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SMARTControl

Smart framework for real-time monitoring and control of subsurface processes in managed aquifer recharge (MAR) applications

Deliverable D4.3

Web-based risk assessment tools

Development and implementation of a web-based tool for QMRA

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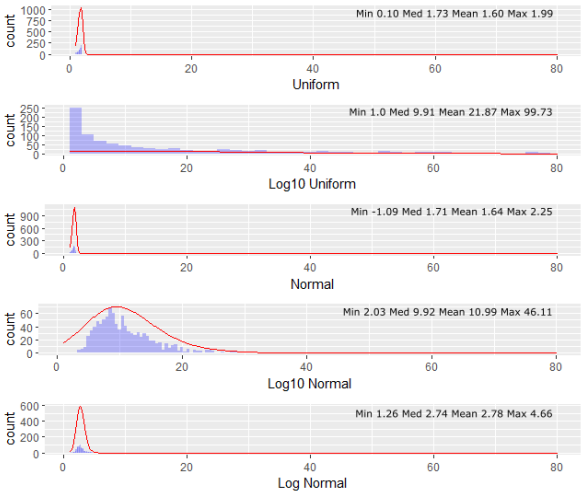

https://www.smart-control.inowas.com

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Short summary

This report describes the main functionalities the SMART-Control web-based tool T1B Quantitative microbial risk assessment. The tool helps to quantify the pathogen occurrence in source water and their removal by various treatment steps at MAR facilities by using a probabilistic approach. The interactive web-based QMRA tool supports the evidence-based risk assessment to minimize water-related infectious diseases.

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ABSTRACT

The main objective of the SMART-Control project is to reduce the risks associated to MAR by the development of an innovative web-based real-time monitoring and control system (RCMS) in combination with risk assessment and management tools. Quantitative Microbial Risk Assessment (QMRA) is recognized as an evidence-based approach to minimize water-related infectious diseases. The risks caused by pathogenic microorganisms can be assessed which supports decision-making related to the microbial safety of water systems. The web-based QMRA tool was developed to support the implementation of QMRA through an interactive, easy-to-use, and guided web-browser based application. The QMRA tool allows the quantification of pathogen occurrence in source water and their removal by various treatment steps and is based on a probabilistic risk assessment.

CONTENT

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1. INTRODUCTION

A. MOTIVATION

Quantitative Microbial Risk Assessment (QMRA) is developed to assess risks caused by pathogenic microorganisms and to support decision-making related to the microbial safety of water systems (Haas et al., 2014). QMRA is widely recognised as an evidence based approach to minimize water-related infectious diseases (WHO, 2016). The QMRA presented here allows the quantification of pathogen occurrence in source water and their removal by various treatment steps. It combines exposure patterns and specific dose-response relationships to calculate the risk of infection or other end-points such as disability-adjusted life-year (DALY). The QMRA presented here is based on a probabilistic risk assessment. The input data is considered to be highly variable and quantified by using Probability Density Functions (PDF). Monte Carlo simulations are applied to generate estimates of the parameters from the PDF.

The QMRA software tool presented herein is developed to support the implementation of QMRA through an interactive, easy-to-use, and guided web-browser based application.

B. QMRA IN THE EUROPEAN LEGISLATION

In EU legislation, risk assessment has been introduced in the Drinking Water Directive (2015/1787) where monitoring of drinking water schemes is based on the principles of risk assessment and risk management (WHO, 2011). In recent years, risk-based approaches on water reuse was developed on behalf of the EU commission (Alcalde-Sanz and Gawlik, 2017). The report was developed by the Joint Research Centre (JRC) and forms the technical basis for the derivation of binding European standards. It addresses the need to promote the reuse of treated wastewater within the EU in order to reduce the pressure on fresh water resources. Water reuse is considered as a possible measure of managing water scarcity and drought. With respect to microbial risks assessment, hygienically relevant indicator organisms were identified. The approach defines treatment targets formulated as Log Reduction Values (LRV) for three relevant groups of pathogenic microorganisms: bacteria, spore formers and viruses. Water professionals received the overall methodology to be appropriate, but the document was considered deficient in some key details. Both the Scientific Committee on Health, Environmental and Emerging Risks (Rizzo et al., 2018) and the European Food Security Agency drew critical conclusion from the evaluation of the JRC report. Rizzo et al. (2018) emphasize that the report does not adequately address the problem of micro pollutants ("contaminants of emerging concern"), the possible spread of antibiotic resistance and possible risks from disinfection by-products. Apart from the technical requirements for water reuse, other issues such as a clear definition of water shortages and the identification of the quantitative demand for reuse, liability issues in the event of contamination and cost regulation for additional treatment and monitoring measures remain unsolved. Moreover, the critical perception of some EU member states, especially with respect to groundwater protection, lead to that aquifer recharge was excluded from this regulation. However, the first European wide regulation on minimum requirements for water reuse in agricultural irrigation came into force in June 2020. The regulation now in force harmonised minimum water quality requirements for reuse of treated urban wastewaters in agricultural irrigation on EU level for the first time.

C. SMART-CONTROL APPROACH

"SMART-Control" is an international research project funded through the Water Joint Programming Initiative (WaterJPI) and implemented by nine institutions from Germany, France, Cyprus and Brazil. The main objective of

the project is to reduce the risks associated to MAR by the development of an innovative web-based real-time monitoring and control system (RCMS) in combination with risk assessment and management tools. The SMART-Control approach relies on coupling a real-time in-situ observation system consisting of state-of-the-art online sensors and an open access web-based groundwater monitoring and modelling platform, developed by the Research Group INOWAS at Technische Universität Dresden, Germany. The platform contains a collection of empirical, analytical and numerical tools for assessing groundwater flow processes with focus on managed aquifer recharge applications (https://www.inowas.com). The INOWAS platform will be amended in the SMART-Control project by four additional simulation tools (Table 1). The resulting system shall provide operators and managers of MAR schemes with automatic decision support tools for monitoring, controlling and prediction of processes occurring during MAR. The approach will be tested and validated at six MAR sites under different environmental and operating conditions. More information about SMART-Control and a complete documentation of tools is available on the project website: https://www.smart-control.inowas.com.

Table 1: Short description of simulation tools developed in the SMART-Control project

No.	Tool name	Tool description
T1	**Initial risk assessment**	The tool represents an easy-to-use instrument to evaluate the viability of a MAR project and the preliminary assessment of human health and environmental risks. The tool has two parts: A) a component for the estimation of groundwater hydraulic residence times during subsurface passage (see Deliverable D4.1); and **b) a component for quantitative microbial risk assessment (QMRA) of MAR schemes, including hazard identification, exposure assessment, dose analysis and risks characterisation**. The risk will be assessed for selected reference pathogens such as bacterial, protozoan and viral pathogens for different hydraulic residence times during MAR.
T2	**Real-time monitoring and control**	This tool aims to facilitate the operational management of MAR sites. The tool includes a web-based monitoring system developed for real-time integration of time series data into the INOWAS modelling platform. Sensors installed at MAR facilities worldwide can be connected to the INOWAS platform to transfer collected data in real time. The data can be visualized, processed, downloaded and prepared for further usage (see Deliverable D4.2).
T3	**Automatic groundwater simulations**	Real-time observations collected from MAR sites can be integrated into a web-based modelling workflow. The system relies on the existing groundwater modelling capabilities of the INOWAS platform, which were expanded by adding additional features. The integration of real-time monitoring data into the simulation workflow will enable fast response time and optimized management, which helps to minimize and control the associated risks.
T4	**Predictions for advanced system management**	The tool allows building climate change and development scenarios for groundwater flow models to predict future boundary conditions and compare them to the present situation using the INOWAS Scenario Analyser. The tool provides a novel way of using real-time, web-based groundwater models to assess the effects of climate change, urbanisation, land use change (irrigation demand) and population growth on spatial and temporal water availability.

This report describes the main functionalities of the new tool **"T1. Initial risk assessment. Part B. Quantitative microbial risk assessment (QMRA)"**.

2. BACKGROUND

In general, QMRA consists of hazard identification, exposure assessment, dose response analysis, and risk characterization to predict the risk of an infection or disease related outcome based on an exposure to the environmental media (Beaudequin et al., 2015; Haas et al., 2014; WHO, 2016).

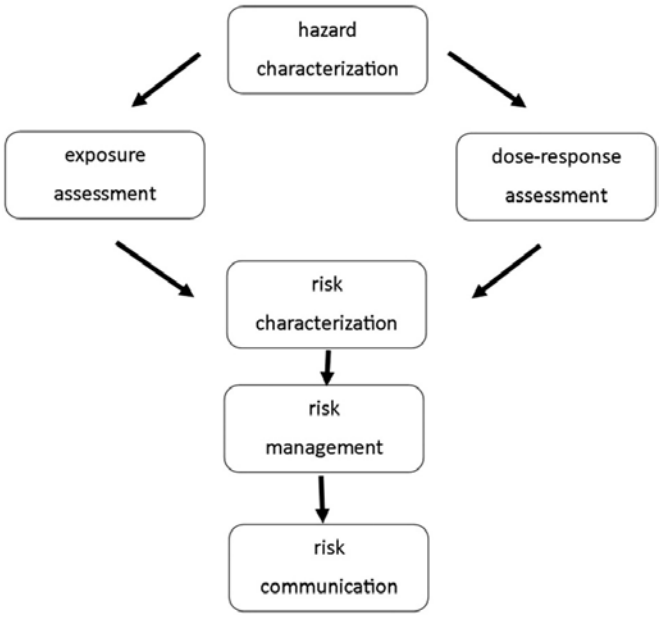

Figure 1: Overview of quantitative microbial risk assessment (Beaudequin et al., 2015)

The first step in QMRA is the hazard identification. Hazard identification consists of identification of the microbial pathogens and the diseases associated to the identified organisms. All potential sources and events that can lead to a breakthrough of pathogens, irrespective if this can be controlled by the operator or not, should be documented for each component of the water systems (WHO, 2011).

Hazardous sources and events are then associated to the specific pathogen characteristic for the source or event, e.g. a failure of upstream wastewater plant may produce other pathogens than a flood event. From a practical point of view, it is not possible to assess all potentially hazardous waterborne pathogens. The selection of reference pathogens is limited by data availability, in particular with respect to human dose–response models and measurements during subsurface passage.

The aim of the exposure assessment is the quantification of the size and the nature of the population exposed to the pathogen(s). It consists of characterising the route of exposure, the distribution of the microorganisms and the duration of the exposure. Exposure routes range from daily drinking water consumption of several litres to accidental ingestion of few millilitres e.g. during irrigation. Exposure assessment and dose-response assessment are mutually dependant. Dose-response assessment in QMRA is the quantification of the relationship between the dose administered and the probability of the severity of health impacts on the exposed population. In QMRA an important concept is that even a single pathogen may be able to cause infection and disease, the so called single-hit principle (WHO, 2011).

Finally, risk characterization is the integration of the data on hazard identification, dose-response and exposure to calculate the risk to human health and its variability and uncertainty. Risk characterization gives information on the probability of an infection to occur and on the severity of the infection presented in terms of DALYs. Disability adjusted life years or disease adjusted life years (DALYs) are used extensively to assess disease burdens associated to a broad range of environmental hazards (WHO, 2016). DALYs not only express the number of years lost due to

premature death, but also the years lived with illness or disability until recovery or death. DALYs are applicable regardless of the type of hazard (microbial, chemical or physical) and allows for comparison of the burden of disease. For potable water consumption, the WHO used a tolerable disease burden of 10^{-6} DALYs pppy (WHO, 2011), which is also used for non-potable purposes (Canada, 2010; NRMMC-EPHC-NHMRC, 2009). The tolerable disease burden of 10^{-6} DALYs pppy means that a city of one million people collectively suffers the loss of one DALY per year.

3. SOFTWARE

The QMRA tool has been included in the INOWAS DSS web platform, which offers a variety of tools related to groundwater modeling with a special focus on managed aquifer recharge (MAR). Because the INOWAS DSS is a browser application, it can be accessed from all over the world without the need of installing extra software or acquiring licenses. The code of the platform is completely open-source and can be accessed on Github: https://github.com/inowas.

The frontend part including user interfaces and visualization of results is developed with the open-source javascript library ReactJS[1]. React is provided by Facebook and is thus widely used in the development of web applications. The concept of reusable components has been used to achieve a sustainable and easy maintainable codebase. Additionally, Redux[2] is used to centralize the state of the application and connect the different components.

The QMRA tool has been previously developed by KWB as a R package[3] called kwb.qmra[4]. OpenCPU[5] is used for running the R scripts for the calculations of the QMRA in the backend. It provides a simple interface between JavaScript on the client-side and R on the server-side part of the tool. Input data is sent from the user interface to the backend with a POST request via Axios[6], a "promised-based HTTP client […] for the browser". The service runs on the INOWAS server and can be reached with the URL: https://opencpu.inowas.com/ocpu/library/kwb.qmra/

The calculation results are received by the front-end and can be downloaded in CSV or JSON format or viewed directly in the browser.

[1] https://reactjs.org/, 22.10.2021
[2] https://redux.js.org/,22.10.2021
[3] https://www.r-project.org/, 22.10.2021
[4] https://kwb-r.github.io/kwb.qmra/, 22.10.2021
[5] https://www.opencpu.org/, 22.10.2021
[6] https://axios-http.com/, 22.10.2021

4. INPUT/OUTPUT PARAMETER

A. INFLOW CONCENTRATION

Inflow concentrations of the pathogen to the treatment scheme are entered as absolute minimum and maximum. concentration per litre and are required for all pathogens that should be used for QMRA. Currently one of the following probability density functions (PDF) can be selected by the user:

i) **Uniform**: provides a constant probability density function, the provided absolute "min" and "max" values are in case minimum concentration is 0 replaced with 0.01; in case maximum concentration is 0 it is replaced with 0.1

ii) **Log_{10} uniform**: same as uniform but all values log_{10} transformed

iii) **Normal**: the required parameters mean and standard deviation are derived from the provided absolute min/max values as follows:

   a. "min": if the minimum concentration is 0 it is replaced with 0.01
   b. "max": if the maximum concentration is 0 it is replaced with 0.1
   c. "mean": (min + max) / 2
   d. "sdev": abs(max - mean) / 1.644854, assuming that 90% of all random values lie between min and max

iv) **Log_{10} normal**: same as normal but all values log_{10} transformed

v) **Log normal:** same as normal but all values log_2 transformed

Total variability in pathogen concentration for inflow concentration is difficult to assess, because it can be unclear whether measurements cover the full range of microbial concentration (possible unobserved values). Low pathogen concentrations and the irregular occurrence of pathogens contributes to the difficulties in capturing this variability. Moreover, some sites may not have any pathogen data and are dependent on assumptions. At data scarce sites, it is recommended to use "log_{10} uniform", because compared to the other it largely overestimate the provided concentration range. In contrast, the "log_{10} normal" distribution could be used for simulating "peak" system behavior as it overestimates the maximum concentration by approximately 250% compared to the maximum value entered by the user. The impact of different PDFs on the inflow concentrations is shown in Figure 2.

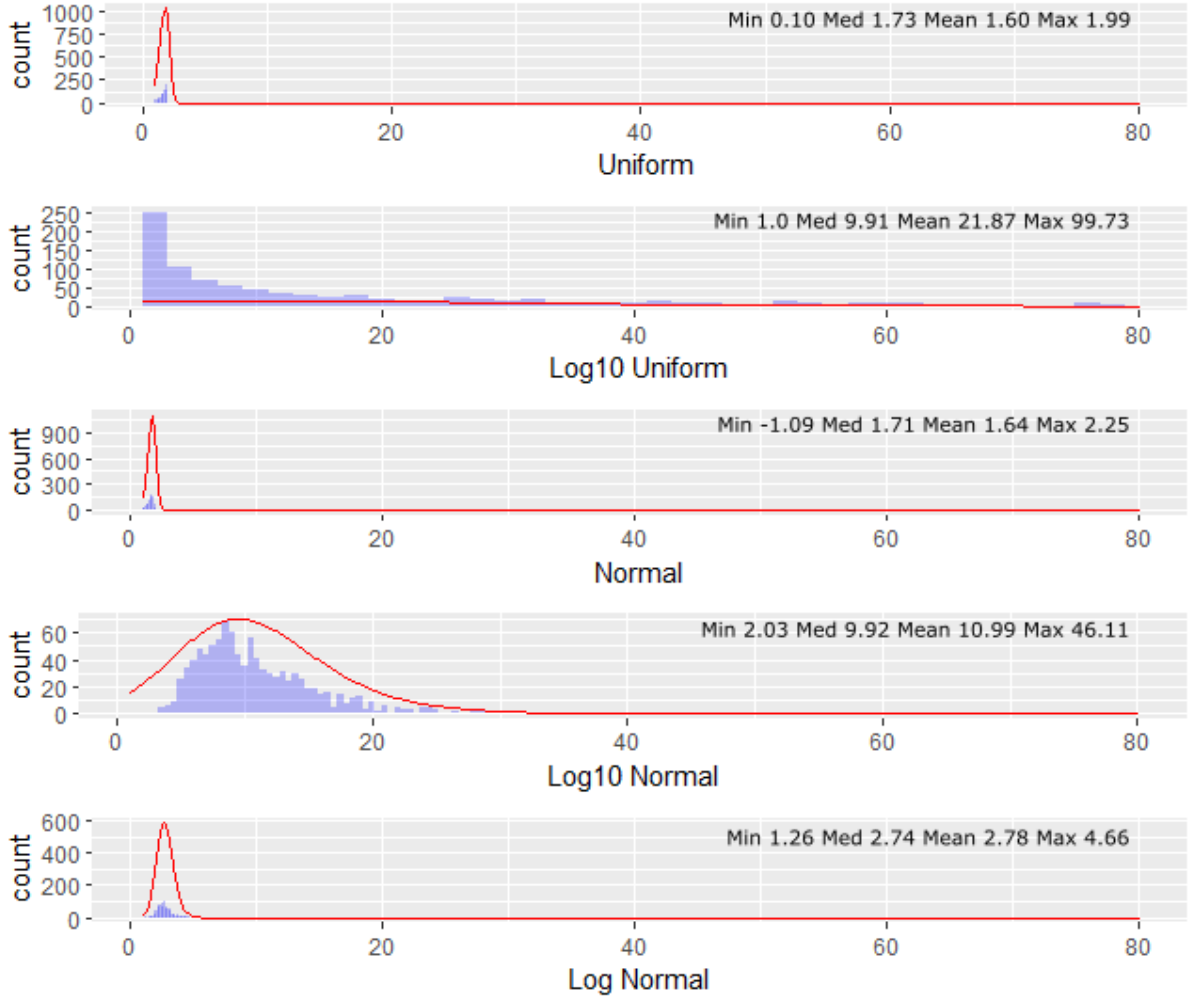

Figure 2: Logarithmic concentration ranges vs count of Probability Density Functions (min log_{10}= 0 and max log_{10} = 2).

For further details the reader is refered to the documentation website of the R function create_random_distribution[7] within the R package kwb.qmra[8].

[7] https://kwb-r.github.io/kwb.qmra/reference/create_random_distribution.html, 22.10.2021
[8] https://kwb-r.github.io/kwb.qmra/, 22.10.2021

B. TREATMENT STEPS

For each treatment process the log_{10}-removals for at least one of the three different pathogen groups (i.e. bacteria, protozoa, viruses) need to be defined. The user can define a new treatment process or select from pre-defined literature based removal performance associated to the different treatment steps. Pre-defined treatments are available by clicking on list icon next to "Add process" button. There are >25 treatment steps available covering the following groups:

- Coagulation, flocculation and sedimentation
- Filtration
- Natural Attenuation
- Pre-treatment
- Disinfection
- Primary and
- Secondary treatment

Natural attenuation e.g. includes bank filtration, soil-aquifer passage and wetlands. Each treatment step is briefly described (Figure 3) and substantiated with literature sources.

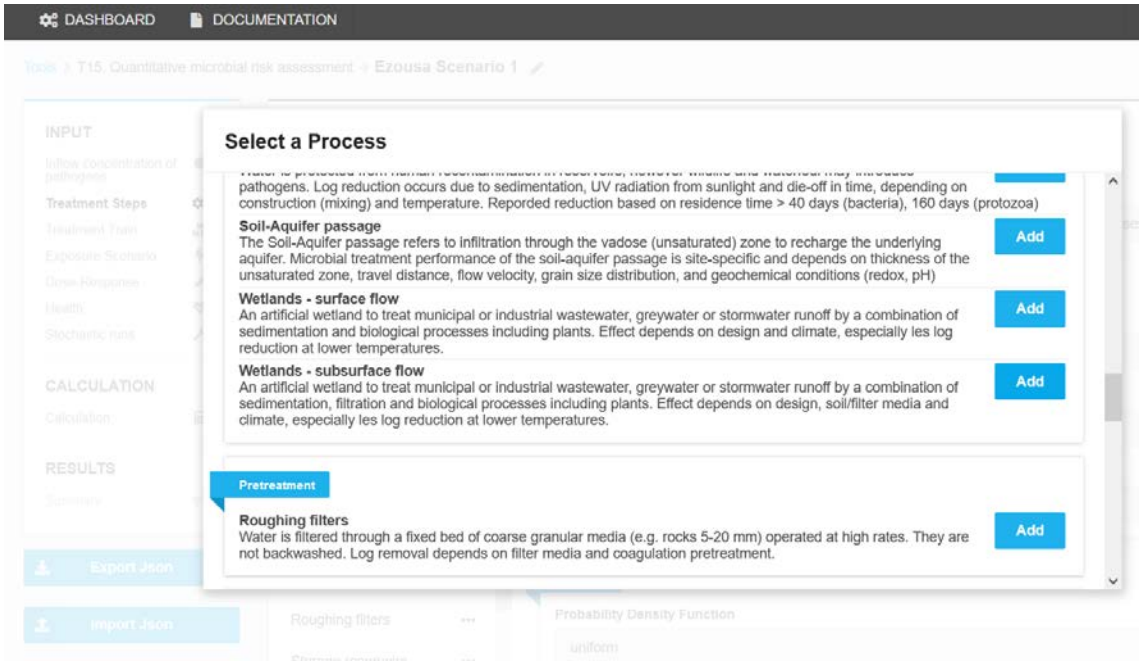

Figure 3: Selection of treatment steps

After selecting the required treatment steps it is necessary to enter Log Removal Values (LRV) for each pathogen and treatment step. The available PDF are limited uniform and normal distribution function (Figure 4).

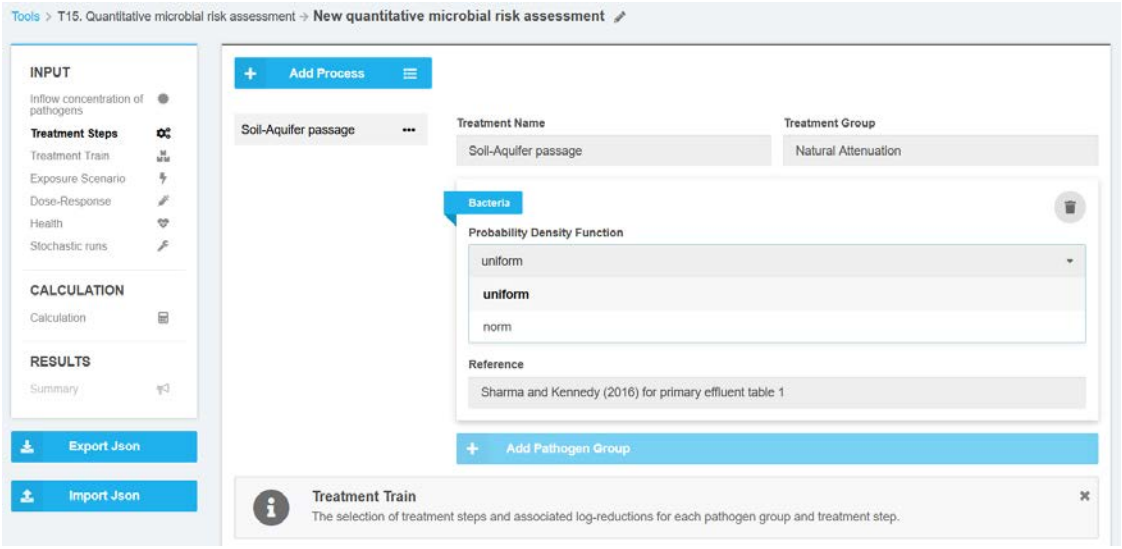

Figure 4: Selection of probability density function for treatment steps

C. TREATMENT TRAIN

Treatment steps can be combined to a treatment train or treatment scheme (Figure 5). The user may construct several treatment trains. All selected treatment trains will be considered in the QMRA calculation. The order of the treatment steps does not play a role in the calculation.

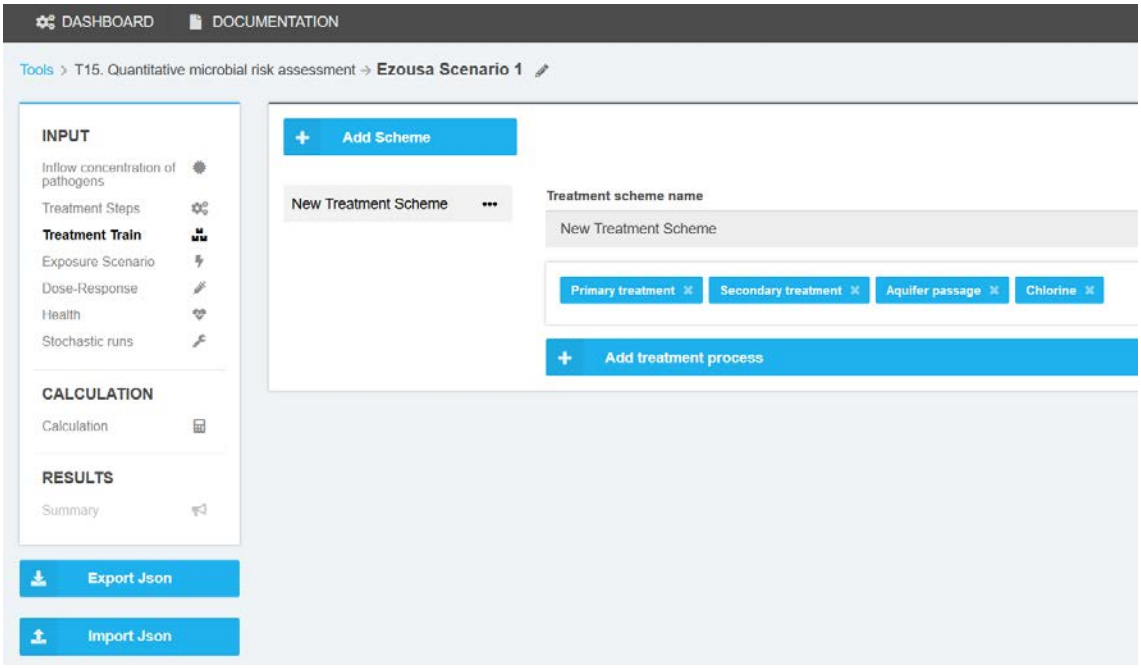

Figure 5: Combination of treatment steps to a treatment scheme

D. EXPOSURE SCENARIO

The number of exposures per year and the ingested volume per event can be defined as fixed value or by following a pre-defined distribution. There are eight pre-defined exposure scenarios from drinking water to irrigation water and domestic end-use. The pre-defined exposure scenarios are accessible by clicking on the "Add Scenario" button. Once selected the exposure scenario can be switched to active by clicking on the "Toogle" button. Only one exposure scenario per simulation can be selected at a time (Figure 6).

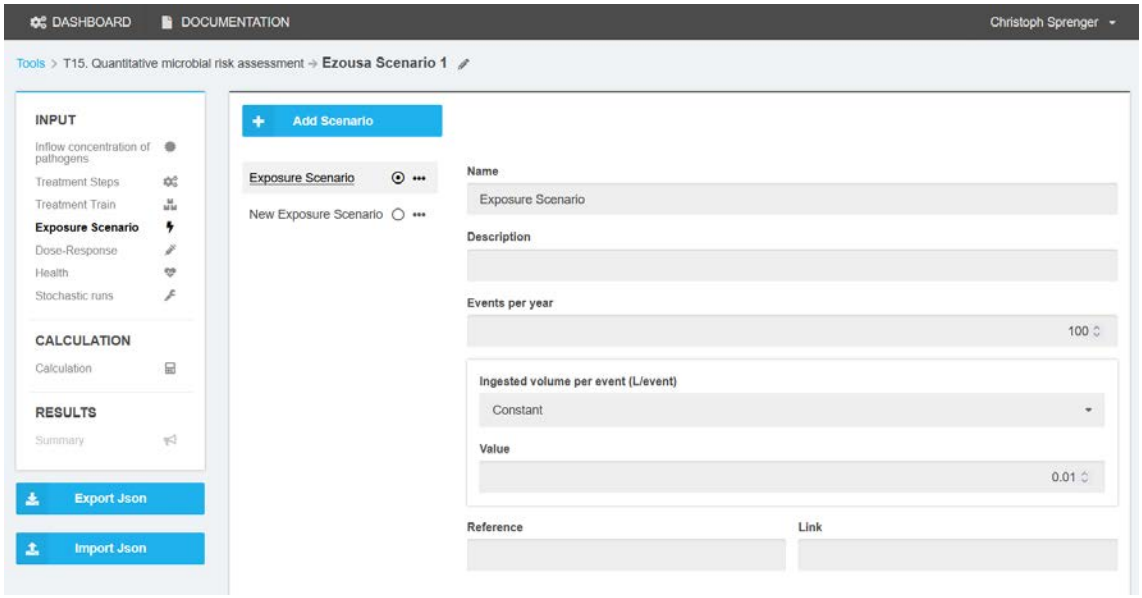

Figure 6: Exposure scenario

E. DOSE-RESPONSE

The dose-response models are based on experimental data. The dose-effect relationships can be approximated for each pathogen by exponential binomial formulae or beta Poisson distributions. Parameters for each pathogen are taken from QMRAwiki (2016)[9] (Figure 7).

[9] http://qmrawiki.canr.msu.edu/index.php/Dose_Response, 22.10.2021

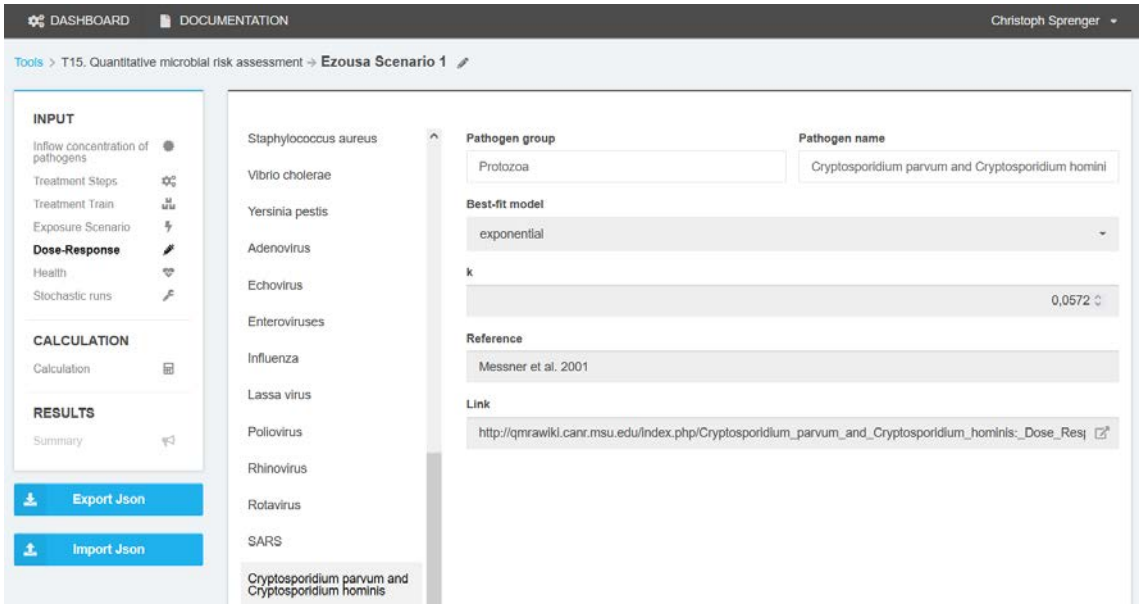

Figure 7: Dose-response relation

Dose-response models are defined for the pathogens that are toggled active in the inflow concentration section.

F. HEALTH

For all pathogens to be used for QMRA, the infection to illness factor and the disability-adjusted life years (DALY) per case need to be defined.

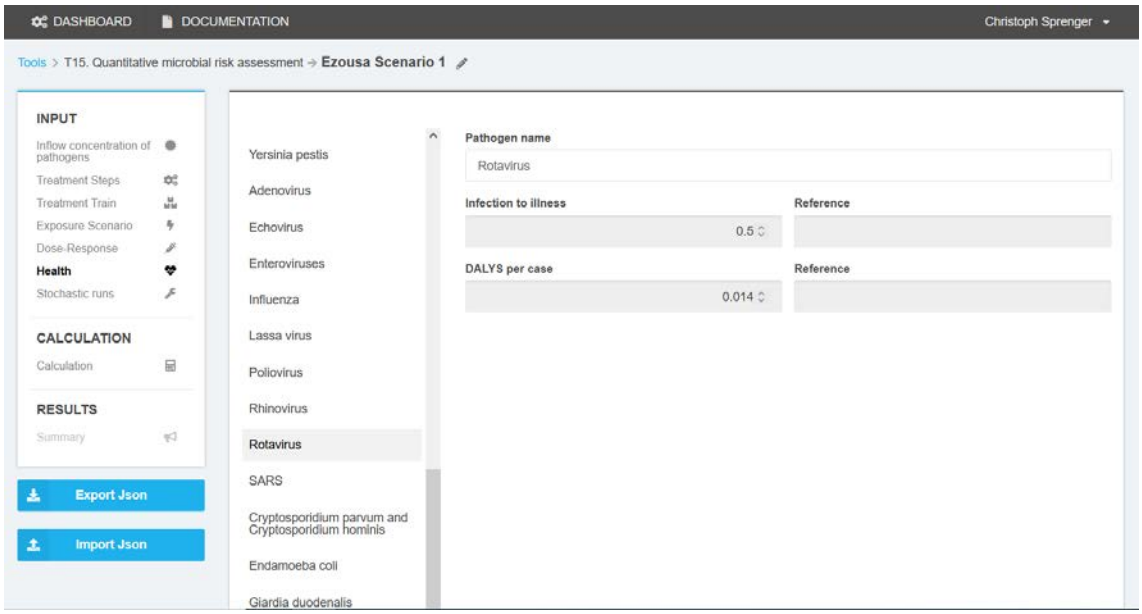

Figure 8: Definition of Health parameters

G. STOCHASTIC RUNS

In Monte-Carlo simulation the number of random distribution generations can be specified here. At least 1000 runs are recommended.

H. RESULTS AND DATA EXPORT

The results are presented in tables and made available for download in json and csv format. A graphical display of results is currently not available. Four files (events, total, stats_total, stats_logremoval) are available for download (Figure 9).

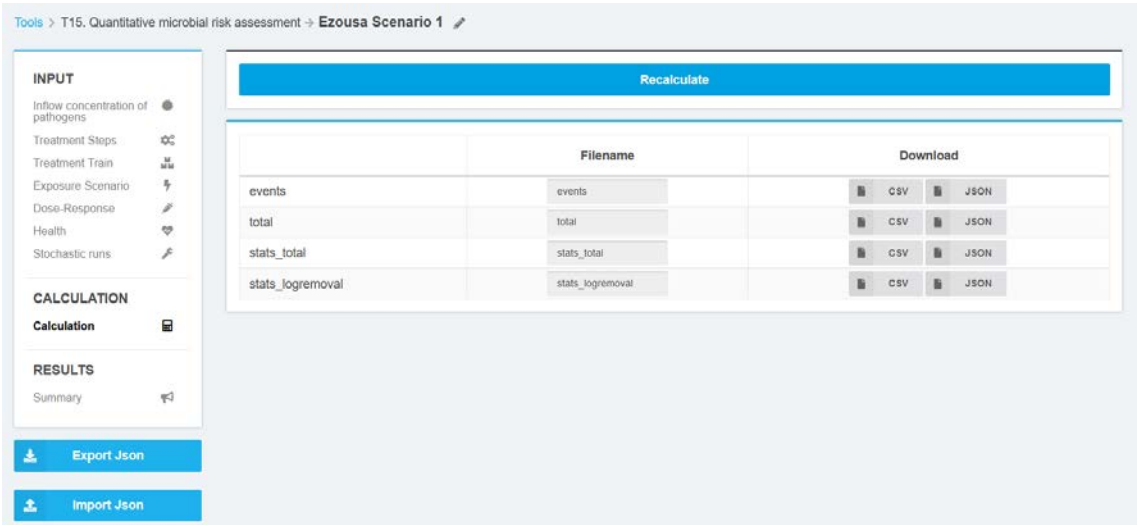

Figure 9: Export of results

The file “events” include the calculated logreduction for each event from each pathogen group. The output file “total” contains the values of the inflow median, logreduction median, volume sum, exposure sum, dose sum, infection probability sum, illness probability sum, and dalys sum for each stochastic run from each pathogen group. The file “stats_total” include aggregated values (min, p05, p25, mean, median, p75, p95, and max) of dalys sum, dose sum, events, exposure sum, infection probability sum, illness probability sum, and dalys sum for each treatment step and pathogen group. The file “stats_logremoval” include aggregated values (min, p05, p25, mean, median, p75, p95, and max) of log removal for each treatment step and pathogen group.

5. CONCLUSIONS

The QMRA tool presented here provides an easy and user-friendly approach to microbiological risk assessment. Due to the many preset parameters, microbial risks at sites with little known information can also be calculated. Based on the findings from the model, problem and risk areas can be identified and protective measures prepared. The embedding in a browser environment allows the calculation without the installation of additional software.

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