TERMS OF REFERENCE FOR A DIRECTED WRC PROJECT

THEMATIC AREA	Water Use
TITLE	An artificial intelligent-augmented multidisciplinary approach for adaptive design and optimization of water and resource recovery facilities - a pathway to a digital twin for water services.

Objectives

General

The primary aim of this study is to develop an AI-augmented, multidisciplinary and transdisciplinary decision support framework for the adaptive design and optimisation of water and resource recovery facilities (WRRFs) using machine learning algorithms to enhance predictive accuracy, enabling scenario-based simulations for resource recovery optimisation. The resulting web-based tool will allow engineers, planners, and policymakers to explore thousands of "what-if" configurations, identify minimal yet impactful retrofits, and design future-proof systems tailored to local socio-technical contexts.

Specific

The specific objectives of the study are:

1. Develop an AI-augmented, multidisciplinary and transdisciplinary decision support tool for the design, optimization, and future-proofing of WRRFs, integrating microbial ecology, mechanistic models, and machine learning for adaptive infrastructure planning.
2. Construct a high-resolution microbial modelling framework by curating and formalizing microbial trait data (e.g., kinetics, stoichiometry, environmental tolerances) into a structured database and ontology for integration with mass-balanced simulation models.
3. Formulate and validate a hybrid simulation engine that combines ontology-driven reasoning with mechanistic modelling to dynamically configure biological treatment processes under varying influent characteristics and operational conditions.
4. Simulate and evaluate scenario-based treatment configurations for wastewater systems exposed to stressors such as climate change, population growth, industrial load variability, and resource recovery mandates, identifying optimal strategies for both new designs and retrofits.
5. Enable real-time learning and continuous system improvement by incorporating live updates of microbial data, new case studies, and process configurations through an open, web-based platform designed for iterative model enhancement and reuse.
6. Support the sustainability and expansion of centralized data and knowledge-sharing platforms, including integration with existing communities of practice and virtual laboratories, to foster collaborative research, training, and innovation across sectors.
7. Promote region-specific and context-aware decision-making, ensuring that system recommendations account for local socio-technical conditions including existing infrastructure, industrial activities, waste sources, climate variability, and regulatory frameworks.

Rationale

Conventional Wastewater Treatment Plants (WWTPs) are typically designed around fixed process configurations, assuming stable influent characteristics and relying heavily on the activated sludge process and biological nutrient removal. While these systems have served reliably for decades, they are now increasingly challenged by:

- The emergence of complex pollutants such as pharmaceuticals, endocrine-disrupting compounds and microplastics.
- Greater influent variability driven by industrial discharges, stormwater inflows, and changing water use patterns.
- Operational and climatic stressors such as resource constraints and climate change impacts.

These challenges often result in inefficient pollutant removal, higher energy and chemical demands, and reduced resilience to disturbances.

Recent advances in microbial ecology and environmental biotechnology have revealed extensive microbial diversity and metabolic potential within wastewater systems, including strains capable of degrading recalcitrant contaminants under varied environmental conditions. However, most widely used modelling frameworks such as the Activated Sludge Models (ASMs) oversimplify microbial communities into broad functional groups and this; (i) fails to reflect the dynamic microbial responses to environmental change. (ii) prevents integration of new, high-resolution microbial trait data (e.g., growth kinetics, metabolic pathways, environmental tolerances) and (iii) limits the ability of engineers and operators to apply this knowledge in design, optimisation, and operational decision-making.

Although artificial intelligence (AI) and machine learning have been applied in process control and fault detection, their integration with microbial modelling especially at the trait level-remains largely unexplored. There is currently no systematic framework for translating microbial trait data into actionable, model-based infrastructure design and optimisation tools.

This project therefore seeks to develop a data-driven, AI-augmented decision-support framework for the design, optimisation, and adaptive operation of WRRFs with the following key elements in mind:

- Curated Microbial Dataset – a structured, high-resolution database of microbial traits relevant to wastewater treatment, including kinetics, stoichiometry, environmental tolerances, and degradation pathways.
- Ontology-Driven Reasoning – a formal microbial-process ontology linking microbial traits with environmental conditions and process functions, enabling logical, context-specific process selection.
- Hybrid Simulation Engine – integration of microbial datasets with mass-balanced mechanistic models (e.g., PWM_SA Gujer matrix) and AI algorithms for parameter estimation and performance optimisation.
- Scenario and Optimisation Tool – a web-based interface enabling engineers, planners, and decision makers to test “what-if” scenarios (e.g., climate change impacts, industrial discharges), evaluate and rank alternative configurations based on pollutant removal, energy use, and resource recovery as well as adapting designs to region-specific socio-technical and environmental contexts.

The system will be continuously expandable, incorporating new data streams such as climate forecasts, settlement patterns, industrial activity profiles, and infrastructure condition data.

Methodology

The study should be implemented through an integrated, phased approach, combining microbiological data curation, semantic ontology development, mechanistic modelling, AI integration and real-world validation. Each phase should be interconnected, ensuring that outputs from one stage feed directly into subsequent stages, culminating in a fully functional AI-augmented decision-support platform for adaptive WRRF design and optimisation. The study phases should, *inter alia*, include the following.

Phase 1: Microbial data collection, curation and database construction.
Phase 2: Ontology development and semantic structuring.
Phase 3: Mechanistic model formulation and hybrid simulation engine.
Phase 4: AI-Augmented configuration optimisation and decision support.
Phase 5: Model validation, demonstration and platform integration.

Deliverables

The following deliverables will be expected:

1. Publicly accessible microbial trait database.
2. Machine-interpretable microbial ontology.
3. Validated hybrid mechanistic simulation engine.
4. AI-enabled web-based decision-support tool.
5. Validated case studies.
6. Sustainable platform in active community of practice.
7. Policy brief based on study findings.
8. Draft final report.
9. Corrected final print ready report.

Outcomes and impacts:

In essence, the study is conceived as a transdisciplinary and multidisciplinary bridge between microbial science, AI technology, and WRRF engineering practice. Hence, the proposed study connects advanced microbiological understanding into design-oriented models and augmenting these with AI optimisation. In this way the study seeks to redefine how infrastructure is planned, retrofitted, and operated in alignment with circular economy principles and climate resilience goals.

Impact Areas:

Water and the Economy, Water and the Environment and Water and Society

Time Frame:

The study is expected to be conducted over a period of 48 months, starting from 01 April 2027 to 31 March 2031.

Total Funds Available: R 2,000,000 inclusive of VAT.