**QMRA TOOLKIT**

Professional Technical Demonstration Guide

Step-by-Step Guide | Professional Diagrams | Comprehensive Tables  
Real-World Scenarios | Regulatory Compliance | Best Practices

**[NIWA EARTH SCIENCES]**

Quantitative Microbial Risk Assessment Toolkit  
Comprehensive Web Application & Desktop GUI Demonstration  
  
Version 2.0  
October 2025  
  
NIWA Earth Sciences New Zealand  
Environmental Health & Water Quality Division

# Executive Summary

This comprehensive technical demonstration guide provides detailed instructions for using the NIWA QMRA Toolkit, a state-of-the-art quantitative microbial risk assessment platform. The toolkit integrates peer-reviewed dose-response models, Monte Carlo simulation, hydrodynamic dilution modeling, and treatment train analysis to deliver professional-grade risk assessments for water quality management.

|  |  |
| --- | --- |
| **Capability** | **Description** |
| **Multi-Pathogen Assessment** | 6 pathogens with peer-reviewed dose-response models |
| **Monte Carlo Simulation** | Up to 100,000 iterations for uncertainty quantification |
| **Treatment Modeling** | Multi-barrier treatment train analysis with LRV |
| **Dilution Integration** | Hydrodynamic model results integration (ROMS/Delft3D) |
| **Multiple Interfaces** | Web app, Desktop GUI, Python API, Command-line |
| **Professional Reports** | Automated PDF/Word report generation for regulatory submissions |

*Table 1: Key Capabilities of QMRA Toolkit*

# System Architecture

The QMRA Toolkit follows a modular architecture design, enabling flexibility, maintainability, and extensibility. The system is organized into distinct layers, each with specific responsibilities.

|  |  |  |
| --- | --- | --- |
| **Layer** | **Components** | **Responsibilities** |
| **Presentation Layer** | Web App (Streamlit) Desktop GUI (Tkinter) CLI | User interface, input validation, visualization |
| **Application Layer** | Risk Characterization QMRA Integration Report Generator | Workflow orchestration, business logic, report generation |
| **Domain Layer** | Dose-Response Models Exposure Assessment Monte Carlo Engine | Core risk calculations, uncertainty analysis |
| **Data Layer** | Pathogen Database Dilution Model Treatment Barriers | Data management, parameter storage, model configurations |
| **Infrastructure Layer** | File I/O Validation Error Handling | System services, logging, exception management |

*Figure 1: QMRA Toolkit System Architecture - Layered Design*

## Data Flow Workflow

|  |  |  |
| --- | --- | --- |
| **Step** | **Process** | **Output** |
| **1** | Load Pathogen Data | Concentration statistics (mean, P95, distribution) |
| **2** | Apply Treatment Train | Post-treatment concentration with uncertainty |
| **3** | Apply Dilution | Environmental concentration at exposure point |
| **4** | Calculate Dose | Ingested dose per exposure event |
| **5** | Dose-Response Model | Infection probability distribution |
| **6** | Health Impact | Illness risk, DALYs, disease burden |
| **7** | Risk Characterization | Annual risk, population impact, compliance |

*Figure 2: QMRA Workflow - Data Processing Pipeline*

# Getting Started: Complete Setup Guide

## Prerequisites Checklist

|  |  |  |
| --- | --- | --- |
| **Requirement** | **Minimum Specification** | **Verification Command** |
| **Python** | 3.11 or higher | python --version |
| **pip** | Latest version | pip --version |
| **pandas** | 2.0+ | pip show pandas |
| **scipy** | 1.11+ | pip show scipy |
| **streamlit** | 1.28+ | streamlit version |
| **Memory** | 4GB RAM minimum | System Information |

*Table 2: System Requirements and Verification*

## Installation Steps - Detailed Guide

**Step 1: Download or Clone Repository**

• Navigate to project location

• If using Git: git clone [repository-url]

• If using download: Extract ZIP to desired location

**Expected Result:** You should see the main project folder with qmra\_toolkit/ subdirectory

**Step 2: Open Command Prompt/Terminal**

• Windows: Press Win+R, type 'cmd', press Enter

• Mac/Linux: Open Terminal application

• Navigate to project directory: cd path/to/project

**Expected Result:** Command prompt should show project directory path

**Step 3: Install Dependencies**

• Run: pip install -r requirements.txt

• Wait for installation to complete (2-5 minutes)

• Watch for any error messages

**Expected Result:** You should see 'Successfully installed' messages

**Step 4: Verify Installation**

• Run: python -c "from qmra\_toolkit.src import pathogen\_database; print('OK')"

• You should see 'OK' printed

• If errors occur, check Python version and dependencies

**Expected Result:** Installation is complete when test imports succeed

**Step 5: Launch Application**

• For Web App: streamlit run qmra\_toolkit/web\_app.py

• For Desktop GUI: python qmra\_toolkit/launch\_enhanced\_gui.py

• Browser should open automatically (web app only)

**Expected Result:** Application interface loads successfully

# Web Application: Complete User Guide

## Interface Overview

|  |  |  |  |
| --- | --- | --- | --- |
| **Interface Element** | **Location** | **Purpose** | **Key Features** |
| **Sidebar Menu** | Left panel | Navigation & settings | Assessment mode selection, settings, help |
| **Main Panel** | Center area | Primary workspace | Input forms, results display, visualizations |
| **File Upload Area** | Top of main panel | Data import | Drag-drop support, file validation, preview |
| **Parameter Forms** | Main panel | Input configuration | Auto-validation, tooltips, example values |
| **Run Button** | Bottom of form | Execute assessment | Progress bar, status updates, error handling |
| **Results Display** | Below run button | Risk metrics | Tables, statistics, compliance status |
| **Visualization Panel** | Below results | Charts & graphs | Interactive plots, download options |
| **Export Options** | Bottom right | Data export | CSV, Excel, PDF, Word formats |

*Table 3: Web Application Interface Elements - Detailed Overview*

# Step-by-Step Demonstration Scenarios

This section provides three complete, real-world demonstration scenarios with detailed step-by-step instructions, expected screenshots, and interpretation guidance. Follow each scenario to gain hands-on experience with the toolkit.

## Scenario 1: Beach Swimming Risk Assessment

|  |  |
| --- | --- |
| **Parameter** | **Value / Description** |
| **Scenario Name** | Recreational Swimming at Takapuna Beach |
| **Pathogen of Concern** | Norovirus GII |
| **Source** | Municipal wastewater outfall, secondary treatment |
| **Distance to Beach** | 100 meters from discharge point |
| **Treatment** | Activated sludge (LRV 3.0) |
| **Dilution** | Hydrodynamic modeling, median 13.6x |
| **Population** | 10,000 summer swimmers |
| **Regulatory Threshold** | ≤ 1×10⁻³ per exposure (WHO 2003) |

*Table 4: Scenario 1 Parameters - Beach Swimming Assessment*

### Detailed Steps

**Step 1: Launch Web Application and Select Assessment Mode**

**Actions:**

□ Open command prompt/terminal in project directory

□ Execute: streamlit run qmra\_toolkit/web\_app.py

□ Wait for browser to open (typically 5-10 seconds)

□ In the sidebar, click 'Quick Assessment' mode

□ Verify that the main panel shows 'Quick Assessment' heading

**Expected Display:** You should see the Streamlit interface with sidebar navigation on the left and main form in center

**Troubleshooting:** If browser doesn't open, manually navigate to http://localhost:8501

**Step 2: Upload Pathogen Concentration Data**

**Actions:**

□ Locate the 'Data Upload' section at top of main panel

□ Click 'Browse files' button

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

□ Select file: treated\_effluent\_pathogens\_2024.csv

□ Click 'Open' to upload

□ Wait for upload progress bar to complete

□ Review the data preview table that appears below upload button

**Expected Display:** Data preview table shows columns: Sample\_Date, Sample\_Type, Norovirus\_copies\_per\_L, E\_coli\_MPN\_per\_100mL, QC\_Flag

**Troubleshooting:** If upload fails, check file exists and is valid CSV format with correct column names

**Step 3: Configure Pathogen Parameters**

**Actions:**

□ In 'Pathogen Selection' section, open dropdown menu

□ Select 'Norovirus' from list

□ Observe that dose-response model auto-populates (Beta-Poisson)

□ In 'Concentration' field, select 'Use mean from uploaded data'

□ Verify calculated mean appears: ~1,542 copies/L

□ Leave dose-response parameters at default (peer-reviewed values)

**Expected Display:** Form shows Norovirus selected, Beta-Poisson model, mean concentration calculated

**Troubleshooting:** If mean doesn't calculate, check that CSV has Norovirus\_copies\_per\_L column

**Step 4: Configure Treatment Parameters**

**Actions:**

□ Scroll to 'Treatment Configuration' section

□ Click 'Load Treatment Scenario' button

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

□ Select: secondary\_treatment.yaml

□ Review loaded treatment barriers (4 barriers displayed)

□ Verify total LRV shows 3.0

□ Calculated post-treatment concentration: 1.54×10³ copies/L

**Expected Display:** Treatment table shows: Screening (0.5), Activated Sludge (2.0), Clarification (0.3), Disinfection (0.2)

**Troubleshooting:** If YAML fails to load, check file format and required fields (name, lrv for each barrier)

**Step 5: Configure Dilution Parameters**

**Actions:**

□ Scroll to 'Dilution Modeling' section

□ Click 'Upload Dilution Data' button

□ Navigate to: qmra\_toolkit/test\_data/dilution\_data/

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

□ In 'Select Site' dropdown, choose 'Site\_100m'

□ Review dilution statistics (median: 13.6x, range: 7.2x - 28.4x)

□ Final environmental concentration calculated: 113.2 copies/L

**Expected Display:** Dilution statistics box shows histogram of dilution factors and selected site statistics

**Troubleshooting:** Ensure CSV has columns: Site\_Name, Dilution\_Factor, Distance\_m

**Step 6: Configure Exposure Parameters**

**Actions:**

□ Scroll to 'Exposure Parameters' section

□ Set 'Exposure Route': Primary Contact (Swimming)

□ Set 'Water Ingestion Volume': 50 mL per event

□ Set 'Exposure Frequency': 20 events per year

□ Set 'Population Size': 10,000 people

□ Review calculated dose: 5.66 organisms per swimming event

**Expected Display:** Exposure form shows all parameters with calculated dose displayed

**Troubleshooting:** All numeric fields must be positive values

**Step 7: Configure Monte Carlo Simulation**

**Actions:**

□ Scroll to 'Monte Carlo Configuration' section

□ Set 'Number of Iterations': 10,000

□ Set 'Random Seed': 42 (for reproducibility)

□ Set 'Confidence Level': 95%

□ Leave uncertainty distributions at defaults

□ Review simulation parameters summary

**Expected Display:** Monte Carlo section shows iteration count, seed, and distribution settings

**Troubleshooting:** More iterations = more accuracy but longer runtime. Use 5,000 for testing, 10,000+ for final

**Step 8: Run Assessment**

**Actions:**

□ Scroll to bottom of form

□ Review all parameters in summary box

□ Click large 'Run QMRA Assessment' button

□ Observe progress bar advancing (0% → 100%)

□ Wait for completion (typically 15-30 seconds for 10,000 iterations)

□ Success message appears when complete

**Expected Display:** Progress bar shows percentage complete, then results panel appears below

**Troubleshooting:** If assessment fails, check error message and verify all required fields are filled

**Step 9: Review and Interpret Results**

**Actions:**

□ Results panel appears automatically below form

□ Review 'Risk Metrics Summary' table

□ Note infection probability per event: ~2.06×10⁻²

□ Note illness probability: ~1.44×10⁻² (accounting for asymptomatic)

□ Note annual risk: ~3.41×10⁻¹ (34.1% per year)

□ Review expected cases: ~144 illness cases per year in 10,000 population

□ Observe compliance status: NON-COMPLIANT (red indicator)

□ Read exceedance factor: 341× above WHO threshold

**Expected Display:** Results table with color-coded compliance (red for non-compliant), bar charts showing distributions

**Troubleshooting:** If results seem unrealistic, double-check input concentrations and dilution factors

**Step 10: Explore Visualizations**

**Actions:**

□ Scroll to 'Visualizations' section below results

□ Review infection risk distribution histogram

□ Examine cumulative distribution function (CDF) plot

□ View box plot showing median, quartiles, and outliers

□ Click 'Download Plot' buttons to save images

□ Toggle between linear and log scales using buttons

**Expected Display:** Three interactive plots: histogram, CDF, and box plot of risk distribution

**Troubleshooting:** If plots don't render, try refreshing page or clearing browser cache

**Step 11: Generate Professional Report**

**Actions:**

□ Scroll to 'Report Generation' section

□ Select report type: 'Regulatory Compliance Report'

□ Select format: PDF

□ Check boxes for: 'Include visualizations', 'Include methodology', 'Include references'

□ Enter report title: 'Takapuna Beach Swimming Risk Assessment 2025'

□ Enter author name and organization

□ Click 'Generate Report' button

□ Wait for processing (30-60 seconds)

□ Download link appears - click to save PDF

**Expected Display:** Report generation form with options, then download link with file size

**Troubleshooting:** Large reports may take longer. Reduce iterations if generation fails

**Step 12: Export Raw Data**

**Actions:**

□ Scroll to 'Export Data' section

□ Select export format: Excel (XLSX)

□ Check options: 'Include metadata', 'Include summary statistics'

□ Click 'Export Results' button

□ Download Excel file

□ Open in Excel/LibreOffice to review

□ File contains multiple sheets: Summary, Raw Results, Parameters, Compliance

**Expected Display:** Export options form, then download link for Excel file

**Troubleshooting:** CSV format is more compatible if Excel fails

### Interpreting Scenario 1 Results

|  |  |  |
| --- | --- | --- |
| **Metric** | **Value** | **Interpretation & Implications** |
| **Single Event Risk** | 2.06×10⁻² | ~2% chance of infection per swim. Relatively high due to norovirus infectivity. |
| **Annual Risk** | 3.41×10⁻¹ | 34% annual infection risk with 20 swims. Nearly 1 in 3 regular swimmers. |
| **Population Impact** | 144 cases/year | Significant public health burden in exposed population. |
| **Compliance** | NON-COMPLIANT | Exceeds WHO threshold by 341×. Additional controls required. |
| **Key Driver** | Treatment LRV | Secondary treatment (LRV 3.0) insufficient for high viral loads. |
| **Recommendation** | UV Disinfection | Additional 4-5 log reduction needed via UV or advanced oxidation. |

*Table 5: Scenario 1 Results - Detailed Interpretation*

# Advanced Topics & Best Practices

## Sensitivity Analysis

Sensitivity analysis identifies which input parameters most strongly influence risk estimates. This is crucial for prioritizing data collection and treatment interventions.

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Baseline Value** | **Test Range** | **Impact on Risk** |
| Raw Concentration | 1.54×10⁶/L | 5×10⁵ - 5×10⁶ | High (3.2× variation) |
| Treatment LRV | 3.0 | 2.0 - 8.0 | Very High (100× variation) |
| Dilution Factor | 13.6× | 7.2× - 28.4× | High (3.9× variation) |
| Ingestion Volume | 50 mL | 25 - 100 mL | Medium (2× variation) |
| Exposure Frequency | 20/year | 10 - 40/year | Medium (1.8× variation) |
| Dose-Response α | 0.04 | 0.02 - 0.08 | Low (1.3× variation) |

*Table 6: Sensitivity Analysis Results - Parameter Importance Ranking*

**Key Finding:** Treatment LRV is the most influential parameter, demonstrating that investment in advanced treatment provides the greatest risk reduction benefit. Improving dilution through outfall relocation or engineering modifications is the second-most effective intervention.

# Troubleshooting Guide

|  |  |  |  |
| --- | --- | --- | --- |
| **Issue** | **Symptoms** | **Likely Cause** | **Solution** |
| **App Won't Launch** | Error message or command fails | Missing dependencies | Run: pip install -r requirements.txt --upgrade |
| **File Upload Fails** | 'Invalid file format' error | Incorrect CSV structure | Check column names match requirements. Use UTF-8 encoding. |
| **Results Show NaN** | Metrics display as NaN or Inf | Zero/negative concentrations | Review input data for invalid values. Ensure concentrations > 0. |
| **Assessment Takes Too Long** | Progress bar stuck or very slow | Too many iterations | Reduce iterations to 5,000 for testing. Close other applications. |
| **Compliance Shows Incorrect** | Status doesn't match calculations | Wrong threshold selected | Verify threshold matches exposure route. Check units (per event vs annual). |
| **Plots Don't Display** | Blank or error where charts should be | Browser compatibility issue | Use Chrome/Firefox. Clear cache. Try incognito mode. |
| **Report Generation Fails** | Error during PDF/Word creation | Insufficient memory | Reduce number of scenarios. Close other applications. Try CSV export instead. |
| **Treatment Config Won't Load** | YAML file rejected | Syntax error in YAML | Validate YAML syntax. Check required fields: name, type, lrv for each barrier. |
| **Dilution Data Not Recognized** | Sites don't appear in dropdown | Missing/incorrect columns | Ensure CSV has: Site\_Name, Dilution\_Factor, Distance\_m columns. |
| **Results Seem Unrealistic** | Risk values too high/low | Input data error or wrong units | Double-check: concentrations in organisms/L, volumes in mL, LRV values 0-10. |

*Table 7: Troubleshooting Guide - Common Issues and Solutions*

**For Additional Support:**  
  
**Email:** reza.moghaddam@niwa.co.nz  
**Documentation:** See QMRA\_TOOLKIT\_USER\_GUIDE.md  
**GitHub:** [Repository URL]

# Appendices

## Appendix A: Quick Reference Commands

|  |  |  |
| --- | --- | --- |
| **Task** | **Command / Action** | **Notes** |
| **Launch Web App** | streamlit run qmra\_toolkit/web\_app.py | Browser opens at localhost:8501 |
| **Launch Desktop GUI** | python qmra\_toolkit/launch\_enhanced\_gui.py | Tkinter window opens |
| **Install Dependencies** | pip install -r requirements.txt | Run from project root |
| **Verify Installation** | python -c "import qmra\_toolkit" | Should complete without errors |
| **Run Test Suite** | pytest qmra\_toolkit/tests/ | Requires pytest installed |
| **Check Python Version** | python --version | Minimum 3.11 required |
| **Update Packages** | pip install --upgrade -r requirements.txt | Updates all dependencies |
| **Find Test Data** | cd qmra\_toolkit/test\_data | Contains all example files |
| **View User Guide** | open QMRA\_TOOLKIT\_USER\_GUIDE.md | Comprehensive documentation |
| **Clear Cache** | streamlit cache clear | If app behavior is unexpected |
| **Generate API Docs** | cd qmra\_toolkit/docs && sphinx-build | Creates HTML documentation |
| **Export Current Session** | Click 'Export Session' in app | Saves all parameters for later |

*Table 8: Quick Reference - Common Commands and Actions*

## Appendix B: Pathogen Database Reference

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pathogen** | **Model Type** | **Alpha (α)** | **Beta/r** | **Illness:Infection** | **Source** |
| **Norovirus** | Beta-Poisson | 0.04 | 0.055 | 0.70 | Teunis 2008 |
| **Campylobacter** | Beta-Poisson | 0.145 | 7.59 | 0.33 | Medema 1996 |
| **Cryptosporidium** | Exponential | — | 0.0042 | 0.70 | DuPont 1995 |
| **E. coli O157:H7** | Beta-Poisson | 0.49 | 5.99×10⁴ | 0.50 | Haas 1999 |
| **Salmonella** | Beta-Poisson | 0.33 | 2.49×10³ | 0.50 | Haas 1999 |
| **Rotavirus** | Beta-Poisson | 0.26 | 0.42 | 0.50 | Ward 1986 |

*Table 9: Pathogen Dose-Response Parameters - Peer-Reviewed Values*

# Conclusion & Next Steps

## Summary

This technical demonstration guide has provided comprehensive, step-by-step instructions for using the NIWA QMRA Toolkit. You have learned how to configure assessments, interpret results, and generate professional reports for regulatory compliance.

## Key Capabilities Demonstrated

• Multi-pathogen risk assessment with peer-reviewed models  
• Monte Carlo uncertainty quantification (10,000+ iterations)  
• Treatment train modeling with multi-barrier LRV analysis  
• Hydrodynamic dilution integration from ROMS/Delft3D models  
• Professional report generation for regulatory submissions  
• Sensitivity analysis for parameter importance ranking

## Best Practices Review

• Always use Monte Carlo simulation (minimum 5,000 iterations) for uncertainty  
• Document all input parameters with sources and dates  
• Validate results against literature values and regulatory benchmarks  
• Conduct sensitivity analysis to identify key risk drivers  
• Generate professional reports with methodology documentation  
• Archive all input data, configurations, and results for reproducibility

## Next Steps

1. Practice with the provided test data scenarios  
2. Adapt scenarios to your specific site conditions  
3. Collect site-specific monitoring data (pathogen concentrations, dilution)  
4. Configure treatment barriers matching your facility  
5. Run assessments and generate reports  
6. Review with stakeholders and regulatory agencies

## Additional Resources

• User Guide: QMRA\_TOOLKIT\_USER\_GUIDE.md  
• API Documentation: qmra\_toolkit/docs/  
• Example Scripts: qmra\_toolkit/examples/  
• Test Data: qmra\_toolkit/test\_data/  
• Scientific References: See Section 8 of User Guide

**END OF TECHNICAL DEMONSTRATION GUIDE**  
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