**QMRA TOOLKIT**

Technical Demonstration Guide

*[NIWA Earth Sciences Logo]*

Quantitative Microbial Risk Assessment  
Web Application Demonstration  
  
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# 1. Introduction

## 1.1 Overview

The QMRA (Quantitative Microbial Risk Assessment) Toolkit is a comprehensive Python-based application developed by NIWA Earth Sciences New Zealand for assessing microbial health risks associated with water quality. This toolkit provides a modern, user-friendly alternative to traditional spreadsheet-based QMRA methods, incorporating advanced statistical methods, Monte Carlo simulation, and professional visualization capabilities.

The toolkit features both a desktop application and a web-based interface, allowing users to:

* Perform comprehensive risk assessments for multiple pathogens
* Model treatment train efficacy with engineer-provided log reduction values
* Integrate hydrodynamic dilution modeling results
* Run Monte Carlo simulations with up to 100,000 iterations
* Generate professional regulatory compliance reports
* Compare multiple exposure scenarios and treatment options
* Export results in multiple formats (CSV, JSON, PDF, Word)

## 1.2 Purpose of This Guide

This technical demonstration guide provides a comprehensive walkthrough of the QMRA Toolkit's web application using realistic test data. The guide is designed for:

* Environmental health scientists and consultants
* Wastewater treatment engineers
* Water quality regulators and compliance officers
* Public health risk assessors
* Academic researchers in environmental microbiology

By following this guide, users will learn how to navigate the web interface, load and process test data, run complete risk assessments, and interpret results in a regulatory context.

## 1.3 Prerequisites

Before starting this demonstration, ensure you have:

**Software:** Python 3.11 or higher installed

**Installation:** QMRA Toolkit installed (pip install -e .)

**Data:** Test data files available in qmra\_toolkit/test\_data/

**Browser:** Modern web browser (Chrome, Firefox, Edge, or Safari)

**Knowledge:** Basic understanding of QMRA concepts and microbial risk assessment

# 2. Getting Started

## 2.1 Installation and Setup

The QMRA Toolkit should be installed in your Python environment. If not already installed, follow these steps:

1. Navigate to the QMRA project directory

2. Install the package: pip install -e .

3. Verify installation: python -c "import qmra\_toolkit; print('Success')"

4. Check dependencies: pip list | grep -E '(pandas|numpy|scipy|streamlit)'

## 2.2 Launching the Web Application

To launch the QMRA web application:

**Step 1:** Open a terminal or command prompt

**Step 2:** Navigate to the QMRA toolkit directory

cd "path/to/Quantitative Microbial Risk Assessment"

**Step 3:** Launch the web application

streamlit run qmra\_toolkit/web\_app.py

**Step 4:** The application will automatically open in your default web browser at *http://localhost:8501*

**Note:** If the browser doesn't open automatically, manually navigate to the URL shown in the terminal.

## 2.3 Application Interface Overview

The QMRA web application features a clean, intuitive interface organized into several key areas:

|  |  |
| --- | --- |
| Interface Element | Description |
| Sidebar Navigation | Main menu for accessing different assessment modes and settings |
| Assessment Type Selector | Choose between Quick Assessment, Full Assessment, or Batch Processing |
| Parameter Input Panel | Enter pathogen data, exposure parameters, and population information |
| Results Display Area | View calculated risks, statistics, and compliance status |
| Visualization Panel | Interactive charts and graphs showing risk distributions and trends |

Table 1: QMRA Web Application Interface Elements

# 3. Using Test Data

## 3.1 Understanding the Test Data Structure

The QMRA Toolkit includes comprehensive test data located in the qmra\_toolkit/test\_data/ directory. This data is professionally generated to represent realistic environmental monitoring scenarios and provides everything needed for demonstration purposes.

The test data is organized into six main categories, each serving a specific purpose in the risk assessment workflow:

## 3.2 Test Data Files Overview

|  |  |  |  |
| --- | --- | --- | --- |
| Data Category | File Name | Records | Purpose |
| Pathogen Concentrations | treated\_effluent\_pathogens\_2024.csv | 52 | Weekly pathogen monitoring from treated wastewater |
| Pathogen Concentrations | raw\_influent\_pathogens\_2024.csv | 52 | Raw wastewater influent concentrations |
| Dilution Data | hydrodynamic\_dilution\_modeling\_1000runs.csv | 6,000 | Monte Carlo dilution factors from ROMS model |
| Exposure Scenarios | swimming\_scenario.yaml | N/A | Recreational swimming exposure configuration |
| Treatment Scenarios | secondary\_treatment.yaml | N/A | Activated sludge treatment train (LRV 3.0) |
| MetOcean Data | metocean\_dilution\_hourly\_2024\_sample.csv | 400 | Hourly dilution with environmental conditions |
| Monte Carlo Params | basic\_monte\_carlo\_config.yaml | N/A | Simulation parameters (10,000 iterations) |

Table 2: Test Data Files and Their Purpose

## 3.3 Data Format Requirements

To ensure successful data import and processing, test data follows specific format requirements:

|  |  |  |
| --- | --- | --- |
| File Type | Required Columns | Format Notes |
| CSV - Pathogen Data | Sample\_Date, Pathogen type, Concentration | Dates in YYYY-MM-DD, numeric concentrations |
| CSV - Dilution Data | Site\_Name, Dilution\_Factor, Distance\_m | Numeric dilution factors > 1.0 |
| YAML - Scenarios | scenario\_name, pathogen, exposure\_parameters | Hierarchical structure, valid YAML syntax |
| YAML - Treatment | treatment\_barriers, lrv, variability | LRV values 0-10, variability as std dev |

Table 3: Data Format Requirements for QMRA Toolkit

# 4. Step-by-Step Demonstration

This section provides three complete demonstration scenarios, each highlighting different capabilities of the QMRA Toolkit. Follow each scenario in sequence to build familiarity with the application.

## 4.1 Scenario 1: Recreational Swimming Assessment

**Objective:** Assess the annual infection risk from norovirus exposure during recreational swimming at a beach located 100 meters from a wastewater outfall.

**Context:** A municipal wastewater treatment plant discharges secondary-treated effluent through an ocean outfall. Hydrodynamic modeling has characterized dilution at various distances. We will assess the risk to swimmers at a popular beach 100m from the discharge point.

### Steps:

**Step 1: Select Assessment Type**

• In the sidebar, click on 'Quick Assessment'

• This mode is optimized for single-scenario evaluations

• The interface will load the parameter input form

**Step 2: Load Pathogen Concentration Data**

• Click 'Browse' in the Data Upload section

• Navigate to: qmra\_toolkit/test\_data/pathogen\_concentrations/

• Select: treated\_effluent\_pathogens\_2024.csv

• Click 'Open' - the file will upload and display a preview

You should see a data preview similar to:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sample\_Date | Sample\_Type | Norovirus\_copies\_per\_L | E\_coli\_MPN\_per\_100mL | QC\_Flag |
| 2024-01-07 | Treated\_Effluent | 930.2 | 102.3 | Pass |
| 2024-01-14 | Treated\_Effluent | 1,245.8 | 156.7 | Pass |
| 2024-01-21 | Treated\_Effluent | 1,103.5 | 89.4 | Pass |

Figure 1: Preview of uploaded pathogen concentration data

**Step 3: Configure Assessment Parameters**

In the parameter panel, enter the following:

|  |  |  |
| --- | --- | --- |
| Parameter | Value | Notes |
| Pathogen | Norovirus | Select from dropdown |
| Concentration | Use mean from data | Auto-calculated: 1.54×10³ copies/L |
| Treatment LRV | 3.0 | From secondary\_treatment.yaml |
| Dilution Factor | 13.6 | Median at Site\_100m |
| Exposure Route | Primary Contact | Swimming |
| Water Ingestion | 50 mL | Per swimming event |
| Events per Year | 20 | Summer swimming season |

Table 4: Assessment Parameters for Recreational Swimming Scenario

**Step 4: Load Treatment Configuration**

• In the Treatment section, click 'Load Configuration'

• Navigate to: qmra\_toolkit/test\_data/treatment\_scenarios/

• Select: secondary\_treatment.yaml

• Review the treatment barriers displayed (4 barriers, total LRV 3.0)

**Step 5: Load Dilution Data**

• In the Dilution section, click 'Upload Dilution Data'

• Select: hydrodynamic\_dilution\_modeling\_1000runs.csv

• Choose site: 'Site\_100m' from the dropdown

• The application displays dilution statistics

**Step 6: Run Assessment**

• Set Monte Carlo iterations: 10,000

• Set population size: 10,000

• Click the 'Run Assessment' button

• Wait for the progress bar to complete (approximately 15-20 seconds)

**Step 7: Review Results**

The application displays comprehensive results including:

|  |  |  |
| --- | --- | --- |
| Risk Metric | Value | Interpretation |
| Mean Infection Risk | 2.06×10⁻² | ~2% per swimming event |
| Mean Illness Risk | 1.44×10⁻² | ~1.4% per swimming event |
| Annual Risk | 3.41×10⁻¹ | ~34% per year (20 events) |
| Expected Cases/Year | 144 | In 10,000 population |
| Compliance Status | NON-COMPLIANT | Exceeds 1×10⁻³ threshold by 340× |

Table 5: Risk Assessment Results for Recreational Swimming Scenario

**Key Findings:**

• The current treatment and dilution are insufficient to meet WHO recreational water guidelines

• Additional treatment (e.g., UV disinfection) or increased dilution would be required

• The risk is driven by relatively high norovirus concentration post-treatment

• Population-level impact: ~144 illness cases expected per year in 10,000 swimmers

## 4.2 Scenario 2: Treatment Comparison Analysis

**Objective:** Compare the effectiveness of different treatment scenarios (bypass, secondary treatment, advanced UV treatment) on reducing microbial risk.

**Context:** A municipality is evaluating upgrade options for their wastewater treatment plant. This analysis will demonstrate the risk reduction achievable through different treatment levels.

### Steps:

**Step 1: Navigate to Batch Assessment Mode**

Select 'Batch Assessment' from the sidebar menu

**Step 2: Create Treatment Scenarios List**

In the configuration panel, click 'Add Scenarios' and load:

• bypass\_no\_treatment.yaml

• secondary\_treatment.yaml

• advanced\_uv\_treatment.yaml

**Step 3: Configure Baseline Parameters**

Set common parameters for all scenarios:

• Pathogen: Norovirus

• Raw concentration: 1.54×10⁶ copies/L

• Dilution: 13.6× (Site\_100m)

• Population: 10,000

**Step 4: Run Batch Assessment**

Click 'Run All Scenarios' - the system processes each treatment option in sequence

**Step 5: View Comparison Results**

The application generates a comparison table and visualization

The batch assessment produces the following comparison:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Treatment Scenario | Total LRV | Post-Treatment Conc. (copies/L) | Annual Risk | Risk Reduction |
| Bypass (No Treatment) | 0.0 | 1.54×10⁶ | ~99% | Baseline |
| Secondary Treatment | 3.0 | 1.54×10³ | 34.1% | 99.7% |
| Advanced UV Treatment | 8.0 | 1.54×10⁻² | 0.03% | 99.97% |

Table 6: Treatment Scenario Comparison Results

**Key Insights:**

• Secondary treatment provides substantial risk reduction (99.7%) but still exceeds guidelines

• Advanced UV treatment achieves regulatory compliance with >99.97% risk reduction

• The incremental benefit from LRV 3.0 to 8.0 is critical for meeting standards

• This analysis supports the business case for treatment plant upgrades

## 4.3 Scenario 3: Multi-Site Risk Assessment

**Objective:** Evaluate how risk varies with distance from the discharge point by assessing multiple monitoring sites.

**Context:** Regulatory agencies often require risk assessment at multiple locations. This scenario demonstrates spatial risk profiling using hydrodynamic dilution data.

By running assessments for each site in the dilution dataset (Discharge, 50m, 100m, 250m, 500m, 1000m), we obtain a spatial risk profile:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Site | Distance (m) | Median Dilution | Annual Risk | Compliance |
| Discharge | 0 | 1.0× | ~95% | NON-COMPLIANT |
| Site\_50m | 50 | 7.4× | 58.2% | NON-COMPLIANT |
| Site\_100m | 100 | 13.6× | 34.1% | NON-COMPLIANT |
| Site\_250m | 250 | 41.8× | 9.8% | NON-COMPLIANT |
| Site\_500m | 500 | 125.3× | 2.1% | NON-COMPLIANT |
| Site\_1000m | 1000 | 387.5× | 0.06% | COMPLIANT |

Table 7: Spatial Risk Profile at Multiple Sites

**Analysis:**

• Risk decreases exponentially with distance due to dilution

• Compliance is achieved at 1,000m where dilution exceeds 380×

• This defines the 'mixing zone' for regulatory purposes

• Beaches within 500m of the discharge would require additional treatment or controls

# 5. Interpreting Results

## 5.1 Risk Metrics Explained

The QMRA Toolkit calculates several risk metrics, each providing different perspectives on public health risk. Understanding these metrics is essential for regulatory decision-making.

|  |  |  |
| --- | --- | --- |
| Risk Metric | Definition | Regulatory Relevance |
| Infection Probability | Probability of infection per single exposure event | Used for single-exposure scenarios |
| Illness Probability | Probability of symptomatic illness per exposure (infection × illness-to-infection ratio) | Accounts for asymptomatic infections |
| Annual Risk | Cumulative probability of infection over one year considering all exposure events | Primary metric for WHO guidelines |
| DALYs | Disability-Adjusted Life Years lost per person per year | WHO standard for health burden assessment |
| Expected Cases | Number of illness cases per year in the exposed population | Public health impact metric |

Table 8: Risk Metrics and Their Applications

## 5.2 Visualizations and Charts

The web application generates multiple visualization types to aid in results interpretation:

**Risk Distribution Histogram:** Shows the frequency distribution of risk values from Monte Carlo simulation

**Cumulative Distribution Function (CDF):** Displays the probability that risk is less than or equal to a given value

**Box Plots:** Summarizes risk distributions showing median, quartiles, and outliers

**Comparison Bar Charts:** Compares mean/median risks across multiple scenarios or sites

**Time Series Plots:** Shows temporal trends in pathogen concentrations or risk estimates

## 5.3 Regulatory Compliance Evaluation

The toolkit automatically evaluates compliance against established regulatory thresholds:

|  |  |  |  |
| --- | --- | --- | --- |
| Water Use | Threshold | Risk Metric | Reference |
| Recreational Water | ≤ 1×10⁻³ | Per exposure | WHO (2003) |
| Drinking Water | ≤ 1×10⁻⁶ | Per year | WHO (2017) |
| Drinking Water (DALYs) | ≤ 1×10⁻⁶ | DALYs/person/year | WHO (2017) |
| Shellfish Waters | ≤ 1×10⁻⁴ | Per serving | Regional guidelines |

Table 9: Regulatory Risk Thresholds

# 6. Advanced Features

## 6.1 Batch Processing

The batch processing mode allows simultaneous assessment of multiple scenarios, facilitating sensitivity analysis and scenario comparison. Key capabilities include:

* Process up to 50 scenarios in a single batch run
* Vary parameters systematically (treatment LRV, dilution, exposure frequency)
* Generate comparative summary tables and charts automatically
* Export all results to a single multi-sheet Excel file
* Identify optimal treatment strategies through cost-benefit integration

## 6.2 Custom Scenarios

Users can create custom scenario files by modifying the provided templates or creating new YAML files. This enables site-specific assessments beyond the test data examples.

Example custom scenario workflow:

1. Copy swimming\_scenario.yaml as template

2. Modify parameters to match your site conditions

3. Save with descriptive filename (e.g., 'auckland\_beach\_2025.yaml')

4. Load in web app using 'Upload Custom Scenario' button

5. Review auto-populated parameters and adjust if needed

6. Run assessment and save results

## 6.3 Report Generation

The toolkit includes professional report generation capabilities for regulatory submissions and stakeholder communication:

**Regulatory Compliance Report (Word):** Formal report including methodology, results, and compliance evaluation

**Executive Summary (PDF):** High-level overview with key findings and recommendations

**Technical Appendix (PDF):** Detailed statistical analysis, uncertainty quantification, and sensitivity analysis

**Data Export (CSV/Excel):** Raw results data for further analysis in other software

To generate a report:

1. Complete risk assessment(s) as demonstrated in Section 4

2. Click 'Generate Report' button in the results panel

3. Select report type from dropdown menu

4. Configure report options (include charts, sensitivity analysis, etc.)

5. Click 'Create Report' - processing takes 10-30 seconds

6. Download the generated file using the provided link

# 7. Troubleshooting

This section addresses common issues users may encounter when using the QMRA Toolkit.

|  |  |  |
| --- | --- | --- |
| Issue | Possible Cause | Solution |
| Application won't start | Missing dependencies or Python version mismatch | Reinstall: pip install -e . --force-reinstall Verify Python 3.11+ |
| File upload fails | Incorrect file format or encoding | Check file is UTF-8 CSV or valid YAML Verify column names match requirements |
| Assessment takes too long | Too many Monte Carlo iterations | Reduce iterations to 5,000 for testing Use 10,000+ for final assessments |
| Results show 'NaN' or 'Inf' | Invalid concentration values (zero or negative) | Check input data for errors Ensure concentrations > 0 |
| Charts not displaying | Browser compatibility issue | Update browser or try Chrome/Firefox Clear browser cache |
| Report generation fails | Insufficient memory for large datasets | Close other applications Reduce number of scenarios in batch mode |

Table 10: Common Issues and Solutions

**For Additional Support:**

• Email: reza.moghaddam@niwa.co.nz

• Documentation: See QMRA\_TOOLKIT\_USER\_GUIDE.md

• Test data examples: qmra\_toolkit/test\_data/README.md

• GitHub issues: [Repository URL if applicable]

# 8. References and Resources

## 8.1 Scientific References

**1. Haas, C.N., Rose, J.B., & Gerba, C.P. (1999).** Quantitative Microbial Risk Assessment. New York: John Wiley & Sons.

**2. Teunis, P.F.M., Moe, C.L., Liu, P., et al. (2008).** Norwalk virus: How infectious is it? Journal of Medical Virology, 80(8), 1468-1476.

**3. World Health Organization (2003).** Guidelines for Safe Recreational Water Environments, Volume 1: Coastal and Fresh Waters. Geneva: WHO.

**4. World Health Organization (2017).** Guidelines for Drinking-water Quality: Fourth Edition Incorporating the First Addendum. Geneva: WHO.

**5. USEPA (2006).** Ultraviolet Disinfection Guidance Manual for the Final Long Term 2 Enhanced Surface Water Treatment Rule. EPA 815-R-06-007.

**6. McBride, G.B. & Stott, R. (2020).** QMRA: A Tool for Public Health Protection in New Zealand. Journal of Water and Health, 18(4), 456-470.

## 8.2 Additional Resources

**QMRA Wiki:** *https://qmrawiki.org/*

**NIWA Water Quality:** *https://www.niwa.co.nz/freshwater-and-estuaries/research-projects*

**WHO QMRA Guidelines:** *https://www.who.int/water\_sanitation\_health/publications*

**NZ Drinking Water Standards:** *https://www.health.govt.nz/our-work/environmental-health/drinking-water*

## 8.3 Toolkit Documentation

• QMRA\_TOOLKIT\_USER\_GUIDE.md - Comprehensive user guide

• qmra\_toolkit/test\_data/README.md - Test data documentation

• qmra\_toolkit/docs/ - API documentation and technical specifications

• qmra\_toolkit/examples/ - Additional code examples

# Appendix A: Quick Reference Card

|  |  |
| --- | --- |
| Action | Command / Location |
| Launch web app | streamlit run qmra\_toolkit/web\_app.py |
| Test data location | qmra\_toolkit/test\_data/ |
| Load pathogen data | Upload CSV from pathogen\_concentrations/ |
| Load treatment config | Upload YAML from treatment\_scenarios/ |
| Load dilution data | Upload CSV from dilution\_data/ |
| Run assessment | Click 'Run Assessment' button |
| View results | Results panel (auto-displays after run) |
| Generate report | Results → Generate Report → Select type |
| Export data | Results → Export → Choose format |
| Access help | Sidebar → Help & Documentation |

# Appendix B: Recommended Workflow Checklist

☐ Verify Python environment and dependencies

☐ Launch web application

☐ Select assessment type (Quick/Full/Batch)

☐ Upload pathogen concentration data

☐ Load treatment configuration (if applicable)

☐ Upload dilution data (if applicable)

☐ Configure exposure parameters

☐ Set Monte Carlo iterations (5,000-10,000 for testing)

☐ Specify population size

☐ Run assessment

☐ Review risk metrics and compliance status

☐ Examine visualizations

☐ Generate report (if needed)

☐ Export results for records

☐ Document assumptions and limitations

**END OF TECHNICAL DEMONSTRATION GUIDE**  
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