Time Dependent Contamination Source Determination:

A Network Subdomain Approach for Very Large Water Networks.*

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Abstract

This paper presents an approach for identifying contamination sources in very large municipal water networks. The vulnerability of municipal drinking water networks to intentional and accidental contaminations requires investigation of alternative protection measures. If a contamination occurs, it is important to identify both the time and location of the contamination source. A dynamic optimization approach for estimating contamination sources was previously presented. The approach developed an origin tracking algorithm that reformulated the partial differential pipe expressions, removing the need to discretize in space. Although this allowed for efficient solutions using a direct simultaneous technique for a network of approximately 500 nodes, the approach does not scale indefinitely to very large networks. This current paper handles very large water networks by performing the optimization on a smaller, subdomain of the entire network. This approach considers the hydraulics and sensor measurements for the entire network, but formulates the dynamic optimization problem for a subset of the network nodes. A subdomain approach is introduced, forming a geographic window around the first sensor to detect contaminant. Numerical results indicate that this subdomain approach is effective at identifying contamination sources. Furthermore, since the required subdomain size is not dependent on the size of the entire network, this approach scales to very large municipal water networks.

1 Introduction

The risk of contamination of water distribution systems through accidental or intentional attacks has motivated the investigation of alternative protection methods, including the use of numerical simulation and optimization algorithms. In the event of a contamination, knowledge about the time and location of the contamination is important to stop the contamination as soon as possible and propose a control strategy. Concentration measurements from a sparse sensor grid can be used to formulate a least squares dynamic optimization problem and invert for the unknown contamination sources. Solving the dynamic optimization problem for unknown, time dependent source terms allows identification of both the time and location of possible contaminant injections.

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Different techniques can be used to solve the dynamic optimization problem, progressing from minimal interfacing with an existing simulator to a more intrusive fully simultaneous technique. Although the fully simultaneous discretization technique produces a very large nonlinear program, in many cases it can be significantly more efficient than sequential techniques [7, 6, 1]. Previous work [6] has indicated that sequential techniques are not appropriate for the solution of the time dependent network source determination problem due to the high cost of calculating derivatives for the time discretized injection profiles. Recent work has presented a reformulation of the pipe constraints, allowing the use of a simultaneous technique for solving the time dependent problem [4].

Efficient numerical results were presented for a network model of approximately 500 nodes, where solution times were under two CPU minutes for all test scenarios. However, this approach performed the optimization over the space of the entire network and will not scale to very large networks. The solution time of large scale optimization tools is governed almost exclusively by the ability to solve the large linear system at each iteration of the optimization. Since the processing and memory requirements are not linear in the number of variables, increasing the problem size can cause a dramatic increase in solution times. Furthermore, with direct factorization techniques, memory limitations place restrictions on the overall size of the linear system that can be solved, restricting the number of network nodes and the number of timesteps that can be considered.

It is important to demonstrate source inversion capabilities for large metropolitan water networks that are much larger than 500 nodes. This paper presents a network subdomain approach where the optimization problem is formulated on a subset of the entire network. Since the time delays associated with paths through water networks are typically long, it is assumed that the entire network would be affected by a contamination. Moreover, it is desirable to invert for the injection location as soon as possible, before the contaminant has had time to dramatically spread through the network. Therefore, shortly following an injection, it is reasonable to assume that there is a subdomain of the entire network that represents the nodes of interest to the inversion problem.

Section 2 presents some background information on the contamination source determination problem, describing the optimization formulation and solution techniques for the entire network problem. Section 3 then presents the subdomain approach for very large water networks. This approach considers hydraulics and sensor measurements from the entire network, selects a subdomain for the optimization, and solves the optimization problem in the space of these selected network nodes only. A modified optimization formulation is presented that applies generally to any set of selected network nodes, allowing the use of any number of techniques to select the nodes of interest. Here, the subdomain is selected based on the geographic location of the network nodes, forming a window around the sensor that first detects contaminant. This approach is demonstrated on an example scenario for a real municipal water network.

2 Background

Water network models are typically represented by a set of nodes and links, where nodes represent junctions, tanks, and reservoirs, and links represent pipes, valves, and pumps. Plug flow is assumed for all pipes, and contaminant reaction is assumed to be negligible, although the model could be formulated with first order decay kinetics. Here it is assumed that network flows are known, either from measurements or numerical simulation and, therefore, are defined inputs to the water quality model. Using the notation described in Table 1 from the Appendix, and introducing unknown time dependent injection terms, $m_k(t)$ at every network node, the least squares estimation for the entire network can be written as,

$$\min_{\substack{m_k(t),\bar{c}_i(x,t),\hat{c}_k(t)\\ \forall i\in\mathcal{P},k\in\mathcal{N}}} \Psi = \sum_{r\in\Theta^\star}\sum_{k\in\mathcal{N}^\star}\frac{1}{2}\int_0^{t_f} w_k(t)\left(\hat{c}_k(t)-\hat{c}_k^\star(t)\right)^2\ \delta(t-t_r)\ dt + \sum_{k\in\mathcal{N}}\int_0^{t_f} m_k(t)^2\ dt \quad (1)$$

s.t.

$$\frac{\partial\bar{c}_i(x,t)}{\partial t} + u_i(t)\frac{\partial\bar{c}_i(x,t)}{\partial x} = 0, \qquad \forall i\in\mathcal{P}, \quad (2)$$

$$\bar{c}_i(x{=}\mathcal{I}_i(t),t) = \hat{c}_{k_i(t)}(t), \qquad \forall i\in\mathcal{P}, \quad (3)$$

$$\bar{c}_i(x,t{=}0) = 0, \qquad \forall i\in\mathcal{P}, \quad (4)$$

$$\hat{c}_k(t) = \frac{\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\ \bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t)}{\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\right) + Q_k^{ext}(t) + Q_k^{inj}(t)}, \qquad \forall k\in\mathcal{J}, \quad (5)$$

$$V_k(t)\frac{d\hat{c}_k(t)}{dt} = \left(\sum_{i\in\Gamma_k(t)} Q_i(t)\ \bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t) - \left[\left(\sum_{i\in\Gamma_k(t)} Q_i(t)\right) + Q_k^{ext}(t) + Q_k^{inj}(t)\right]\hat{c}_k(t), \qquad \forall k\in\mathcal{S}, \quad (6)$$

$$\hat{c}_k(t{=}0) = 0, \qquad \forall k\in\mathcal{S}, \quad (7)$$

$$m_k(t) \geq 0, \qquad \forall k\in\mathcal{N}. \quad (8)$$

The first term in the objective measures the difference between calculated and measured node concentrations, and the second term regularizes the problem, forcing a numerically unique solution. The network links are modeled using constraint equations (2-4), network nodes are modeled using constraint equations (5-7), and

the injection terms are bounded to be positive by (8). External flows, $Q_k^{ext}, k \in \mathcal{N}$, pipe velocities, $u_i(t), i \in \mathcal{P}$, and volumetric flow rates, $Q_i(t), i \in \mathcal{P}$, are known inputs to the model coming from the hydraulic analysis. In practice, flow rates, $Q_k^{inj}, k \in \mathcal{N}$, of the injection terms will not be known, but it is assumed that the contaminant injections will not dramatically affect the network flow conditions, and these flow terms are set to a small number relative to other network flow rates.

The only unknowns in the optimization problem are the pipe concentrations, $\bar{c}_i(x,t), i \in \mathcal{P}$, the node concentrations, $\hat{c}_k(t), k \in \mathcal{N}$, and the mass injections, $m_k(t), k \in \mathcal{N}$. The solution values for the the injection terms, $m_k(t)$, are the profiles of interest, where positive values indicate a potential contamination time and location. Problem (1-8) presents an infinite dimensional optimization problem subject to algebraic, ordinary differential, and partial differential constraints. A review of techniques for solving differentially constrained problems can be found in [1].

A direct simultaneous technique has been used to solve problem (1-8) [4]. The partial differential pipe expressions are a function of both time and space, and straightforward application of the simultaneous technique produces an Eulerian type discretization in time and space. Unfortunately, this would result in a nonlinear program that is too large for current optimization tools that use direct factorization techniques. Lagrangian solution methods are the current industry standard for simulation of chemical transport in water distribution networks [5], but it is not clear how to formulate this model in a simultaneous setting, or how to efficiently calculate derivatives.

Instead, to allow the use of a simultaneous discretization technique, an origin tracking algorithm was presented that reformulated the partial differential pipe expressions (2-3) into a system of algebraic equations with time delays. Based on the water quality method presented by Liou and Kroon [2], the origin tracking algorithm exploits the efficiency of the Lagrangian technique, but provides a straightforward mathematical representation of the pipe time delays. While traditional Lagrangian methods use the known hydraulic information and track the actual concentration value of fluid elements as they move through the network, the origin tracking algorithm instead tracks the origin of each fluid element in the pipe. Any element of fluid in the pipe originated from one of three possible sources; either it entered from one of the two connected nodes, or it was present in the pipe initially. The algorithm records the origin of each fluid element as it enters the pipe. As flow conditions push elements past the pipe boundaries, knowledge of the origins of these elements is sufficient to describe the time delays between pipe boundary concentrations and connected nodes. This algorithm removes the need to discretize in space and allows the use of a simultaneous technique, discretizing in time alone. For a more detailed description of this work, refer to Laird et al [4].

3 A Subdomain Approach

The direct simultaneous solution method with the origin tracking algorithm has successfully inverted for the time and location of contamination sources on a relatively complex, medium sized network model of approximately 500 nodes. Due to the limitations of direct linear solvers, it becomes significantly more expensive to solve the full network problem for increasingly larger networks. The challenge in this current work is to invert for contamination sources in very large networks where solving the optimization problem on the entire network is not possible. Instead, hydraulics and sensor measurements are considered from the entire network, then a subdomain of the entire network is selected, and the optimization problem is formulated and solved for this subdomain.

The subdomain is identified by choosing some subset of *selected* nodes out of the entire set of network nodes. It is first necessary to rewrite problem (1-8) for this subset of selected nodes. The node concentrations, $\hat{c}_k(t)$, injection terms, $m_k(t)$ and node expressions, (5-8), are only necessary for selected nodes as well. Given a set of selected nodes, it is straightforward to determine which pipes need to be considered. If pipe i is connected to a selected node at each end, the pipe itself is *selected* and must be modeled. Therefore, the variables, $\bar{c}_i(x,t)$ and expressions (2-4) are included for all selected pipes. On the other hand, if pipe i is not connected to any selected nodes, it is unselected and can be completely excluded from the model. Difficulty arises when pipe i is connected to a selected node at one end and an unselected node at the other. This pipe is still classified as unselected and does not need to be modeled, but it represents a boundary to the subdomain. Since the flow conditions for the node at this boundary must be rectified, the flow into the subnetwork from this pipe is treated as a known external source and the node expressions must be altered to reflect this change.

Using the notation described in Table 1 in the Appendix, and defining $p_i(\bar{c}_i(x,t), \hat{c}_{k_i(t)}(t)) = 0$ to represent expressions (2-4), the optimization problem in the space of the selected subdomain is given by,

$$\min_{\substack{m_k(t),\bar{c}_i(x,t),\hat{c}_k(t),\\ \forall i\in\mathcal{SP},k\in\mathcal{SN}}} \Psi = \sum_{r\in\Theta^\star}\sum_{k\in\mathcal{SN}^\star}\frac{1}{2}\int_0^{t_f} w_k(t)\,(\hat{c}_k(t)-\hat{c}_k^\star(t))^2\;\delta(t-t_r)\,dt + \frac{\rho}{2}\sum_{k\in\mathcal{SN}}\int_0^{t_f}(m_k(t))^2 dt \tag{9}$$

s.t.

$$p_i(\bar{c}_i(x,t), \hat{c}_{k_i(t)}(t)) = 0, \qquad \forall i\in\mathcal{SP}, \tag{10}$$

$$\hat{c}_k(t) = \frac{\left(\sum_{i\in\mathcal{S}\Gamma_k(t)} Q_i(t)\;\bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t)}{\left(\sum_{i\in\mathcal{S}\Gamma_k(t)} Q_i(t)\right) + \left(Q_k^{ext}(t) + \sum_{i\in\mathcal{U}\Gamma_k(t)} Q_i(t)\right) + Q_k^{inj}(t)}, \qquad \forall k\in\mathcal{SJ}, \tag{11}$$

$$V_k(t)\frac{d\hat{c}_k(t)}{dt} = \left(\sum_{i\in\mathcal{S}\Gamma_k(t)} Q_i(t)\ \bar{c}_i(x{=}\mathcal{O}_i(t),t)\right) + m_k(t)$$

$$- \left[\left(\sum_{i\in\mathcal{S}\Gamma_k(t)} Q_i(t)\right) + \left(Q_k^{ext}(t) + \sum_{i\in\mathcal{U}\Gamma_k(t)} Q_i(t)\right) + Q_k^{inj}(t)\right]\hat{c}_k(t), \quad \forall k \in \mathcal{SS}, \quad (12)$$

$$\hat{c}_k(t{=}0) = 0, \quad \forall k \in \mathcal{SS}, \quad (13)$$

$$m_k(t) \geq 0, \quad \forall k \in \mathcal{SN}. \quad (14)$$

Here, the pipe constraints are written for the selected pipes in $\mathcal{SP}$, the junction constraints for the selected junctions in $\mathcal{SJ}$, the tank constraints for the selected tanks in $\mathcal{SS}$, and the injection bounds for all selected nodes in $\mathcal{SN}$. The objective has been modified to sum the concentration errors for the selected sensor nodes in $\mathcal{SN}^\star$ and to regularize over the injection terms in $\mathcal{SN}$. Finally, the mass balances for the junctions and tanks have been modified to include the unselected inlet pipes as external sources.

In the event of a contamination, a subdomain of the entire network can be selected and the solution techniques described in Section 2 can be used to solve the smaller, reduced network problem (9-14).

The formulation presented is general enough for any set of selected network nodes and any subdomain selection technique must satisfy the following goals:

1. The resulting nonlinear program must be small enough for current optimization techniques, therefore the selection technique must choose a reasonable number of nodes from the network.

2. This source inversion problem uses real time sensor measurements from the network and needs to be solvable in an online setting. Therefore, any preprocessing to select the network subdomain must be efficient for large networks.

3. The algorithm must select a subdomain that sufficiently represents the area of interest to the source inversion problem. This can be difficult since the actual source is, of course, not known.

Here, a simple geographical window is used to select the network subdomain. The geographical location of first sensor to detect contaminant is identified. Then, the n closest nodes to this location are selected for the subdomain, where the value of n is chosen large enough to represent the area of interest, but small enough to produce a solvable nonlinear program. Of course, there is no explicit guarantee that this subdomain will include the actual contamination locations, but if a contamination source is identified on the boundary of the subdomain, the window could be expanded or moved. Furthermore, since solutions have already been demonstrated on networks of 500 nodes, it is likely that this window can be made sufficiently large.

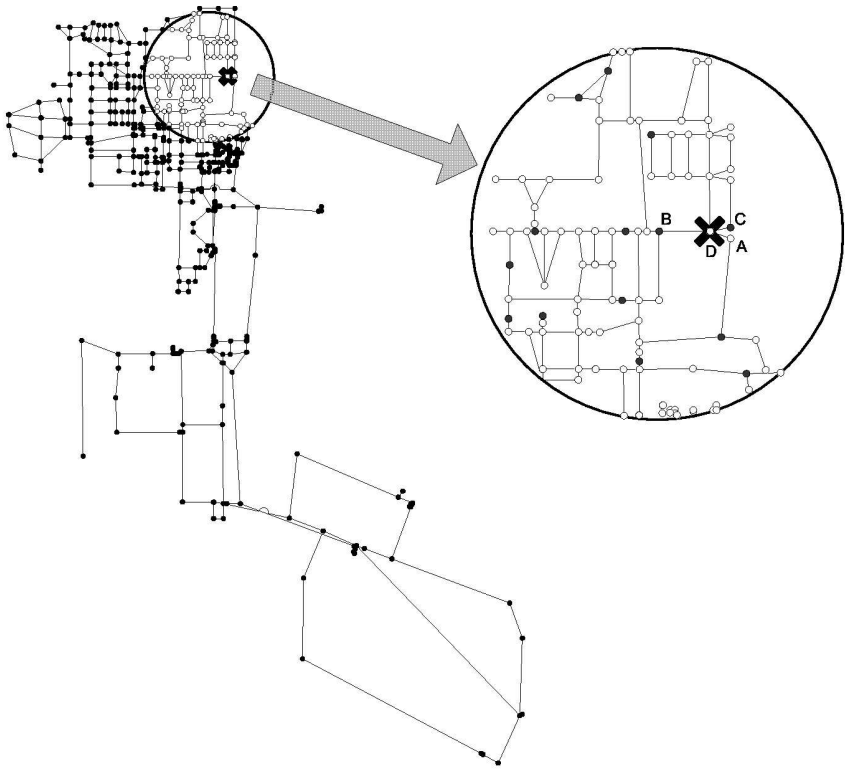

Figure 1: Example Water Network. This figure shows the entire water network. The hollow nodes mark the 100 node subdomain considered in the optimization and X marks the simulated injection location. The inset figure shows increased detail on the subdomain, where shaded nodes indicate sensor locations.

4 Numerical Results

The effectiveness of the subdomain approach is demonstrated on a real municipal water network, shown in Figure 1, with 50 randomly placed sensors. The attack scenario is simulated using EPANET [5] where an hour long injection is simulated at hour 4 from the node indicated by X. The simulated hydraulic information and sensor measurements for the entire network are given to a formulation tool. This tool identifies the geographical location of the first sensor node to detect contaminant. Then, the nearest 100 nodes are selected as the network subdomain, illustrated by the hollow nodes in Figure 1. The inset diagram shows this subdomain in more detail, where shaded nodes indicate installed sensors.

The optimization is formulated at hour 8, 4 hours following the initial contamination, and uses the previous 8 hours of simulation data. Specifying this horizon information and a 5 minute integration timestep, the formulation tool performs the origin tracking algorithm and writes the time discretized nonlinear program in AMPL [3] format. AMPL is an optimization modeling language that provides first and second order derivatives using automatic differentiation. This nonlinear program is then solved using IPOPT [8], a large scale, interior point, optimization tool. Equation (14), once discretized, produces a large number of variable

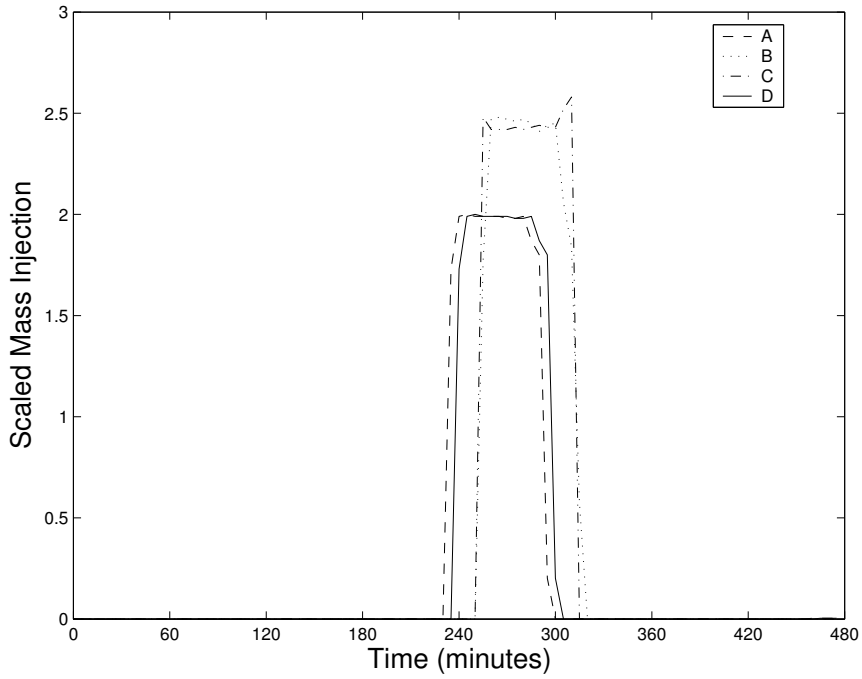

Figure 2: Optimization Solution. This figure shows the solution profile for significant contamination injections. All four injection locations are neighboring, and the subdomain formulation has predicted the precise time of the actual injection at node D.

bounds, and interior point algorithms provide an alternative to active-set strategies for these problems.

The discretized nonlinear program contains 43200 variables, 33600 equality constraints, and 9600 variable bounds and converges on a 2.2 GHz Pentium 4 machine in less than 30 seconds. The solution of the injection profiles are shown in Figure 2, where only the injection terms with significant values are included. Of course, it is desirable to identify a single unique injection location, but with the non-uniqueness caused by the network structure and sensor configurations, this may not be possible. This solution illustrates four possible injection locations at nodes A through D, as shown in Figure 1. Location D is the actual simulated injection point, and it is important to note that locations A through C are all neighboring nodes of D. The formulation has accurately pinpointed the area of the attack. The optimization problem makes no assumption about the initial time or duration of the attack. Yet it has accurately predicted the initial time and length of potential contaminations. The solution indicates that the injection at node D begins at 240 minutes (hour 4) and has a duration of one hour, the exact attack scenario that was simulated.

5 Conclusions and Future Work

These numerical results illustrate the effectiveness of the formulation and the subdomain approach in identifying contamination sources. Not only was the contamination region identified, but the injection time and duration for each possibility

were also determined. Furthermore, this result is illustrated using 50 randomly placed sensors and a contaminant injection duration of only one hour. Optimally placed sensors and longer injection durations should further increase the effectiveness of the inversion.

These results were illustrated using a 100 node subdomain of the entire 500 node network model. It is worth noting that the use of this approach on a larger network does not necessarily require a proportionally larger subdomain. Since the larger network represents a larger area and longer time delays, the size of the required window may not increase at all. Rather, the required number of subdomain nodes is determined by the model granularity, the sensor configuration, and the effectiveness of the algorithm selecting the subdomain. Furthermore, reasonable solution times have been previously demonstrated on the complete 500 node network, therefore, solutions are possible with subdomains much larger than 100 nodes. The authors believe that this network subdomain approach will perform equally well when the entire network is much larger than 500 nodes.

This paper presents a rudimentary algorithm for selecting the subdomain of interest based on geographical location. Future work includes the investigation of more advanced techniques for selecting this subdomain. If possible contamination sources are found on the boundary of the subdomain, it is possible that the subdomain may need to be expanded or moved. The subdomain can be expanded up to acceptable computational limits of the direct linear solver. Also, the window itself can easily be moved, solving the formulation again, until the identified contamination sources are interior to the subdomain. Multiple windows could also be used in a single optimization, each over a different period of time. This requires a multistage approach, where the first window is used for $t = [0..t_1]$, the second for $t = [t_1..t_2]$, etc. Multiple windows could also be solved in parallel. Using distributed parallel processing, each window can be solved independently, with an external algorithm to resolve the connected boundaries.

In conclusion, these preliminary results indicate the potential of simultaneous optimization techniques for efficient, effective identification of contamination sources in municipal drinking water networks. The subdomain approach allows consideration of very large water networks, and reasonable solution times allow its use in a real time setting. Finally, although the simultaneous optimization formulation using the origin tracking algorithm has only been demonstrated on the contamination source inversion problem, its importance extends to other applications, including real time optimization of operating conditions.

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Appendix

Table 1: Notation for Continuous Optimization Formulations (1-14)

Variable	Comments
$\mathcal{P}$, $\mathcal{J}$, $\mathcal{S}$	the complete sets of all pipes, junctions, and storage tanks
$\mathcal{SP}, \mathcal{SJ}, \mathcal{SS}$	the complete sets of all selected pipes, junctions, and storage tanks
$\mathcal{UP}, \mathcal{UJ}, \mathcal{US}$	the complete sets of all unselected pipes, junctions, and storage tanks
$\mathcal{N}, \mathcal{SN}, \mathcal{US}$	the complete set of all nodes, $\mathcal{N} = \mathcal{J} \cup \mathcal{S}$, selected nodes, $\mathcal{SN} = \mathcal{SJ} \cup \mathcal{SS}$, and unselected nodes, $\mathcal{UN} = \mathcal{UJ} \cup \mathcal{US}$
$t \in [0..t_f]$	time
$x \geq 0$	displacement along a pipe
$\bar{c}_i(x,t), i \in \mathcal{P}$	contaminant concentration in pipe i at displacement x and time t
$\hat{c}_k(t), k \in \mathcal{N}$	contaminant concentration of node k at time t
$m_k(t), k \in \mathcal{N}$	unknown contamination mass injection
$\mathcal{N}^\star, \mathcal{SN}^\star, \Theta^\star$	the set of nodes with installed sensors, $\mathcal{N}^\star \subseteq \mathcal{N}$ the set of selected nodes with installed sensors, $\mathcal{SN}^\star = \mathcal{N}^\star \cap \mathcal{SN}$, and the set of all sample times
$\hat{c}_k^\star(t), k \in \mathcal{N}^\star$	measured contaminant concentrations, these values will not be known continuously in time, but rather at discrete sampling points, $t_r, r \in \Theta^\star$
$w_k(t), k \in \mathcal{N}^\star$	time dependent weight for the concentration errors. A flow based weighting function is used, shifting the error measure from a concentration basis to a mass basis
$\Gamma_k(t), \mathcal{S}\Gamma_k, \mathcal{U}\Gamma_k, k \in \mathcal{N}$	the set of all pipes flowing into node k at time t, and the set of all selected and unselected pipes flowing into node k at time t
$\mathcal{I}_i(t), \mathcal{O}_i(t), i \in \mathcal{P}$	displacement along pipe i where fluid is entering and leaving the pipe respectively, these designations are time dependent and change with the flow direction
$k_i(t), i \in \mathcal{P}$	the index of the node connected at the inlet of pipe i, this designation is time dependent and changes with the flow direction
$u_i(t)$	known fluid velocity in pipe i
$Q_i(t), i \in \mathcal{P}$	the known volumetric flow rate in pipe i at time t
$Q_k^{ext}(t), k \in \mathcal{N}$	the volumetric flow rate for known external sources (e.g. reservoir flow)
$Q_k^{inj}(t), k \in \mathcal{N}$	the volumetric flow rate of the unknown contaminant mass injection, $m_k(t)$, in practice this value will not be known and they are set to a small quantity relative to other network flow rates
$V_k(t), k \in \mathcal{S}$	the volume in tank k at time t
$\delta(t)$	Dirac delta function