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Modelling the potential for water quality failures in distribution networks: framework (I)

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ABSTRACT

The deterioration of water quality can adversely affect consumers' health as well as the aesthetic properties of water (taste, odour, colour). To date, little consideration has been given to the impact of deteriorating (ageing) water mains on water quality as a major decision driver for the renewal/rehabilitation of water mains. The main objective of this research was to identify major deterioration mechanisms in distribution networks that may contribute to water quality failures (WQF) and develop a model to quantify overall potential for WQF as a function of this deterioration. Numerous factors affect water quality in the distribution network and interactions among them are complex and often not well understood. Water quality failures in distribution networks are relatively scarce, which makes it difficult to establish statistically significant generalizations. In such data-sparse circumstances, expert knowledge and judgement can serve as a supplement or even as alternative source(s) of information. This paper discusses major deterioration mechanisms that may contribute to WQFs in distribution networks, and proposes a modelling framework using fuzzy-based methods. The following two papers in this series will provide a mathematical formulation of the proposed model and its application using two case studies, respectively.

Key words | distribution networks, fuzzy-based methods, potential for water quality failure, water quality models

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MECHANISMS FOR WATER QUALITY DETERIORATION

A typical modern water supply system comprises the water source (aquifer or surface water including the catchment basin), treatment plants, transmission mains and the distribution network, which includes distribution pipes, storage tanks and pumping stations. While water quality can be compromised at any component, failure at the distribution level can be extremely critical because it is closest to the point of delivery and, with the exception of an occasional point of use filtering device, there are virtually no safety barriers before consumption.

The management of water quality encompasses a variety of factors, in both the design and the operation stages. In the design stage, water source(s) is/are selected and the appropriate water treatment facilities are identified. In the operational stage, several measures are required to maintain an acceptable level of water quality, including water quality monitoring/sampling protocols, minimization of 'water age' in the distribution network, administration of effective cross-connection control programmes, maintenance of an adequate balance between residual chlorine and disinfection by-product (DBP) formation, inspection and maintenance of storage tanks and, finally, monitoring and control of the impact of deteriorated water mains on the water quality in the network (Leland 2002). In this research project the focus was on the latter aspect of water quality management.

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The causal relationships between factors affecting water quality in the distribution network due to deteriorating water mains are quite complex and intertwined. Diagnostic of contamination events in water distribution networks is a difficult task because of several factors. A water distribution network can comprise (depending on the size of the water utility) thousands of kilometres of pipes of different ages and materials. The operational and environmental conditions under which these pipes function may vary significantly depending on the location of the pipes within the network. Further, field data are not generally available since the pipes are not readily accessible and visible, making it relatively difficult and expensive to collect data on their performance and deterioration. In addition, some factors and processes affecting pipe performance are not completely understood. Finally, it is often difficult to determine or validate an exact cause for water contamination or waterborne disease outbreak because such episodes are often investigated long after their occurrence has ended (Sadiq *et al.* 2003).

The water distribution network can be perceived as a complex chemical reactor in which various processes occur simultaneously. The water quality in the distribution network is an outcome of these processes, continuously changing both temporally and spatially. The *Guidance Manual for Maintaining Distribution System Water Quality* (Kirmeyer *et al.* 2000) makes the analogy between water and a perishable product, where shelf life, packaging and preservatives are analogous to 'water age', distribution pipes and disinfection residuals in the distribution network, respectively. Figure 1 provides a simplified conceptual map that partially captures this complexity (Sadiq *et al.* 2003). It illustrates the interactions between the bulk water, the pipe and its surrounding environments and operational factors.

Referring back to the analogy between the water distribution network and a chemical reactor, one can envisage the degradation of water quality as a result of two conceptual processes, namely, the introduction of 'quality-effecting factors' into the reactor and the physico-chemical/microbiological reactions that continuously occur inside the reactor. The 'quality-effecting factors' may be introduced into the reactor in a variety of ways, as described below. The reactions inside the reactor are governed by 'quality-effecting factors' as well as by the physicochemical and biological characteristics of the main medium in the reactor, which in our analogy is bulk water.

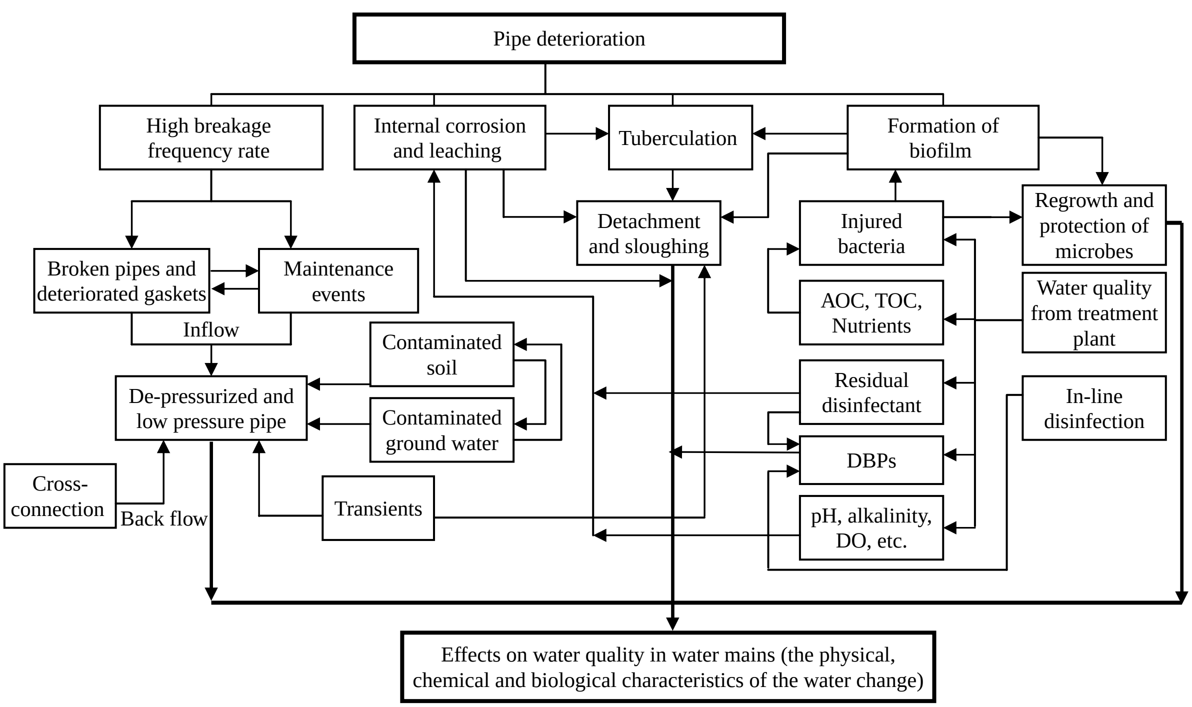


Figure 1 | Conceptual map for water quality failures in water mains (Sadiq *et al.* 2003).

Several mechanisms can compromise water quality within a distribution network. These include (Kleiner 1998):

- intrusion of contaminants into the distribution network through system components whose integrity is compromised or through misuse or cross-connection or deliberate introduction of harmful substances in the water distribution network;
- formation of corrosion by-products and leaching of chemicals from the internal pipe surface;
- regrowth of microorganisms in the distribution network;
- formation of disinfection by-products (DBPs) and loss of residual disinfectants;
- permeation of organic compounds from the soil through plastic components into the distribution network.

As water travels through pipes, its quality undergoes various transformations, affected by the properties of the finished water, flow velocity, water temperature, pipe material, condition of the inner surfaces of the pipes walls, and deposited materials (i.e. sand, iron, manganese). The USEPA White Papers (2004) also lists 'water age' (or residence time) as a major contributory factor to bulk water quality deterioration in distribution networks. However, contrary to specific water quality deterioration mechanisms, 'water age' affects water quality only indirectly, because most of the deterioration processes are time dependent and increasing 'water age' leads to poor water quality in the distribution network (Committee on Public Water Supply Distribution Systems 2005).

WATER QUALITY FAILURES (WQFS)

In this as well as in the subsequent papers, the term water quality failure (WQF) means a potential hazard/threat or an actual non-compliance with regulations (or guidelines or self-imposed limits) of one or more water quality indicators, or customer complaints, or a possible failure to meet the water quality objectives set by a water utility (see water quality regulations relevant to distribution systems in Table 1). Water quality failures can be classified as microbiological (M-WQF), physicochemical (P-WQF) or aesthetic water quality failures (A-WQF).

Microbiological water quality failure (M-WQF) can occur through several pathways and sources and is potentially the single most devastating type of water quality event that can occur in the distribution network. Typically, the maintenance of residual disinfectant in the distribution network at a target level is used to protect against microbiological failure, and therefore loss of residual disinfectant is considered an indicator for a possible water quality failure. The US EPA Total Coliform Rule (TCR) is promulgated to protect public water supplies from adverse health effects associated with disease-causing pathogens, which may enter into the distribution network through pathway(s) identified earlier. The TCR requires monitoring of total coliforms in water distribution networks, and in the case of positive test results, it requires verification through the testing of faecal coliform or *E. coli*. A positive verification implies MWQF.

The US EPA Surface Water Treatment Rule (SWTR) covers all water supply systems that use surface water or groundwater under the direct influence of surface water. This rule is intended to protect against exposure to pathogens such as *Giardia lamblia* and *Legionella* viruses. The SWTR requires that the disinfectant (residual chlorine) dose be at least $0.2\,\mathrm{mg\,l^{-1}}$ at the point of entry and disinfectant residual be detectable in all parts of the distribution network. Any failure to meet the prescribed residual disinfectant limits is considered a MWQF. Similarly, the US EPA the Stage 1 D/DBPR (disinfectants/disinfection by-products rule) establishes maximum residual disinfectant levels (MRDL) for chlorine, chloramine and chlorine dioxide, and maximum contaminant level (MCL) for DBPs (trihalomethanes, haloacetic acids). The rule requires the removal of specified percentages of organic materials (precursors), which can react with disinfectants to form DBPs. These limits can also be associated with physicochemical water quality failures (P-WQF). Details of these regulations can be found on the US EPA website (http://www.epa.gov/).

Craun & Calderon (2001) compiled data about US waterborne disease outbreaks over the period 1971–1998. More than 18% of outbreaks reported in public water systems (PWSs) were caused by chemical and microbiological contaminants entering the distribution network or as a consequence of aggressive water that was corrosive to

Table 1 | Water quality parameters and associated regulations for water distribution network* (modified after Kirmeyer *et al.* 2000)

WQI	Sampling location	Regulatory limit	Regulation
Disinfectant residual	At the entering point in the distribution network	$> 0.2\,\mathrm{mg\,l^{-1}}$ on continuous basis	SWTR
Turbidity	After direct and conventional filtration	≤ 0.3 NTU (95% of the time)	IESWTR†
		≤ 1 NTU (maximum)	
Disinfectant residual	Distribution network	MRDL chlorine $4.0\,\mathrm{mg\,l^{-1}}$, MRDL chloramine $4.0\,\mathrm{mg\,l^{-1}}$, annual average	Stage 1 D/DBPR
Disinfectant residual or HPC bacteria count	Distribution network	Detectable level of disinfectant residual or HPC bacteria $\leq 500\,\mathrm{cfu\,ml^{-1}}$ in 95% of the samples collected each month for any two consecutive months	SWTR
TTHM (Total THMs)	Distribution network	$80\,\mathrm{\mu g\,l^{-1}}$, running annual average based on quarterly samples	Stage 1 D/DBPR
		$80\,\mathrm{\mu g\,l^{-1}}$, LRAA based on quarterly samples	Stage 2 D/DBPR
HAA_5	Distribution network	$60\,\mathrm{\mu g\,l^{-1}}$, running annual average based on quarterly samples	Stage 1 D/DBPR
		$60\,\mathrm{\mu g\,l^{-1}}$, LRAA based on quarterly samples	Stage 2 D/DBPR
Total coliform	Distribution network	$<5\%$ positive (large systems)	TCR
Lead and Copper	Customer's tap	Pb: $0.015\,\mathrm{mg\,l^{-1}}$ at 90%	LCR
		Cu: $1.3\,\mathrm{mg\,l^{-1}}$ at 90%	
pH	Representative points in the distribution network	Each system determines optimized corrosion control	LCR

*In addition, US EPA has established National Secondary Drinking Water Regulations that set non-mandatory water quality standards for 15 contaminants. The US EPA does not enforce these secondary maximum contaminant levels (SMCLs). They are established only as guidelines to assist public water systems manage their drinking water for aesthetic considerations, such as taste, colour and odour. These contaminants are not considered to present a risk to human health at the SMCL.

†Interim Enhanced Surface Water Treatment Rule (IESWTR) is designed to improve control of microbial pathogens and prevent inadvertent reductions in microbial safety as a result of DBP control efforts. The IESWTR is promulgated to improve public health by increasing the level of protection from exposure to *Cryptosporidium* and other pathogens in drinking water supplies through improvements in the filtration at water treatment plants.

HAA_5: haloacetic acids; HPC: heterotrophic plate counts; RAA, LRAA: running annual average, locational running annual average; MRDL: maximum residual disinfectant rule; TTHM: total trihalomethanes; D/DBP: disinfectant/disinfection by-product rule; LCR: lead and copper rule; SWTR: surface water treatment rule; TCR: total coliform rule; IESWTR: interim enhanced surface water treatment rule.

plumbing systems within buildings and homes (M-WQF and P-WQF). Their study concluded that distribution networks contributed to a significant number of waterborne disease outbreaks, caused illness among large populations (i.e. widespread) and also caused illness that results in hospitalization and even death (i.e. severe).

Kirmeyer *et al.* (2000) identified and ranked important water quality concerns and issues with respect to public and utility perception and satisfaction. They also identified various studies in Europe and North America, which ranked public expectations regarding water quality concerns (Table 2). Utilities representing various jurisdictions in Canada and the USA ranked *microbial safety* as the highest priority, followed by *disinfectant residual* maintenance, *taste and odour*, *corrosion control* and *DBP formation* (two rightmost columns in Table 2). Each water quality issue/concern may be related to a multitude of sources and mechanisms of contamination and requires various remedial and mitigative decision actions (interventions) to maintain water quality at an acceptable level. Therefore, high uncertainties are inherent in any measure of risk that may be assigned to the distribution network.

Table 2 | Ranking of major water quality concerns in distribution networks

Water quality issues and concerns	Primary concerns*	Stanford (1996)†	Smith (1997)	Osborn (1997)‡	Kirmeyer et al. (2001)	
					Customer	Utilities
Microbial safety	M-WQF	X	3	1	1	1
Free of excess chlorine residual	P-WQF				2	
Taste and odour (T&O)	A-WQF	X	1	2	3	3
Good appearance	A-WQF	X	2		4	
Uniform water quality	A-WQF				5	
Disinfectant residual	M-WQF					2
Corrosion control	P-WQF; AWQF					4
DBPs formation	P-WQF					5
Others			4			

*P-WQF: physicochemical WQF; M-WQF: microbiological; A-WQF: aesthetic WQF.
†No ranking was provided.
‡AwwaRF 357 Project: Customer Survey, e-mail to K. Martel, 30 September 1997.

Taste and odour (T&O) as well as appearance (e.g. discoloured or red water) problems are aesthetic water quality failures (AWQF), which are a major concern to water utilities because of customer complaints and public perception of the water quality (Table 2). Taste and odour could point to biological activities, higher disinfectant levels, presence and continuing reactions of DBPs, leaching of materials and blending factors (Khiari *et al.* 2002). Suffet *et al.* (1993) reported that 65% of the T&O problems in 388 water utilities surveyed across the USA occurred in the distribution networks.

WATER QUALITY MODELLING IN DISTRIBUTION NETWORKS

Several factors make water quality modelling in distribution networks a very complex and challenging task. These factors include the aforementioned interactions between quality of the water entering the network, residence time, material type, size and condition of the pipes, external environment and operational conditions. Further, concentrations of contaminants may continuously change over time and space because of simultaneous occurrences of physicochemical, biochemical and biological processes in the network.

Although research on water quality modelling in distribution networks started appearing in the literature in the early 1970s, it only gained a significant boost in the last 15–20 years as a result of advances in affordable computing power and the development of new mathematical computing techniques. For example, water utilities are increasingly relying on hydraulic simulators coupled with water quality modules (e.g. EPANET) to predict indicators such as residual chlorine and DBPs in the distribution network. The effective use of properly calibrated models can help establish monitoring protocols, maintain water quality in the distribution network through improved design and operational practices, and ultimately lead to a better decision-making process to replace/renew ageing pipes. In addition, water quality models can help attain control over operational parameters (e.g. pH and chlorine dose), enable the study of the effects of upgrading physicochemical treatment processes and help generate operational and water quality knowledge for epidemiological studies (Rodriguez *et al.* 2000).

Recently, *ASCE Journal of Water Resources Planning and Management* published a special issue on 'Drinking water distribution systems security', which included 13 technical papers encompassing a wide spectrum of techniques to model the deliberate injection of chemical or biological contaminant into the distribution networks (Ostfeld 2006). These innovative tools can also be useful for modelling water quality deterioration in distribution networks. Similarly, *Urban Water Journal* also published a special issue on 'Water quality in distribution systems', which included six technical papers on this topic (Maksimovic & Butler 2005). Distribution networks modelling can be divided into four major areas of application: (1) water quality parameters; (2) hydraulics; (3) pipe failure/deterioration; and (4) risk/reliability.

Modelling of water quality parameters in the distribution network generally uses reaction kinetics of physico-chemical, biochemical or biological processes. Goodrich (1989) provided a summary of various kinetic reactions that occur within the distribution network, including those associated with decay of disinfectants, DBP formation, and biofilm adhesion, growth and detachment. Other kinetics models to predict chlorine decay include power-law decay (*n*th order), first order decay with stable components, power-law decay with stable components (nth order) and parallel first order decay models. The effective use of kinetic approaches for water quality modelling is very helpful in the initial evaluation of the distribution network. These models can determine the locations of critical concentrations of residual disinfectants and DBPs as well as predict internal corrosion and biofilm growth and detachment processes in the distribution network. A wealth of literature is available on a series of experimental studies conducted on biofilm growth kinetics in the laboratory and at bench scale levels (LeChevallier 1991). In addition, empirical models use multivariate regression and neural network to relate DBP concentrations to various combinations of explanatory variables, including water quality and operational parameters associated with disinfection (Sadiq & Rodriguez 2004*a*).

Initial efforts to develop water quality models for contaminant transport and fate in distribution networks used a steady state hydraulic modelling approach. Subsequent efforts used a dynamic modelling approach: for example, dynamic water quality model (DWQM), which was used to predict chloroform, trihalomethane (THM) and hardness in the distribution network (US EPA 1999). Subsequent to the development of DWQM, Rossman (1994) and Rossman *et al.* (1994) developed a model based on mass transfer, for the prediction of chlorine decay in the distribution network. As mentioned above, the model used first order kinetics for the bulk water and at the pipe wall. The EPANET software (a network hydraulics simulation program developed by Rossman) was used as platform for this model. EPANET uses extended period simulation (quasi-dynamic approach) to solve both hydraulics and water quality behaviour at predefined nodes in the network. EPANET has proved useful to predict both total THM and disinfection residuals in the network. Recently, Munavalli & Kumar (2004) proposed a hybrid method, EDMNET, based on the Lagrangian time-driven method (TDM) and Lagrangian event-driven method (EDM), which appears to have a better prediction power than both TDM and EDM methods individually. Most existing commercial software applications contain water quality modules, which are coupled with hydraulic simulators.

There is a large body of literature available on work related to pipe failure/deterioration in a distribution network. Comprehensive reviews of published work on two types of model, namely mechanistic (physical-based) and statistical models, have been reported in Rajani & Kleiner (2001) and Kleiner & Rajani (2001), respectively.

In the above three applications, the modelling efforts focus on a specific aspect of a distribution network, whereas in risk-based analysis, all aspects of a distribution network are considered simultaneously. The approach discussed in this paper falls within this latter area of application.

Risk-based analysis

The attractiveness of risk-based models stems from the fact that risk can be viewed as a common denominator that allows us to consider non-commensurate properties (effects and objectives, such as pressure, contaminant intrusion, structural reliability) in a single measure, defined as a composition of *likelihoods* and *consequences*. Risk-based models generally include hydraulic simulations with considerations of pipe breakage data, soil conditions, contaminant sources, pipe location and so on. Table 3 provides a non-exhaustive list of risk-based models and their associated attributes.

Besner *et al.* (2001) developed a framework that integrates a hydraulic model with a database representing water quality indicators and pipe condition (breakage rate data) at various locations in the network. One of the objectives of this research was to include structural, operational and water quality indicators to predict the microbial quality of the water. Lindley (2001) superimposed the *likelihood* of failure events (intrusion) with 'population at risk' to prioritize the rehabilitation of water mains.

Table 3 | Recent applications of risk-based water quality modelling for distribution networks

Reference	Model type	Model output	Parameters/inputs/data	Risk type
Besner *et al.* (2001)	Hydraulic simulator, GIS, pipe breakage rate data base	Overlaying layers of different indicators (pressure), residual chlorine etc.	Pipe age, diameter, C-factor, length, pipe break data, material, velocity, pressure, Reynolds number, residence time	Health/public safety
Lindley (2001)	Hydraulic simulator, probabilistic methods	Intrusion susceptibility	Pressure, pathway and contaminant source	Reliability-based; health/public safety
Mamlook & Al-Jayyousi (2003)	Fuzzy logic	Leakage detection	Pipe age, pipe material, operational aspects and demand patterns	Reliability-based
Howard *et al.* (2004)	Point scoring method, GIS	Risk maps	Pipe age, diameter, length, material, pressure and soil corrosion, source of contaminants, population at risk	Health/public safety
Vairavamoorthy *et al.* (2004, 2007)	GIS, fuzzy logic	Intrusion susceptibility	Potential pollution areas, contaminant concentration, pipe condition state	Reliability-based
Sadiq *et al.* (2004, 2007, 2008)	Fuzzy logic	Aggregative risk	Various water quality failure mechanisms in distribution system	Reliability-based
Makropoulos & Butler (2004, 2005, 2006); Makropoulos *et al.* (2003)	GIS, fuzzy logic	Risk maps (based on risk attitude)	Soil corrosivity, pipe attributes (age, material, diameter), pressure, location sensitivity	Reliability-based; health/public safety

Vairavamoorthy *et al.* (2004) adopted fuzzy composite programming to prioritize water mains for renewal in the distribution network, based on risk of contaminant intrusion. Mamlook & Al-Jayyousi (2003) proposed a fuzzy synthetic evaluation technique to detect leakages in the distribution network. Sadiq *et al.* (2004, 2007, 2008) proposed a framework to determine 'aggregative' risk associated with water quality failure in the distribution network. Each risk item was defined using a product of the *likelihood* of a failure event and its *consequence*. Both likelihood and consequences of a failure event were defined using fuzzy numbers. Makropoulos & Butler (2004, 2006) proposed a novel approach to develop a prioritization strategy for distribution network rehabilitation using multi-criteria, spatial decision-making. The proposed approach included a fuzzy rule-based model and OWA (ordered weighted averaging) operators, which were coupled with a GIS (geographical information system). The main feature of this approach was the incorporation of 'risk attitude' as one of the spatial variables in the GIS layer, in which OWA operators were used to assign consequences to various locations in the distribution networks based on their perceived importance.

Table 4 provides a summary of techniques/methods used directly or indirectly for water quality modelling in distribution networks. This summary has two tiers: the first tier lists the major application areas (hydraulics, pipe failure, water quality and risk/reliability) and provides the relative usage frequency (i.e. low, medium, high) of each method/technique in each major application area; and the second tier identifies common responses that are generally used as indicators in each application area. This table is meant to be only illustrative and not complete.

Limitations

The two major limitations of the existing techniques/methods are: a) interactions among various factors are

Table 4 | Summary of methods used in water quality modelling arena (Sadiq *et al.* 2009)

Modelling techniques/ methods/approaches	Usage frequency in major application areas and categories: Hydraulics	Pipe failure	Water quality	Risk/reliability
Analytical	M	H		L
Numerical	H			L
Kinetics-based			H	
Regression-based		M	H	
Statistical*		L	M	L
Soft computing†		L	L	L
Probabilistic		M	L	H
Mechanistic/physical		H		
Response/indicators	**Hydraulics**	**Pipe failure**	**Water quality**	**Risk/reliability**
Water age	X			
Pressure	X			X
DBPs			X	X
Total coliform			X	X
HPCs			X	
Residual chlorine			X	
Organics			X	
Internal corrosion			X	
Health risk		X	X	
External corrosion		X		X
Pipe breaks		X		X
Leakage	X	X		X
Biofilm			X	

*Other than regression.
†ANN, fuzzy logic, evidential reasoning etc.
Notes: L = low; M = medium; H = high.

generally not taken into account (i.e. factors are assumed to impact water quality independently); and b) the contributions of the various factors towards the estimation of total risk are assumed to be additive (linear). These two assumptions reflect a general effort in the modelling literature to reduce complexity. In addition, existing approaches handle uncertainties associated with data and models cursorily. The methodology developed in this research endeavours to transcend these limitations.

MODELLING COMPLEX SYSTEMS

The level of uncertainty associated with a system is proportional to its complexity, which arises as a result of vaguely known relationships among various entities, and randomness in the mechanisms governing the domain. Ross (2004) described complex systems such as environmental, socio-political, engineering or economic systems, which involve human interventions, and where vast arrays of inputs and outputs could not all possibly be captured analytically or controlled in any conventional sense. Moreover, relationships between causes and effects in these systems are often not well understood but can be expressed empirically. Typical complex systems consist of numerous interacting 'factors' or 'concepts'. Complex systems are highly non-linear in behaviour and the combined effects of contributing factors are often sub-additive or super-additive. The modelling of complex dynamic systems requires methods that combine human knowledge and experience as well as expert judgement. When significant historical data exist, model-free methods such as artificial neural networks (ANN) can provide insights into cause–effect relationships and uncertainties through learning from data (Ross 2004). But, if historical data are scarce and/or available information is ambiguous and imprecise, soft computing techniques can provide an appropriate framework to handle such relationships and uncertainties. Such techniques include probabilistic and evidential reasoning (Dempster-Shafer theory), fuzzy logic and evolutionary algorithms (Makropoulos & Butler 2004).

Most water distribution systems have only a limited number of water quality failures (WQF) each year, making statistically significant generalizations difficult. The rarity of WQF belies their seriousness, as each failure indicates the potential for harmful public health effects and increased public mistrust and complaints. In such data-sparse circumstances, expert knowledge and belief can serve as an alternative representation of a domain. Various computational techniques may be appropriate to predict potential WQFs in ageing water mains. Table 5 provides a qualitative comparison between five soft computing techniques including artificial neural networks (ANN), decision trees (DT), fuzzy rule-based models (FRBM), Bayesian networks (BN)

Table 5 | Comparison of various techniques to model complex systems (Sadiq et al. 2009)

	Soft computing techniques				
Attributes	**DT**	**FRBM**	**ANN**	**BN**	**CM/ FCM**
Network capability	N*	L†	N	H‡	VH§
Ability to express causality	H	M	N	H	VH
Formulation transparency	H	H	N‖	H	VH
Ease in model development	H	M	M	M	VH
Ability to model complex systems	M	H	VH	H	VH
Ability to handle qualitative inputs	H	H	N	H	VH
Scalability and modularity	VL	L	VL¶	H	VH**
Data requirements	H	L	VH	M	L††
Difficulty in modification	VH	H	M	L	N
Interpretability of results	VH	VH	VH	VH	H
Learning/training capability	H	M‡‡	VH§§	H‖‖	H¶¶
Time required for simulation	L	L	H	L	L
Maturity of science	VH	H	H	VH	M
Ability to handle dynamic data	L	H	H	H	M
Examples of hybrid models (ability to combine with other approaches	H	VH***	VH***	H	H†††

*Structure is hierarchical.
†Dimensionality is a major problem and formulation becomes complicated for network systems.
‡Can manage networks but cannot handle feedback loops, therefore referred to as directed acyclic graphs (DAG).
§Can handle feedback loops.
‖Generally referred to as black box models.
¶ANN needs to be retrained for new set of conditions.
** Very easy to expand, because algorithm is in the form of matrix algebra.
††Minimal data requirement, because causal relationships are generally soft in nature.
‡‡Clustering techniques, e.g. Fuzzy C-means.
§§Algorithms, e.g. Hebbian learning.
‖‖Algorithms, e.g. evolutionary algorithms and Markov chain Monte Carlo.
¶¶Training algorithms are available which have been successful in training ANNs.
*** Examples are available in the literature to develop models using hybrid techniques, e.g. neuro-fuzzy models.
†††Has a potential to be used with other soft techniques.
Notes: Ratings: N = no or negligible; VL = very low; L = low; M = medium; H = high; VH = very high; Soft computing techniques: ANN = artificial neural networks; DT = decision tree; FRBM = fuzzy rule-based models; BN = Bayesian networks; CM/FCM = cognitive maps/fuzzy cognitive maps.

and cognitive maps/fuzzy cognitive maps (CM/FCM). Central to this comparison is an assessment of how each technique treats inherent uncertainties and its ability to handle interacting factors that encompass issues specific to water distribution networks. In this research FCM was adopted as the method of choice, and its application is described in detail in the following sections.

Fuzzy cognitive maps (FCMs)

A FCM is a cyclical graph comprising nodes and arcs (edges) (Figure 2). A FCM illustrates a cause/effect representation between interacting entities within a system. These cause/effect relationships determine the behaviour of the system. The nodes in FCM represent factors (or concepts) of the system, which may be inputs, outputs or intermediate products. The arcs represent causal relationships between nodes. In FCM each node (factor) can interact with any number of nodes (factors). Typically, a FCM is constructed to represent the best available knowledge and judgement of the complex system under consideration.

Figure 2 illustrates a simple FCM that consists of six factors C_i ($i = 1, 2, \ldots, 6$). Weight $w_{ij} \in [-1, 1]$ represents the nature and strength of the relationship between 'causal factor' i and 'effect factor' j and the sign represents the type of causation. This scheme may give rise to the following

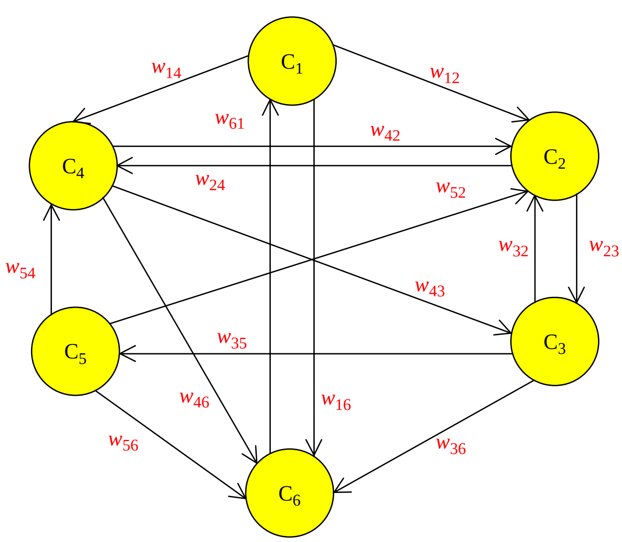


Figure 2 | An example of a fuzzy cognitive map (FCM).

three types of interaction between the ith (cause) and the jth (effect) factors:

$w_{ij} > 0$ a positive causality, where an increase in the value of i causes an increase in the value of j and vice versa;

$w_{ij} < 0$ a negative causality, where an increase in the value of i causes a decrease in the value of j and vice versa;

$w_{ij} = 0$ no causal relationship between i and j.

The value of factor C_i is denoted A_i'. The actual calculations in FCM are performed using A_i, which is a normalized value of A_i', i.e. mapped over a continuous interval [0, 1]. The transformation of A_i' to A_i can be linear or non-linear, depending on the nature of the factor. A_i can also be expressed directly either by a crisp or a fuzzy (linguistic) value (such as high or medium, etc.) but that should range over a unit interval [0, 1].

Koško (1986) proposed a method to calculate the value of each (receiving) factor in an FCM based on the total influence of the interconnected (causal) factors, where the value of the following function is normalized in the interval of [−1, 1]

$$A_j^t = f\left(k_1^i \sum_{\substack{i=1 \\ i \neq j}}^{n} A_i^{t-1} w_{ij} + k_2^j A_j^{t-1} \right) \quad 0 \le k_1^i \le 1 \text{ and } 0 \le k_2^j \le 1 \tag{1}$$

where A_j^t is the value of factor C_j at time step t, A_i^{t-1} is the value of factor C_i at time step $t-1$, w_{ij} is the weight (strength) of the causal impact exerted by factors i ($i = 1, 2, \ldots, n$) on factor j, and $f(\circ)$ is a threshold function. The expression in the brackets (Equation (1)) represents the total impact that is exerted on C_j by all other factors in the FCM. Theoretically, every node in the network can connect to every other node; however, for practical reasons, graphical representations normally show only non-zero w_{ij} and we say that nodes i and j are interconnected only when $w_{ij} \neq 0$. Moreover, the influence coefficient k_1^i provides an additional weight for the combined impact of interconnected factors in the configuration of the new value of factor A_j. The coefficient k_1^i will be close to a value of unity when the impact of interconnected factors is high and close to zero when the impact is low. Coefficient k_2^j

expresses the influence of the value of A_j at time $t-1$ (using past history similar to Markov process). Influence coefficients k_1^i and k_2^j may have different values for each receiving concept j. The selection of coefficients k_1^i and k_2^j depends on the nature and type of each factor. Initially, Kosko (1986, 1997) assumed that the value of the receiving factor j at the previous time step $(t-1)$ did not participate in the calculation of the value of j at timestamp t, therefore implying $k_2^j = 0$. It is common practice to assume that the influence of the interconnected concepts is high, and therefore coefficient $k_1^i = 1$.

Two types of non-linear threshold function $f(\circ)$ are commonly used in FCMs (Figure 3); incidentally, these functions are also used in ANN. The first is the uni-polar sigmoid function, where $\lambda > 0$ determines the steepness of the continuous function $f(\circ)$, whose value is constrained to the interval [0, 1].

$$f(x) = \frac{1}{1+e^{-\lambda x}} \tag{2}$$

The other common non-linear threshold function is the tangent hyperbolic function, which transforms the value of the function to the interval $[-1, 1]$.

Inferencing in FCMs is performed using matrix operations instead of explicit *if–then* rules found in traditional expert systems. The inference process is numerical or semi-numerical; therefore FCMs offer much greater flexibility than other causal frameworks. The FCM is a process model, which can use knowledge of expert opinion and belief

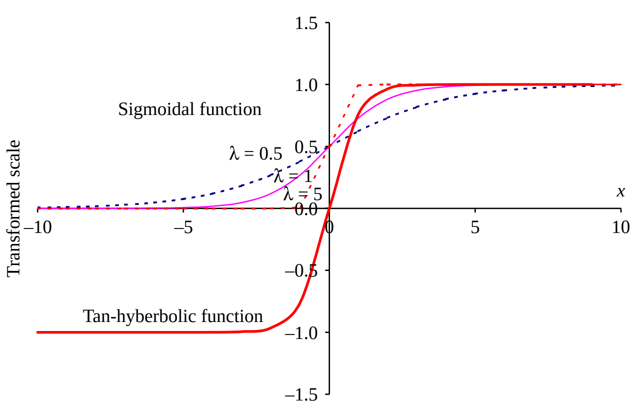


Figure 3 | Common non-linear threshold functions.

(qualitative and soft) and/or existing (quantitative and hard) data. Knowledge extracted from these sources may contradict or differ in terms of describing factors and expressing their causal relationships. Various FCMs can be combined into one, which means that opinions from different experts can act synergistically in the system. Several FCMs can be combined to obtain an aggregated FCM by merging adjacency matrices, which may contain different causal values of the same relationship and additional concepts usually representing different beliefs of experts.

Conventional FCMs have three major limitations. The following discussion describes these limitations and the ways to overcome them.

Constant relationship

Traditional FCMs do not allow causal relationships between two factors (represented by w_{ij}) to vary dynamically, as is often the case in real life. This limitation can be overcome by using the *dynamic causal weight*, $w_{ij} = w_{ij}(A_i^t)$, which is a weight whose value depends on the state value of its 'causal factor'. Khan & Khor (2004) proposed fuzzy rules to describe causal relationships, in which the state value of its 'causal factor' depends on the value of 'effect factors'. For example, the negative causality (monotonically decreasing) can be represented by fuzzy rules such as: 'If C_i is high then C_j is low' (equivalent to $w_{ij} < 0$ in traditional FCM). Conversely, positive causality (monotonically increasing) can be represented by fuzzy rules such as: 'If C_i is low (high, medium) then C_j is low (high, medium)' (equivalent to $w_{ij} > 0$ in traditional FCM). Non-monotonic causal relationships can also be dealt with efficiently through fuzzy rules, such as: 'If C_i is low (high, medium) then C_j is low (low, medium or high)'.

Lack of a temporal dimension

As different causal relationships may have different levels of time delay (response time can vary from minutes to weeks or even longer), traditional FCMs cannot effectively describe the dynamics of processes. This limitation can be addressed by the usage of dynamic cognitive networks (DCNs), which are an extension of FCM. Miao *et al.* (2001)

proposed DCNs based on time delayed functions. In this framework, the dynamic weights are functions of the state value of the cause concept C_i and of time, which is akin to order kinetics in stoichiometry (accounting or maths used in chemistry, e.g. zero order, first order, second order kinetics and so on).

Co-occurrence of multiple causes

Traditional FCMs cannot deal with a process in which the co-occurrence of multiple causes (such as expressed by 'AND' conditions) is required to trigger a single 'effect factor': for example, 'If C_i is low and C_k is high then C_j is low'. If 'AND' conditions are required inferencing can be done using a fuzzy rule-based model (FRBM) and/or the fuzzy measures theory (FMT). The inferencing mechanism in traditional FCMs is a simple weighted sum, which is a linear function that is subsequently normalized using a non-linear threshold function as described earlier (Equation (2)). Multiple causal inputs to an effect factor can inflict insensitivity in the FCM model, whereby a change in any important causal link does not significantly impact the effect factor. This insensitivity is exacerbated in networks with feedback loops (Carvalho & Tome 2002). The following approach is proposed in this research to avoid this issue:

If the FCM model is not to have feedback loops (i.e. if factor i is affected, directly or indirectly, by factor j, then factor j cannot be affected, directly or indirectly, by concept i), the cognitive map reduces to a directed acyclic graph (DAG), in which no iterations are required to reach equilibrium. Therefore, the iteration activation value A^t can be replaced by A in Equation (1). The need for a non-linear threshold function $f(\cdot)$ can also be eliminated if the causality (w_{ij}) is defined by rules or any other function; for example, $w_{ij}(A'_i)$ (Khan & Khor 2004).

As stated above, fuzzy rule-based models (FRBM) and fuzzy measures theory (FMT) are two possible ways to inference in the case of multiple causal nodes ('AND' action). A fuzzy rule-based model has to be the 'multi input single output' (MISO) kind to capture the 'AND' action. However, dummy nodes have to be introduced into the network in order to handle effectively possible dimensionality problems, as will be described in subsequent sections.

In the case of fuzzy measures theory, inferencing can be performed using either Choquet or Sugeno integrals (Sugeno 1974). Fuzzy measures theory is a plausible choice to handle redundancy present in various causal nodes. The use of fuzzy MISO model and FMT using Choquet integral is discussed in the following sections.

Fuzzy rule-based models (FRBM)

In FRBM, relationships between variables are represented by means of fuzzy *if–then* rules of the form '*If* antecedent proposition *then* consequent proposition'. The antecedent proposition is always a fuzzy proposition of the type 'X is A' where X is a linguistic variable and A is a linguistic constant term. The proposition's truth-value (or membership value), which is a real number between 0 and 1, depends on the degree of similarity between X and A. This linguistic model (Mamdani 1977) has the capacity to capture qualitative and imprecise/uncertain knowledge in the form of *if–then* rules such as:

$$\boldsymbol{R_i}: \text{if } X \text{ is } A_i \text{ then } Y \text{ is } \boldsymbol{B_j} \; i = 1, 2, \ldots, L \quad j = 1, 2, \ldots, N \tag{3}$$

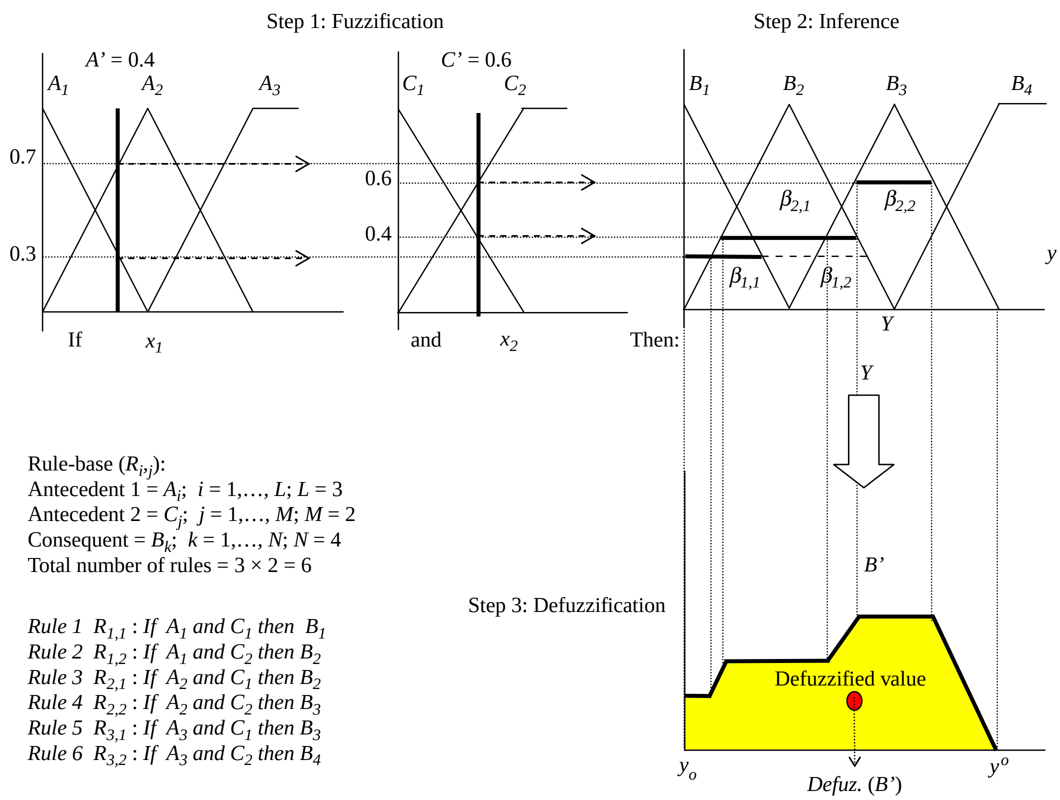
where R_i is the rule number i, X is the input (antecedent) linguistic (fuzzy) variable and A_i is a fuzzy subset, which corresponds to an antecedent linguistic constant (one of L in set A). Similarly, Y is the output (consequent) linguistic (fuzzy) variable and B_j is a fuzzy subset, which corresponds to a consequent linguistic constant (one of N in set B). A fuzzy rule can be regarded as a fuzzy relation; that is, simultaneous occurrence of values X and Y. For example, Equation (3) can be applied as follows:

> '**If** HPCs level is *medium* **then** microbiological water quality failure potential is low'where X denotes levels of HPCs, A denotes a fuzzy linguistic constant (a fuzzy subset) *medium* over the universe of discourse of HPC levels (e.g. *low*, *medium*, *high*), Y denotes microbiological water quality failure potential, B denotes a fuzzy linguistic constant (or a fuzzy subset) *low* in the universe of discourse of microbiological water quality failure, and rules R defines their fuzzy relationship.

This type of fuzzy relationship becomes a little more involved when X is not exactly equal to *medium* but rather has a membership of, say, $\mu_{A_2}(x) = 0.5$ to *low* and $\mu_{A_3}(x) = 0.5$ to *medium*. It is clear that since the HPC concentration is less than *medium* the microbiological water quality failure will likely be less than *low*. A detailed description of the Mamdani inference process is shown in Figure 4 and the formulation is provided in Appendix A.

Fuzzy measures theory (FMT)

A significant aspect of aggregation in a multi-criteria decision analysis is the assignment of weights to the different factors. Until recently, the most common aggregation methods have been based on averaging operators, such as weighted arithmetic means or quasi-linear means; however, these methods have limitations. None of these



x_1 has support (membership > 0) in A_1 and A_2, and x_2 has support in C_1 and C_2, consequently only the first four rules are 'fired' (or activated).

- Rule 1: $\mu_{A_1}(x_1) = 0.3, : \mu_{C_1}(x_1) = 0.4 \Rightarrow \beta_{1,1} = 0.3 \wedge 0.4 = 0.3 \Rightarrow \mu_{B_1}(y) = 0.3$
- Rule 2: $\mu_{A_1}(x_1) = 0.3, : \mu_{C_2}(x_1) = 0.6 \Rightarrow \beta_{1,2} = 0.3 \wedge 0.6 = 0.3 \Rightarrow \mu_{B_2}(y) = 0.3$
- Rule 3: $\mu_{A_2}(x_1) = 0.7, : \mu_{C_1}(x_1) = 0.4 \Rightarrow \beta_{2,1} = 0.7 \wedge 0.4 = 0.4 \Rightarrow \mu_{B_2}(y) = 0.4$
- Rule 4: $\mu_{A_2}(x_1) = 0.7, : \mu_{C_2}(x_1) = 0.6 \Rightarrow \beta_{2,2} = 0.7 \wedge 0.6 = 0.6 \Rightarrow \mu_{B_3}(y) = 0.6$
- For every subset B_k choose maximum membership, i.e., $\mu_{B_2}(y) = 0.4$
- Define quality ordered weights (q_k) for every subset B_k (assume $q_1 = 0$; $q_2 = 0.3$; $q_3 = 0.7$; $q_4 = 1$)

$$Defuz.(B') = \left(\sum_{k=1}^{N} \mu_{B_k}(y) \bullet q_k \right) = 0.3 \times 0 + 0.4 \times 0.3 + 0.6 \times 0.7 + 0 \times 1$$

$Defuz.(B') = 0.54$

Figure 4 | Fuzzy rule-based model: making inference using two 'causal factors'.

operators is able to address interaction between causal factors, which makes them unsuitable when such interactions are important. It is now widely accepted that additivity, which is inherent in these operators, is actually absent in many real situations, and therefore is often not a suitable proposition (Ross 2004).

Complex interactions between factors (i.e. sub- and super-additivity) can be expressed using a non-additive set function that permits us to define weights for a 'subset of factors' rather than for an individual 'factor'. Sugeno (1974) proposed to replace the *additivity* property by a weaker one–*monotonicity*. He developed a set of non-additive monotonic operators and called them *fuzzy measures*. It is important to note that fuzzy measures are not related to fuzzy sets (Sugeno 1974). A description of fuzzy measures and its inference using Choquet integral is shown in Figure 5 and the formulation is provided in Appendix B.

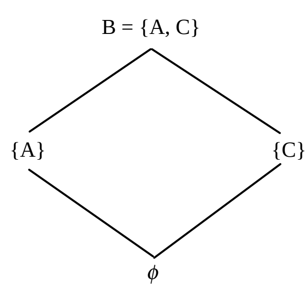
DEVELOPMENT OF THE PROPOSED FRAMEWORK

Presently, several decision models exist for water main renewal. Most models consider pipe structural integrity and/or hydraulic performance as the key decision criteria for rehabilitation and renewal of water mains. As mentioned earlier, water quality and pipe deterioration mechanisms are intertwined, where ageing pipes may affect the quality of the water, and aggressive water can deteriorate pipe inner surfaces. Therefore, it is very difficult to isolate the impacts of ageing water mains on the water quality in the distribution network. This research explores the role of water quality considerations as a decision driver for the rehabilitation and renewal of water mains. The results of this study will help to gain better understanding of the impact of 'ageing' water mains on the potential for water quality failure.

The term 'potential' for water quality deterioration mechanisms or water quality failures may refer to the *possibility* or *likelihood* of occurrence of these events. The scale for this potential is defined over a continuous interval [0, 1] similar to probability. The terms 'risk' and 'probability' are intentionally not used in order to avoid confusion. The difference between possibility (likelihood) and probability is that possibility refers to *what can happen* whereas probability refers to *what will happen*. We have also avoided using the terms 'likelihood' and 'possibility' as they have specific meanings in Bayesian theory and

Fuzzy measures	μ_i
μ (ϕ)	0.0
μ ({A})	0.6
μ ({C})	0.5
μ (B) = μ ({A, C})	1.0

Lattice representation for the power set B



The values for factors A and C are 0.4 and 0.6, respectively, i.e.,

$A_{(\{A\})} = A' = A_1 = 0.4$ $\quad$ $A_{(\{C\})} = C' = A_2 = 0.6$

Re-ordering is required to use Choquet integral. The activation values in descending orders are:

$A_{(1)} = 0.6$ $\quad$ $A_{(2)} = 0.4$ (where parenthesis shows the ordinal position)

Using Equation (B6), the value for B can be determined as follows:

$A_{\{B\}} = B' = [A_{(\{C\})} - A_{(\{A\})}] \times \mu(\{C\}) + [A_{(\{A\})}] \times \mu(\{C, A\})$

$B' = [0.6 - 0.4] \times 0.5 + [0.4] \times 1 = 0.1 + 0.4 = 0.50$

Figure 5 | Fuzzy measures theory: making inference using two 'causal factors'.

possibility theory, respectively. But, the essence of the term 'potential' used in this research is very similar to possibility or likelihood.

A two-tiered framework is proposed for the prediction of 'potential for water quality failures' in a given pipe segment (Figure 6). Note that a pipe segment is any pipe length or an alternative unit of acceptable measure where pipe conditions are assumed homogeneous. Tier I of the framework comprises six FCMs, corresponding to the seven WQ deterioration mechanisms described earlier, namely contaminant intrusion, internal corrosion, leaching, biofilm formation, disinfectant loss and THM formation, and permeation. These lower (Tier I) level FCMs are also called 'modular FCMs'. Input factors are divided into five major categories that include pipe attributes, site-specific conditions (environs), operational and hydraulic factors, water quality indicators and mitigative decision actions (interventions). Various input factors from each of these categories can contribute to any of the modular FCM (e.g. a disinfection practice can contribute simultaneously to biofilm formation, disinfectant loss and THM formation modules). Outputs from the modular FCMs are fed as inputs to a 'supervisory FCM' (Tier II), which in turn predicts the potential for WQ failure in each of three domains: namely, aesthetic, physicochemical and microbiological. The potentials in the three domains are in turn aggregated to provide the overall potential for water quality failure in the distribution pipe segment (Figure 6).

The second paper in this three-part series describes in detail the mathematical formulation of the proposed model and the third paper uses case studies to provide the details for model applications. Figure 7 illustrates schematically the 5-steps involved in the development of the framework, which are described in detail below.

Knowledge acquisition

Knowledge acquisition consisted of four distinct activities: preliminary analyses; literature review; surveys/interviews; and solicitations of expert opinions. The preliminary analyses broke down items along categorical lines, which helped identify contributing factors. In-depth literature review followed the preliminary analyses. The result of these analyses provided a more comprehensive understanding of the items associated with water quality. Use of too many input factors in any model deteriorates the accuracy because of noise and/or conflict in the data, therefore the selection of a sufficient subset of input data was a major challenge. With this understanding, expert judgement was used to organize available information as

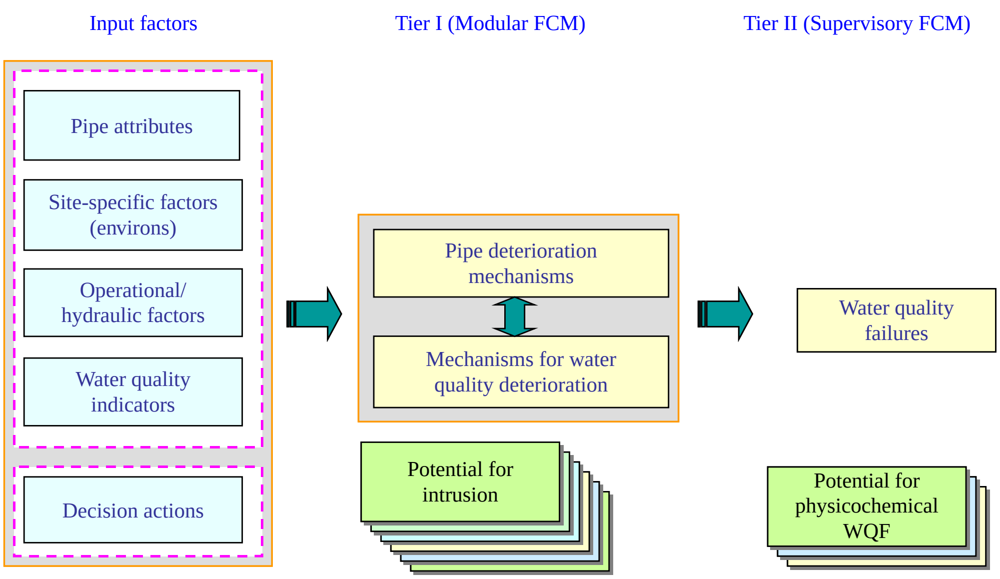


Figure 6 | Assessing the potential for water quality failures in ageing water mains: framework.

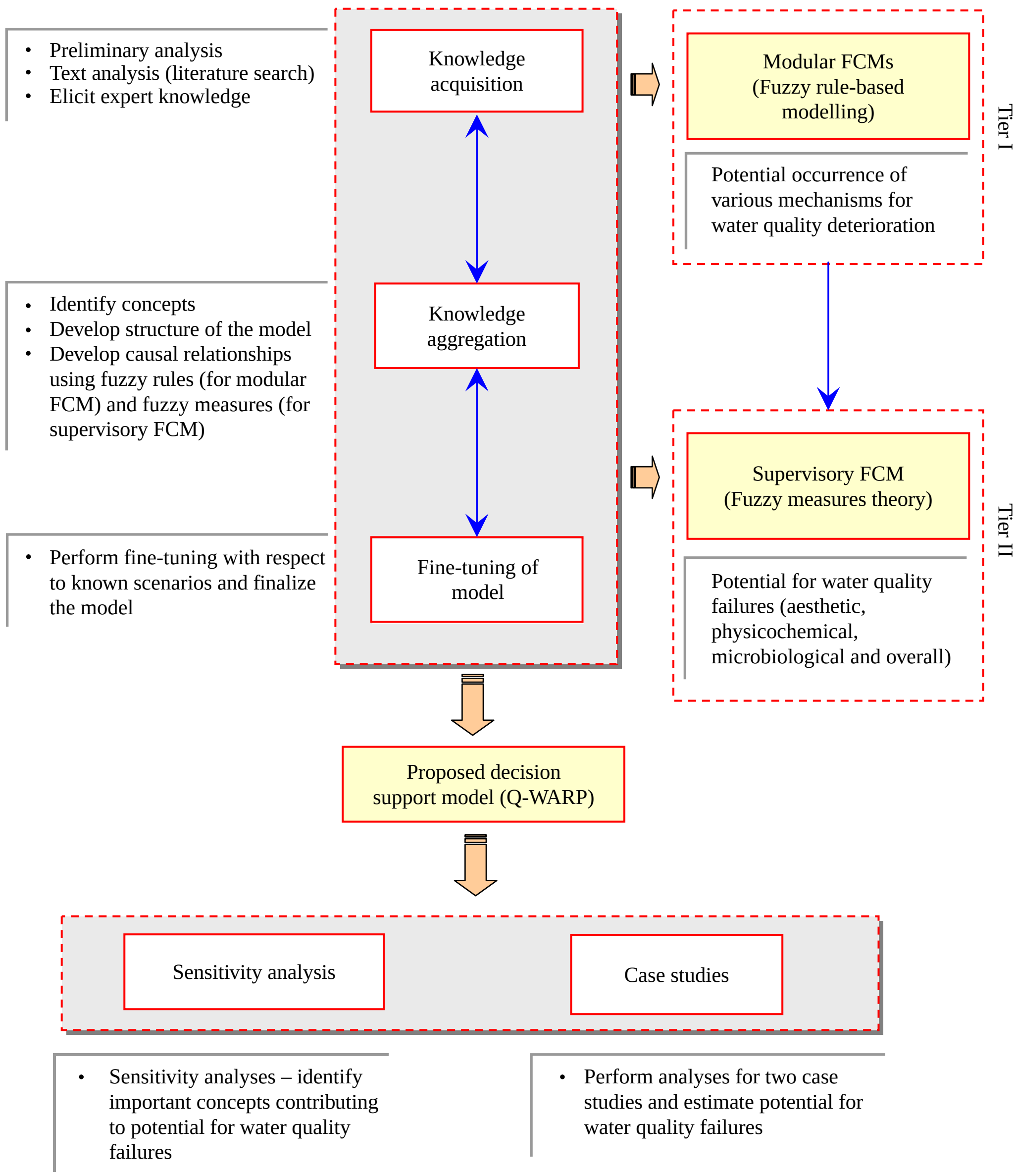


Figure 7 | Steps involved in the proposed research.

well as identify knowledge gaps. More than 50 key factors were identified, which play key roles in explaining water quality deterioration in ageing water mains.

Knowledge aggregation

Basic input factors, transformation functions, and rule sets were identified and the structure of the proposed model was developed such that it takes into account the entire body of the acquired knowledge. Causal relationships were established using fuzzy rules (at Tier I level) or fuzzy measures (at Tier II level). The main reason for using two different inferencing methods was that at the supervisory level, the causal relations are mainly governed by redundant factors, which can be more efficiently explained through fuzzy measures theory.

Fine-tuning of the model

Numerous simulations were conducted for known scenarios and the causal relationships revised to avoid discrepancies or counter-intuitive outcomes. Once the structure of the model was finalized and 'reasonably' trained, then the model became ready to explore hidden patterns nascent or embodied in the model.

Sensitivity analyses

Sensitivity analyses were conducted to determine the contributions, and to rank input factors that affect a specific water quality deterioration mechanism. A new sensitivity analyses technique was developed in this research, details for which are provided in the second paper.

Case studies

Two case studies including City of Philadelphia (USA) and the City of Ottawa (Canada) were carried out. Analyses helped to verify the historical occurrences of water quality failures in those networks.

SUMMARY AND CONCLUSIONS

Deterioration of water quality in distribution networks causes health-related as well aesthetic concerns. To date, little consideration has been given to the impacts of deteriorating water mains on the quality of distributed water, as a decision driver for the rehabilitation of water mains. The main objectives of this research were, firstly, to identify deterioration mechanisms in water mains that may cause water quality failures in distribution networks and, secondly, to integrate the effects of these mechanisms in a proof-of-concept model capable of quantifying the resulting overall potential for water quality failure.

Water quality failures that compromise either the safety or the aesthetics of water within distribution networks can be caused directly or indirectly by the following mechanisms:

- intrusion of contaminants through deteriorated system components, misuse or cross-connection, or deliberate introduction of harmful substances;
- internal corrosion due to an oxidation–reduction reaction that releases by-products;
- leaching of chemicals from pipe or lining as a result of the dissolution of the exposed material;
- biofilm formation and regrowth of microorganisms on the internal surface;
- loss of disinfectant and formation of disinfection by products (DBPs);
- permeation of hydrocarbon compounds through the walls of plastic pipes and appurtenances.

Many mechanisms affecting water quality in the distribution network are partially or only intuitively understood. Furthermore, existing modelling approaches do not consider interdependencies among contributing factors. These interdependencies can significantly affect the results of any modelling effort. Finally, aleatory (natural heterogeneity, variability) and epistemic (ignorance or lack of knowledge) uncertainties associated with data and models (respectively) are not dealt with in a rigorous way. Fuzzy cognitive maps (FCMs) are illustrative causative representations of complex systems. FCMs draw causal representations among all identified factors of any specific system. A complex system represented by FCM can incorporate human experience, judgement, understanding and knowledge of the system, and has the capability to effectively deal with issues of complexity and uncertainty.

The objectives of this research were achieved in a five step process that included: knowledge acquisition; knowledge aggregation and development of model; fine-tuning; sensitivity and scenarios analyses; and finally performing two case studies. The proposed two-tiered framework can be used to predict the potential for water quality failures in a given pipe segment. At the lower or modular (Tier I) level, input factors were used to predict potential for various mechanisms causing water quality deterioration, which includes contaminant intrusion, internal corrosion, leaching, biofilm formation, disinfectant loss and THM formation, and permeation. In the supervisory (Tier II) level, these water quality deterioration mechanisms were used for the assessment of potential for aesthetic, physicochemical, microbiological and overall water quality failures. The second paper in this series will provide the details of the steps used for the development of the models.

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APPENDIX A: FORMULATION FOR FUZZY RULE-BASED MODEL

The full relationship between X and Y according to rule i can be computed in one of two basic ways using fuzzy implications or fuzzy conjunctions (Mamdani 1977). In the proposed approach, the Mamdani method is used, in which conjunction $A \wedge B$ is computed by a *minimum* (and type t-norm or conjunctive) operator. The interpretation of conjunction $A \wedge B$ is 'it is true that A *and* B simultaneously hold'. The relationship is symmetric and can be inverted: Each rule is regarded as a fuzzy relation denoted by R_i $(X \times Y) \rightarrow [0, 1]$.

$$R_i = A_i \times B_j, \quad \text{i.e. } \mu_{R_i}(x, y) = \mu_{A_i}(x) \wedge \mu_{B_j}(y) \tag{A1}$$

The *minimum* operator is applied to the Cartesian product space of X and Y (i.e. for all possible pairs of X and Y). The union of all fuzzy relations R_i comprises the entire relationship between X and Y and is given by the disjunction $A \vee B$ (*union*, *maximum*, or type, s-norm) operator of the L individual relations (rules) R_i $(i = 1, \ldots, L)$:

$$R = \overset{L}{\underset{i=1}{\Upsilon}} R_i, \quad \text{i.e. } \mu_R(x, y) = \max_{i=1,2,\ldots,L} [\mu_{A_i}(x) \wedge \mu_{B_j}(y)] \tag{A2}$$

Remembering that each relationship R_i is symmetric and can be inverted, the entire rule-set is now encoded in the fuzzy relation (rule) set $\boldsymbol{R}$. Equation (A2) can be restated as

$$y = x \circ R \tag{A3}$$

where the output of the linguistic model is computed by applying the *max–min* composition (denoted by the operator '$\circ$') to the input or antecedent proposition.

Suppose that A' is an input fuzzy number (or a singleton), which is mapped on set A, and B' is an output fuzzy number which is mapped on a set B, such that:

$$\mu_B(y) = \max_X [\mu_{A'}(x) \wedge \mu_R(x, y)] \tag{A4}$$

Substituting μ_R (x,y) from Equation (A2), the above expression can be rearranged as

$$\mu_B(y) = \max_{i=1,2,\ldots,L} \left(\max_X [\mu_{A'}(x) \wedge \mu_{A_i}(x)] \wedge \mu_{B_j}(y) \right) \tag{A5}$$

Defining $\beta_i = \max_X [\mu_{A'}(x) \wedge \mu_{A_i}(x)]$ as the degree of fulfilment of the antecedent of the ith rule, the output fuzzy set of the linguistic model becomes

$$\mu_B(y) = \max_{i=1,2,\ldots L} \lfloor \beta_i \wedge \mu_{B_j}(y) \rfloor \tag{A6}$$

The above algorithm is SISO Mamdani inference (Equations (A1) through (A6)) and can be extended to the MISO model. For example, for two causal concepts:

$$R_{i,j} : \text{If } x_1 \text{ is } A_i \text{ and } x_2 \text{ is } C_j \text{ then } y \text{ is } B_k; \quad \begin{aligned} i &= 1, 2, \ldots, L \\ j &= 1, 2, \ldots, M \\ k &= 1, 2, \ldots, N \end{aligned} \tag{A7}$$

This is a special case of SISO model, where the antecedent proposition is obtained as the Cartesian product of fuzzy sets A and C, therefore the degree of fulfilment is given by:

$$\beta_{i,j} = \left\{ \max_{X_1} [\mu_{A_i}(x_1) \wedge \mu_{A'}(x_1)] \wedge \max_{X_2} \left[\mu_{C_j}(x_2) \wedge \mu_{C'}(x_2) \right] \right\} \tag{A8}$$

Consider an effect concept B, which is connected by two causal concepts A and C. The 'AND' sign represents that both A and C are simultaneously required for B to occur. The details of the inferencing are shown graphically in Figure 4. The process is shown in three distinct steps: namely, fuzzification, inference (a rule base and an inference engine) and defuzzification. Assume that causal concepts A and C are activated at levels of $A' = 0.4$ and $C' = 0.6$, respectively. The rule set consists of six rules (3×2) and input activation values (A') and (C') fire the first four rules to determine output B' which is defined over the universe of discourse Y.

The *defuzzification* provides a discrete (crisp) value of an effect B (i.e. B'). The crisp value approximates the deterministic characteristics of the fuzzy reasoning process based on the output fuzzy set $\mu_{B_k}(y)$, which helps convert the uncertainty into an applicable action when solving real-world problems. The defuzzification step described in Figure 4 uses quality ordered weights (q_k) for every subset B_k (Sadiq & Rodriguez 2004*b*). These weights are simply multiplied to corresponding output fuzzy set $\mu_{B_k}(y)$, and a weighted score is the defuzzified value B'.

APPENDIX B: FORMULATION FOR FUZZY MEASURE THEORY

For a discrete universal set $X = \{x_1, x_2, \ldots, x_n\}$, a fuzzy measure on X is a set function, such that $\mu: (2^n - 2) \to [0, 1]$ satisfying the following conditions (where n is the cardinality of a discrete set):

$$\text{Condition 1}: \mu(\phi) = 0, \mu(X) = 1 \text{ (where } \phi \text{ is a null subset)}$$

$$\text{Condition 2}: S \subseteq T \Rightarrow \mu(S) \le \mu(T) \text{ (monotonicity condition)}$$

For example, let set $X = \{x_1, x_2, x_3\}$. The cardinality of X is 3. In addition to null set ϕ and universal set X, there are total $2^3 - 2 = 6$ subsets to X, these include, $\{x_1\}$, $\{x_2\}$, $\{x_3\}$, $\{x_1, x_2\}$, $\{x_1, x_3\}$, $\{x_2, x_3\}$. For any subset $S \subseteq X$, $\mu(S)$ can be viewed as the weight or strength of the subset S for the particular decision problem under consideration. Thus, in addition to the usual weights on criteria taken separately (e.g. $\{x_1\}$, $\{x_2\}$, $\{x_3\}$), weights on any combination of criteria (e.g. $\{x_1, x_2\}$, $\{x_1, x_3\}$, $\{x_2, x_3\}$) can also be defined. Monotonicity means that adding a new element to a subset cannot decrease its importance (Marichal 1999). For example, if $S = \{x_1\}$, and $\mu(\{x_1\}) = 0.5$, and if $T = \{x_1, x_2\}$ then $\mu(\{x_1, x_2\}) \ge 0.5$ to fulfil the monotonicity condition. The fuzzy measure $\mu(\{x_1, x_2, x_3\})$ of a universal discrete set X (or sample space) is always unity (this is similar to probability theory, in which the probability sum of all outcomes for an event is 1).

The assessment of fuzzy measures by human experts is a daunting task, since the non-additivity property of a fuzzy measure requires the consideration of $(2^n - 2)$ subsets. Sugeno (1974) proposed a so-called λ-fuzzy measure, which identifies the fuzzy measure of combined attributes from single attributes, expressed as:

$$\mu(A \cup B) = \mu(A) + \mu(B) + \lambda\mu(A)\mu(B); \quad (\lambda > -1) \tag{B1}$$

The parameter λ is used to describe an interaction between factors that are combined. According to the value of λ, the above equation can be interpreted as:

If $\lambda > 0$, then $\mu(A \cup B) > \mu(A) + \mu(B)$ (super-additive),
if $\lambda = 0$, then $\mu(A \cup B) = \mu(A) + \mu(B)$ (additive), and
if $\lambda < 0$, then $\mu(A \cup B) < \mu(A) + \mu(B)$ (sub-additive).

Super-additive relationship implies a synergy effect or strengthening dependency between factors, meaning that the combined contribution of factors A and B is greater than the sum of their contributions. Sub-additive relationship implies a redundancy condition or weakening dependency between factors, meaning that the combined contribution of factors A and B is lower than the sum of their contributions. Additive relationship implies independence between factors. Sugeno's λ-fuzzy measure can be generalized for $X = \{x_1, x_2, \ldots, x_n\}$ as follows:

$$\mu(\{x_1, x_2, \ldots x_n\}) = \frac{1}{\lambda}\left[\prod_{i=1}^{n}(1 + \lambda\mu(\{x_i\})) - 1\right]; \lambda \ne 0 \tag{B2}$$

The value of λ is obtained through the boundary condition, $\mu(X) = 1$, which yields a polynomial equation with respect to λ, given by:

$$1 + \lambda = \prod_{i=1}^{n}(1 + \lambda\mu(\{x_i\})) \tag{B3}$$

As Sugeno (1974) has shown, there exists a unique λ, which is greater than '-1' and not equal to zero, satisfying Equation (B3). The fuzzy measure of a given set $S \subset X$ is computed as:

$$\mu(S) = \frac{1}{\lambda}\left[\prod_{\forall x_i \in S}(1 + \lambda\mu(\{x_i\})) - 1\right] \tag{B4}$$

Sugeno (1974, 1977) also introduced the idea of *fuzzy integrals* to develop tools capable of integrating all values of a function in terms of the underlying fuzzy measure (μ). An integral for fuzzy measures in a sense represents an aggregation operator, which, contrary to the weighted arithmetic means, describes interactions between factors ranging from redundancy (negative interaction, i.e. sub-additive) to synergy (positive interaction, i.e. super-additive). Several classes of fuzzy integrals exist, among which the most representatives are those suggested by Choquet and Sugeno (Marichal 1999).

The Choquet integral $C_\mu(X)$, first proposed by Schmeidler (1986), is based on an idea introduced in capacity theory by Choquet (1953). $C_\mu(X)$ is an aggregation operator, where the integrand is a set of n values

$x = \{x_1, x_2, \ldots, x_n\}$. The Choquet integral of a function X with respect to μ is defined by:

$$C_\mu(X) = \sum_{i=1}^{n} [x_{(i)} - x_{(i+1)}] \cdot \mu(\{x_{(1)}, x_{(2)}, \ldots, x_{(i)}\}) \tag{B5}$$

where $x_{(1)} \geq x_{(2)} \geq \ldots \geq x_{(n)}$ represent the order of x_i in set X in descending order. The values for $x_1, \ldots, x_n$ in our case can be replaced by activation values of causal nodes. Therefore, for a set of causal factors $\{A_1, A_2, \ldots, A_n\}$ impacting on factor C_j, the Choquet integral will determine activation value A_j as the following:

$$A_j = \sum_{i=1}^{n} [A_{(i)} - A_{(i+1)}] \cdot \mu(\{A_{(1)}, A_{(2)} \ldots A_{(i)}\}) \tag{B6}$$

where $\mu(\{A_{(1)}, A_{(2)} \ldots A_{(i)}\})$ are fuzzy measures similar to causal weights (w_{ij}). Interested readers should refer to Grabisch (1996) for details.

We use the same example for describing the inference procedure in FMT as was used for FRBM. Figure 5 shows how the activation values from A (i.e. $A' = A_1$) and C (i.e. $C' = A_2$) feed into an effect concept B. Therefore, the sample space for $B = \{A, C\}$. The power set $2^{|B|}$ requires the definition of four fuzzy measures as given in Figure 5, where $|B|$ is the cardinality of sample space, which is 2. The fuzzy measures here are derived arbitrarily based on semantics (expert judgement). However, alternative objective methods based on data, λ-fuzzy measure and heuristics can be used to derive these measures (Grabisch 1996).

Lattice representation of the power set of B is shown in Figure 5. It can be noticed in our example that the fuzzy measures are sub-additive, because $\mu(\{C\}) + \mu(\{A\}) \geq \mu(\{A, C\})$. It shows that causal nodes A and C are not independent in the impact they deliver to node; that is, there is some redundancy between them. As $\mu(\{C\})$ and $\mu(\{A\}) \leq \mu(\{A, C\})$ that represents the monotonicity of the fuzzy measures. Therefore, under these conditions, the 'effect factor' B will have a value of 0.5 (using Equation (B6)).