

Quick User Guide to QMRAcatch

General description

QMRAcatch is a microbial water quality model for simulating target microbial concentrations in a river, a floodplain river and / or a floodplain compartment. Quantitative microbial risk assessment (QMRA) is performed based on predefined dose-response functions for Enterovirus, Norovirus, *Campylobacter jejuni, Cryptosporidium parvum, Giardia lamblia,* or based on user defined dose-response functions for any type of pathogen. QMRAcatch simulates the required pathogen reductions from the compartments which have to be achieved by bank filtration and further disinfection steps to meet a defined infection risk target. Simulations are daily for a period of one year. Input parameters consist of river discharge (Q), source concentration (C₀) and microbial log₁₀ removal of wastewater discharges (WWTPs), number of visitors and animals in the floodplain compartment, water temperature, rainfall depth, release rate, runoff rate, probability of defaecation of visitors and dimensions of each compartment. Mean and 95-percentiles of concentrations in wastewater and in faeces, log₁₀ removal, quantity and weight of faecal droppings, and excretion probability of predefined statistical distributions have to be set by the user. The simulations are performed by the Monte Carlo method, i.e. random values are drawn from the statistical distributions.





1. Simulating microbial concentrations in the river, the floodplain river and the floodplain

Concentrations of the selected microorganism in the river are computed based on a plug flow reactor type model. At the point of interest (intake for drinking water production or recreational area), they vary depending on the up-stream distance of one to five wastewater treatment plants (WWTPs, Figure 1). Concentrations of the selected microorganism in the floodplain river and the floodplain are computed based on continuously stirred reactor type models assuming spatially uniform and completely mixed conditions over daily time intervals. Concentrations in all compartments are computed based on dilution, mixing and temperature-dependent die-off. Rainfall, infiltration, release



and runoff determine microbial concentrations in the floodplain and the floodplain river. During flood events (i.e. river discharges exceed a certain threshold) a part of the floodplain is flooded by inflow of river water. This area is computed based on a width of the floodplain river and a slope of the floodplain. All faecal deposits are assumed to be released in this area and animals are assumed to leave this area until the flood has receded.



Figure 2 Conceptual model for 1) simulating daily microbial concentrations in the river, the floodplain river and the floodplain

2. QMRA: setting the required log_{10} reduction of target microbial pathogens to meet a certain health risk target (Figure 3)

The required reduction of pathogens by riverbank filtration, or other treatment methods for compliance with the selected infection risk target can be set. The Monte Carlo simulations can be repeated 10 000 to 1 000 000 times. Results include the 95-percentiles of the required log_{10} reductions, i.e. the reductions that have to be achieved by the respective treatment system over 95 % of the time. For the detailed model description including the model equations see Schijven et al. (2015).



Figure 3 Conceptual model for 2) performing the QMRA. The output of QMRA is an infection risk estimate, and, in addition, the required log₁₀ reduction of pathogens to comply with a set health risk target



Generating plots, saving and reading data in QMRAcatch

Plots

All plots (i.e. concentration time series and logos) can be saved in QMRAcatch as graphical images by right-clicking and then *Safe Graphic As* in all common graphic formats. Plots of simulated concentrations can be displayed in linear and plot scale by checking either *Lin* or *Log* on the left panel of the QMRAcatch screen.

Save and read files

On the bottom of the home screen (Figure 1), there are options to save and load settings made by the user. Hydrologic and microbial data can be read from spreadsheet files with specific format rules (Figure 4 and 6). Examples spreadsheets are provided on the website.

- In the first row, all settings and simulated concentrations can be saved into a file by clicking on the button *Settings+simulations*, choosing the file directory and file name and pushing the *Save* button.
- In the second row, settings can be loaded from a previously saved file.
- In the third row, the hydrologic data can be loaded. The format of the data file is as shown in Figure 4. On each day in a year (1-365) have to be set: main river discharges, water temperatures, floodplain river discharges and water temperatures, floodplain river volumes, rainfall depth, flooded area and flooded volume. Derx et al. (2016) describes how floodplain river discharges can be determined if no observation data is available.
- In the fourth row, the microbiologic data can be loaded with format as shown in Figure 5. Dates and values of observed concentrations of the selected indicator can be set for: each WWTP, the Main river and the Floodplain river compartment. When plotting graphs of the simulated time series, the observed mean, 95-percentile, α and β parameters of the Gamma distribution (taking into account non-detects) are shown below the respective values of the simulated time series. The observed values are shown as circles in the graph (non-detects are not shown in plot-scale).

	А	В	С	D	E	F	G	Н	1	J
1		Main river		Floodplain			Floodplain			
2	Day	q m3/s	oC	q m3/s(mr=	оС	m3	mm prec	m2	m3	
3	1	1534	3.254167	0.25	5.254167	250000	1.080297	0	0	
4	2	1712	3.6	0.25	5.6	250000	0.111308	0	0	
5	3	1635	3.454167	0.25	5.454167	250000	0	0	0	
6	4	1537	3.391667	0.25	5.391667	250000	0	0	0	
7	5	1391	3.333333	0.25	5.333333	250000	0	0	0	

Figure 4 Spreadsheet format (.xlsx or .xls) for hydrologic data



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		12/01/11 16/02/11	2000000 460000							24/01/11 21/02/11	2500 660	24/01/11 21/02/11	30 0	
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		04/05/11	560000							10/05/11	20	10/05/11	20	
		06/07/11	169000							19/07/11	620	19/07/11	250	
		03/08/11	118000							13/09/11	400 480	13/09/11	230	
		05/10/11	93000 550000							15/11/11 06/12/11	600 540	15/11/11 06/12/11	0 190	
		29/11/11 06/12/11	540000 740000									24/01/11 21/02/11	230 20	
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> > Micro	biology data	a (2)							ſ			10/05/11	1200	9

Figure 5 Spreadsheet format (.xlsx or .xls) for microbiologic data

Getting started

- Choose one type of microorganism (pathogen/indicator).

The following list of pathogens and indicators are available: Enterovirus, Norovirus, Campylobacter (jejuni), Cryptosporidium (parvum), Giardia (lamblia), E.coli, HF183, other (see below). For more information on HF183 see (Derx et al. 2016).

- Check the number of wastewater treatment plants (**WWTP**), 0 to 5, contributing to the simulated microbial concentrations in the river compartment.
- Enter the number of boar, deer, birds and visitors in the **floodplain** [per day].
- Drinking water **consumption:** choose mean and standard deviation values in L/d (predefined or set manually).

Other types of microorganisms

- For this case the parameters for the temperature dependent inactivation, a₀ and a₁, have to be set manually, as explained by Schijven et al. (2015).
- Check if the microorganism is zoonotic. This will require setting contamination source concentrations of boar, deer and birds, if their numbers are set to a value greater than zero.
- Check if the microorganism is pathogenic. For a pathogenic microorganism, the dose-response relationship must be set. The user can choose either an exponential 1-parameter relationship, or, the hypergeometric model with model parameters α and β (Schijven et al. 2015, Teunis and Havelaar 2000).



Quick User Guide Home Contamination sources Water system QMRA drinking water QMRA bathing water About QMRAcatch IECHNISCHE UNIVERSITÄT WIEN 藏 Pathogen/indicato ersity Other Enterovirus Norovirus -**QMRA**catch Campylobacter Cryptosporidium Giardia Deposition HUMAN E. coli HF183 BIRDS HUMAN Flow 1 2 3 QMRA bathing water Floodplain FLOOD Runoff FLOODPLAIN RIVI LMH 0 deer QMRA drinking water LMH 0 birds Riverbank LMH 0. visitor ANIMAL filtration Infiltra Consumption in(CI) 0.28(0.019- 1.3) GROUNI VATER -1.85779 Settings+simulations N:\Documents\Enterovirus_setsim_270816_1027.xls σ Save Settings+simulations N:\Documents\Enterovirus_setsim_270816_1027.xls Health based target Clear Hydrologic data Load Microbiologic data Load Plot scale 💿 Lin 🔘 Log

Figure 6 Choosing other types of microorganisms

Contamination sources

Wastewater treatment plants (WWTPs)

QMRAcatch Pathogen/indicator HF183 •					
WWTP V 1 V 2 V 3 V 4 V 5 Floodplain L M H 150 boar L M H 240 deer L M H 900 birds L M H 900 visitors	WWTPs Fecal droppings WWTP1 WWTP2 WWTP3 Wastewater treatment plant Upstream distance L M H 193 km Discharge L M H 2.232 m ³ /s Overflow L M H 3 BV	WWTP4 WWTP5 HF183 Raw wastevaster.titL Treatment.Log10 Overflow water.titL	Mean L M H 100000 L M H 2.63 L M H 194000 Plot con	95% 000 L M H 5820 L M H 2.15 00000 L M H 5820 centrations in wastewate	0 000 000
Consumption NL US WHO Set μean(CI) 0.28(0.019-1.3) μ -1.02779 σ 1.07487 Health based target 10 ⁻⁵ 10 ⁻⁴ 10 ⁻³ 10 ⁻² Plot scale OLin € Log	Randomize overflow events Hising degree L M M 1 (I-fully mixed) 0.1=10x concentration)	0 WWTPS-HF18	3_165344_2208	Bild - Wolfram Math	ematica 11.0 - Treat tean 1.4 × 108 770 5% 7.4 × 108 7.0 amma ¢ 0.2 0.22 amma ¢ 7.1 × 10 ⁸ 1.6 ×

Figure 7 Contamination sources – Wastewater treatment plants (WWTPs)

- For each checked WWTP have to be set:

The upstream distance from the point of interest (PI)

Mean discharge rates over a year

Number of overflows / year

Mixing degree; is the the fraction of the river width at the PI that the discharged wastewater of the WWTP has fully mixed with.



- For the selected target pathogen/indicator the respective raw wastewater concentrations, achieved log₁₀ removal by wastewater treatment and overflow water concentrations have to be set (mean and 95-percentiles).
- The computed raw and treated target microbial concentrations in wastewater can be plotted (Figure 7).

Faecal droppings

	Home	Contamination sou	rces	Water s	system	QMRA drinking water	QMRA bathing water	About	
QMRAcatch									
Pathogen/indicator Campylobacter									
WWTP		WWTPs Fecal drop	pings	;					
Floodplain		Boar D	eer E	Birds H	luman				
LMH 0. birds		Weight of	dropp	ping,g	(2)	Mean	95% LMH 200.		
Consumption		Campylol	t drop bacter,	pings/da ./g	y/Boar	LMH 10.	LMH 20 000 000		
NL US WHO Set Mean(CI) 0.28(0.019- 1.3)		Depositio	e n, #/da	ау		LMH 0.01 1.7×10 ¹⁰	5.5×10 ¹⁰		
σ 1.07487									
Health based target									
Plot scale 🔘 Lin 🔘 Log									

Figure 8 Contamination sources – Faecal droppings

When boar, deer, or birds are considered, the weight of dropping (g), number of droppings / day / animal, the source concentrations (microbial particles/g) and the prevalence have to be set. Default values and references for some parameters are given in Schijven et al. (2015) and (Derx et al. 2016). The calculated total number of target microorganism per day is shown based on the set values.

When visitors are considered, a probability of defaecation replaces the number of droppings / day.

Water system - Main River + Floodplain River

The main river water system includes settings for the discharges (m^3/s) , the average width (m), water depth (m) and slope (-) of the main river and Manning coefficient $(s/m^{1/3})$ of the river bed.

The floodplain river water system further includes settings for the discharges from the main to the floodplain river and the groundwater exfiltration into the floodplain river.

Water temperatures of the main river and floodplain river are calculated based on a triangular distribution over a year. The user has to set the date and values of the minimum and maximum water temperatures. Alternatively, daily values for water temperature can be used from hydrologic data by checking the option *Use data* (Figure 10, see Section on how to Save and read files).



River flow discharges

Discharges of the main river can be simulated based on ARMA processing (Schijven et al. 2015). Mean monthly discharge values have to be set. For setting a mean yearly discharge, use same values for all months. Set ARMA parameters a (-), β (-), v (m³/s)² and press *Randomize ARMAprocess*. The generated time series is shown on the top right of the screen. Alternatively, daily values for river discharges can be used from hydrologic data by checking the option *Use data* (Figure 10, see Section on how to Save and read files).

Discharges from the main river to the floodplain river

a) Use data

Daily values for floodplain river discharges can be used from hydrologic data by checking the option *Use data* (Figure 10, see Section on how to Save and read files).

b) Set

Fraction of the main river discharge (qmr) minus a threshold discharge of the main river at which the main river connects to the floodplain river.

c) Advanced set

A polynomial regression function dependent on main river discharges can be entered.

	Home Contamination sources Water system QMRA drinking w	water QMRA bathing water About
QMRAcatch	Main river + Floodplain River Floodplain	
	Discharge of Main river(qmr, m ³ /s)	Main river
Pathogen/indicator	🔘 Use data 🔘 Set	5000
Campylobacter 🔻	JFMA 1756. 2251. 3148. 2014. MJJA 2252. 2147. 1766. 3866.	4000 ⁵⁰ 3000 ⁶⁰ 2000
WWTP □ 1 V 2 □ 3 ■ 4 ■ 5	$\begin{array}{c} \alpha \\ \hline Randomize \\ \alpha \\ \beta \\ \hline M \\ H \\ 0. \end{array}$	1000 J F M A M J J A S O N D
Floodplain	V L M H 100 000.	Floodplain River
LMH 150 boar	Main river width L M H 250. m	30
LMH 0. deer	Main river depth LMH 4. m	20 20
LMH 0. birds	Manning coefficient for river bed	^m _E 15
LMH 2000 visitors	Sand Gravel 0.05	
Consumption	Main river bed slope LMH 0.004 m/m	JEMANJJASOND
NL US WHO Set	Discharge from Main to Floodplain river(m ⁻ /s)	Water temperature
Mean(CI) 0.28(0.019- 1.3)	0.01 ×(gmr-LMH 2000,)	30
μ -1.85779	Groundwater to Floodplain River L M H 0.25 m ³	s 20
0 1.07487	Water temperature	·c
Health based target	🔘 Use data 💿 Set	10
10-5 10-4 10-3 10-2	Date (d/m) D-°C FR-°C	
Plot scale 🔘 Lin 🔘 Log		Plot concentrations in main river
		Plot concentrations in floodplain river

Figure 9 Water System: Main river + floodplain river





Figure 10 Water system: main river + floodplain river using loaded hydrologic data

Water system - Floodplain

The floodplain water system includes settings for daily precipitation, length, width, depth of the floodplain river, Manning coefficient and slope of the floodplain river bed, area, horizontal angle and area of the floodplain (Figure 11).

Daily precipitation values are calculated by means of a stochastic rainfall model, see Schijven et al. (2015) for details. The user has to set the mean rainfall rate (events per day) and mean rainfall depth (mm) and the month of maximum rainfall. Alternatively, daily values for precipitation can be used from hydrologic data by checking the option *Use data* (Figure 10, see Section on how to Save and read files).

The flooded area is calculated in QMRAcatch based on set values of width, depth, length, the discharge and flow velocity of the floodplain river and the slope of the floodplain and floodplain river, see Schijven et al. (2015) for details.

Further settings are required for the release rates of microbial particles from faecal deposits per day, the evaporation and runoff (both fractions of precipitation). A sink term for the infiltration is calculated (also fraction of precipitation) by subtraction of the evaporation and runoff from precipitation (Figure 11).

When pushing the button on the bottom of the screen the simulated concentrations of the selected microorganisms in infiltration water are plotted.





Figure 11 Water system: floodplain

QMRA drinking water

At this point the concentrations of a selected pathogen or indicator have been simulated in the *Water systems*, i.e. the Main River, the Floodplain River and the Floodplain.

Under this tab QMRA outcomes are shown. The simulated concentrations and set values for consumption (Section Getting Started) are fed into the dose-response models of the selected pathogen. The dose-response models are incorporated in the model program code for the listed pathogens (see Schijven et al. (2015) for details) or taken from the set model parameters as described in the Section Getting started – Other types of microorganisms.

For each compartment the user presses the respective button (*Main river, Floodplain river, Floodplain)*. The required log_{10} treatment by bank filtration (+ further disinfection steps) are simulated for meeting the set health based target (Section Getting Started). Mean and 95-percentiles are simulated. The treatment systems are commonly designed based on 95-percentiles which have to be achieved over 95% of the time.

The next step is to calculate the infection risks from drinking water which was treated according to the previously simulated settings. The user can set ratios for each compartment that are contributing to the composition of well water.

For calculating the infection risks from drinking water, the number of Monte Carlo samples can be varied from low (L) to high (H) numbers. The simulations are repeated this number of times. If the results are sensitive to the number of samples, high values should be used.





Figure 12 Quantitative microbial risk assessment (QMRA) for drinking water usage

QMRA bathing water

At this point the QMRA will be performed for bathing in the Main River and in the Floodplain River. The user can set the minimum bathing water temperature. Only the days are considered with water temperatures greater than this value. The user can further select *Man*, *Woman*, or *Child*, differing by their given volumes of swallowed water per event. An event is referred to an occasion that a person goes swimming. The simulated concentrations from the prior steps and set values for consumption are fed into the dose-response models of the selected pathogen. The models are integrated into the model program code for the list of pathogens (see Schijven et al. (2015) for details) or taken from the set model parameters as described in the Section Getting started – Other types of microorganisms.

By pushing *Recalculate infection risks* the mean and 94-percentile infection risks are calculated and displayed below the target value for the Main River (left) and the Floodplain River (right).

For calculating the infection risks, the number of Monte Carlo samples can be varied from low (L) to high (H) numbers. The simulations are repeated this number of times. If the results are sensitive to the number of samples, high values should be used.



	Home	Contamination sources	Water system	QMRA	drinking water	QMRA bathing v	vater	About	
QMRAcatch Pathogen/indicator Campylobacter									
WWTP 1 2 3 4 5 Floodplain 6 6 M H 0 boar 5 M H 0 birds 5 M H 0 visitors 5 Consumption Mill Us WHO Set Mean(CI) 0.26(0.019-1.2) μ -1.65779 σ 1.07487 1.07487 Health based target 10-5 10-2 Plot scale Un Log		Minimum bathing w: Volume of swallowe Main Woman (Infection risk/person Main river -4 -6 -8 -10 Recalcula	ater temperatur d water per even Child Campylob Target 0 Mean 0 95% 0 te infection risk	e nt 0001 000018	L M H 18 Average 27. ml Floodplain river -1 -2 -3 -4 -5 -6 L M H 10 000	Camp Target Mean 95%	vlobact 0.00 0.11 0.65 arlo sa	er 01 mples	

Figure 13 Quantitative microbial risk assessment (QMRA) for bathing water usage

Technical manual

The technical manual and other reference can be downloaded for free following the link in the *About* section.

References

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