Modelling formation of disinfection by-products in water distribution: optimisation using a multi-objective evolutionary algorithm

Mohanasundar Radhakrishnan, Assela Pathirana, Kebreab Ghebremichael and Gary Amy

ABSTRACT

Concerns have been raised regarding disinfection by-products (DBPs) formed as a result of the reaction of halogen-based disinfectants with DBP precursors. In order to appreciate the chemical and biological tradeoffs, it is imperative to understand the formation trends of DBPs and their spread in the distribution network. However, the water at a point in a complex distribution system is a mixture from various sources, whose proportions are complex to estimate and requires advanced hydraulic analysis. To understand the risks of DBPs and to develop mitigation strategies, it is important to understand the distribution of DBPs in a water network, which requires modelling. The goal of this research was to integrate a steady-state water network model with a particle backtracking algorithm and chlorination as well as DBPs models in order to assess the tradeoffs between biological and chemical risks in the distribution network. A multi-objective optimisation algorithm was used to identify the optimal proportion of water from various sources, dosages of alum, and dosages of chlorine in the treatment plant and in booster locations to control the formation of chlorination DBPs and to achieve a balance between microbial and chemical risks.

Key words | biological risk, chemical risk, disinfection by-products, genetic algorithm, multiple objective optimisation, particle back tracking algorithm

Mohanasundar Radhakrishnan (corresponding author)
Gary Amy
Department of Urban Water Supply and Sanitation,
UNESCO-IHE Institute for Water Education,
Delft,
The Netherlands
E-mail: *Mohanasundar@gmail.com*

Assela Pathirana
Department of Water Science and Engineering,
UNESCO-IHE Institute for Water Education,
Delft,
The Netherlands

Kebreab Ghebremichael
Patel School of Global Sustainability,
University of South Florida

Gary Amy
King Abdullah University of Science and Technology,
Saudi Arabia

INTRODUCTION

Disinfection is the most important step in drinking water treatment and is unquestionably important in the supply of safe drinking water (WHO 2006). Disinfectant residual maintenance in the distribution system is practised mainly to minimise bacterial growth and biofilm formation, to act as an additional safeguard against exogenous pathogenic intrusion, and to act as an indicator for system integrity (Laurent *et al.* 2005). Chlorine and its compounds are the most commonly used disinfectants for the treatment of water and its popularity is due to its high oxidising potential, high half life, and relatively low cost (Gopal *et al.* 2007).

However, disinfection can pose a chemical threat due to the formation of carcinogenic disinfection by-products (DBPs) in the presence of precursors such as natural organic matter (NOM) and bromide (Br^-). Chlorination DBPs such as trihalomethanes (THM) and haloacetic acids (HAA) are well known carcinogenic substances and there is a growing body of epidemiological evidences showing that these compounds are linked to cancer (Gopal *et al.* 2007). This necessitates the creation of checks and balances to control the usage of disinfectants to minimise the health risk due to DBPs. It must be noted that the reduction of chlorine would compromise the microbial safety of water. Hence, a balance between biological and chemical risk has to be achieved. Ideally, an overall risk assessment must be carried out considering the microbial risk due to inadequate disinfection and the long- and short-term risks due to DBPs.

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DBPs formation and speciation is a complex phenomenon and depends on many factors such as NOM concentration and characteristics, water quality parameters (e.g. pH and background inorganic matrix, especially bromide concentration), chlorination conditions (e.g. temperature, chlorine dose and contact time) and ratios of bromide/DOC (dissolved organic carbon) and bromide/chlorine concentrations (Singer 1999; Ates *et al.* 2007a, b). Numerous water quality models are available to predict the formation of DBPs based upon water quality parameters. DBPs models such as USEPA models (Amy *et al.* 1998) and kinetic models (Sohn *et al.* 2004) are among the widely used models. They are based on bench scale assessments under laboratory conditions and predict the formation of DBPs based on water quality and treatment conditions. However, they do not take into account practical considerations such as mixing of water from different sources in a network and the formation kinetics of DBPs based on studies under real distribution system conditions. DBP formation in distribution networks can be modelled by combining DBPs models with network hydraulic tools such as EPANET 2.0 (Rossman 2000; USEPA 2000; Seyoum 2006). In addition to hydraulic analysis, EPANET 2.0 can also perform computations such as determining water age, tracing the water source, and water quality computations such as the formation or decay of chemicals such as chlorine. However, it cannot perform the analysis of a number of chemicals at a time, which is essential to determine the kinetics of DBPs in the network. Thus, this study has been able to combine the strength of the hydraulic capability of EPANET 2.0 and the statistical DBP models by creating an external module to link the two models. The number of paths taken by water, the proportion of water through these paths and the age of water in various paths is not computed by EPANET 2.0. From EPANET 2.0, an average water age at the nodes is estimated and used by the water quality models. An EPANET 2.0 based tool, a particle backtracking algorithm (PBA), has been used to determine these parameters (Zierolf *et al.* 1988). PBA is a Lagrangian model for simple networks without tanks, which tracks the travel of water particles in reverse time and finds all the paths from an input location (source) to the output location (Bhave & Gupta 2006). PBA concisely describes the output concentration (co) as a linear function of the input strength (Shang *et al.* 2002).

$$c_o(t_o) = \sum_{j=1}^{N} \gamma_j c_i(t_o - t_j)$$

where N = number of paths between input and output; t_o = output time; c_j = water quality at source input; t_j = time delay for travel path j; and γ = impact coefficient for travel path.

In the presence of reservoir tanks, the computational effort can be very large as PBA generates huge numbers of paths when tanks are draining (Shang *et al.* 2002). The complexities involving multiple water sources and multiple chemical species can be handled by using innovative tools such as the PBA developed by Shang *et al.* (2002) and EPANETMSX (Shang *et al.* 2008) – an extension of EPANET 2.0 which models chemical reactions between multiple chemical and biological species. These tools enable water quality estimation using multiple input parameters along all the different travel paths from various sources.

This research focuses on: (i) integrating statistical chlorine residual and DBPs models (Amy *et al.* 1998), with the hydraulic model of EPANET 2.0 (Rossman 2000) along with a PBA (Shang *et al.* 2002) and a multi-objective optimisation (MOO) algorithm non-dominated sorting genetic algorithm (NSGA-II) (Deb 2001); (ii) mapping the chemical and biological risks in the distribution system corresponding to DBPs and pathogens; and (iii) assessing the formation of DBP in the distribution system with multiple water sources. In order to achieve these objectives, it is necessary to integrate a hydraulic model that analyses the flows in a water distribution network with DBP models, and an optimisation algorithm. This study does not focus on the different treatment methods or different levels of treatment to minimise the risks. The water treatment cost has been approximated for conventional water treatment using prevailing market rates.

METHODS

In this study, a modelling tool has been developed for identifying the trade-off between chemical (carcinogenic) and biological (microbial) risks. In theory, it is possible to

calculate both biological and chemical risks in financial terms. However, it should be understood that these two risks are very different. The former manifests itself as an immediate cost while the latter refers to long term. The levels of uncertainty involved in estimating the two quantities are also very different. A better approach of optimisation would be to come up with a series of optimal solutions with different chemical and biological risk levels, or a two-dimensional Pareto-optimal front with chemical risk and biological risk (or their cost equivalents) as objective functions. For example, with the biological risk level of x, suppose that there are number of (sub-optimal) solutions for chemical risk y_1, $y_{2,} \ldots y_n$. If the value y_i is the smallest level of risk in this set, one can call y_i the optimal solution for chemical risk with a (fixed) biological risk of x. However, when x varies, the optimal solution y_i also varies. Therefore, we end up with a Pareto-optimal front of optimal solutions, which can be called optimal solutions for y with varying x. The results of such an optimisation are similar to the one shown in Figure 1. Decision makers are able to interpret such a representation without any background on optimisation and modelling, in order to make final recommendations.

The NSGA-II developed by Deb (2001) has been used to perform the necessary MOO to obtain the Pareto-optimal front of biological risk versus chemical risk. Genetic algorithms (GA) is an optimisation method based on Darwinian theory of evolution. NSGA-II is an algorithm that extends GA to MOO. It employs an elitist preservation strategy and uses an explicit diversity preserving mechanism and

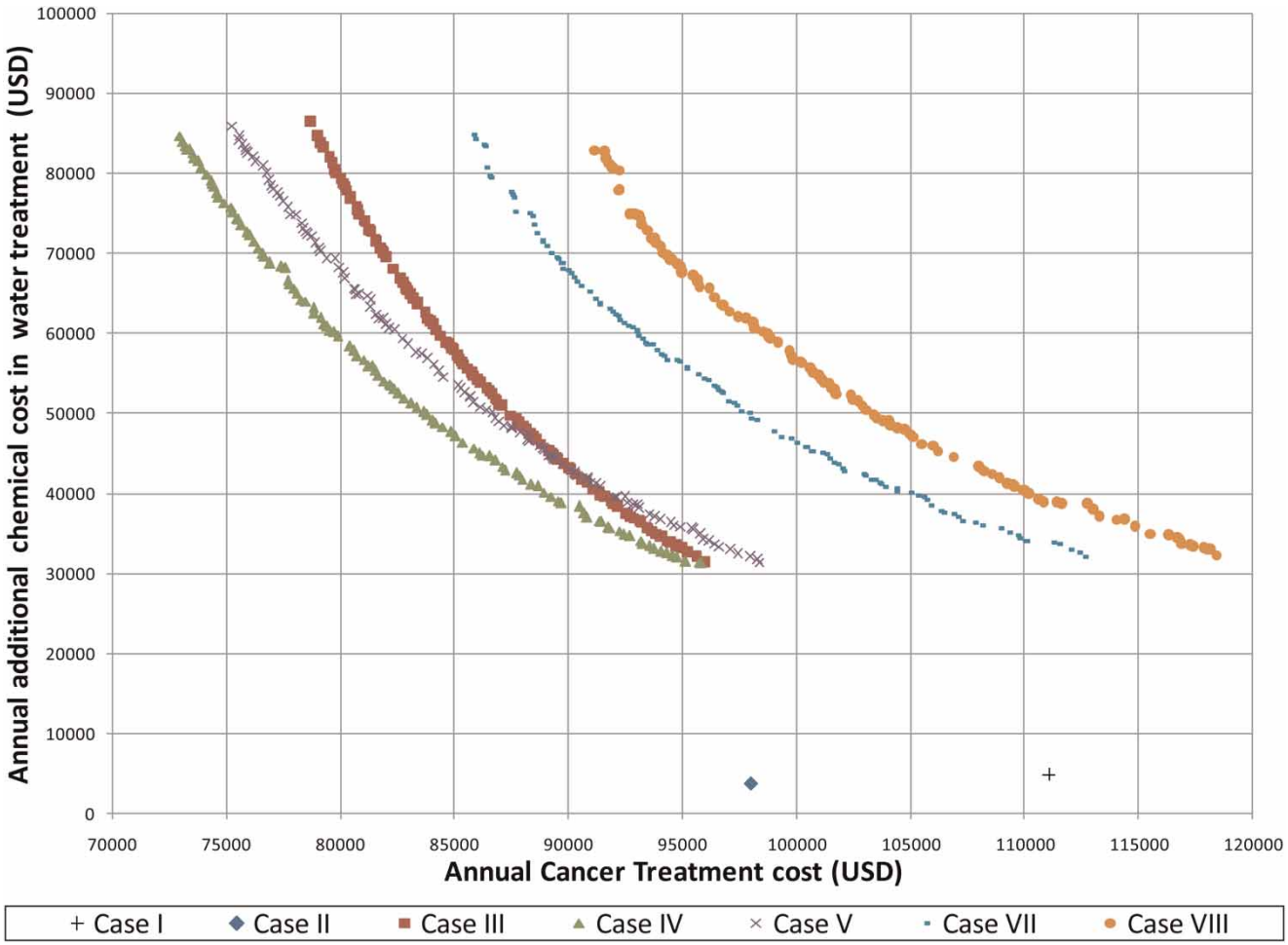


Figure 1 | Water and cancer treatment cost comparison for Minneriya network in various cases under consideration.

produces Pareto-optimal solutions (Salazar *et al.* 2006). The average annual cancer treatment cost per patient has been based on the research of Chowdhury (2010).

Predictions of THMs, HAAs and chlorine decay have been made using the statistical DBP models developed by Amy *et al.* (1998). The models incorporate water quality parameters such as DOC, pH, Br^- and temperature; and treatment conditions such as chlorine dose and reaction time. Separate models have been developed for raw water as well as alum-coagulated and iron-coagulated water. In this study, alum-coagulated water models have been used including temperature and pH correction factors developed by Shon *et al.* (2004). Residual chlorine has been computed using the chlorine decay model developed by Amy *et al.* (1998). Hydraulic analysis of the network performed using the EPANET 2.0 model (Rossman 2000).

In addition to integrating the hydraulic and chemical models, a MOO algorithm based on biological safety and chemical risks has been linked to control DBPs in the network and to minimise the chemical risk.

A tool has been integrated in C/C++ programming language comprising NSGA-II (Deb 2001) for optimisation, hydraulic EPANET toolkit functions (Rossman 2000), PBA (Shang *et al.* 2002), chlorine and DBPs computations models (Amy *et al.* 1998), cancer risk estimation (Sohn 2001) and DOC removal model (Zhu 1995, as cited by Sohn 2001). The developed tool was used to analyse water quality in networks with booster chlorination and to predict the spread of arsenic in the network due to deliberate or accidental contamination. The model implementation has been arranged in two parts: the risk model and the optimiser, as shown in Figure 2. In the risk model, water quality parameters are direct input values whereas alums and chlorine doses as well as reservoir head are input values generated by the optimiser.

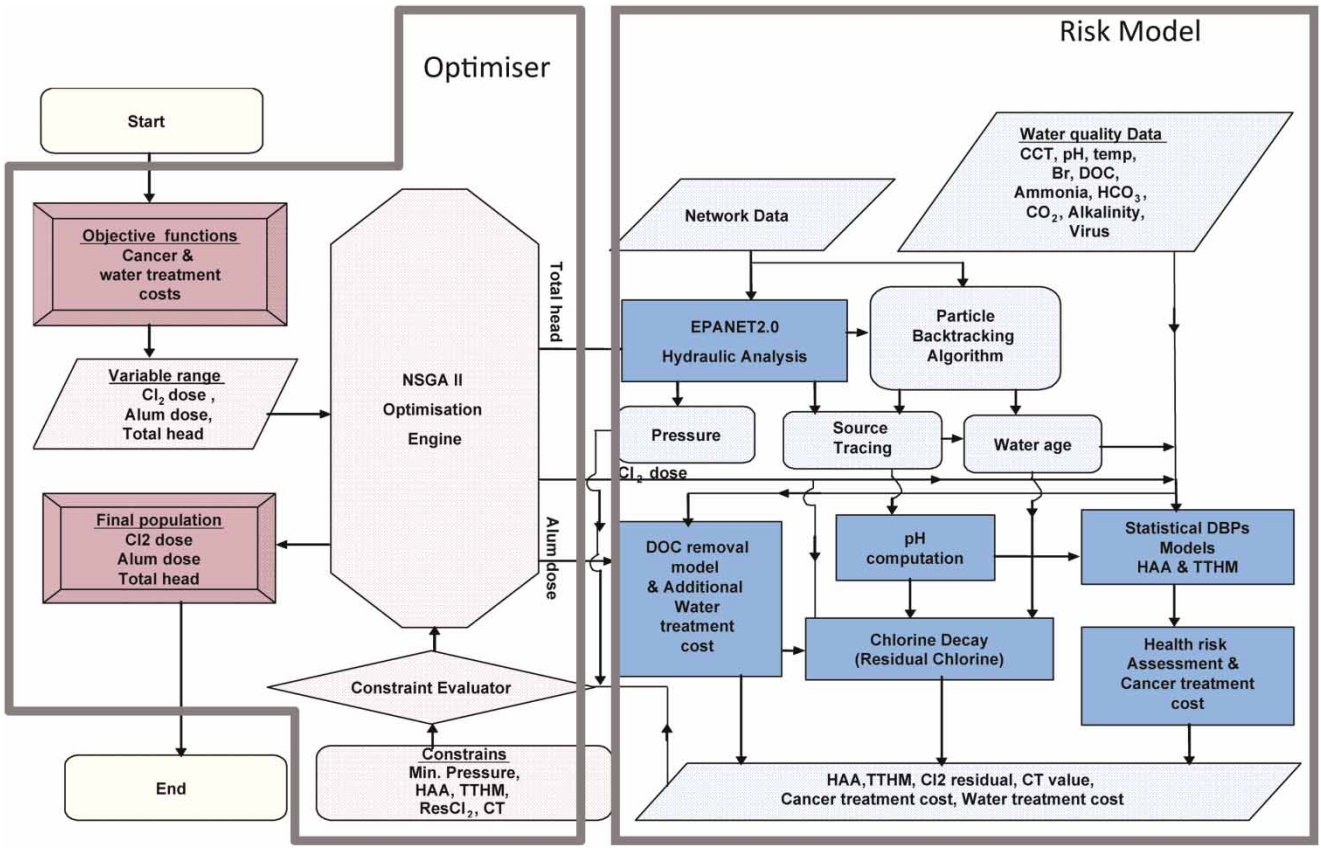


Figure 2 | Flow diagram for integration and system optimisation.

The objective of the optimiser in this context is to minimise costs. The objectives, real variables and constraints for the Optimiser are presented in Table 1. Pareto optimal solutions have been generated by the NSGA-II after a number of iterations.

Case study

The developed tool was tested on a distribution network in Minneriya, in Sri Lanka (Wanigasekara 2009). The network consisted of a single source and 89 nodes (Figure 3). The hydraulic and water quality analyses were carried out for 72 h (run time). CT values have been based on residual chlorine available at the node by considering only bulk phase reactions. For optimising the flow from the reservoirs in the network with multiple sources, the head of the reservoirs can be changed but, in the scenarios under consideration, the reservoir heads were fixed due to the hydraulic complexities of the network.

The following scenarios were :

- Case I – Arbitrary chorine dose at source
- Case II – Chlorine dose optimisation at source
- Case III – Alum coagulation optimisation at source
- Case IV – Chlorine and alum optimisation at source
- Case V – Chlorine optimisation at source and booster chlorination
- Case VI – Chlorine dose optimisation at booster chlorination with less chlorine at source

Table 1 | Objectives, real variables and constraints for optimiser

Objective functions	• Minimize cancer treatment cost
	• Minimize water treatment chemicals cost
Real variables	• Alum dose at water treatment plant
	• Chlorine dose at water treatment plant
	• Head of reservoir at water treatment plant
	• Chlorine dose at booster chlorination
Constraints	• Pressure≥minimum desired pressure
	• Residual chlorine >0.2 mg/L (WHO 2006)
	• CT value>required CT value (USEPA 1999)
	• HAA6 <0.060 mg/L (USEPA 1998)
	• TTHM <0.080 mg/L (USEPA 1998)

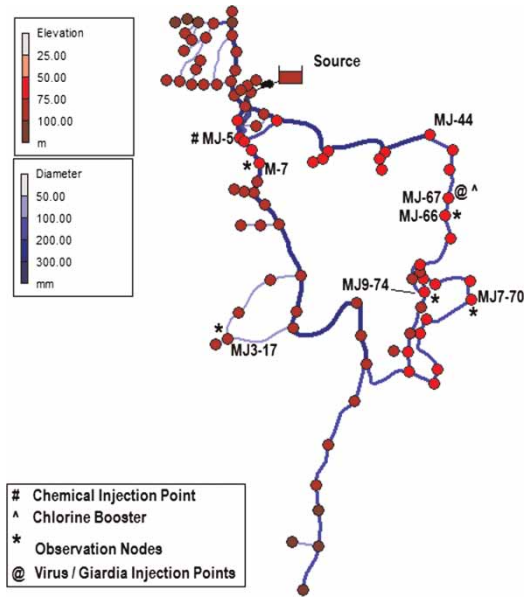


Figure 3 | Minneriya water distribution network – Sri Lanka.

- Case VII – Alum, chlorine and flow optimisation with multiple water sources
- Case VIII – Alum, chlorine and flow optimisation with multiple water sources and booster chlorination
- Case IX – Chemical perturbation

RESULTS AND DISCUSSION

Consistency check of the optimiser

After a number of trial runs and consistency checks, optimisation parameters: population size, number of generations, probability of crossover of real variables, and probability of mutation of real variables were selected to be 128, 50, 0.7 and 0.1, respectively. In order to check if the NSGA-II optimisation produced consistent results, an optimisation test case was run five times with different randomisations. The results showed that the average annual cancer treatment cost was USD \$82,600±430, whereas the average water treatment cost was USD \$55,800±1,080 for all of the five cases. Hence, it was concluded that the optimiser produced consistent results in repeated runs.

Upon optimising all the cases under consideration, the best populations, i.e. alum dose and chlorine dose

complying with the constraints for each case, have been generated. The corresponding water treatment cost and cancer treatment cost for each of these populations have also been computed (Figure 1). The results show that the water treatment cost is lower when chlorine dose is optimised without alum addition (Case II). Optimising alum and chlorine doses at source (Case IV) results in lower water treatment costs compared to other cases where either only one of the chemicals is optimised at the sources (Cases III) or when booster chlorination is included (Cases V and VIII). The least cancer treatment cost was observed when both coagulant and chlorine were optimised at source (Case IV). The results of chemical risk are presented in the form of a contour plot for each case (Figures 4–6). Chemical risk for Case V follows similar pattern as Case IV, but in the vicinity of the booster locations, higher risks are observed due to the high residual chlorine. Analyses for water age, residual chlorine, CT values, THM and HAAs have also been performed and contour plots were prepared (results not shown). From the results it has been observed that chemical risk varied with changes in alum dose, chlorine dose, presence of booster chlorine, and additional source.

Arbitrary dose versus optimised doses of chlorine and alum

An arbitrary chlorine dose of 3 mg/L was assumed for Case I to compute the chemical risk. However, the optimum chlorine dose recommended by the model was 2.34 mg/L (Case II). In both cases there was no additional alum dosage. It was observed that the chemical risk was less in Case II compared to Case I. In Case III, the chlorine dose was fixed at 2.34 mg/L and alum dose was optimised. The optimised alum dose was found to be 47.5±14.5 mg/L. In Case IV both alum and chlorine doses were optimised with values of 46.4±15.2 and 2.2±0.1 mg/L, respectively, and the chemical risk was found to be the least when both alum and chlorine doses were optimised.

Optimisation of chlorine at source versus booster chlorination

It was observed from Figure 5 that the presence of booster chlorine increased the chemical risk in the surrounding nodes. After optimisation, the chlorine dose required at the booster chlorinators was close to the minimum set point of 0.4 mg/L, which clearly indicates that booster chlorination was not necessary in this particular network. In Cases VI an attempt was made to identify locations of booster steps by reducing chlorine dose at source to less than 2 mg/L. It was observed that residual chlorine at several scattered nodes was less than 0.2 mg/L (Figure 7),

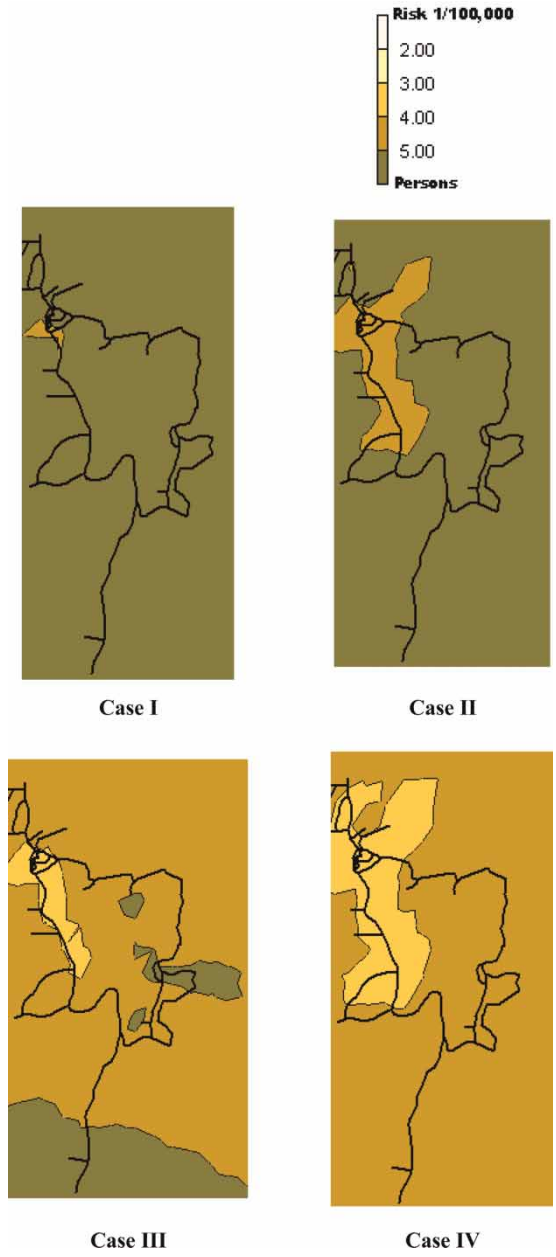


Figure 4 | Chemical risks in Case I, II, III, IV.

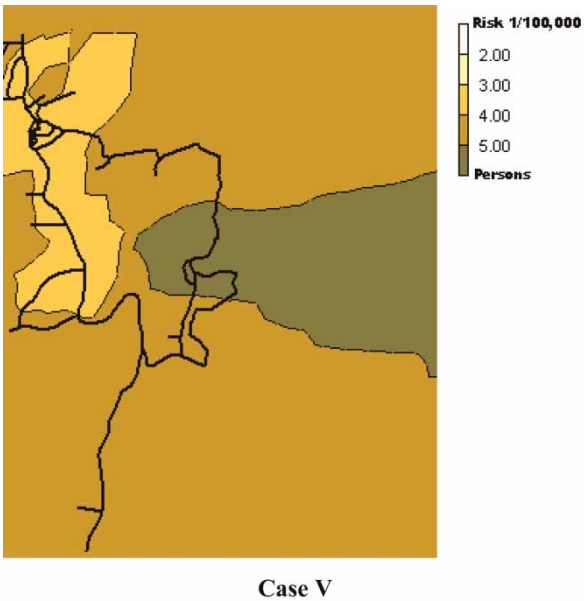


Figure 5 | Chemical risks in Case V.

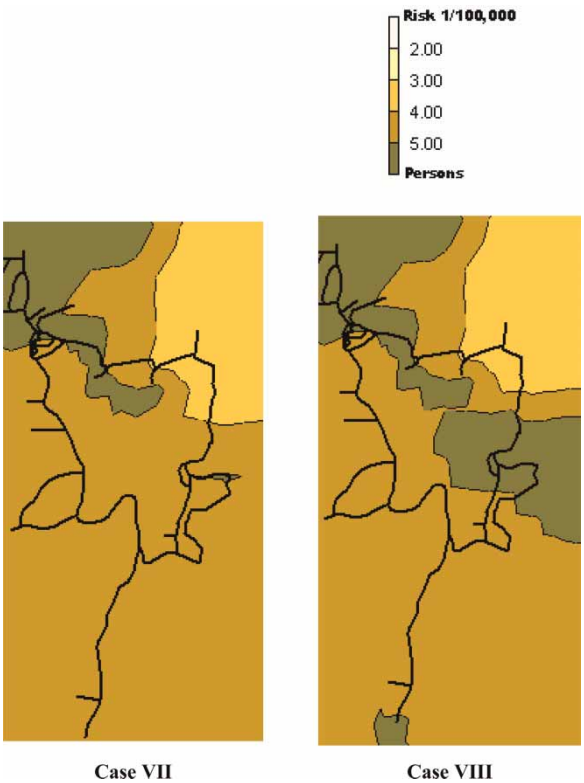


Figure 6 | Chemical risk in Cases VII and VIII.

which implies that either several booster chlorinators should be implemented or the chlorine dose should be increased at the source. The latter solution was more attractive and feasible for this network, in particular, as it is a relatively small network.

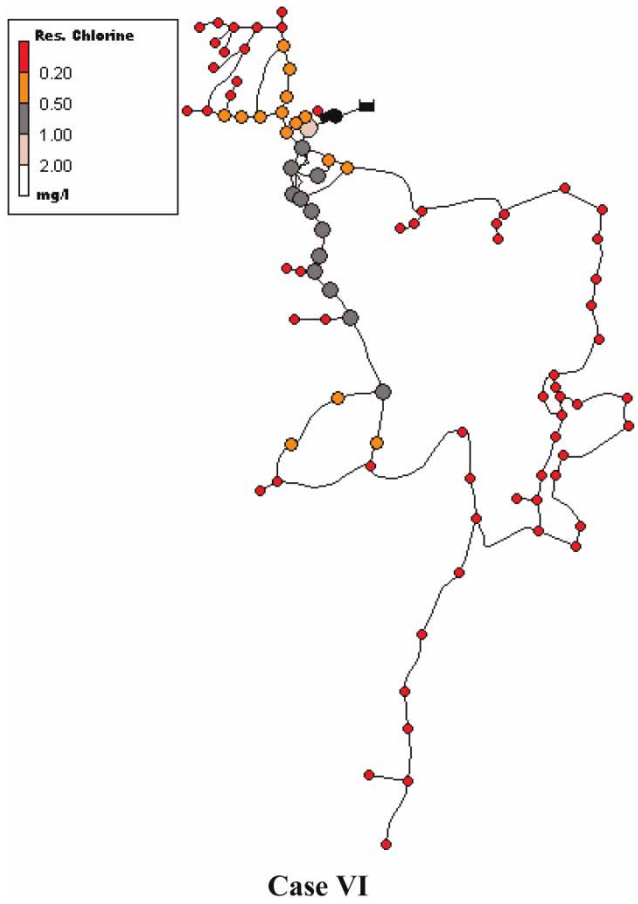


Figure 7 | Residual chlorine in Case VI.

Single source versus multiple sources

In the case of multiple water sources (Case VII and Case VIII), it was observed that the chemical risk reduced substantially in spite of a higher amount of DOC from the additional source. The reduction in DBPs is mainly due to reduction in water age, which is the result of pumping additional water from the second source to the distribution system.

Node specific solutions

A reference node has been selected to evaluate the different cases outlined in the study. Water quality and risk parameters were computed at node MJ9-74 (Figure 3), which

received approximately 40% of its water from source 1 and 60% from source 2. Most of the other nodes received about 90% of their water from either of these sources.

The variation in residual chlorine values and chemical risk for five cases are shown in Figure 8. It can be clearly seen that the residual chlorine and chemical risk follow patterns of water age. While a direct relationship was observed between chemical risk and water age, chlorine residual had an inverse relationship. The residual chlorine for all the optimised cases was lower compared to that of Case I (arbitrary dose), however, in all cases residual chlorine was more than the minimum required (0.2 mg/L). Figure 8(b) shows that the chemical risk in Case IV was the lowest compared to all other cases, and the fact that it is lower than in Case V (with booster chlorination) indicates that there is no need for booster chlorination in the particular network if chlorine and alum dose are optimised at the treatment plant.

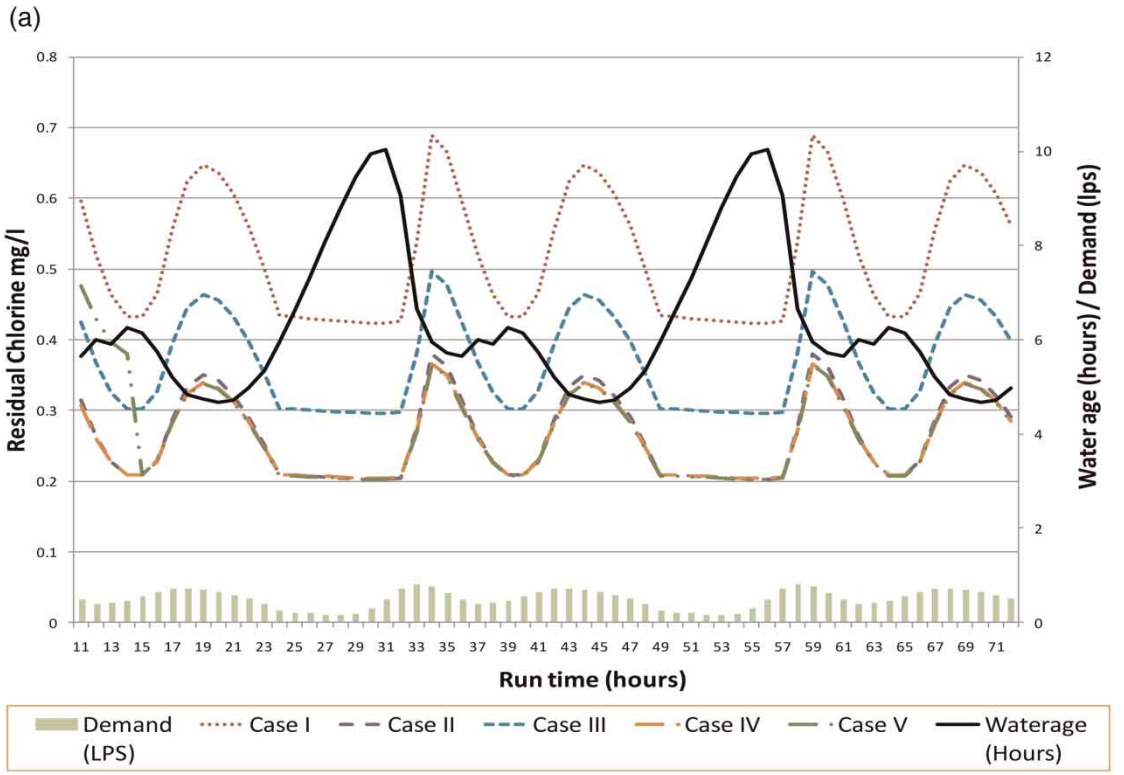
Chemical perturbation and spread

Injection of a toxic chemical in the network has been simulated to analyse the extent of its spread and duration of its presence in the system (Case IX). This information is important to assess water security from the perspective of the impact of potential lethal concentrations arising from an intentional chemical perturbation. In order to simulate this condition, 10 kg of arsenic has been injected into the system during peak demand at node MJ-5. This node is the critical juncture where the inflow from the source enters the network and the trunk mains branch off from this point. The lethal dose (LD_{50}) value for arsenic is 1 mg arsenic/kg body weight, which is approximately 35 mg/L in water (Dart 2004). The results showed that spiked arsenic remained in the system in higher concentrations (1–57 mg/L) for about 9 h, i.e. from 08:00 to 17:00 h, after which it was found only in trace concentrations in nodes with less demand and at dead ends. Figure 9 shows that near the point of injection arsenic concentrations were higher than the LD50 until the first 9 h whereas, at distant locations, an increase in arsenic concentration was observed at a later time. Figure 10 shows the concentrations of arsenic at three nodes during the entire simulation period. Node M-7 is close to the point of arsenic injection. Node MJ3-17 is a node in a secondary loop away from the point of injection, whereas Node MJ7-70 is one of the farthest nodes from the point of injection where the water age is high and the demand is low. The pattern of spread has been unique at each of these points. There was a spike at M-7 much higher than LD50 for some time, after which there was no trace, whereas at MJ3-17 the arsenic concentration increased beyond LD50 for a short period. However, at MJ7-70, the concentration had a gradual build up and drop spreading over 6 h.

Predicting the extent of spread and duration of spread is useful in isolating areas of toxicity and to carry out flushing to remove the contaminant from the system.

Effect due to demand fluctuations

Case IV has also been simulated for variation in demand in order to understand the variation in microbial, cancer risk and its effect. Demand multiplier of the network has been varied between 0.8 and 1.2 and also by means of spiking the demands in the reference node (MJ9-74) and in certain nodes (MJ5-26 and MJ-65) in the vicinity of the reference node. Significant changes in the water age (Figure 11) and risks have been observed due to change in demand for the entire network. It could be inferred that the variation in demand has a certain effect on the risk assessment and the subsequent optimisation that would lead to the change in optimisation levels. The varying seasonal demands could also have the same effect. The exact quantification of the risks and its variation merits further detailed study for the confirmation of the same. Even though the change in water age has been significant for spiked demands at certain nodes, this is not likely to affect the overall annual increase in the risks and also the overall optimisation scheme. Also, the sensitivity of the models has been tested by introducing a water tank that served as a hydraulic and water quality hot spot. The rapid filling of the tank during the initial hours and slow discharge from it due to network hydraulics lead to high water ages in the tank in the range of 58–60 h and to a higher dose of alum and chlorine. Optimisation in this case has not been possible due to the tremendous increase in computational load due to the iterative calculations that PBA (Shang *et al.* 2002) performs for computing water quality in the Water tanks.



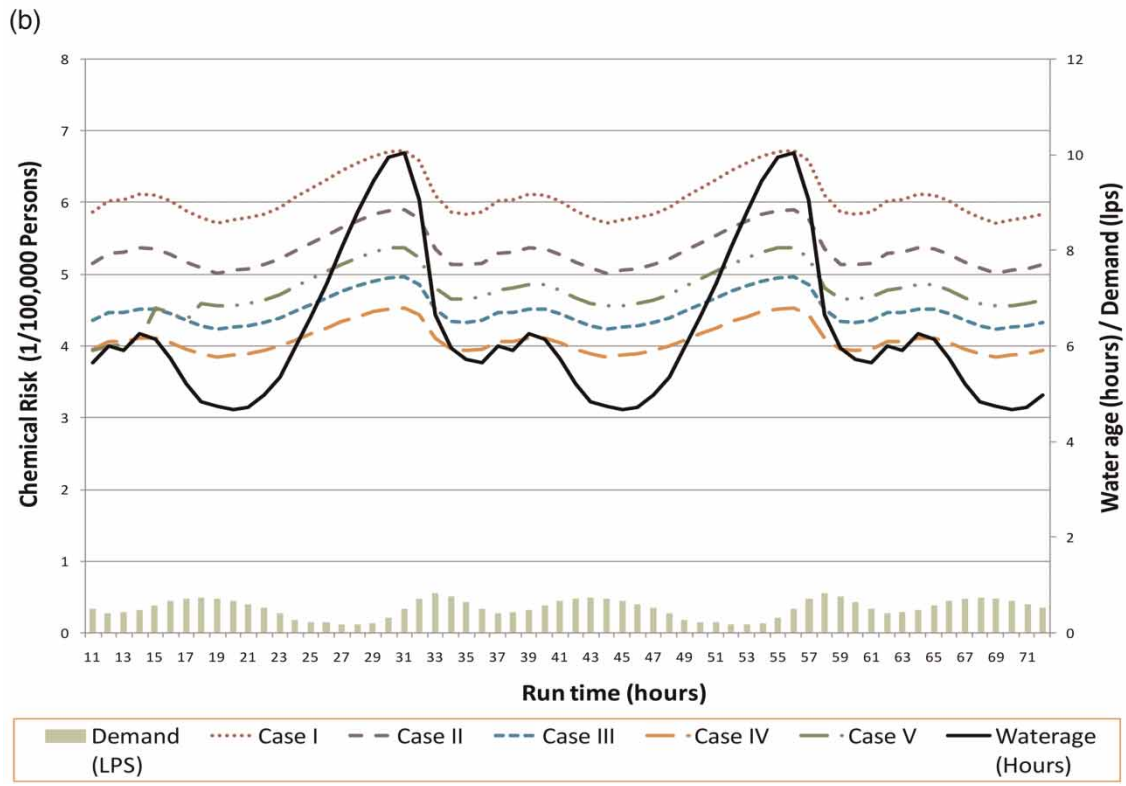


Figure 8 | Residual chlorine and chemical risk in node MJ9-74 (Figure 2) in various cases under consideration.

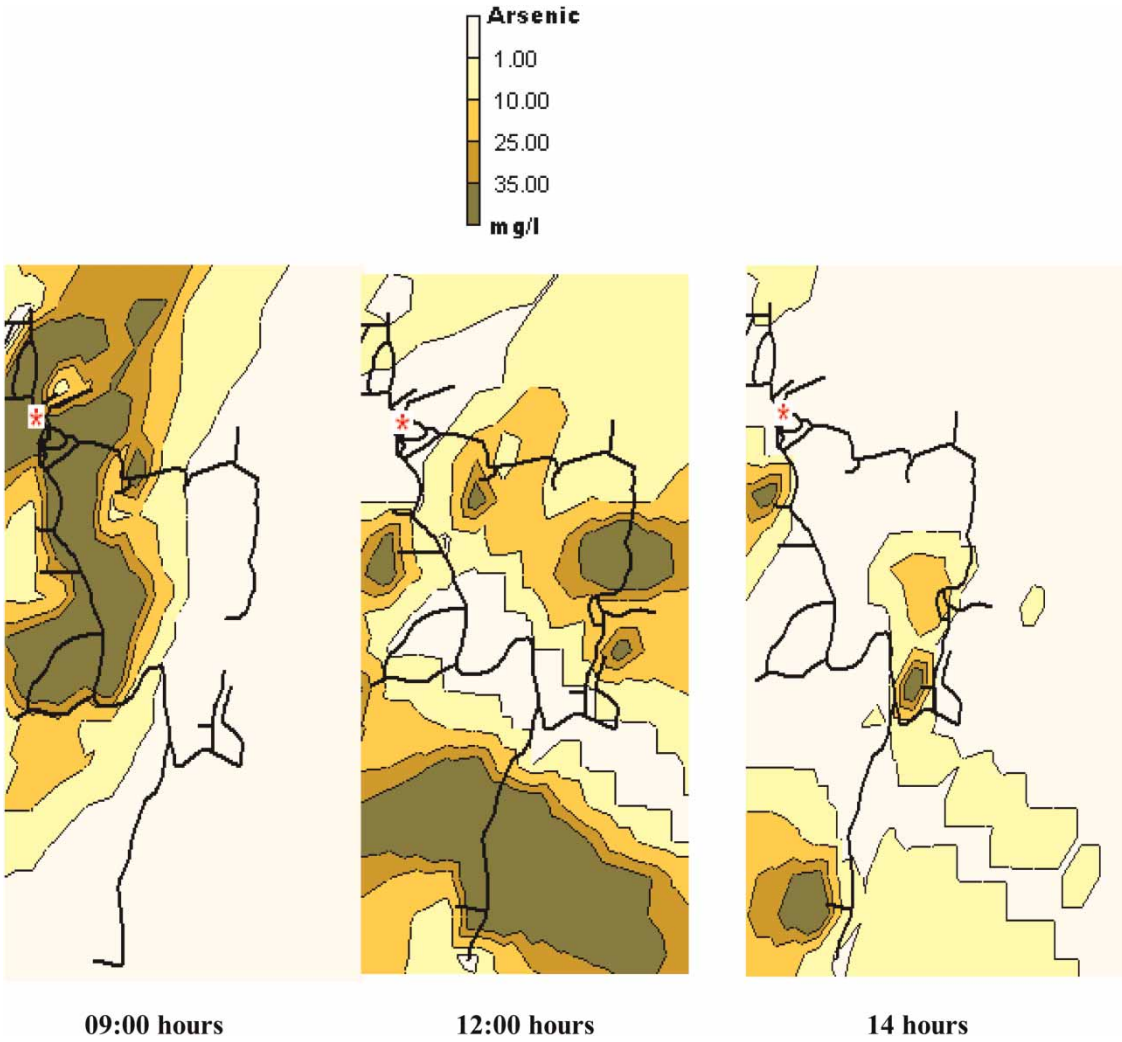


Figure 9 | Arsenic spread in the network at various time. * Point of arsenic injection.

Limitations and recommendations

We tested the model on small distribution systems as a proof of concept and agree that the results would have been more informative if the model was tested on several bigger distribution systems for extended periods, preferably for a year or more with diurnal and seasonal variations in demand. However, numerical optimisation schemes used in the study demand thousands of repeated simulations, which stress the computing resources even for a small network. A single optimisation run for the distribution system under study required about 22 h on a dual core 2.53 GHz platform. It is indeed possible to apply the system for more detailed, complex networks and longer simulations without any changes in the model. However, the optimisation schemes would take several weeks of continuous computing on a normal personal computer. The other alternative is to go for a parallel processing approach, which needs some trivial changes in the model code (evolutionary algorithms are well-known for easy parallelisation). However, this is left for future research. The optimisation module is only capable of solving networks based on continuous supply and demand driven approach and modifications are necessary for intermittent supply. Further, the computational time could be much higher for networks with tanks as the PBA generates huge numbers of paths when tanks are draining (Shang *et al.* 2002).

It has already been mentioned that DBPs models such as USEPA models (Amy *et al.* 1998) and kinetic models

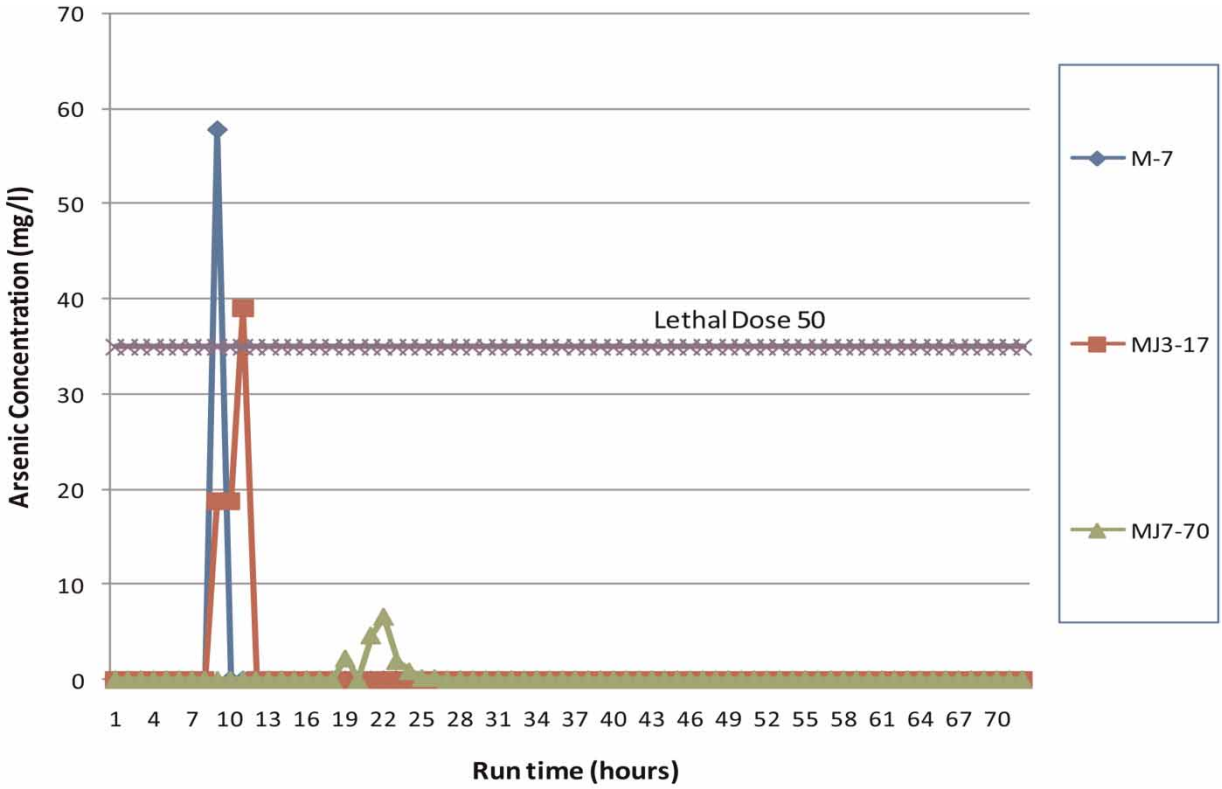


Figure 10 | Arsenic spread at the nodes at various locations in the network.

(Sohn *et al.* 2004) though widely used but are based on bench scale assessments. The water residence times in distribution system and its impact on disinfectant residuals and THM formation has been studied by Simard *et al.* (2011) who have recommended the calibration of hydraulic network based on the residence time obtained using tracer studies. Due consideration has been already given to the kinetic DBPs models developed by Sohn *et al.* (2004) during the development of the risk analysis module. Results obtained from both the models – chlorine concentration, THMs, HAA6 – have been checked and variations have been found to be within acceptable limits for the range of water quality parameters under consideration. The kinetic models have not been adopted in spite of it being found more stable than USEPA models developed by Amy *et al.* (1998) due to the fact that Sohn *et al.* (2004) have developed the kinetic model for the TTHM and HAA6 and not for the individual species. It is recommended that the incorporation of kinetic models for individual DBPs species will certainly enhance the accuracy of the results.

Also, due to the limited availability of time and resources, only the bulk water reactions in the pipeline have been considered and the wall reactions have not been considered. The limitations at the DBPs prediction and incorporation enhanced hydraulic parameters, such as variation and demand, could be overcome though much focused research needs to be conducted extensively on these limitations. Integrity of water quality and negation of biological risk in a municipal water supply system has always been paramount and care has been taken in developing the optimisation module in not overriding this principle. There has always been a risk of trade off whenever biological risk is computed in monetary terms and it has been precisely due to these reasons that the required residual chlorine values and CT values have been used as constraints in the optimiser and not as variables.

Many water distribution networks in developing countries face the problem of low-pressure conditions and intermittent supply (Vairavamoorthy *et al.* 2008) that does not yield well for demand driven analysis which is the

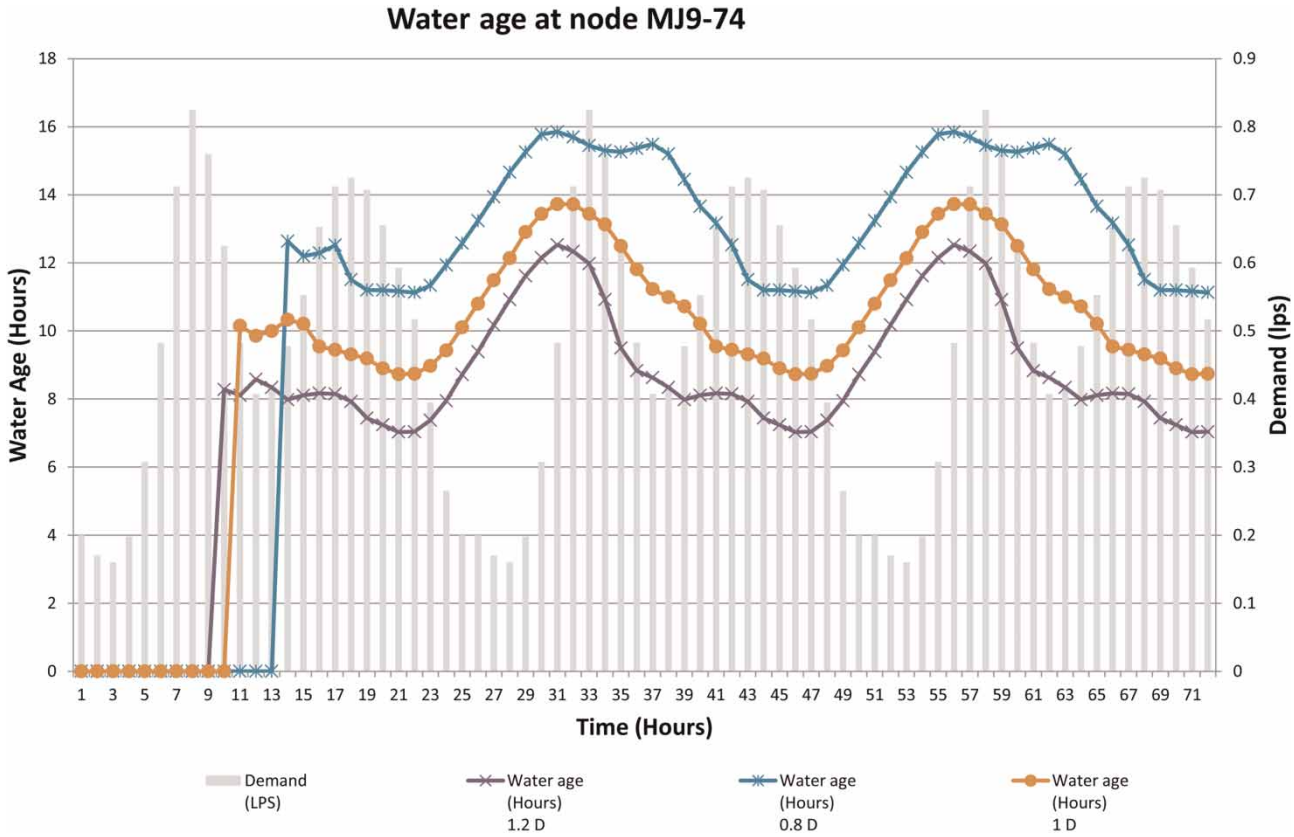


Figure 11 | Variation in water age due to demand fluctuations.

traditional practice in water-distribution systems analysis. While this analysis has been carried out using demand-driven hydraulic analysis, which is clearly a limitation applying the findings to low-pressure networks, it is straightforward to conduct a similar study using pressure sensitive demand hydraulics (Pathirana 2010).

CONCLUSIONS

A modelling approach for reduction of chemical risk due to DBPs and microbial risk in distribution networks employing MOO together with an integrated chlorine decay, DBPs formation, and hydraulic models is presented. Vulnerability assessment of distribution networks in respect of exogenous chemical and microbial contamination have also been carried out. A tool has been developed by integrating the models and NSGA-II and has been tested using a real distribution network with the objective of lowering the potential cancer treatment cost and water treatment cost by varying alum and chemical dose at the water treatment plant, and by varying the chlorine dose at booster chlorine locations without compromising the CT values required for microbial inactivation. Provision for varying the quantity of water from different sources has also been built into the tool as a measure to control DBPs in case of varying water quality from multiple sources in a network.

Based on the results from the case study in Sri Lanka, the research concludes that it is possible to determine optimised chlorine and alum dosages, and thereby minimise carcinogenic risk due do chlorination DBPs without compromising microbiological safety. Employing effective water quality algorithms such as a PBA can be helpful in solving problems arising out of water mixing from different sources and changes in water quality due to stagnation. Enhancement of water quality such as booster chlorine injection can be done in an effective manner with the help of a backtracking algorithm. Also, this approach is very

useful in identifying mitigation measures and precautions in case of chemical or microbiological attack in the system. Coupled with online water quality monitoring and feedback stations in the system, a safe distribution network can be made operational and water security assured. Furthermore, the usage of optimisation techniques such as NSGA-II enables one to select an optimal solution from a wide range of possible solutions. The modelling approach used in this study in combination with strategically placed valves can be used to implement water safety plans.

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