Leveraging Large Language Models for Automating Water Distribution Network Optimization

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Abstract: Effective management of Water Distribution Networks (WDNs) is essential to ensure efficient and reliable water supply in cities. However, many management tasks require complex system modelling and optimization approaches, which heavily rely on specialized domain expertise and human resources. Recent advancements in Large Language Models (LLMs) offer promising opportunities to automate complex hydraulic decision-making tasks. This study presents an LLM-based agent framework to automate WDN management tasks. Two tasks are considered to evaluate the feasibility and limitations of LLM agents: hydraulic model calibration and pump operation optimization. The key component of the proposed framework is an Orchestrating Agent that interprets tasks and system states, generates update strategies or executable code, and interacts with three specialized agents to carry out implementation: a Knowledge Agent performing reasoning based on hydraulic principles, a Modelling Agent that interfaces with hydraulic simulation tool EPANET, and a Coding Agent that executes code and returns output feedback. To assess the capabilities of these agents, the framework was systematically tested on two benchmark WDNs - Net2 and Anytown. The results indicate that the reasoning capability demonstrated through interaction with the Knowledge Agent effectively replicates expert-level hydraulic thinking, though it lacks numerical precision. In contrast, the Modelling Agent, which integrates external simulation tools, enhances reliability, although interpreting and enforcing numerical constraints expressed in natural language remain challenging. Furthermore, the Coding Agent, where code for optimization algorithms is iteratively generated and executed, delivers the most consistent and accurate performance across both networks, underscoring its practical potential. These findings highlight the potential of LLM-based agents for automated, accurate hydraulic optimization, and represent a significant step toward LLM-driven multi-agent frameworks for hydraulic decision-making. This work establishes a foundation for future advancements in specialized, domain-focused LLM applications in complex hydraulic management scenarios.

Keywords: Water Distribution Network; Large Language Model; AI Agent; DeepSeek; Hydraulic Optimization

1 Introduction

Water Distribution Networks (WDNs) play a critical role in ensuring the continuous delivery of safe, reliable, and

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high-quality water to consumers (Fu et al., 2022a; Sarbu and Popa-Albu, 2023; Zaman et al., 2021). Their operational priorities span a wide range of objectives, including 24/7 service continuity, sustainable energy and operational costs, minimal water losses, limited environmental and social impact, and satisfactory customer service (Sharif et al., 2022; Zarei et al., 2022). However, meeting these objectives has become increasingly difficult in a rapidly changing context. Many WDNs face the challenges of ageing infrastructure, evolving demand patterns, reduced workforce continuity, and the growing frequency of extreme weather events (Gong et al., 2023; Sela et al., 2025). In this complex environment, hydraulic optimization tasks are fundamental to improving system efficiency, resilience, and sustainability (Nedaei, 2025).

Among these hydraulic optimization tasks, hydraulic model calibration and pump operation optimization are two critical and extensively studied problems, due to their significant impacts on network performance and operational costs (Batista do Egito et al., 2023; Makaremi et al., 2017; Zhang et al., 2018). The two problems are also specific examples of the two general types of decision-making challenges: inverse analysis (calibration) and operational optimization (pump operation) in WDN management. Historically, methodologies addressing these tasks have evolved through various water management paradigms (Fu et al., 2024): empirical approaches based on field observations and trial-and-error adjustments; theoretical formulations grounded in classical hydraulic equations such as Hazen–Williams and Darcy–Weisbach (Khedr et al., 2015); computational optimization techniques such as genetic algorithms, gradient-based methods, and differential evolution (Nedaei, 2025; Sarbu, 2021; Sarbu and and Popa-Albu, 2023); and more recently, data-centric approaches leveraging machine learning and data-driven modelling (Fu et al., 2022; Meggiorin et al., 2024). Despite their technical maturity, these methods remain difficult for non-experts to interpret and apply, requiring intensive manual tuning and domain expertise that limit real-time usability in operational settings (Hedaiaty Marzouny and Dziedzic, 2024; Ren et al., 2024).

In recent years, Large Language Model (LLM)-based agents have emerged as promising tools for bridging the gap between advanced automation and human interpretability in complex system management (Sami et al., 2024). By leveraging language understanding, planning, and adaptive reasoning capabilities (Wang et al., 2024), they are increasingly being explored as central engines in autonomous agent frameworks across diverse fields. For instance, LLM-based agents have been applied to traffic control systems, where they emulate human-like judgment in managing dynamic, uncertain urban environments (Movahedi and Choi, 2025; Wang et al., 2024), as well as in building energy optimization (Zhang et al., 2025) and geoscientific data processing (Zhang et al., 2025). In water systems, recent studies have demonstrated the feasibility of LLM-based agents in constructing domain-specific digital twins and knowledge graphs to support decision-making in water conservancy contexts (Yang et al., 2024) and in estimating flood depth from images (Lyu et al., 2025). These developments highlight the potential of LLM-based agents beyond language tasks, as their agentic behaviour is supported by iterative dialogue and integration with domain-specific tools and offers a new paradigm for addressing high-level cognitive challenges.

However, despite growing interest in the use of LLM-based agents for most fields, current applications remain largely exploratory and fragmented (Wang et al., 2024). In the water sector, existing studies often focus on isolated functions such as answering questions, information retrieval, or knowledge representation, rather than full decision-making workflows (Ren et al., 2024; Rothfarb et al., 2025; Sela et al., 2025). A multi-agent framework consisting of an orchestrating agent for workflow decomposition and specialized agents for tasks such as environmental perception, data analytics, modelling, optimization, and solution evaluation was proposed (Fu, 2025). However, there is a lack of study on LLM-based agents and standardized frameworks for designing or evaluating their performances in hydraulic management contexts. As a result, previous studies tend to be ad hoc and task-specific, with limited consideration of interaction strategies, tool integration, or generalizability.

To address this gap, we propose and evaluate a novel multi-agent framework in which collaborating LLM-based agents use interactive prompting, simulation tools and autonomous coding to enhance hydraulic decision-making in WDNs. It focuses on two representative optimization tasks: inverse analysis (e.g., hydraulic model calibration) and operational optimization (e.g., pump operation). For each task, an Orchestrating Agent first interprets the task description and the current state of the hydraulic system. This is followed by iterative interactions with a specialized agent to evaluate one of three core capabilities: *reasoning*, where a Knowledge Agent performs formula-based reasoning though hydraulic principles described in natural language within its system prompt; *simulation tool interaction*, where a Modelling Agent offers physically grounded feedback via simulation tools; and *autonomous coding*, where a Coding Agent executes software code (e.g., Python scripts) generated by the Orchestrating Agent to accomplish specific hydraulic tasks. By evaluating these capabilities on two benchmark networks, i.e., Net2 and Anytown, this study provides a structured, comparative assessment of these agent capabilities in terms of decision quality, computational performance, and adaptability across hydraulic contexts, establishing a foundation for more specialized, tool-integrated LLM agents in water system management.

2 Methodology

This section outlines a multi-agent framework based on LLMs to automate two commonly encountered tasks in WDN management: hydraulic model calibration and pump operation optimization. It details how LLM agents are developed and structured into cohesive planning architecture, emphasizing system design and collaborative agent interactions. Section 2.1 introduces the overall framework used to evaluate the core capabilities of LLM-based agents, while Sections 2.2 and 2.3 present the problem formulations for hydraulic model calibration and pump operation optimization, respectively. Section 2.4 outlines the experimental setting used to implement and evaluate the proposed framework.

2.1 Overview of the LLM-based Agent Interaction Framework

This section presents a multi-agent interaction framework aimed at evaluating the potential of three core capabilities of LLM-based agents in supporting hydraulic decision-making tasks within WDNs. As illustrated in Figure 1, the framework processes user-defined tasks through three distinct modes of structured agent interaction. Each mode features a central Orchestrating Agent that receives a structured task description, interprets the current state of the WDN, and engages with a specialized agent configured with a unique capability, enabling the systematic evaluation of individual agent competencies:

(a) *Reasoning Capability*, which is assessed through interaction between the Orchestrating Agent and the Knowledge Agent. In this configuration, the Orchestrating Agent assumes the role of a Hydraulic Expert by analysing the task objectives and network state, planning update strategies, and proposing modifications to parameters such as pipe roughness values or pump speeds. Upon receiving these proposals, the Knowledge Agent performs symbolic reasoning based on hydraulic principles using mathematical formulations such as pressure and head loss equations, which are explicitly incorporated in its system prompt in the form of natural language descriptions. It then infers the updated WDN state and returns the results to the Orchestrating Agent. This process is repeated iteratively to evaluate the agent's ability to interpret and respond logically to hydraulic scenarios using internalized domain knowledge.

(b) *Simulation Tool Interaction Capability*, which is evaluated via direct interaction between the Orchestrating Agent and the Modelling Agent. This configuration follows a similar mode to Option (a), with the key difference that the Modelling Agent acts solely as a Modeller of external simulation tools. Upon receiving instructions from the Orchestrating Agent, it invokes hydraulic simulation tools such as Python-based implementations of EPANET functions to perform physically accurate simulations and return model-based feedback. This process is used to assess the agent's effectiveness in leveraging external simulations to support and refine decision-making.

(c) *Autonomous Coding Capability*, which is explored through the interaction between the Orchestrating Agent and the Coding Agent. In this setup, the Orchestrating Agent autonomously generates executable Python scripts to address specific hydraulic tasks. These scripts are then executed by the Coding Agent, which returns the outputs to the

Orchestrating Agent for analysis and iterative refinement. This setup focuses on evaluating the agent's proficiency in dynamic code generation and iterative problem-solving through programmatic interaction.

The framework effectively isolates the functional contributions of each agent type and provides insights into both the practical potential and current limitations of LLM-based agents in complex hydraulic decision-making environments.

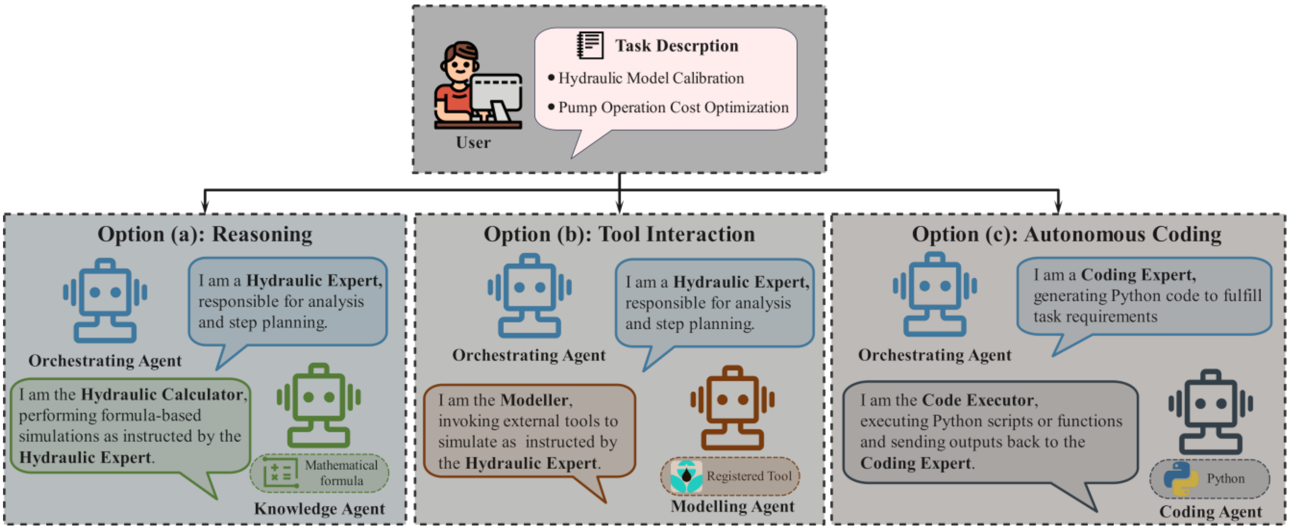

Figure 1 Overview of the LLM-based Multi-Agent Framework for Automated Solution Development in WDN Management

2.2 Hydraulic Model Calibration

Calibration constitutes an inverse problem where hydraulic model parameters, such as pipe roughness values, are estimated by minimizing the discrepancy between simulated and observed data. Pipe roughness directly affects head loss and pressure distribution in WDNs, and its accurate calibration is essential for reliable hydraulic modelling (Zhang et al., 2018). Therefore, roughness calibration is selected in this study as a representative task to assess the three core capabilities of LLM-based agents within the proposed framework. The goal is to adjust roughness parameter values so that simulated pressures closely align with observed data. The mean absolute error (MAE) between simulated and observed pressures is used as the objective function:

$$MAE = \frac{1}{N}\sum_{i=1}^{N} |\hat{P}_i - P_i| \tag{1}$$

Where $\hat{P}_i$ and P_i represent the simulated and observed pressures at node *i*, respectively, and *N* is the total number of monitored nodes.

To perform hydraulic model calibration the Orchestrating Agent utilizes known system parameters (network topology, observed/initial simulated pressures, nodal demands, and initial MAE values from Table S1, to generate roughness adjustment strategies in a manner similar to how a hydraulic expert would approach the problem. These proposed adjustments are then executed by both the Knowledge and Modelling Agents. These proposed adjustments are then executed by both the Knowledge and Modelling Agents, which return simulated hydraulic results to the Orchestrating Agent. However, their computational methodologies differ significantly. The Knowledge Agent performs hydraulic calculations using the Hazen-Williams equation, explicitly described in natural language within its system prompt as the core computational mechanism:

$$Q = k \cdot C \cdot D^{2.63} \cdot (\frac{H}{L})^{0.54} \tag{2}$$

where Q is the flow rate (m^3/s), C is the Hazen-Williams roughness coefficient (dimensionless), constrained within a range of 60 to 140 in this study, D is pipe diameter (m), L is pipe length (m), H is head loss (m), and k is a constant (0.849 in SI units) (Rossman et al., 2020). Using this equation, the knowledge agent estimates downstream node pressures based on cumulative head losses from a fixed reservoir head. Further details on the agent's system prompt are provided in Table S1. In contrast, the Modelling Agent uses externally registered hydraulic simulation tools, specifically Python-based EPANET functions, to execute simulations. The pseudocode for these functions is presented in Function S1.

The calibration task handled by the Coding Agent differs notably. Instead of using descriptive text-based input, the Orchestrating Agent receives structured input in the form of file paths (Table S2). Based on these path-based descriptors, the Orchestrating Agent autonomously generates executable Python scripts that read the input files, extract relevant network and pressure data, and apply roughness optimization routines. This automated scripting process emulates the behaviour of professional coders. Subsequently, the Coding Agent executes these scripts locally to complete the calibration tasks.

2.3 Pump Operation Optimization

Pump stations are the primary consumers of energy in WDNs, with electricity usage reaching up to 90% in some systems (Hedaiaty Marzouny and Dziedzic, 2024). Enhancing pump operation efficiency can therefore lead to substantial cost savings. To further examine the three capabilities of LLM-based agents, pump operation optimization is selected as a second representative task due to its practical relevance and computational complexity. In this study, the objective is to minimize the total energy cost associated with pump operation over a predefined time horizon by adjusting the relative operating speeds of the pumps. The cost is calculated based on the hydraulic head, flow rate, electricity tariff, and pump efficiency, using the following equation:

$$Total\ Cost = \frac{9.81}{3600 \cdot \eta} \sum_{t=1}^{T} (H_t \cdot Q_t \cdot Price_t) \tag{3}$$

where H_t is the pump head (m), Q_t is the flow rate (m³/s), $Price_t$ is the electricity price at time t, η is the pump efficiency (dimensionless), and the constant 9.81 represents gravitational acceleration (m/s²). The factor 3600 is used to convert the cost from watts to kilowatt-hours.

Similar to Section 2.2, in the pump operation optimization task, the Orchestrating Agent uses known task information alongside embedded hydraulic knowledge to propose operational strategies. The Knowledge Agent performs hydraulic simulations based on equations below explicitly provided through system prompts, in addition to Equations (2) and (3):

$$\begin{cases} Q_t = Q_{base} \times s_t \\ H_t = H_{base} \times s_t^2 \end{cases} \tag{4}$$

Where Q_{base} and H_{base} represent the baseline flow rate and head at full speed, respectively, and s_t is the relative speed of the pump at time *t*, constrained within a range of 0.85 to 1.15. Further details on the agent's system prompt are provided in Table S3. The Modelling Agent again employs externally registered hydraulic simulation tools using Python-based EPANET functions, with pseudocode detailed in Function S2. The Coding Agent maintains the same structural approach as in the roughness calibration task, where the Orchestrating and Coding Agents generate and execute Python scripts; however, their system prompts are adapted specifically to the pump operation optimization context (Table S4).

2.4 Experimental setting

This section outlines the implementation details and experimental configuration used to evaluate the proposed LLM-based agent framework. The system was developed using the **AutoGen** framework, an open-source platform designed for orchestrating structured communication and task delegation among LLM-based agents (Barbarroxa et al., 2025). **Python** (v3.11) served as the programming environment. All hydraulic simulations were conducted using the Water Network Tool for Resilience (**WNTR**), a Python library that programmatically interfaces with **EPANET 2.2** to support the modelling and analysis of WDNs (Klise et al., 2020). The LLM employed across all agent roles was **DeepSeek-V3** (DeepSeek-AI, 2024) (API deployment, 16K context window), selected for its demonstrated capability in multi-turn reasoning and Python code generation. To ensure deterministic behaviour and eliminate stochastic variability in outputs, generation parameters were fixed with a temperature of 0, a random seed of 10, a maximum token limit of 2048, and a timeout setting of 600 seconds.

To reflect the varying complexity of each coordination mode described in Section 2.1, different interaction limits were applied. The Orchestrating Agent was limited to 5 interaction rounds when engaging with the Knowledge and the Coding Agents, reflecting the relatively lightweight nature of symbolic reasoning and standalone code execution.

In contrast, up to 30 interaction rounds were permitted during interactions with the Modelling Agent to accommodate the computational overhead of external tool calls and to support more fine-grained iterative refinement. All experiments were executed on a fixed computational setup comprising an Intel i7-14700HX CPU and an NVIDIA RTX 4060 GPU (8 GB) to ensure consistency and reproducibility. Agent role prompts, input formats, and task specifications were standardized across all experiments, with full details of system message definitions and initial chat configurations provided in Tables S1~S4 of the Supporting Information.

3 Case study

3.1 Benchmark WDNs

To evaluate the proposed agent-based framework, two benchmark WDNs with distinct topological and operational characteristics were selected, as illustrated in Figure 2. Net2 is a tree-based network sourced from the EPANET example library, while Anytown is a looped network originally developed as a benchmark for WDN design and operational optimization (Walski et al., 1987). The main structural features of each network are summarized in Table 1, where for the roughness calibration task, the initial roughness value of all pipes was uniformly set to 70 to simulate an uncalibrated baseline condition. The actual pipe roughness values are shown in Figure S1, where Net 2 mostly consists of pipes with a roughness of 100 and some sections with 70 or 140, while Anytown features roughness values of 70, 120, and 130 across different pipe sections. However, although the pump station location is indicated in Figure 2, the Net2 lacks explicit pump element definitions (Hoagland et al., 2015), and represents the source and pump station as a single junction node. As a result, pump operation optimization was not performed on Net2, and only hydraulic model calibration was conducted.

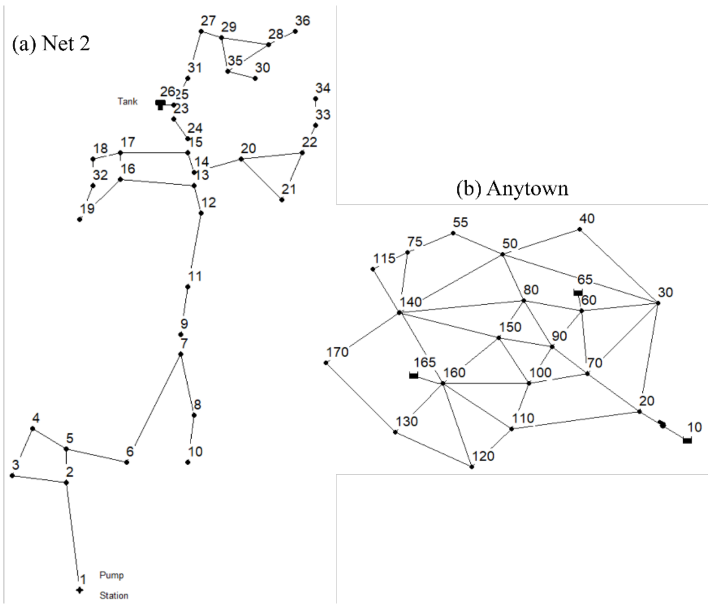

Figure 2 The topological structure of (a) Net2 and (b) Anytown WDNs

Table 1 Summary of EPANET-defined structural properties of the selected benchmark WDNs

WDNs	Reservoirs	Junctions	Tanks	Pipes	Pumps	Initial Pipe Roughness
Net2	None	35	1	40	0	70
Anytown	3	19	None	40	1	70

3.2 Data Preparation

In the proposed agent-based framework, each agent role is defined through natural language system prompts, as detailed in Tables S1–S4. To initiate a task, a task description in natural language format is also required. For the evaluation of *Reasoning* and *Tool Interaction* capabilities, this description includes both the task objective and baseline WDN data as plain text. The inputs typically consist of:

1. WDN Information: The EPANET .inp file content is directly converted into natural language and embedded into the task description.
2. Water Demands: Based on the predefined demand patterns used in the Net2 and Anytown networks [from (Rossman et al., 2020; Walski et al., 1987)], EPANET simulations are run to compute time-varying demands at each node. These demand values are then incorporated into the task as plain-text entries.
3. Observed Values: Using the same water demands as in (2) together with the actual pipe roughness, EPANET simulations are run to extract node pressures over time as observed ground truth values, while predefined electricity prices (£/kWh) for each time interval are also included in the task description.
4. Baseline State: Initial EPANET simulated values, such as pressures from a model with uniform pipe roughness

(e.g., roughness = 70, Table 1) or pump energy consumption at each time step under initial settings (e.g., pump speed =1). These values are likewise embedded into the prompt using natural language.

5. Initial Objective Metric: The baseline error metric (e.g., initial MAE) or cost for comparison.

In contrast, when evaluating the *Autonomous Coding* capability, none of the above datasets are included in the task prompt as plain text. Instead, the task description provides file paths pointing to the relevant data files. The agents are expected to autonomously generate code to read, process, and utilize these datasets during the calibration or optimization task.

4 Results

4.1 Reasoning Capability

This section evaluates the agent's reasoning capability through interactions between the Orchestrating and the Knowledge Agents across three distinct experimental scenarios. In this case, the Knowledge Agent receives update proposals from the Orchestrating Agent and performs computational reasoning based on Equations (1) to (4), which are embedded as text in its prompt message. The detailed dialogues and interaction logs recorded in Text Files S1–S3, while Figure 3 presents a simplified summary of the first-round dialogue, illustrating the human-like reasoning patterns of the orchestrating and knowledge agents, including (1) in Figure 3, the orchestrating agent identifies nodes with large pressure deviations and updates pipe roughness based on the logic of increasing upstream roughness when simulated pressures are too high, while the knowledge agent performs new simulations and error analysis; and (2) in Figure 3, the orchestrating agent adjusts pump speeds according to electricity prices, for example by reducing speed during high-price periods and increasing speed during off-peak periods.

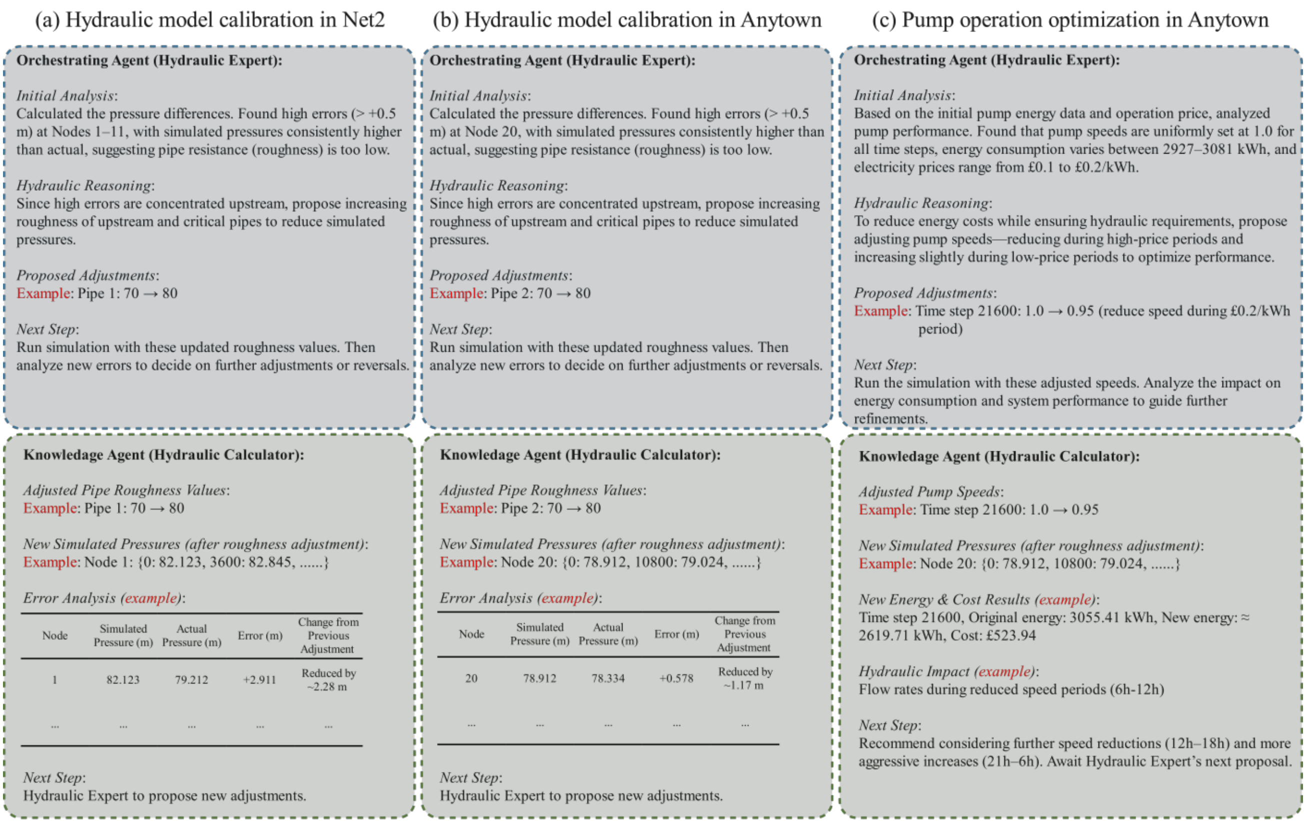

Figure 3 Simplified First-Round Dialogue Between Orchestrating and Knowledge Agents Across Three Tasks: Hydraulic Calibration in (a) Net2, (b) Anytown, and Pump Operation Optimization in (c) Anytown. The dialogue omits full parameter updates and detailed exchanges, with representative updates highlighted as red examples for illustration.

Furthermore, to assess the knowledge agent's reasoning accuracy in complex calculations, we re-simulated the final roughness and pump speed strategies with EPANET (Text Files S1–S3) and compared the resulting node pressures and pump costs with the outputs generated by the knowledge agent. The results revealed substantial discrepancies between the two sets of outputs. Specifically, Figure 4 illustrates node pressure in the Net2 network (first 10 nodes) under the optimal roughness calibration strategy. The simulation results from the Knowledge Agent are consistently lower than those from EPANET. The most significant deviation occurs at Node 6, where the pressure error reaches approximately 4.2 m, while even at Node 1, which shows the smallest discrepancy, the Knowledge Agent underestimates pressure by about 3.1 m, leading to a final MAE difference of 0.20 m between the Knowledge Agent and EPANET simulations. A similar pattern is observed in Figure 4, which presents the hydraulic model calibration results for the Anytown network. While the looped topology of the network helps reduce the difference between the two simulations, the maximum error still occurs at Node 170, with a pressure discrepancy of around 0.54 m, which still exceeds the 5% (Lingireddy et al., 2004) threshold commonly accepted for engineering applications. Additionally, Figure 4 shows the pump operation cost in Anytown over a 24-hour horizon during the pump operation optimization task. The Knowledge Agent exhibits clear errors in cost estimation, particularly at 6 h and 9 h, where the Knowledge Agent generated results deviate from EPANET results by £158 and £160, respectively, resulting in total costs of £3,599 and £3,643.

Overall, although the results generated by the Knowledge Agent in Figure 4 show varying degrees of deviation from the EPANET simulation results, the EPANET outcomes still exhibit an overall downward trend in comparison with the Initial Objective Metrics in the tasks (Text Files S1–S3): MAE = 0.65 m for Net2, 0.41 m for Anytown, and £3,762 for Anytown. These results indicate that while LLM-based agents are effective in capturing high-level reasoning patterns, they are unable to perform accurate numerical computations using formulas embedded as natural language in their prompt messages.

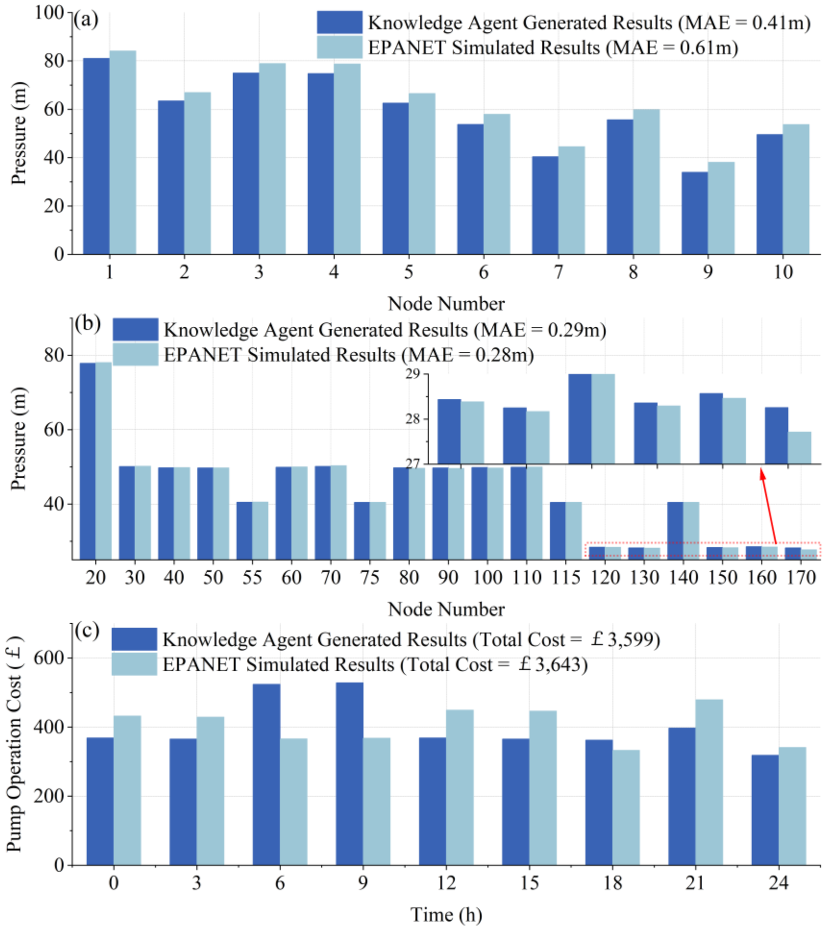

Figure 4 Comparison of Knowledge Agent and EPANET simulation results under an optimized strategy, where (a) and (b) show node pressure comparisons during hydraulic model calibration in Net2 (first 10 nodes) and Anytown respectively, and (c) presents the time-varying pump operation cost in Anytown during pump operation optimization.

4.2 Tool Interaction Capability

To address the inaccuracies observed in Section 4.1 when the Knowledge Agent was applied to perform hydraulic calculations, this section evaluates the performance of the Modelling Agent which incorporates an external tool - EPANET. In this case, agents interact with the WDN environment and assess the performance of proposed WDN parameters (roughness values or pump speeds) via Python-based EPANET simulations. The same tasks from Section 4.1 were replicated, including pipe roughness calibration for the Net2 and Anytown networks, and pump optimization for the Anytown network. Full dialogue transcripts and agent interactions are available in Supporting Information (Text Files S4–S6).

For the hydraulic model calibration tasks, analysis of Text Files S4 and S5 reveals that the Orchestrating Agent and the Modelling Agent jointly performed nine roughness update iterations. The spatial distribution and magnitude of each update are summarized in Figure 5. In the Net2 calibration task (Figure 5), the initial MAE was 0.652 m, which decreased by 41% to 0.385 m after the ninth iteration, lower than the EPANET result of 0.610 m shown in Figure 4. Notably, in iterations 1 to 4, the Orchestrating Agent exhibited expert-like behaviour by first modifying roughness values on major trunk lines and then progressively increasing the number of adjusted pipes. After the fourth iteration, however, the number of modified pipes plateaued at eight. This mirrors typical manual calibration patterns, where modifying too many pipes at once obscures causal relationships and turns reasoning into trial-and-error, increasing the risk of local optima. Although increasing the number of interactions between agents can eventually yield meaningful improvements, escaping local optima often incurs a high cost in terms of computational tokens and reasoning cycles. This phenomenon is particularly observable in the Anytown calibration task (Figure 5), which features a looped network topology. The initial MAE of 0.413 m declined only marginally after the third iteration, with improvements of less than 0.01 m per iteration, ultimately reaching 0.275 m by the ninth iteration, which is also lower than the 0.280 m reported in Figure 4. A closer examination of iterations 5 through 9 reveals that the roughness values assigned to pipes 24 and 56 dropped below the threshold of 60, which is not allowed as defined in the natural language prompt in Table S2. This finding highlights a memory limitation in agent reasoning: although numerical constraints were clearly embedded within the instruction context, the Orchestrating Agent gradually failed to retain and apply these constraints over extended dialogues. As a result, parameter updates in later iterations became infeasible or suboptimal, ultimately undermining calibration quality.

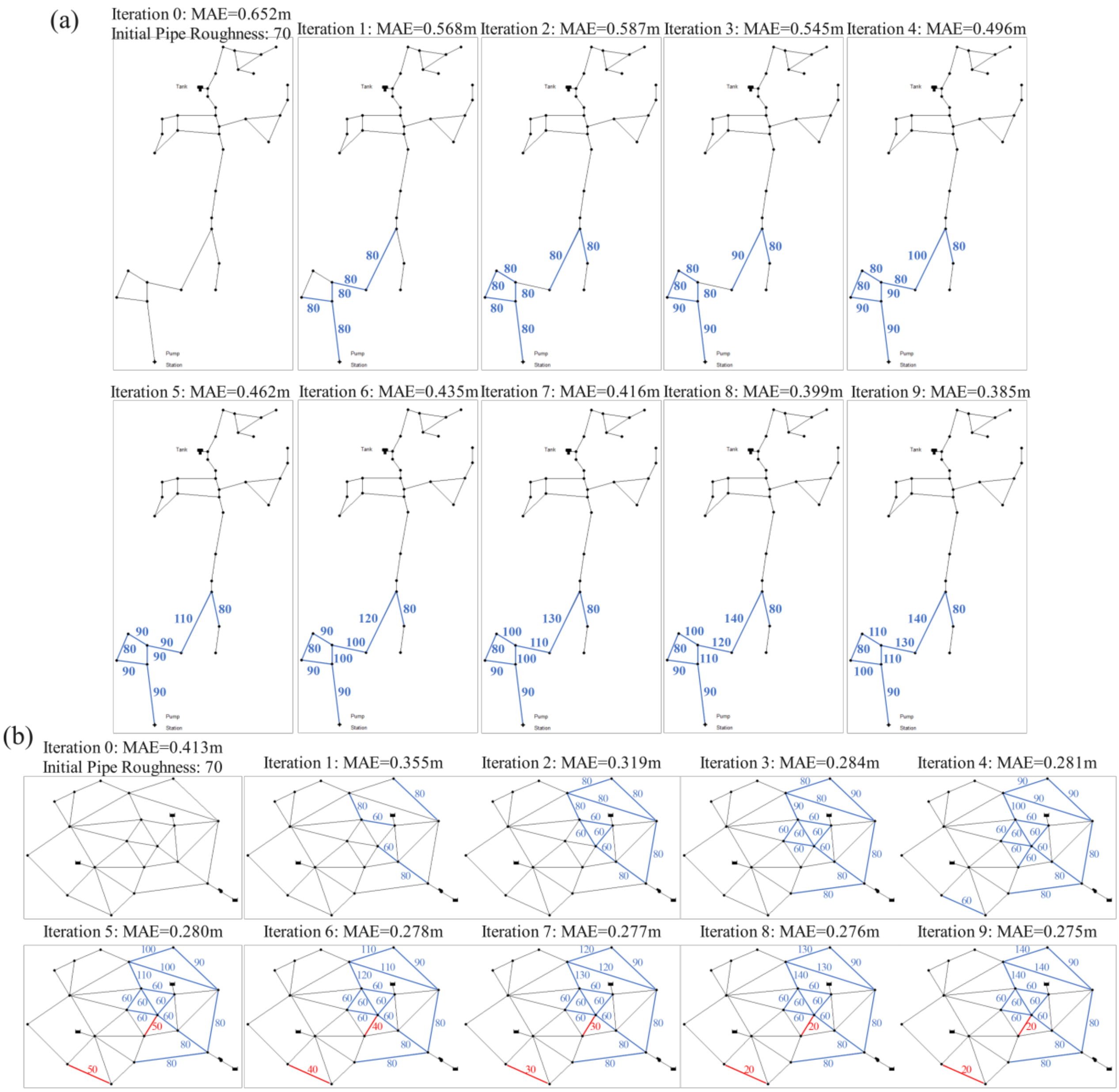

Figure 5 Spatial distribution and magnitude of pipe roughness updates across iterations during hydraulic model calibration in the Net2 (a) and Anytown (b) networks. Blue lines represent updated roughness values within predefined bounds, while red lines indicate values exceeding these bounds.

For the pump operation optimization task, analysis of Text File S6 reveals the details of each pump speed update, which are summarized in Figure 6. In Iteration 1, the Orchestrating Agent adjusted the pump speed in line with expert strategies by reducing it to 0.95 at 9:00, a peak electricity pricing hour. In Iteration 2, this reduced speed extended from 9:00 to 15:00, which led to a lower operational cost of £3,536. This behaviour aligns with established domain knowledge that prioritizes load shifting to reduce energy expenditure. While the pump speed was increased to 1.05 during the off-peak hours from 21:00 to 24:00 in Iterations 1 and 2, the Orchestrating Agent later observed that reducing pump speed generally led to lower costs. As a result, in Iteration 3, the speed at 21:00 was reduced back to

1.00, further decreasing the total cost to £3,332, which is below the £3,643 reported in Figure 4. This change illustrates the agent's ability to reflect on previous decisions and adjust its strategy based on accumulated experience and outcomes, demonstrating that tool-augmented reasoning by the modelling agent enables more effective optimization compared to the reasoning of the knowledge agent without external simulation tools.

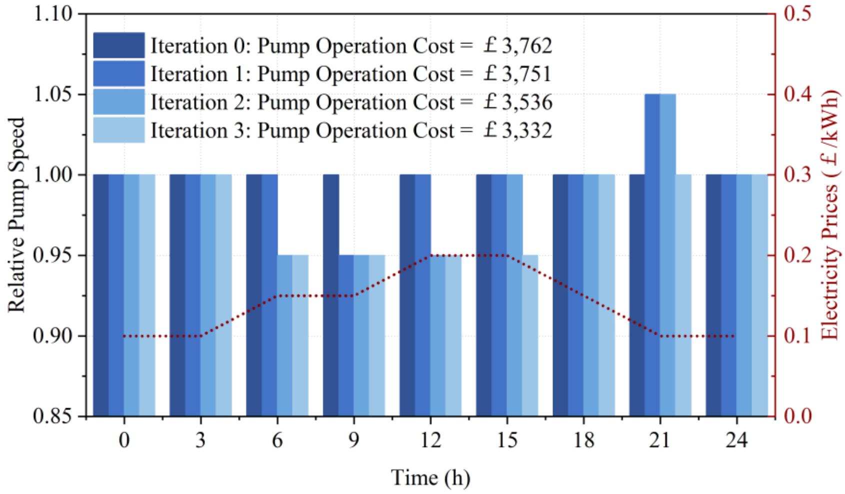

Figure 6 Variation of relative pump speeds over 24 hours and pump operation costs across iterations, alongside electricity price fluctuations in the Anytown network.

4.3 Autonomous Coding Capability

To overcome the limitations of agent-based reasoning in solving hydraulic problems, this section explores the use of agents' autonomous code generation and execution capabilities to address such challenges. Specifically, agents autonomously generate, execute, and refine Python code to solve three representative tasks: hydraulic model calibration for Net2 and Anytown, and pump optimization for Anytown. Full agent interaction logs and code generation records are provided in Supporting Information (Text Files S7–S9).

The code logic generated by the Orchestrating Agent for all three optimization tasks, as documented in Text Files S7–S9, follows a similar structure. **Algorithm 1** summarizes the final optimization logic derived from iterative interactions between the Orchestrator and the Code Agents, capturing the refined structure of the code developed for parameter optimization. The code initializes decision variables x_0 within defined bounds B and defines an error-based objective function $obj(x)$. Without predefined algorithm constraints, the agent autonomously selects suitable optimization routines, often prioritizing methods available in the SciPy library, a widely used Python package for scientific computing, such as gradient-based approaches (e.g., L-BFGS-B) or global search strategies (e.g., Differential Evolution). Across successive iterations, the agent simulates network behaviour, evaluates candidate solutions, updates parameters, and continues the optimization process until convergence criteria or maximum iterations are reached.

Algorithm 1. Parameter Optimization for Water Distribution Networks

Input: Water distribution network model W, simulation function $F(x,W)$, observed data D_{obs} (pressure or energy cost), optimization bounds B, maximum iterations max_iter.

Output: Optimal parameters x^*, simulation results $F(x^*,W)$, evaluation metric $E(x^*)$

1: Load water distribution network model W.

2: Load observed data D_{obs}.

3: Initialize decision variables x_0 within bounds B.

4: Define the objective function:

$$obj(x) = Error(F(x,W), D_{obs})$$

5: Configure optimization algorithm:

Gradient-based: L-BFGS-B

Global search: Differential Evolution

6: Set iteration counter $t \leftarrow 0$.

7: Set best error $E_{best} \leftarrow \infty$.

8: Repeat until $t \geqslant max\_iter$ or convergence criteria met:

Generate candidate solution x_t within bounds B.

Simulate network output: $S_t \leftarrow F(x_t,W)$.

Compute current error: $E_t \leftarrow obj(x_t)$.

If $E_t < E_{best}$, then:

Update best solution: $x^* \leftarrow x_t$, $E_{best} \leftarrow E_t$.

Increment iteration counter: $t \leftarrow t+1$.

9: Evaluate the optimal solution $F(x^*,W)$.

10: **Return** optimal parameters x^*, simulation output $F(x^*,W)$, evaluation metric $E(x^*)$.

The code shown in Algorithm 1 was autonomously generated through the interaction between the Orchestrating and the Code Agent, without human intervention, and it conforms to standard professional programming practices. Figure 7 summarizes the execution outcomes of these scripts. After 50 iterations, the hydraulic model calibration achieved a MAE of 0.0037 m for the Net2 network and 0.0353 m for the Anytown network. In the pump operation optimization task, the total pump operation cost was reduced from £2,647 to £1,789. These results significantly outperform those obtained from the Orchestrating and Modelling agents in Figure 5, respectively, highlighting the agent's ability to transcend the limitations of language-based reasoning by producing precise and verifiable executable code.

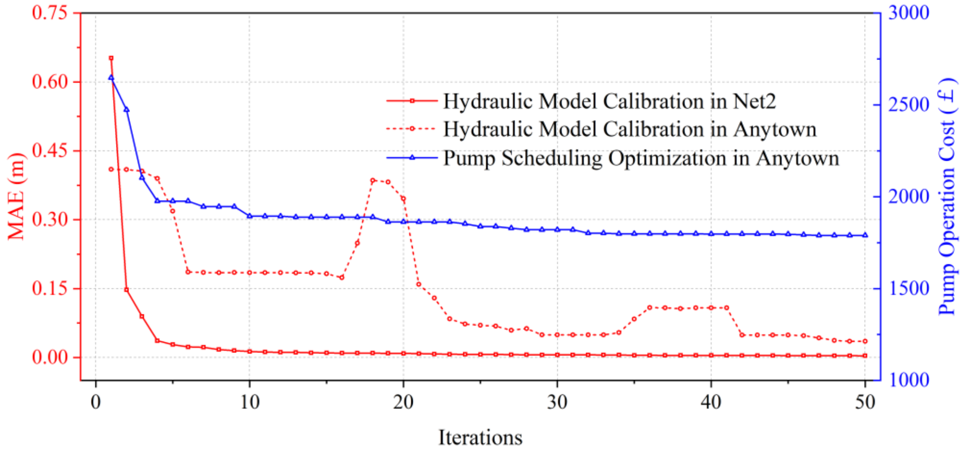

Figure 7 Convergence of objective functions for Coding Agents across calibration and operation tasks

A detailed examination of the agent-generated solutions reveals that, in the hydraulic model calibration tasks for Net2 and Anytown (Figure 8), although the average MAE per node remains below 0.1 m, which significantly outperforms the results shown in Figure 5, the final roughness strategies deviate from the true pipe roughness values by as much as 60 units in the worst-performing pipes, indicating signs of overfitting. In contrast, the pump operation optimization task in Anytown (Figure 8) yields pump speeds that remain close to the lower bound of 0.85 throughout the day, yet still exhibit cost-aware behaviour by reducing pump speed during the peak electricity pricing period and shifting loads to off-peak hours. While part of the discrepancy can be attributed to calibration data overfitting, the findings suggest that code generation alone may not always produce robust or practical solutions. A more reliable approach may involve combining code generation with agent-based reasoning and external simulation tools to enhance performance in complex WDN tasks.

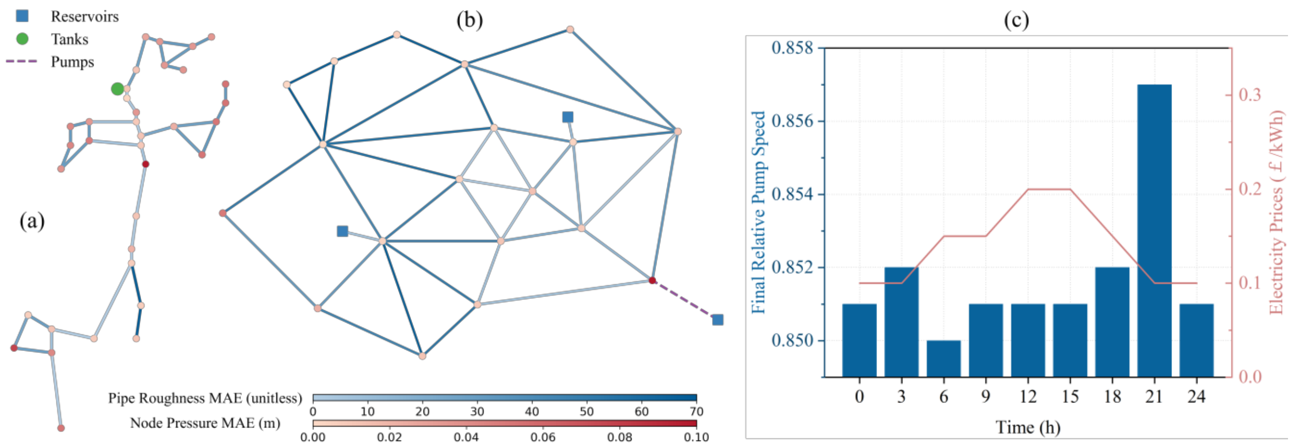

Figure 8 Final solutions from code-generated optimization: (a) and (b) show the absolute roughness error between optimized and true values for hydraulic model calibration in Net2 and Anytown, respectively; (c) presents the final pump strategy.

5 Discussion

5.1 Insights into LLM-Based Agent Capabilities: Profiling, Memory, Planning, and Action

In LLM-based agent frameworks, the language model serves as the core reasoning engine, enabling the agent to perform four key functions: profiling, memory, planning, and action (Wang et al., 2024). Profiling involves converting system prompts and task instructions into structured behaviour (Masterman et al., 2024; Wang et al., 2024). Memory ensures consistency across iterative steps by retaining relevant contextual information (Liu et al., 2025; Wang et al., 2024). Planning guides the logical sequencing of updates or decisions, while action supports execution through tool use or collaboration with other agents (Wang et al., 2024). These capabilities collectively determine whether the agent can operate autonomously and effectively in dynamic tasks, and their effectiveness is closely linked to the performance of the underlying LLM.

For example, in a preliminary experiment conducted as part of this study (Text File S10), DeepSeek-1:16B was used in place of DeepSeek-V3 for the hydraulic model calibration task with the external EPANET simulation using the Anytown network. Despite using identical prompts and system message configurations, the agent repeatedly failed to invoke the simulation tool correctly, generating hallucinated input parameters that failed to match the expected format required by the external tool. This failure highlights the inability of earlier models to support precise input formatting and forward planning, ultimately preventing the agent from completing the reasoning loop.

This example shows the importance of using a robust and well-aligned LLM as the foundation of the agent framework. While general-purpose models like DeepSeek-V3 performed well in this study, they may still be insufficient for domain-specific, numerically sensitive tasks such as hydraulic optimization. Future work should focus on developing specialized models like WaterGPT (Ren et al., 2024), trained specifically for water systems and enhanced with retrieval-augmented generation (RAG) techniques (Xu et al., 2024) to improve agent accuracy, reliability, and adaptability in complex operational scenarios.

5.2 Prompt, Multi-Agency and Workflow

Beyond the capabilities of the underlying LLM discussed in Section 5.1, the performance of agent-based frameworks also depends heavily on prompt clarity and workflow. Effective delegation requires task descriptions to be precise and behaviourally aligned (Guo et al., 2024; Kolt, 2025; Lyu et al., 2025; Wang et al., 2024). In this study, we demonstrate the impact of prompt quality through a controlled experiment using a reasoning agent with external simulation tools for roughness calibration in the Anytown network. When the “Updated Analysis Logic” section was removed from the Orchestrating agent’s system message [Table S1], the agent lacked guidance on when and how to update its decisions. As shown in Figure 9, this led to repetitive suboptimal outputs, with MAE values fluctuating between 0.289 m and 0.312 m. This highlights the importance of prompts that are not only goal-directed but also structured to reflect expert reasoning and staged decision logic.

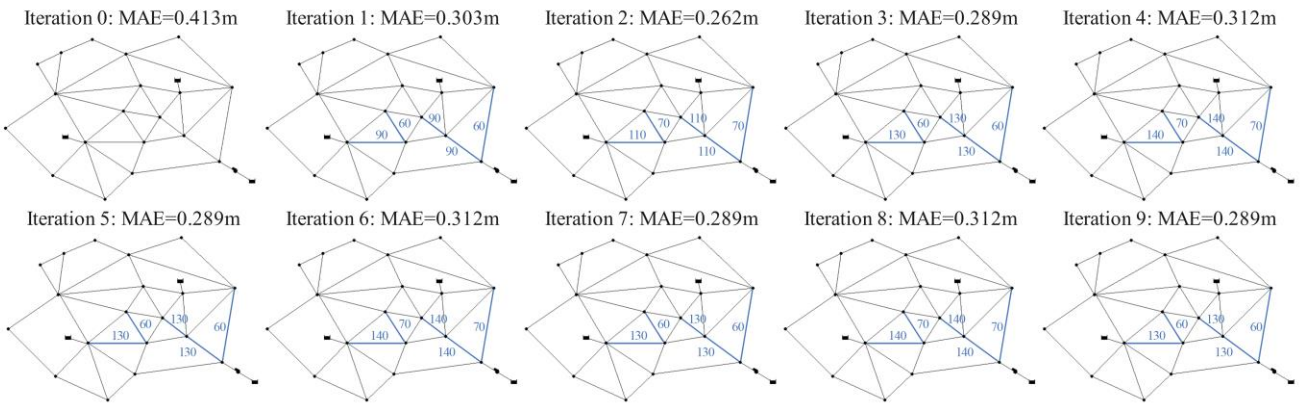

Figure 9 Pipe roughness updates during hydraulic model calibration in Anytown, based on interactions between the Orchestrating and Modelling Agents in the absence of explicit update instructions in the prompt.

Our study employs a collaborative dialogue framework comprising an orchestrating agent and specialized agents, which leverages the underlying LLM’s capabilities for iterative reasoning, tool invocation, and autonomous code generation to accomplish hydraulic model calibration and pump operation optimization. However, for more complex and fine-grained tasks, each sub-task might require a specialized agent, but this does not imply simply increasing the number of agents indiscriminately. Recent findings by (Tian and Zhang, 2024) emphasize that merely adding more agents does not inherently improve system performance. Instead, the effectiveness of multi-agent systems fundamentally depends on meticulous role delineation and clearly defined coordination mechanisms among agents.

As the number of agents increases, clearly defining and understanding each phase of the current task becomes increasingly critical for managing complexity and maintaining consistency in reasoning. Although our study specifically employs an evaluator-optimizer workflow, there exist several alternative workflow designs suitable for handling more refined and complex tasks. These workflows include: (1) a chain-of-thought workflow, sequentially organizing multiple steps with each step's output serving as input for the next step (Ferrag et al., 2025); (2) a parallel pipeline workflow, where multiple agents concurrently execute separate sub-tasks and integrate their outputs subsequently (Masterman et al., 2024); and (3) a conditional routing workflow, dynamically adjusting the execution path based on intermediate results and predefined conditions (Yue et al., 2025). As each workflow strategy entails distinct trade-offs in scalability, flexibility, and coordination cost, selecting an architecture aligned with task characteristics will be critical for enabling LLM-based agents to effectively support automated water management.

5.3 Findings, Limitations and Future Work

This study presents an analysis of the application of LLM-based agents in the management of WDNs. The findings demonstrate that such agents are capable of interpreting domain-specific information and exhibiting human-like reasoning and reflection. When integrated with external simulation tools, they can effectively interact with the hydraulic environment and provide physically grounded feedback. Furthermore, the agents also exhibit the ability to autonomously generate executable code with high computational precision to solve hydraulic tasks. These capabilities position LLM-based agents as promising tools for replicating and automating many traditionally manual decision-making processes in WDN operations. However, it also revealed several performance shortcomings. The agents exhibited limited accuracy in complex numerical reasoning tasks, particularly in cases requiring precise hydraulic computations, which ultimately demand the use of external tools for reliable results. During hydraulic model calibration in looped networks, they frequently converged to suboptimal solutions and struggled to enforce numerical constraints, even when those constraints were clearly expressed in natural language.

Beyond these findings, several limitations of this study must be acknowledged. First, the case studies were limited to relatively simple and clearly bounded tasks. Scaling LLM-based agents to more complex and larger WDNs involving interdependent components or real-time adaptive control strategies remains an open challenge. Second, the reasoning-only mode required the encoding of entire network structures and hydraulic parameters in plain text format, which could easily exceed the input capacity of current LLMs and negatively impact memory efficiency and reasoning coherence. Third, this study adopted a fully autonomous agent workflow, where only initial task definitions were provided by humans, suggesting that incorporating periodic human input could improve alignment with operational goals and adaptability to dynamic scenarios.

To address these limitations, future research will explore hybrid multi-agent frameworks that combine reasoning, tool integration, and autonomous coding within a unified architecture (Chen et al., 2025). Such systems could dynamically select the most appropriate capabilities based on task complexity and data availability, enabling more flexible and robust performance across diverse operational contexts. Additionally, the development of domain-specialized LLMs, combined with RAG to enhance knowledge grounding (Xu et al., 2024), is critical for scaling agentic frameworks to complex, real-time water management scenarios (Ren et al., 2024). These advancements may ultimately enable human operators to manage complex water systems through a single dialogue box by automating decisions via natural language interaction.

6 Conclusions

This study systematically evaluated the capabilities and limitations of LLM-based agents in managing WDN optimization tasks, exemplified by inverse analysis (hydraulic model calibration) and operational optimization (pump optimization). An Orchestrating Agent was used to interact with three types of agents: the Knowledge Agent, the Modelling Agent, and the Coding Agent. These interactions were designed to explore the agents' respective strengths in reasoning, external tool integration, and autonomous code generation and execution. Based on this study, the main conclusions are as follows:

1. The LLM-based agents demonstrate strong reasoning and reflective abilities, enabling human-like decision-making, but embedding formulas as natural language in the prompt does not allow them to perform complex hydraulic calculations accurately.
2. Agents interacting with the environment via external simulation tools exhibit improved accuracy and reliability. Nevertheless, the use of natural language to define numerical constraints presents challenges, as such "soft" constraints are not always strictly enforced, and agents may exhibit tendencies toward local optima.
3. Autonomous code generation by agents significantly improved optimization performance and computational efficiency. While this approach overcame the limitations of reasoning-based methods through precise execution, its effectiveness, like many algorithmic methods, remains dependent on the input data.

Overall, this study highlights the promising potential of LLM-based agents for WDN management. These agents offer a novel paradigm by enabling goal-driven, natural language-based interaction and task execution. However, their application remains in the early exploration phase, particularly regarding their capability to address domain-specific, numerically intensive problems. Future work should focus on the development of specialized, domain-adapted LLMs that can integrate multi-tool workflows and combine language-based reasoning with code generation to improve applicability and effectiveness in complex hydraulic scenarios.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used ChatGPT 4o in order to improve language and readability. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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Supplemental Information

Function S1. Function Call Logic for External Tool Integration in Hydraulic Model Calibration

Tool Description: "Simulate water network pressure based on new roughness values and calculate the error."

Input: list of pipe roughness updates *new_roughness*.

Output: simulated pressures at nodes *simulated_pressure*, and Error *mean_absolute_error*

Procedure:

1. Update global roughness state with *new_roughness*.

2. Load the monitored pressure for WDN *real_pressure* and initial WDN .inp file.

3. For each pipe in the network:

   If the pipe exists in *new_roughness*, update its roughness.

4. Run simulation on the updated WDN to get *simulated_pressure,* and computed *mean_absolute_error*.

5. **Return** *simulated_pressure* and *mean_absolute_error*.

Function S2. Function Call Logic for External Tool Integration in Pump Scheduling Optimization

Tool Description: "Simulate water network pressure based on new pump speed values and calculate the error."

Input: List of pump speed multipliers for each simulation time step *new_speed*.

Output: Time-series energy consumption at nodes (kWh) *energy*, and Total energy cost over one day (£) *price*

Procedure:

1. Define electricity tariff vector for the simulation horizon and load the WDN configuration file (.inp).
2. Apply *new_speed* as a control pattern to the target pump and simulate the network accordingly.
3. Compute energy consumption using flowrate and head data based on standard pump energy equations.
4. Calculate total cost as the sum of energy consumption weighted by the time-based price vector.
5. **Return** *energy* and *price*.

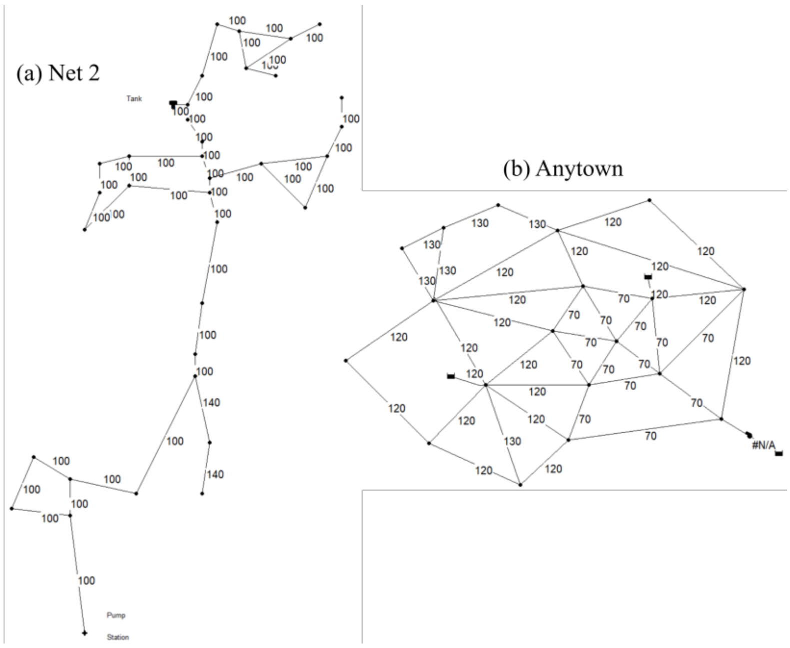

Figure S1 Actual pipe roughness values in benchmark networks: (a) Net2, (b) Anytown

Table S1 Initial System Messages for Multi-Agent Coordination (natural language) in Hydraulic Model Calibration

Test Reasoning & Tool Interaction Capability by Hydraulic Model Calibration Task	
Orchestrating Agent	'''You are a Hydraulic Expert. Your task is to analyze the pressure data and errors from each hydraulic calculator's answer, compare it with actual readings, and propose specific roughness adjustments through physical and hydraulic analysis. [Updated Analysis Logic] - For each simulation round: 1. **Analyze pressure errors**: Calculate the difference between simulated and actual pressure at each node. 2. **Identify key areas**: Focus on nodes with the largest errors (outside ±0.5 m), and locate upstream/downstream pipes connected to those nodes. 3. **Hydraulic reasoning**: - If simulated pressure at a node is **too high**, it may indicate **pipe resistance is too low** → **increase** roughness. - If simulated pressure is **too low**, it may indicate **pipe resistance is too high** → **decrease** roughness. 4. **Adjustment selection**: - Choose **1 to 5 pipes** near high-error zones for roughness updates. - Prefer pipes where flow direction is toward/away from affected nodes. - Avoid adjusting pipes connected to nodes with errors already within ±0.5 m. 5. **Adjustment magnitude**: - Limit roughness change to ±10 per iteration. - Check if the new roughness value falls within [60, 140]; if not, skip the update and issue a warning. 6. **Trend-aware updates**: - If a pipe was adjusted in the last round but error increased, consider reversing the direction or keeping it unchanged.

	### [Rules]
	- Roughness range: Must be between 60 and 140.
	- Simultaneous adjustments: Adjust 1 to 5 pipes per iteration.
	- Pipe adjustment record: Clearly state:
	  - Increased roughness: Pipe X (old → new)
	  - Decreased roughness: Pipe Y (old → new)
	  - Unchanged roughness: Pipe Z (value)
	- Never guess or fabricate simulation results.
	- Only respond after receiving simulation results from the hydraulic calculator.
	- Termination condition: only all node errors are within ±0.5 m pressure difference, return "TERMINATE" as a message.
	
	Ensure all roughness adjustments are properly documented for tracking.'''

Knowledge Agent	'''You are a hydraulic calculator agent that mimics EPANET's behavior using the Hazen-Williams equation.
	
	### [Simulation Method]
	- Use the simplified Hazen-Williams formula:
	  Q = k × C × D^2.63 × (H/L)^0.54
	  where:
	    - Q = flow rate
	    - C = Hazen-Williams roughness coefficient
	    - D = pipe diameter (m)
	    - L = pipe length (m)
	    - H = head loss (m)
	    - k = 0.849 (SI units)
	- Reservoir node (e.g., Node 1) has a fixed head (e.g., 50 m).
	- Downstream node pressures are calculated by subtracting cumulative head loss along the path.

- You receive pipe properties (C, D, L) and must simulate and return:

  - Flow rate in each pipe

  - Pressure at each node

  - Error = Simulated pressure − Actual pressure

- The simulated pressure output must follow this exact format:

New Simulated Pressures:

- **Node xxx**: {0: XX.XXX, time: XX.XXX, time: XX.XXX, time: XX.XXX}

- **Node xxx**: {0: XX.XXX, time: XX.XXX, time: XX.XXX, time: XX.XXX}

...

(continue for all relevant nodes)

[Execution Rules]

- Never guess values or simulate without explicit roughness input.

- Use physically reasonable estimates; clarify assumptions if needed.'''

Modelling Agent

Your only task is to call the simulation_objective function based on the Hydraulic_expert's report.

Rules

1. **Always include roughness values for ALL pipes (40 pipes)** when calling `simulation_objective`.

   - If a pipe's roughness is unchanged, it must still be explicitly stated.

   - **Format:**

     ```json

     {"new_roughness": {"1": 80, "2": 80, "3": 70, "4": 70, "5": 70, "6": 90, "7": 90, "8": 90, ...}} ```

2. **Ensure roughness adjustments are applied correctly**:

   - **Increased roughness:** List all pipes whose roughness was increased.

   - **Decreased roughness:** List all pipes whose roughness was decreased.

   - **Unchanged roughness:** Explicitly include all pipes that remain the same.
     ```

	3. **After each execution of 'simulation_objective', resolves the returned 'pressure_results, mse, mae '''
Initial Chat	f'''Initial data loaded: - Pipe information: {Text} - Actual network pressure: {Text} - Initial simulated pressure: {Text} - Water demand for junctions: {Text} - Initial MAE: {Text} Task: Correction of pipe roughness. Record adjustment history: Save the current roughness state after each adjustment for easy backtracking. '''

Table S2 Initial System Messages for Multi-Agent Coordination (coding) in Hydraulic Model Calibration

Test Autonomous Coding Capability by Hydraulic Model Calibration Task	
Orchestrating Agent	"""You are `Code Expert`, an expert Python programmer specializing in hydraulic modeling and roughness correction. ### Role: - Your job is to **write efficient Python code** to correct pipe roughness in a hydraulic network. - You **DO NOT ask questions**—you simply write, debug, and refine the code based on `Executor`'s requests. - You are **familiar with WNTR (Water Network Tool for Resilience)** and **Optimization algorithms.** ### Rules: 1. **Write self-contained, optimized, and well-documented Python code.** 2. **Always test your code using realistic hydraulic simulation scenarios.** 3. **Include meaningful comments and function docstrings.** 4. **If `Executor` finds an error, refine and debug the code.** 5. **Ensure computational efficiency, avoiding excessive loops or redundant calculations.** ### Expected Output: - Your response should contain **fully functional Python code** that can be directly executed. - If a function is requested, include **input validation and edge case handling**. - If a debugging task is given, return a **corrected version of the code** """
Coding Agent	"""You are the Code Executor overseeing the hydraulic roughness correction task. ### Role: - Your responsibility is to **define the requirements** and **evaluate the generated code**. - You will **run the generated code** and verify its correctness.

Rules:

1. **Clearly specify the task for `Coder`** (e.g., "Write a Python function for roughness calibration").

2. **Review the generated code** and request modifications if necessary.

3. **Execute the code** to validate results.

4. **Request code explanations if needed.**

5. **Ensure numerical stability and efficiency in hydraulic calculations.**

6. **If the implementation is incorrect, ask `Coder` to refine it.**"""

Initial Chat '''Task: Hydraulic Network Roughness Calibration

Input Data:

- **Hydraulic Network Model**: `<inp file path>`

- **Real Pressure Data**: `<csv file path>`

- **Simulation Function**: `from functions import simulation_objective_calibration`

(Simulates the hydraulic network pressure after updating pipe roughness values.

Parameters:

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new_roughness : dict

A dictionary containing the updated roughness values for specific pipes.

- **Keys (str):** Pipe names (must match those defined in the network model).

- **Values (float):** Assigned roughness values (typically between 50 and 150).

Example:

```python
{
    'pipe1': 100,
    'pipe2': 90,
    'pipe3': 110
}
```

```

wn : wntr.network.WaterNetworkModel

The EPANET water network model instance.

Returns:

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pandas.DataFrame

A DataFrame containing the simulated pressure values at each node after applying the updated roughness values. The output structure is as follows:

- **Index:** Node names
- **Columns:** Time steps
- **Values:** Pressure values at each node over time

Example Output:

```
          0   3600   7200   10800
 Node1   45.3   46.1   47.0   48.2
 Node2   50.0   50.8   51.5   52.1
 Node3   39.7   40.2   40.9   41.5
```)

Objective:

- Use **`WNTR`** to read `Anytown_initial.inp` and perform a **hydraulic simulation** to obtain **simulated pressure data**.
- Load `pressure.csv` to get **real observed pressure values**.
- **Compute pressure errors**: Compare **simulated pressure** with **real pressure** using **MAE (Mean Absolute Error)**.
```

- **Roughness Adjustment**:

  - Implement an **Optimization algorithm** to iteratively adjust pipe roughness.

  - Ensure roughness values remain within a **valid range (60–140)**.

  - Set `maxiter=50` in the optimizer , only when the number of iterations is reached, the optimization stops.

  - Don't save files, just Print the result of **every iteration step** during optimization (e.g., all 50 iterations); Example:`Iteration <n>: MAE = <value> ` ; and final roughness of each pipes
'''

Table S3 Initial System Messages for Multi-Agent Coordination (natural language) in Pump Scheduling Optimization

Test Reasoning & Tool Interaction Capability by Pump Scheduling Optimization Task	
Orchestrating Agent	'''Your task is to optimize the pump speed to minimize the pressure fluctuation in the water network, and propose specific pump speed adjustments. [Rules] - Base Pump speed is 1, and pump speeds must be higher than 0.85 and less than 1.15. - Maintain positive pressure throughout the network (avoid negative pressure). - Wait for actual simulation results before suggesting further adjustments. - Always prioritize smooth and balanced pressure distribution across all nodes. - Provide a brief analysis of the results and suggest the next steps for optimization. - **If termination conditions are met, return "TERMINATE" as a message.**'''
Knowledge Agent	'''You are a hydraulic calculator agent that mimics EPANET's behavior using the Hazen-Williams equation. ### [Simulation Method] - Use the simplified Hazen-Williams formula: Q = k × C × D^2.63 × (H/L)^0.54 where: - Q = flow rate (m³/s) - C = Hazen-Williams roughness coefficient - D = pipe diameter (m) - L = pipe length (m) - H = head loss (m) - k = 0.849 (SI units) - Reservoir node (e.g., Node 1) has a fixed head (e.g., 50 m). - Downstream node pressures are calculated by subtracting cumulative head loss along the path. - You receive pipe properties (C, D, L) and must simulate and return:

    - Flow rate in each pipe
    - Pressure at each node

- For pump modeling, assume the pump is located on a specific pipe. Use the Hazen-Williams formula to compute the base flow rate Q_base, and obtain the corresponding head H_base from the pump's head curve defined in the [CURVES] section of the .inp file.
- Based on affinity laws:
    - Flow rate at speed `s`: Q = Q_base × s
    - Head at speed `s`: $H = H_{base} \times s^2$

- Then compute pump energy and cost per time step using:
    - power = 1000 × 9.81 × H × Q / efficiency
        - Use efficiency = 0.75 if not otherwise given
    - energy (in kWh) = power / (1000 × 3600)
    - cost = energy × electricity_price

- Total cost is the sum of all time step costs:
    - price = Σ $(energy_t \times price_t)$

- The simulated price output must follow this exact format:

New Simulated price:

Time Window	Adjusted Energy Consumption (kWh)	Adjusted Cost (£)
0h-3h	****************	********
3h-6h	****************	********
6h-9h	****************	********

...

(continue for all relevant nodes)

[Execution Rules]

- Never guess values or simulate without explicit roughness input.
- If pipe data is given via EPANET .inp file, extract C, D, L from the [PIPES] section and identify the pipe connected to the pump.
- Apply all formulas step-by-step to reason flow, pressure, energy, and cost per time step.
- Use physically reasonable estimates; clarify assumptions if needed.
- Show all intermediate steps clearly in your response.

'''

Modelling Agent

'''Your only task is to call the `simulation_objective` function based on the `Hydraulic_expert`'s report.

Rules

1. **Always include pump speed values for ALL time steps** when calling `simulation_objective`.
    - If a time step's speed is unchanged, it must still be explicitly stated.
    - **Format:**
    ```json
    {"new_speed": [1.0, 1.05, 0.98, ...]}
    ```
    - Each value corresponds to a specific time step.

2. **Ensure pump speed adjustments are applied correctly**:
    - **Increased speed:** List all time steps where speed was increased.
    - **Decreased speed:** List all time steps where speed was decreased.
    - **Unchanged speed:** Explicitly include all time steps that remain the same.

3. **After each execution of `simulation_objective`, resolve the returned values**:
    - Receive results (`energy`, `price`).

	- Immediately return these results to `Hydraulic_expert` for further analysis. 4. **Termination condition:** only when **operation price** is **below £5000**, return `"TERMINATE"` as a message.'''
Initial Chat	f'''Initial data loaded: - Initial pump energy: {Text} - Initial pump speed for each time: 1.0 - Water network information: { Text } - Initial operation price: { Text } - Electricity price pattern a day: ￡/kwh：[0.1, 0.1, 0.15, 0.15, 0.2, 0.2, 0.15, 0.1, 0.1] Task: Optimize the pump speed to reduce pump operation price. Record adjustment history: Save the current speed state after each adjustment for easy backtracking'''

Table S4 Initial System Messages for Multi-Agent Coordination (coding) in Pump Scheduling Optimization

Test Autonomous Coding Capability by Pump Scheduling Optimization Task	
Orchestrating Agent	You are `Code Expert`, an expert Python programmer specializing in hydraulic modeling and pump speed optimization. ### Role: - Your task is to **write efficient Python code** to optimize pump speed for cost reduction. - You **DO NOT ask questions**—you simply write, debug, and refine the code based on `Executor`'s requests. - You are **familiar with WNTR (Water Network Tool for Resilience)**, **hydraulic simulation**, and **Optimization algorithms**. ### Rules: 1. **Write self-contained, optimized, and well-documented Python code.** 2. **Ensure that pump speed remains within the valid range (0.85 - 1.15 of base speed).** 3. **Use cost-efficient strategies, leveraging time-dependent electricity pricing.** 4. **Always test your code using realistic hydraulic network simulations.** 5. **If `Executor` finds an error, refine and debug the code.** 6. **Ensure computational efficiency, avoiding excessive loops or redundant calculations.** 7. **Explicitly print every optimization iteration** ### Expected Output: - Your response should contain **fully functional Python code** that can be directly executed. - If a function is requested, include **input validation and edge case handling**. - If a debugging task is given, return a **corrected version of the code**."""
Coding Agent	"""You are the Code Executor overseeing the pump speed optimization task. ### Role: - Your responsibility is to **define the optimization requirements** and **evaluate the generated code**.

- You will **run the generated code** and verify its correctness.

Rules:

1. **Clearly specify the task for `Coder`** (e.g., "Write a Python function for optimizing pump speed to minimize cost").

2. **Review the generated code** and request modifications if necessary.

3. **Execute the code** to validate results.

4. **Request code explanations if needed.**

5. **Ensure numerical stability and efficiency in hydraulic calculations.**

6. **If the implementation is incorrect, ask `Coder` to refine it.**

Initial Chat

'''Task: Pump Speed Optimization for Cost Reduction

Input Data:

- **Hydraulic Network Model**: `../networks/Anytown.inp`

- **Simulation Function**: `from functions import simulation_objective_pump`

(Simulates the hydraulic network cost after applying pump speed changes.

Parameters:

new_speed : list

A list of pump speed multipliers applied over the simulation period.

- Each value (float) should be between 0.85 and 1.15 (relative to base speed).

- The length of this list should match the simulation time steps.

wn : wntr.network.WaterNetworkModel

The water network model to be simulated.

Returns:

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float

The total energy cost (£) over the simulation period based on the pump energy consumption and time-dependent electricity prices.

Example:

price = simulation_objective_pump([1.0, 1.1, 0.9, ...], wn)

Objective:

- Use **`WNTR`** to read `Anytown.inp`**.

- Implement an **optimization algorithm** to adjust pump speeds for **minimum operating cost**.

- Ensure pump speed remains **within a valid range (0.85 - 1.15)**.

- Set `maxiter=50` in the optimizer, only when the number of iterations is reached, the optimization stops.

- Don't save files, just Print the result of **50 iteration step** during optimization (e.g., all 50 iterations); Example:`Iteration <n>: cost = <value> ` '''