5E-06	fraction
silt density	0.000486	2.65	1.325	3.975	g/cm^3
MWCNT-POM collision efficiency	0.000245	0.000001	5E-07	1.5E-06	fraction
MWCNT-silt collision efficiency	5.6E-05	0.000001	5E-07	1.5E-06	fraction
particulate organic matter (POM) density	4.53E-08	1.5	0.75	2.25	g/cm^3
MWCNT-POM settling velocity	0	0.25	0.125	0.375	m/day
sand density	0	2.65	1.325	3.975	g/cm^3
clay density	0	2.65	1.325	3.975	g/cm^3
free MWCNT density	0	2.1	1.05	3.15	g/cm^3
free MWCNT final time load	0	0.1	0.05	0.15	kg/day
MWCNT-clay density	0	2.1	1.05	3.15	g/cm^3
free MWCNT settling velocity	0	0.001	0.0005	0.0015	m/day
MWCNT-silt settling velocity	0	1.4	0.7	2.1	m/day
MWCNT-clay settling velocity	0	0.16	0.08	0.24	m/day
MWCNT-silt density	0	2.1	1.05	3.15	g/cm^3

4.6.4 Discussion

82. WASP8 is a deterministic and dynamic modeling tool that couples the water flow and quality functionality of WASP with nanomaterial transformation processes such as homo- and heteroaggregation. WASP8 is run using a GUI and can be parameterized by importing data from spreadsheets or from other databases, parameters can also be manually adjusted in the GUI. Despite its large number of parameters, WASP8 scores a 2/5 on the difficulty rating because it is run in a GUI and comes with many user guides. WASP8's features include a high level of modularity that comes with a large number of parameters. The modeling tool is spatially explicit, and requires a large number of physical or spatial parameters on the water system that it models including water flow rates, and other physical properties of the sediment in the water system. The modeling tool uses vetted hydrological computation methods, and computes the quality and flow in the water system dynamically by re-evaluating model parameters at each time-step. Because of its depth of modeling features, but also lack of environmental compartments such as soil and air, the model scores a 0.88 for its applicability criteria score. The uncertainty analysis reveals that WASP8 produces output with a variance that is large for some locations of the river system. The output of the uncertainty analysis also reveals that levels of MWCNT in sediment in the last time step remains constant with no variance. The sensitivity

analysis reveals some parameters that have no effect on the output. The sensitivity analysis also reveals that some parameters have a peculiar shape to the sensitivity response.

4.7 LearNano

4.7.1 Functional assessment

4.7.1.1 MECHANISTIC ASSESSMENT

4.7.1.1.1 AUTHOR: Yoram Cohen, Haoyang Haven Liu

4.7.1.1.2 VERSION: N/A

4.7.1.1.3 ACCESSIBILITY:

Table 52. Accessibility information for LearNano.

COST	Free
MODEL ACCESS SOURCE	
DOCUMENTATION SOURCE	https://www.beilstein-journals.org/bjnano/articles/6/97

4.7.1.1.4 DEPENDENCIES:

N/A

4.7.1.1.5 INSTALLATION:

1) Sign up for an account on nanoinfo.org
2) Click on LearNano application link.

4.7.1.1.6 FOLDER AND FILE STRUCTURE:

N/A

4.7.1.1.7 USAGE:

Summary:

1) Graphical interface is intuitive.
2) Input parameters are specified in the web application.
3) Results are available in web application exportable to csv or spreadsheet.
4) User guide is well written.

Difficulty Rating:

Table 53. Difficulty rating for LearNano.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.7.1.1.8 FEATURES:

1) Life-cycle inventory assessment (LCIA), MFA
2) **Domain:** Sediment, Water, Soil, Air
3) **Scope:** Medium-high modularity. Limited connectivity for compartment definition.
4) **Supporting documentation:** includes user-guides, and publication.
5) The model is **not dynamic,** steady-state, deterministic, and accounts for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.67

4.7.1.1.9 PROVIDED EXAMPLE:

1) Scenario(s):
   - Flow of nanomaterials locally in Los Angeles US
   - Flow of nanomaterials globally in 12 countries including Switzerland, US, and Canada
   - TiO_2, CeO_2, SiO_2, CNT
   - Using market study data, among other data from a database
   - Used in sequence with MendNano model
2) Results:
   - No comparison with previous studies
   - Novel predictions (unchecked)

4.7.1.2 THEORETICAL ASSESSMENT

4.7.1.2.1 ASSUMPTIONS:

Table 54. Summary of assumptions made by LearNano.

Model Feature	Assumption
Compartment	- Non-spatial blocks - Sources, stocks, and sinks
Transfer	- Differential mass balance - Transfer coefficients based on market study
Transformation	- None
Substance	- Production volume from product applications
Time	- Steady-state - Long term average - Deterministic evolution of simulation

4.7.1.2.2 ALGORITHMS:

1) Algebraic solution of mass balance equations using fractional distribution

   * Source code unavailable; algorithm details are limited.

4.7.1.2.3 INPUT PARAMETERS

Table 55. Summary of input parameters for LearNano.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name	Web App, DB
Compartment Property	- Source, stock, or sink - Production volume - Product application - Real region	Web App, DB
Transfer	- Fraction	Web App, DB
Transfer Property	- Pseudo first order rate processes - Transfer fractions - Comes from market study	Web App, DB
Transformation	- None	None
Transformation Property	- None	None
Release	- Amount	Web App, DB
Release Property	- Initial	Web App, DB
Substance	- Defined by name	Web App, DB
Substance Property	- N/A	
Temporal	- Steady-state	Web App
Temporal Property	- Deterministic long-term average (steady-state)	GUI, DB

4.7.1.2.4 MODEL OUTPUT:

Table 56. Summary of model output for LearNano.

Output Type	Output unit	Summary Note	Output Format
Single value	tons	In one compartment	Web App
Diagram	tons	Sankey. In each compartment	Web App

4.7.1.2.5 NANOMATERIAL APPLICATIONS:

[Al_2O_3 ,CNT, CeO_2 ,Cu, Fe, Nanoclays, Ag, SiO_2, TiO_2, ZnO, C60]

4.7.2 Uncertainty analysis

83. The uncertainty analysis couldn't be performed because of unresolved problems to obtain the model output, and source code of the model.

4.7.3 Sensitivity analysis

84. The sensitivity analysis couldn't be performed because of unresolved problems to obtain the model output, and source code of the model.

4.7.4 Discussion

85. LearNano is a web-based MFA tool that uses the life-cycle inventory assessment (LCIA) method to estimate flows of material into compartments such as sediment, air, soil, and water (among other market-related compartments). LearNano provides an easy to use graphical user interface that allows users to customize exposure scenarios from a number of pre-organized input parameters that are supplied by several databases. Documentation is provided and the user-guide is well written. Because of how easy it is to use, LearNano scores a 1/5 for difficulty rating. However, its ease of use

comes at a cost of modularity and modeling features. The model is steady-state and accounts for changes in the long-term. LearNano scores a 0.67 for its applicability criteria score. Since the tool is a web-based application, the source code is not provided which limits the transparency of the tool to the documentation. Moreover, unresolved errors were encountered when using the model, which lead to the unsuccessful retrieval of the output. Many unsuccessful communication attempts were made to the authors, and to the support team of the website. Thus, because of unresolved problems with obtaining the model output, the sensitivity and uncertainty analysis could not be performed.

4.8 MendNano

4.8.1 Functional assessment

4.8.1.1 MECHANISTIC ASSESSMENT

4.8.1.1.1 AUTHOR: Yoram Cohen, Haoyang Haven Liu

4.8.1.1.2 VERSION: N/A

4.8.1.1.3 ACCESSIBILITY:

Table 57. Accessibility information for MendNano.

COST	Free
MODEL ACCESS SOURCE	https://nanoinfo.org/#!/mendnano/
DOCUMENTATION SOURCE	https://pubs.acs.org/doi/pdf/10.1021/es405132z

4.8.1.1.4 DEPENDENCIES:

N/A

4.8.1.1.5 INSTALLATION:

1) Sign up for an account on nanoinfo.org
2) Click on LearNano application link.

4.8.1.1.6 FOLDER AND FILE STRUCTURE:

N/A

4.8.1.1.7 USAGE:

Summary:

1) Graphical interface is intuitive.
2) Input parameters are specified in the web application.
3) Results are available in web application exportable to csv or spreadsheet.
4) User guide is well written.

Difficulty Rating:

Table 58. Difficulty rating for MendNano.

<- Easy to use ---------- Difficult to use ->				
1	2	3	4	5

4.8.1.1.8 FEATURES:

1) EFM
2) **Domain:** Sediment, Water, Soil, Air
3) **Scope:** Medium-high modularity. Limited number of compartments.
4) **Supporting documentation:** includes user-guides, and publication.
5) The model is **dynamic,** steady-state, deterministic, and accounts for **long-term** changes.
6) **Default parameters** are provided for several scenarios. **User-overrides** are possible.

CRITERIA SCORE: 0.94

4.8.1.1.9 PROVIDED EXAMPLE:

1) **Scenario(s):**
   - Flow of nanomaterials locally in Los Angeles US
   - Flow of nanomaterials globally in 12 countries including Switzerland, US, and Canada
   - TiO_2, CeO_2, SiO_2, CNT
   - Using market study data, among other data from a database
   - Used in sequence with LearNano model
2) **Results:**
   - No comparison with previous studies
   - Novel predictions (unchecked)

4.8.1.2 THEORETICAL ASSESSMENT

4.8.1.2.1 ASSUMPTIONS:

Table 59. Summary of assumptions made by MendNano.

Model Feature	Assumption
Compartment	- Spatial blocks with volumes - Soil, sediment, air, water - Subject to meteorological and environmental conditions
Transfer	- Differential mass balance - Transfer coefficients based on market study
Transformation	- Aggregation as a simple factor defined as fraction of nanomaterial attached to particulate matter. - Dissolutions and general reactions in water
Substance	- Nanomaterial and other particulate matter - Particle size distributions
Time	- Steady-state or dynamic - Time-series with daily time step - Deterministic evolution of simulation

4.8.1.2.2 ALGORITHMS:

1) pre-developed ODE solver from MATLAB (unkown) – for solution of mass balance equations
2) Iterative daily time step – for simulation dynamics

4.8.1.2.3 INPUT PARAMETERS:

Table 60. Summary of input parameters for MendNano.

Parameter Type	Summary Note	Parameter Format
Compartment	- Defined by name	Web App, DB
Compartment Property	- Soil, Water, Sediment, Air - Uptake compartments (biota, vegetation) - Physical properties (Volume, Density) - Real region	Web App, DB
Transfer	- Defined by process - Rate	Web App, DB
Transfer Property	- Pseudo first order rate processes - Fractional distribution - Stoke's law	Web App, DB
Transformation	- Defined by process - Rate	Web App, DB
Transformation Property	- Pseudo first order rate processes - Fractional distribution - Stoke's law - Dissolution constants - Other reaction constants	Web App, DB
Release	- Rate	Web App, DB
Release Property	- Initial - Regular - Functional	Web App, DB
Substance	- Defined by name and type	Web App, DB
Substance Property	- Nanomaterial or particulate matter - Particle size distribution - Density	
Temporal	- Steady-state or dynamic	Web App
Temporal Property	- Iterative time-step (daily) - Re-evaluation of model parameters	Web App, DB

4.8.1.2.4 MODEL OUTPUT:

Table 61. Summary of model output for MendNano.

Output Type	Output unit	Summary Note	Output Format
Single value	ng/L µg/kg ng/m^3	Concentration in each compartment	Web App
Series	Conc vs time	Multivariate (for each compartment)	Web App

4.8.1.2.5 NANOMATERIAL APPLICATIONS:

[Al_2O_3 ,CNT, CeO_2 ,Cu, Fe, Nanoclays, Ag, SiO_2, TiO_2, ZnO, C60]

4.8.2 Uncertainty analysis

86. The uncertainty analysis couldn't be performed because of unresolved problems to obtain the model output, and source code of the model.

4.8.3 Sensitivity analysis

87. The sensitivity analysis couldn't be performed because of unresolved problems to obtain the model output, and source code of the model.

4.8.4 Discussion

88. MendNano is a web-based environmental fate modeling tool from the same developers as LearNano, and is hosted on the same website. The model is a dynamic fate modeling tool that iteratively solves as system of differential equations that describes the kinetic behaviour of nanomaterial transfers between compartments such as sediment, air, water, and soil. MendNano provides an easy to use graphical user interface that allows users to customize exposure scenarios from a number of pre-organized input parameters that are supplied by several databases. Documentation is provided and a user-guide is well written. Because of how easy it is to use, The model scores a 1/5 for difficulty rating. The model is dynamic, deterministic and accounts for changes in the long-term. MendNano scores a 0.94 for its applicability criteria score due to its depth of modeling features. Since the tool is a web-based application, the source code is not provided which limits the transparency of the tool to the documentation. Moreover, unresolved errors were encountered when using the model lead to the unsuccessful retrieval of the output. Thus, because of unresolved problems with obtaining the model output, sensitivity and uncertainty analysis could not be performed. Since the output could not be retrieved, the score of 1/5 for user-friendliness is appropriate only in the case that the errors can be resolved. Otherwise, MendNano's user-friendliness should be overlooked in favor of other models whose output can be collected.

5 RECOMMENDATIONS

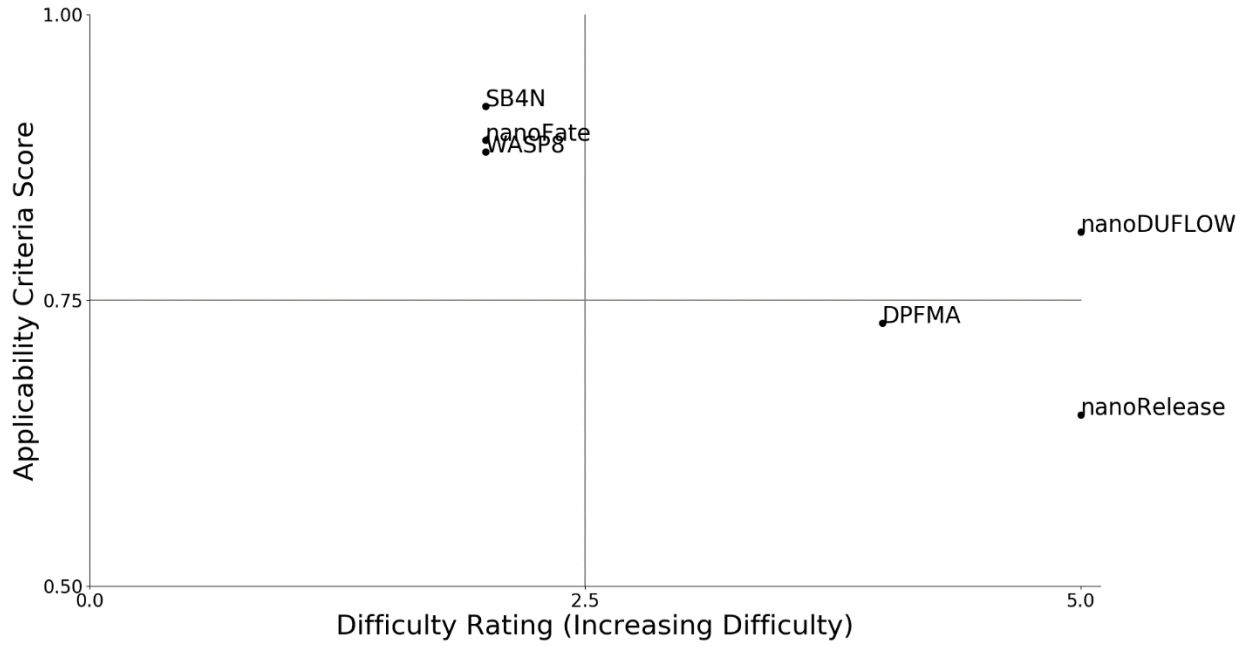


Figure 15. Summary of functional assessment metrics for all models

Note: The X-axis shows the difficulty rating in increasing difficulty on a scale of 1 to 5. The Y-axis shows the applicability criteria score for each model calculated as described in the methods for the functional assessment. Each model is shown as a dot and labelled by name. Quadrant lines are shown for visual purposes. SB4N = SimpleBox4nano.

5.1 Recommendations based on the functional assessment

89. Figure 15 above places the modeling tools on a plot according to their difficulty ratings and their applicability criteria scores. The purpose of this figure is to help recommend to a user, a modeling tool based on the scope and user-friendliness. As no tool scored below 0.5 for the applicability criteria, the cut-off is the midpoint between 0.5 and 1.0. However, the cut-off is quantitatively arbitrary and serves only as a visual aid. The cut-off for the difficulty rating is the midpoint of the rating, and like the applicability cut-off, serves only as a visual aid. The tools that are easiest to use, that do not require any coding knowledge are found on the left side of the figure; SB4N, nanoFate, and WASP8. The tools that provide the most depth with respect to their scope are found on the upper portion of the plot; nanoFate, WASP8, SB4N, and nanoDUFLOW. If you are a user that does not have coding knowledge, this plot recommends to use the tools found in the upper-left quadrant; SB4N, nanoFate, or WASP8. If you are a user that has coding knowledge, this plot recommends any of the tools on the right side of the plot; DPMFA, nanoDUFLOW, or nanoRelease. Interestingly, MFA type tools such as DPMFA, or nanoRelease do not score as high as the other modeling tools on the applicability criteria due to the lack of physical or chemical processes in the theoretical structure of the models. However, it is important

to note that despite the low score for MFA type tools, the benefit is that they do not require as much input parameter data. Thus, models that have more depth to their scope (like the EFM or hydrology models) score higher, but have the drawback that they require more input parameter data to fuel the model. Therefore, there may exist a situation where a user is prompted to use a tool that has less depth to its scope, but requires less data. Where the data is plentiful, it is always recommended to use the tool that scores higher. Hydrology models like WASP8 or nanoDUFLOW require explicit spatial data, and are recommended for situations where a user may be required to model a river system or other water systems. Where spatial data is scarce, it is recommended to use a screening tool such as SB4N that requires only a few spatial parameters. Where market data is available, and there is a lack of chemical or physical data, it is highly recommended to use an MFA type model such as DPMFA or nanoRelease. DPMFA, or nanoRelease do not require explicit knowledge of the chemistry or physics of the nanomaterial, but due to vetted algebraic techniques, can solve a suitable screening-level prediction of concentrations in environmental compartments such as air, water, soil, or sediment. To be clear, these vetted algebraic techniques are used to solve systems of equations that present a simplification of material flow that does not take into consideration physical and chemical processes. It is because of this simplification that MFA type models are considered screening-level. Moreover, MFA and EFM type models can be used independently. However, where the data permits, MFA models should be used to define initial input flow volumes for EFM type models.

5.2 Recommendations based on the uncertainty analysis

90. For the uncertainty analysis, we did not have access to real life data, and thus the estimation of errors was made artificially. The uncertainty analysis would have importance for decision-making if the estimated errors for the parameters are quantified from real data, or have some rationale behind them that would attribute some degree of validity. Quantification of the uncertainty in the output is valuable only if uncertainty is explicitly taken into account, and understood when making a regulatory decision with respect to risk assessments. For example, we may consider that a quantity of material in water is a risk only when 95 % of its PDF is found symmetrically around a given value of interest. In the previous example, quantification of the uncertainty in the output would prove a useful method for informing such a decision. Specifically, the current study would recommend models whose output yields a level of variance that seems reasonable with respect to variance in input parameters. For example, DPMFA, nanoRelease, SB4N, and nanoDUFLOW all produce outputs that vary when faced with input parameter variance. On the other hand, nanoFate and WASP8 have some outputs that either vary minutely or not at all. However, the proportion of variance in the output with respect to variance in the input is difficult to predict due to the complexity of the models, so these recommendations must be interpreted with caution.

5.3 Recommendations based on the sensitivity analysis

91. The sensitivity analysis proves to be a useful method for probing the relationship between input parameter values and the output. It reveals areas in the model that require further understanding. For example, in the case of nanoRelease where for some parameters there is a sudden drop to zero sensitivity for a range of parameter values. The sensitivity analysis also shows the sensitivity response of the system with respect to a given range of parameter values. For example, in DPMFA, the shape of the response for the transfer coefficients appears to be a rectangular parabola. While in a number of other models, the shape of the response for some parameters is linear or quasi-linear, exponential, or parabolic with a local maximum sensitivity around a particular value of the parameter. Calculating the overall sensitivity and presenting the results in a table sorted in descending order is also useful. Such a table allows users to see what parameters are more sensitive on the output. The overall sensitivity

table also displays parameters that have a net zero effect on the output. For those parameters that have a net zero effect on the output, there is a possibility that the model can be simplified by removing the need to specify a numeric value for this parameter. However, before such simplifications can be made, more testing should be conducted with respect to the parameter of interest. Additionally, the sensitivity analysis conducted in this study proves a useful analysis for finding bugs or sensitivity in parameters where it is expected that these parameters be insensitive. For example in the case of SB4N, a bug was found where the output erroneously depended on the octanol/water partition coefficient. This bug was fixed and a new version of SB4N was provided and re-analyzed. The analysis of the new SB4N version revealed that the previous bug was fixed, now properly displaying zero sensitivity to the octanol/water partition coefficient. The SB4N example also shows the importance of testing a variety of parameters not only to find expected behaviour, but unexpected behaviour as well. In the current study, it is recommended to use a model whose input parameters display a predictable sensitivity response. Such models with predictable sensitivity responses are DPMFA, nanoFate, SB4N, and nanoDUFLOW.

5.4 Overall recommendations

92. We recognize there are great differences in authorizations between OECD member countries, thus the recommendations we provide in this document should be taken into consideration individually with specific regulations from different countries. Models that are recommended overall are models that have been recommended in each of the above sections (5.1, 5.2, and 5.3). Such models are DPMFA, SB4N, and nanoDUFLOW. Thus, we have three models, and coincidentally one of each of the model types (see section 2.1.1) evaluated. Based on the current study, DPMFA seems to be an MFA model suitable to estimate material flows from the technosphere to environmental compartments for a variety of scenarios. Moreover, DPMFA is transparent with respect to its source code and documentation, and is thus easy to implement new scenarios and analyze new model implementations. SB4N is an EFM model suitable to estimate screening level estimates of nanomaterial concentrations in environmental compartments based on a number of nano specific pseudo-first order kinetic processes. Additionally, SB4N is run in an Excel spreadsheet that provides transparency with respect to input parameters and calculations. nanoDUFLOW is a river model implementation of a specific river system, but with some effort and knowledge of the DUFLOW modeling studio can be modified to model any river system. Thus, due to the amount of effort it would take to implement new river systems with nanoDUFLOW, it is recommended to use this tool in cases where the risk of exposure is high to provide more reliable site specific estimations of nanomaterial concentrations in river systems.

93. Table 62 below presents some useful summary points from the model assessments. Data requirements are based on number of parameters required to run the model. All of the models have provided the input parameters for the default scenarios that they represent. However, if new scenarios were to be developed, the level of data requirements indicated in this table would provide the user with a rough estimate on the number of numeric parameters required to run the model.

Table 62.Summary of assessments and analyses.

Tool Name	Tool Type	Data Requirements*	Applicability Score	Difficulty Score	Dynamic	Stochastic	Spatially Explicit
DPMFA	MFA	Medium (180)	0.73	4	Yes	Yes	No
nanoRelease	MFA	Low (63)	0.65	5	Yes	Yes	No
nanoFate	EFM	Medium (182)	0.89	2	Yes	No	Yes
SimpleBox4nano	EFM	High (288)	0.92	2	Yes	No	Yes
nanoDUFLOW	EFM/River	High (8478)	0.81	5	Yes	Yes	Yes
WASP8	EFM/River	High (439)	0.88	2	Yes	No	Yes
LearNano	MFA	N/A	0.67	1	No	No	No
MendNano	EFM	N/A	0.94	1	Yes	No	Yes

*Total number of numeric parameters indicated in parentheses.

6 CONCLUSION

6.1 General conclusions of the current study

94. In conclusion, this report contains the details and the results of the functional assessments for each modeling tool that are summarized by two metrics: the difficulty rating and the applicability criteria score. This report also contains the details and results of the uncertainty and sensitivity analysis. Functional assessments were not performed on WASP7 nor on Rhone/Rhine model due to inaccessibility to the model files. Sensitivity and uncertainty analysis were not performed on LearNano nor on MendNano due to unresolvable error messages preventing the collection of the output. The uncertainty analysis is successful for every tested model (not including MendNano and LearNano), and is summarized by quantified metrics in the distribution of output values from Monte Carlo simulations. The sensitivity analysis is also successful for every tested model (not including MendNano and LearNano), and is summarized by a sensitivity score calculated for a range of parameter values. Validation against real monitoring data was not completed due to a lack of monitoring data. Modeling tools are recommended on the basis of the metrics provided by the functional assessment, whereas recommendations on the basis of sensitivity and uncertainty analysis would require further analysis. The modeling tools are all based on well-known chemical and physical principles, and the algorithms provide sound mathematical processes that solve for their respective output quantities and concentrations. The particular models themselves are applicable only to the scenario that those specific parameters describe. The modeling tools, however, in a more general sense, can be applicable to a number of different scenarios given the proper parameterization. For example, a model given spatial parameters, and describing the quality of the environmental compartments in Switzerland may be suitable for Switzerland, but not for Canada. In general, chemical and physical parameters describing the nanomaterial can be shared between the models and tools for any scenario, but property data describing the quality of the environmental compartments of a particular geographical region are valid only for scenarios using that region. Thus, for a modeling tool to be applicable in a specific country, we may prefer data describing the physical space and quality of environmental compartments in this country.

6.2 Recommendations for further analysis in future studies

95. For recommendations to be possible based on sensitivity and uncertainty analysis, the following analysis would need to be completed: both the Monte Carlo Simulations and the systematic sensitivity testing would need to be re-done where the error ranges represent real uncertainties reported from experimental measurements of the input parameters. In the current study, approximations to the error ranges (i.e. +/- 50% of the default) limits the applicability of the sensitivity and uncertainty analysis to demonstrative purposes. Thus, the present analysis demonstrates what could be done in the case where real errors for input parameters are used. In the case where real errors are used, the model that yields the lowest uncertainty (i.e. lowest standard deviation, or smallest coverage interval) would be preferred over the others. In the case where input mass flow volumes differ drastically between scenarios, normalization of the uncertainty output can provide a basis for comparison of standard deviations (provided that the distributions for the outputs of each model are the same, i.e. both have

the same distribution type). If some of the models in this study are considered further to be used in regulatory assessments, it is recommended to do a more in-depth uncertainty and sensitivity analysis. This more in-depth analysis would include all possible input parameters (not just a selection of parameters like it was done in the current study). A more in-depth analysis would also consider several scenarios for each modeling tool, and possible default scenario parameterizations that can be applied across all models for comparison.

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8 APPENDIX

8.1 Assessment overview

96. Below is a **template** of the factsheet's sub-headings including a description of the information you can find under each heading for any given model. The purpose of this template is to provide clearly defined categories under which each model can be assessed in the most objective way possible. Thus, in the name of objectivity and comparability, each modeling tool is assessed in the same way. Each individual assessment follows the template below, as the information for any assessment is organized under the section sub-headings that define the assessment sections. Two main sections: the **Mechanistic Assessment**, and the **Theoretical Assessment** are defined as a means to organize the sub-categories with respect to the kind of information that can be found within those categories. The mechanistic assessment contains information relevant to the installation, usage and scope of the modeling tools, and also provides information about what scenarios have been previously modeled using the tools. The theoretical assessment provides information about the assumptions, the algorithms, kinds of input parameters, as well as the type of model output. The template below is provided for transparency, and for reference about what kind of information can be found under each section sub-heading.

4.x.1.1 MECHANISTIC ASSESSMENT:

4.x.1.1.1 AUTHOR:

GOAL: *Credit to the author.*

- Author name(s)

4.x.1.1.2 VERSION:

GOAL: *Documentation for reproducibility.*

- Version of the model being evaluated

4.x.1.1.3 ACCESSIBILITY:

GOAL: *Provide source to users.*

- Is it free of charge to download?
- Where can the user find the model?

4.x.1.1.4 DEPENDENCIES:

GOAL: *Inform users on computer requirements and other programs.*

- Necessary or optional additional programs to help run the model
- Example dependencies: R, Python, MATLAB, Other packages

4.x.1.1.5 INSTALLATION:

GOAL: *Provide users with an overview of the installation process.*

- Summary of installation process
- Verification of installation

4.x.1.1.6 FOLDER AND FILE STRUCTURE:

GOAL: *Provide users with correct folder structure for proper functioning of application.*

- Required folder structure for certain models
- Path specifications

4.x.1.1.7 USAGE:

GOAL: *Provide user with an at-a-glance feel for how to use the program.*

- Summary of usage based on difficulty rating criteria
- Difficulty rating
- Highlights use of graphical interface, scripting, or spreadsheet
- Highlights specification of input parameters, and collection of output results

4.x.1.1.8 FEATURES:

GOAL: *Provide user with an at-a-glance feel for what features the model offers.*

- Summary of general features
- Category: MFA or EFM
- Product applications
- Spatial and temporal resolutions
- Compartments, transformation, transport etc.
- Applicability criteria score

4.x.1.1.9 PROVIDED CASE STUDY:

GOAL: *Summary of the case study provided by the author in a publication*

- Summary of scenario(s) design
- Summary of results

4.x.1.2 THEORETICAL ASSESSMENT

4.x.1.2.1 ASSUMPTIONS:

GOAL: *Inform the user on what is assumed in the model.*

- Theory (Principles or Laws)
- Mathematical principles
- Qualitative assumptions about physical or chemical processes
- Summarized in a table

4.x.1.2.2 ALGORITHMS:

GOAL: *Inform the user on what algorithms are used in the model.*

- Name of algorithm, or reference to standards (like an ordinary differential equation (ODE) solver)
- Probabilistic sampling algorithms
- Calculations
- Iterative processes

4.x.1.2.3 INPUT PARAMETERS:

GOAL: *Inform the user on the kinds of input parameters.*

- What kind of parameter is it?
- What computer format is it stored in?
- What is the source of the parameter?

4.x.1.2.4 MODEL OUTPUT:

GOAL: *Inform the user on the kinds of output from the model.*

- What is the output type?
- What are the units?
- What computer format is it stored in?

4.x.1.2.5 NANOMATERIAL APPLICATIONS:

GOAL: *Inform the user on what nanomaterials can be modeled by the model.*

- What nanomaterials has the developer used in a study involving the model.

8.2 Parameter database and database manager (PDBM)

8.2.1 Purpose of PDBM:

97. The purpose of the input parameter database is to ease the process of collecting and organizing input parameters for downstream analysis. PDBM is meant to be used as a data manipulation and organization tool within a command-line terminal alongside

8.2.2 Implementation:

98. PDBM is an applied database management system whose functionality is specific to input parameter data for exposure models implemented in Python 3.8 (Python Software Foundation[37]). PDBM leverages the functionality of the Pandas DataFrame (McKinney, 2010[38]) as the main data structure for manipulation and organization of the database.

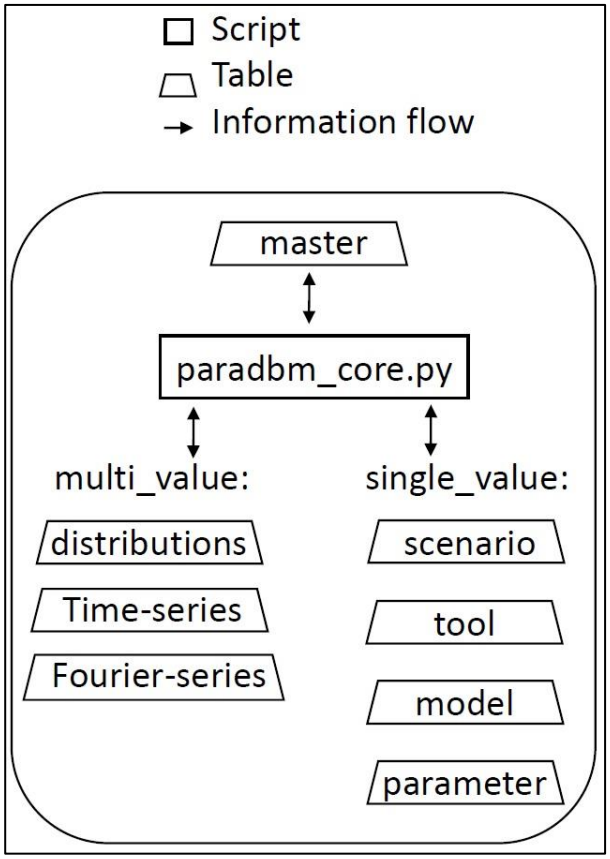

Figure 16 Schematic Depiction of the PDBM Structure and Flow of Information

Note:Legend is shown above the schematic; rectangular boxes represent scripts, trapeze boxes represent tabes containing records, and arrows show flow of information between scripts or tables.

99. PDBM stores data in a file folder system containing Excel spreadsheets. Below is an illustration of the database structure:

8.2.2.1 Features:

100. PDBM's features divides into two sets of functionalities; the implicit functionality that occurs automatically, and the explicit functionality that can be used at the command of the user. Below is a summary of the features PDBM provides. PDBM is not limited to this functionality, and is in continual evolution and development.

8.2.2.2 Implicit Functionality:

(1) **Unique Identification:** PDBM implicitly assigns and automatically logs a unique identification number key to any new record inserted into both the master table and any sub-table in which the record is located.

(2) **Auto-Save:** For any change made to the master table, PDBM automatically writes those changes to memory.

8.2.2.3 Explicit Functionality:

(1) **Open/Close:** Open or close the master table, any number of sub-tables, or any number of other tables.

(2) **Insert/Delete Record:** Insert one or more new records with or without accompanying entry values, or delete existing record rows.

(3) **Insert/Delete Entry:** Insert a new entry column with accompanying entry values, or delete an existing entry column.

(4) **Replace Record:** Replace the entry values for an existing record with new entry values.

(5) **Replace Entry:** Replace an entry value for a particular entry for one record.

(6) **Push Table:** Push the changes made in the master table to any of the sub-tables.

(7) **Filter:** Filter rows or columns based on search criteria.

(8) **Save:** Write any table to memory.

8.2.2.4 Record Entries:

101. PDBM currently stores 31 record entry types used to store specific information about the tools, scenarios, models, or parameters. The entry types are described below including a naming convention for each entry type, and the type of value that is stored under that entry type. Akin to PDBM's functionality, the entry types and naming conventions are mutable to accommodate new kinds of information.

Table 63. Description of record entries in PDBM.

Number	Name	Type	Sub tables	Naming Convention	Description	Use
1	id_key	Integer	All	N/A	Unique identifier for a record in the master table	Automatically updated
2	id_scenario	Integer	scenario	N/A	Unique identifier for a record in the scenario sub table	Automatically updated
3	id_model	Integer	model	N/A	Unique identifier for a record in the model sub table	Automatically updated
4	id_tool	Integer	tool	N/A	Unique identifier for a record in the tool sub table	Automatically updated
5	id_distribution	Integer	distribution	N/A	Unique identifier for a record in the distribution sub table	Automatically updated
6	id_time_series	Integer	time series	N/A	Unique identifier for a record in the time series sub table	Automatically updated
7	reference_parameter	list of reference integers as string	parameter	'[ref_1,ref_2,ref_3]' , with ref_1 2, and 3 being the integers	Reference number to identify a cluster of related parameters	Assign reference numbers manually as needed
8	reference_tool	list of reference integers as string	model	'[ref_1,ref_2,ref_3]' , with ref_1 2, and 3 being the integers	Reference number to identify one or more tools used by a model	Assign the id_tool of the tool to which you wish to refer the model
9	reference_scenario	list of reference integers as string	model	'[ref_1,ref_2,ref_3]' , with ref_1 2, and 3 being the integers	Reference number to identify one or more scenarios used by a model	Assign the id_scenario of the scenario to which you wish to refer the model
10	reference_model	list of reference integers as string	parameter	'[ref_1,ref_2,ref_3]' , with ref_1 2, and 3 being the integers	Reference number to assign a set of parameters to one or more models	Assign the id_model of the model to which you wish to refer the set of parameters
11	table_push	string	All	'sub_table_name' e.g. 'parameter', or 'tool'	Name of the table to which the record should be pushed	Assign the sub table name as needed. Table push is also used to filter for sub table entries from the master table.

Number	Name	Type	Sub tables	Naming Convention	Description	Use
12	name_common	string	All	The generic naming convention follows this logic: object_{adjectives}_[process] Objects are either compartments or substances Processes are either transfers or transformations Adjectives are differentiation terms and vary depending on the record The naming convention for name_common depends on the table_push: **Scenario:** country_name_{substance, local or global} **Tool:** Tool_full_name_{abbreviation} **Model:** model_name_{dynamic or steady state} **Parameter:** **Compartments:** Main compartment names are: System_exterior Ecosphere: Air, Water, Soil, Sediment Technosphere: Production, Manufacture, Consumption Compartment_name_{sub_compartment,descriptor} e.g. water_{surface,fresh}, water_{deep,marine}, soil_{deep,urban} e.g. manufacture_{polymer_composites} **Compartment Properties:** Compartment_name_{compartment_adjectives}_[property_name] soil_{surface,urban}_[density] **Transfers:** Initial_compartment_name_{compartment_adejctives}_[transfer_name]_final_compartment_name_{compartment_adjectives} **Transfer Properties:** transfer_name_[transfer_property] **Transformations:**Transformations happen on substances Initial_substance_name_{substance_adjectives}_[transformation_name]_final_substance_name_{substance_adjectives} **Transformation properties:** Transformation_name_[transformation_property] **Substances:** Substance_name_{substance_adjectives} e.g. titanium_dioxide_{TiO2,nano,dissolved} **Substance Properties:** Susbstance_name_{substance_adjectives}_[substance_property] **Releases:** compartment_name_{compartment_adjectives}_[release_name] **Release Properties:** release_name_[release_property_name]	Common name of the record to be used for programing operations	Assign the names manually as best you can according to the above conventions. Use the naming convention for comparison, automaton, and filtering.

Number	Name	Type	Sub tables	Naming Convention	Description	Use
13	name_original	string	All	'name of the object as declared by author'	Name of the record object as declared by the author	Assign the name as declared by the author Use the name for reference and disambiguation
14	source	string	All	source_name_[source_type] Source_types: web doi name_year	Source of the record object	Assign the source and source type Use for reference
15	descriptor	string	All	'any descriptive statement'	A descriptive statement to make the record object understandable by a human	Add a description as you wish
16	type_parameter	string	parameter	**Compartment**: compartment_property **Transfer**: transfer_property **Transformation**: transformation_property **Substance**: substance_property **Release**: release_property **Temporal**: temporal_property **Meta**: meta_property	Types of parameter record objects to be used for operations	Follow the convention Use for filtering and comparison
17	type_value	string	parameter	[1] mean [2] median [3] mode [4] variance [5] error_other [6] factor_other [7] range '[low_val]_[high_val]' **string [8] numeric [9] time_series [10] distribution [11] nominal [12] bound **Probability distribution suffixes:** _{distribution_type} _{normal} _{lognormal} _{uniform} _{triangular} _{Weibull} _{binomial} _{beta} _{other}	Value types for parameter record objects to be used for operations	Follow the convention Use for filtering and comparison

Number	Name	Type	Sub tables	Naming Convention	Description	Use
18	code_common	string	parameter	N/A	Name of the variable used for scripting in excel, R, or Python	Variable name for reference to scripts
19	code_original	string	parameter	N/A	Name of the variable used for scripting in excel, R, or Python as declared by the author	Use for reference to original code
20	value_default	string, integer, float	parameter	N/A	Numeric or nominal value of the parameter	Use for formatting and passing to downstream scripts for analysis
21	use_math	string	parameter	Use code_common as variables in the equations Use Python syntax for math operations	The mathematical use or formula that the parameter fits into	Use for reference
22	use_computation	string	parameter	N/A	The use of the parameter in the computational model	Use for reference
23	substance_name	string	scenario	substance_name_{substance_adjectives}	The name of the substance to be modeled	Use for reference
24	continent_name	string	scenario	N/A	The name of the continent	Use for reference
25	country_name	string	scenario	N/A	The name of the country	Use for reference
26	region_name	string	scenario	N/A	The name of the region (like a province, or a state)	Use for reference
27	time_period	string	scenario	[initial_yyyy_mm_dd]_[final_yyyy_mm_dd]	The time period of the scenario	Fill in the resolution as it is available e.g. [2003]_[2005], [2003_05]_[2005_07], [2003_05_21]_[2005_05_09]
28	path_exec	string	tool	'path/to/executable/'	The computer location of the executable file for the tool	Use for scripting and automation to run the model from the system
29	type_tool	string	tool	EFM, MFA, others?	The type of tool	Use for reference
30	unit	string	parameter	Use Python syntax for math notation e.g. **Yes:** kg/(m**3) **No:** kg/m^3	The units of the parameter value	Use for reference
31	version	string	tool	'v3.0.1' or 'v2020_03_05'	The version of the tool logged in the record	Use for reference