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Abstract

For the detection of contaminations in urban water supply networks we introduce a continuous optimal control model governed by partial differential equations. We derive a linear mixed-integer model by discretization of the dynamics of the partial differential equations and by approximations to the cost functional. Finally, we present numerical results for artificial and real-world networks.

1 Introduction

Since the early days of Newton and Leibnitz, phenomena involving physical laws such as growth and decay, transport of mass, or conservation of energy are described by differential equations. In our days, continuous models based on partial differential equations (PDEs) are used in various areas of applications, for example, in the simulation of production processes, the understanding of traffic flow in street networks, or the simulation and control of the energy transport from power plants to customers. PDEs provide the finest level of description for many physical and economical processes. In particular, for simulations of large quantities, only the continuous formulations of the PDE models can provide an accurate description of the underlying physical process. Usually, these models rely on quantities such as density (parts per length) and flux (parts per time unit), where the involved parts are not considered individually, but as a continuum. Moreover, we distinguish between simulation and optimization in the following sense. The *simulation* of a physical process is given by a solution to the PDE model under some fixed parameters, e.g., workload of machines, state of compressors in gas networks or demands in water pipeline systems. Thus, simulation means just solving the PDE model, which in itself can be difficult and time-consuming. On the other hand, the *optimization* of processes which are described by a continuous PDE model tries to identify an optimal set of parameters or optimal states in the system, with respect to an objective function or functional. There are now several approaches to achieve this task. The perhaps most simple one is the so-called black-box approach, which is applicable to any simulation process. It consists in successively simulating the PDE model and afterwards gradually changing the input parameters until an "optimal" solution is found. Of course, this heuristic only leads to local optimal solutions without any solution guarantee. Additionally, this approach can be very time consuming in practice.

The new aspect of our work is to introduce a relationship between continuous models and mixed integer programming (MIP) models. The advantage of this MIP approach to PDE models is twofold. First, in many cases MIPs can be solved even for large scale instances in reasonable time by state-of-the-art numerical solvers. Second, the solutions come with a quality warranty, that is, either optimality is proven or an estimation of the optimality gap for the best-known solution is returned. Linear mixed-integer programming can be applied in many ways to continuous PDE models. Below we present a case study related to water quality management. There, we derive a simple PDE model including all major effects and achieve a linear mixed-integer reformulation by a discretization of the PDE model.

The article is organized as follows. We introduce to water quality management in Section 2. We present in Section 3 the continuous water contamination model and in Section 4 the corresponding MIP model. Numerical results for the MIP model are given in Section 5. In Section 6 other areas of application are described. We end up with conclusions in Section 7.

2 Water quality management

Water quality management has many facets. Here we consider the transport of a containment in water networks. Water networks can be understood in a broad sense ranging from municipal water networks supplying a major city up to networks of rivers. Since water is the source of life, the control of water quality has always been a topic of interest. Possible threats to water quality are intentional or accidental contaminations by industry, farms or individual persons. We discuss the problem of identifying sources of containments from given measurements. The networks under investigation are of large scale, which makes it impossible to prevent containments by physical security. We also assume that the measure stations are expensive, such that only a small number of sensors exists throughout the network, which provide information on possible containments. Based on this information we want to identify the origin of the containment. A fast and reliable determination of the sources allows to start activities to prevent further containment. To this end, we present a model for simulating the spreading of the containment within the network, and extend it to an optimization problem for identifying the sources' locations.

The literature on propagation of water and containments through pipes and networks is rich and mathematical approaches for simulation can be found, for example, in [GuLe2003], [GLS2003], [RBA1993], and the references therein. The first researchers who studied the inverse problem, i.e., finding the sources and transient inflow profiles that correspond to given measurements, were Laird, Biegler, and van Bloemen Waanders (see [LBV2006a], [LBV2006b], [LBVB2005]). They formulate the problem as a continuous optimization problem which is similar to our approach. The main difference to the approach presented in the sequel is that they solve the problem using non-linear optimization techniques. Since the resulting non-linear programming problems are of enormous size, only small instances can be solved to optimality.

3 The Continuous PDE Model

Before we introduce the source detection problem, we provide a model for transport of containment inside the network, similar to the model presented in [LBVB2005].

3.1 Simulation

We model the water network as a finite graph $(\mathcal{V}, \mathcal{A})$ with node set $\mathcal{V}$ and arc set $\mathcal{A}$. We cannot consider each atom of the containment individually, since there are too many of them. Hence it is natural to analyze the flux f^j of the contamination on arc j. *Flux* means the amount of containment per unit time. The flux depends on the *density* (or *concentration*) c^j of the containment, i.e., the amount of containment per unit length. We assume that the containment is totally dissolved in water. If u^j denotes the *velocity* (or *speed*) of water in arc j (in length per time), then the flux of containment is given by $u^j \cdot c^j$. Since the whole water network system is dynamic, the density itself is not a constant, but depending on and changing with the time t. It is also depending on the space, because the density of the containment can be different in different parts of the network (it can even vary within one arc). If we model the arcs as one-dimensional (i.e., the atoms of the containment cannot overtake each other), then a single coordinate $x \in [a^j, b^j]$ is sufficient to uniquely determine every location within the arc. Hence we have $c^j = c^j(x,t)$ and $u^j = u^j(x,t)$, and thus

$$f^j(c^j(x,t)) = u^j(x,t) \cdot c^j(x,t). \tag{1}$$

$c^j(x,t)$ describes the concentration of the containment at position x at time t, and $u^j(x,t)$ describes the velocity, also depending on the position and the time. Note that the signum of $u^j(x,t)$ indicates the direction of the flow. For $u^j(x,t) > 0$ the flow is in direction of the arc, for $u^j(x,t) < 0$ the water flows in the opposite direction. We assume that for every time step t we either have $u^j(x,t) \geq 0$ or $u^j(x,t) \leq 0$, that means, the direction of the flow does not change within the arc.

At time t the amount of containment in a section of some arc j between positions x_1 and x_2 is given by

$$\int_{x_1}^{x_2} c^j(x,t)\,dx = \text{amount of containment between } x_1 \text{ and } x_2 \text{ at time } t. \tag{2}$$

In the same way, we can express how many containment flows through position x during a time interval from t_1 to t_2:

$$\int_{t_1}^{t_2} f^j(c^j(x,t))\,dt = \text{amount of containment passing position } x \text{ during } t_1 \text{ and } t_2. \tag{3}$$

Now we have a *mass balance*, that is, the amount of containment on the arc between x_1 and x_2 at time t_2 equals the amount of containment in this section at time t_1 plus the *inflow* at x_1 minus the *outflow* at x_2 during the time interval from t_1 to t_2. We assume that no water is lost or produced during the transport. Expressed as an equation, the material balance can be stated as

$$\int_{x_1}^{x_2} c^j(x,t_2)\,dx = \int_{x_1}^{x_2} c^j(x,t_1)\,dx + \int_{t_1}^{t_2} f^j(c^j(x_1,t))\,dt - \int_{t_1}^{t_2} f^j(c^j(x_2,t))\,dt. \tag{4}$$

From the *fundamental theorem of calculus* we obtain

$$c^j(x,t_2) - c^j(x,t_1) = \int_{t_1}^{t_2} \frac{\partial}{\partial t} c^j(x,t)\,dt, \tag{5}$$

$$f^j(c^j(x_1,t)) - f^j(c^j(x_2,t)) = -\int_{x_1}^{x_2} \frac{\partial}{\partial x} f^j(c^j(x,t))\,dx, \tag{6}$$

which implies

$$\int_{x_1}^{x_2} c^j(x,t_2)\,dx - \int_{x_1}^{x_2} c^j(x,t_1)\,dx = \int_{x_1}^{x_2}\int_{t_1}^{t_2} \frac{\partial}{\partial t} c^j(x,t)\,dt\,dx, \tag{7}$$

$$\int_{t_1}^{t_2} f^j(c^j(x_1,t))\,dt - \int_{t_1}^{t_2} f^j(c^j(x_2,t))\,dt = -\int_{t_1}^{t_2}\int_{x_1}^{x_2} \frac{\partial}{\partial x} f^j(c^j(x,t))\,dx\,dt. \tag{8}$$

Combining these results with the material balance equation (4) yields

$$\int_{x_1}^{x_2}\int_{t_1}^{t_2} \frac{\partial}{\partial t} c^j(x,t)\,dt\,dx + \int_{t_1}^{t_2}\int_{x_1}^{x_2} \frac{\partial}{\partial x} f^j(c^j(x,t))\,dx\,dt = 0. \tag{9}$$

If we assume that equality (9) holds for every segment x_1, x_2 in the processor and for each time interval t_1, t_2, and if the function $c^j(x,t)$ and its partial derivatives of order one are continuous functions, then from an elementary integration property of continuous functions we obtain that

$$\frac{\partial}{\partial t} c^j(x,t) + \frac{\partial}{\partial x} f^j(c^j(x,t)) = 0. \tag{10}$$

Moreover, the containment can react with the surrounding according to some chemical laws expressed for the sake of simplicity in an additional equation as

$$\frac{\partial}{\partial t} c^j(x,t) = R^j(c^j(x,t)), \tag{11}$$

where R^j is a function depending only on the density of the containment and the arc (i.e., the size of the water pipe's cross section). In the case under consideration we use a decay of containment over time and, to be more precise, we assume that

$$\frac{\partial}{\partial t} c^j(x,t) = -rc^j(x,t), \tag{12}$$

for some constant $r \ll 1$.

It remains to prescribe the coupling of the network pipes at nodes $v \in \mathcal{V}$. Denote by A^j the cross section area of the water pipe. Denote by

$$\delta^+(v,t) := \{(w,v) \in \mathcal{A} : u^{(w,v)}(x,t) > 0\} \cup \{(v,w) \in \mathcal{A} : u^{(v,w)}(x,t) < 0\} \tag{13}$$

the set of incoming arcs to v, and by

$$\delta^-(v,t) := \{(v,w) \in \mathcal{A} : u^{(v,w)}(x,t) > 0\} \cup \{(w,v) \in \mathcal{A} : u^{(w,v)}(x,t) < 0\} \tag{14}$$

the set of outgoing arcs. By $e^j(t)$ we denote the coordinate of the arc's outflow end, that is, $e^j(t) := b^j$ for $u^j(x,t) > 0$ and $e^j(t) := a^j$ for $u^j(x,t) < 0$. The amount of water leaving the arc is proportional to the cross section area and the velocity, that is, it is proportional to $A^j|u^j(e^j(t),t)|$. We assume that at each node v the total incoming flux

$$\sum_{j \in \delta^+(v,t)} A^j|u^j(e^j(t),t)| \tag{15}$$

is distributed proportional to the ratio of the outgoing fluxes

$$\frac{A^i|u^i(e^i(t),t)|}{\sum_{j \in \delta^-(v,t)} A^j|u^j(e^j(t),t)|}, \quad \forall\, i \in \delta^-(v,t). \tag{16}$$

That is, in the simplest possible case of water pipes of the same diameter and having the same velocity, we would observe a distribution with the same flow on each outgoing pipe. Since the containment is dissolved in the water, it is natural to assume that the concentration traveling along with the water flow is distributed exactly as the water flow itself. At the node $v \in \mathcal{V}$ we prescribe the inflow of the containment by functions $q^v(t)$. Hence, we obtain

$$c^i(e^i(t),t) = \frac{q^v(t) + \sum_{j \in \delta^+(v,t)} A^j|u^j(e^j(t),t)|c^j(e^j(t),t)}{\sum_{j \in \delta^-(v,t)} A^j|u^j(e^j(t),t)|}, \quad \forall\, i \in \delta^-(v,t). \tag{17}$$

This setting guarantees conservation of the containment through nodes, because adding all incoming arcs $i \in \delta^-(v,t)$ yields the flow conservation condition

$$q^v(t) + \sum_{j\in\delta^+(v,t)} A^j |u_j(e^j(t),t)| c^j(e^j(t),t) = \sum_{j\in\delta^-(v,t)} A^j |u^j(e^j(t),t)| c^j(e^j(t),t). \tag{18}$$

Finally, we assume that initially at $t = 0$, no containment is present on the arcs of the network,

$$c^j(x,0) = 0. \tag{19}$$

3.2 Optimization

For the presented model we formulate the source inversion problem. Given measurements of containment $\bar{c}^j(x,t)$ for $j \in \mathcal{A}_{meas}$ we try to identify sources q^v for $v \in \mathcal{V}$ such that the time evolved concentrations c^j coincide with the measurements on arcs $j \in \mathcal{A}_{meas}$. Moreover, we identify the time-evolution of these sources, i.e., we are looking for functions $t \to q^v(t)$.

We introduce an objective function measuring the distance between the predicted contamination and its measured value. There are several possible choices to define a measure for the distance between predicted and measured contamination. For example, [LBV2006a] proposed to measure the time and spaced averaged quantity

$$\sum_{j\in\mathcal{A}_{meas}} \int_0^T \int_{a^j}^{b^j} \left(c^j(x,t) - \bar{c}^j(x,t)\right)^2 \, dx \, dt \tag{20}$$

Therein, T denotes the total time horizon of the measurements. We assume that the measurements $\bar{c}^j$ are given for all points in space and time on pipe $j \in \mathcal{A}_{meas}$. If we only have information on a single point $\bar{x}^j$ of this pipe, then a possible objective functional might also be given by

$$\sum_{j\in\mathcal{A}_{meas}} \int_0^T \left(c^j(\bar{x}^j,t) - \bar{c}^j(\bar{x}^j,t)\right)^2 \, dt + \rho \sum_{v\in\mathcal{V}} \int_0^T q^v(t) \, dt \tag{21}$$

for some $\rho > 0$. This penalize the number of sources and its intensity, see again [LBVB2005] and the references therein.

In view of the latter mixed-integer approximation we propose the following objective functional also measuring the difference between simulated and measured contamination and penalizing the number of sources:

$$\sum_{j\in\mathcal{A}_{meas}} \max_{t\in(0,T)} (c^j(\bar{x}^j,t) - \bar{c}^j(\bar{x}^j,t)) + \rho \sum_{v\in\mathcal{V}} \max_{t\in(0,T)} q^v(t). \tag{22}$$

4 A Linear Mixed-Integer Model

For a numerical solution of the continuous model in the case of large scale networks and in near real-time, we reformulate this model as a linear mixed-integer program. We first transform the partial differential equations for the transport (10) and the decay (12) into a set of linear constraints. For the time derivative we use the *forward difference approximation*

$$\frac{\partial}{\partial t} c^j(x,t) \approx \frac{c^j(x,t+\Delta t) - c^j(x,t)}{\Delta t}, \tag{23}$$

whereas for the spatial derivative we take the *backward difference approximation*

$$\frac{\partial}{\partial x} c^j(x,t) \approx \frac{c^j(x,t) - c^j(x-\Delta x,t)}{\Delta x}. \tag{24}$$

We introduce a discretization for the time as $t_n := n\Delta t$ for $n \in \{0,1,\ldots,N\}$, where Δt is a constant step size (see below), and $N = \lceil T/\Delta t \rceil$. From now on, the time is not running continuously, but in discrete time steps.

For each arc j of the water network we introduce three variables $c_t^{j,in}, c_t^{j,mid}$ and $c_t^{j,out}$, corresponding to the containment concentration at three points inside the water pipe. The direction of the flow plays an important role, so we make a distinction between the cases $u^j(x,t) \geq 0$ and $u^j(x,t) \leq 0$. In the first case, we take $c_n^{j,in} := c^j(a^j,t_n), c_n^{j,mid} := c^j(\frac{a^j+b^j}{2},t_n)$, and $c_n^{j,out} := c_j(b^j,t_n)$, and in the second case we have $c_n^{j,in} := c^j(b^j,t_n)$, $c_n^{j,mid}$ as before, and $c_n^{j,out} := c_j(a^j,t_n)$. Accordingly, we use $u_n^{j,in}, u_n^{j,mid}, u_n^{j,out}$ as abbreviations for the function values $u^j(x,t)$ at the corresponding coordinates. Note that by this settings, we implicitely introduced a spatial discretization of $(\Delta x)^j := \frac{b^j-a^j}{2}$. Using these variables and the difference approximations (23) and (24), the so-called *upwind discretization* of (10) reads

$$c_{n+1}^{j,mid} = c_n^{j,mid} - \frac{\Delta t}{(\Delta x)^j} u_n^{j,mid} \left(c_n^{j,mid} - c_n^{j,in}\right), \tag{25a}$$

$$c_{n+1}^{j,out} = c_n^{j,out} - \frac{\Delta t}{(\Delta x)^j} u_n^{j,out} \left(c_n^{j,out} - c_n^{j,mid}\right). \tag{25b}$$

To avoid numerical problems, that is, for the *stability* of the discretization, the *CFL condition*

$$\frac{\Delta t}{(\Delta x)^j}|u^j(x,t)| \leq 1 \tag{26}$$

is required (named after Courant, Friedrichs, and Lewy). To fulfill the CFL condition we thus set

$$\Delta t := \min_j \left(\frac{(\Delta x)^j}{\max\limits_{x,t} |u^j(x,t)|} \right). \tag{27}$$

Using (23) we obtain the following discretization for the decay equation (12):

$$\frac{c^j(x,t+\Delta t) - c^j(x,t)}{\Delta t} = -rc^j(x,t), \tag{28}$$

or

$$c^j(x,t+\Delta t) = (1 - r\Delta t)c^j(x,t). \tag{29}$$

Putting together (25) and (29), we arrive at

$$c_{n+1}^{j,mid} = (1 - r\Delta t) \left(c_n^{j,mid} - \frac{\Delta t}{(\Delta x)^j} u_n^{j,mid} \left(c_n^{j,mid} - c_n^{j,in} \right) \right), \tag{30a}$$

$$c_{n+1}^{j,out} = (1 - r\Delta t) \left(c_n^{j,out} - \frac{\Delta t}{(\Delta x)^j} u_n^{j,out} \left(c_n^{j,out} - c_n^{j,mid} \right) \right). \tag{30b}$$

We remark that the proposed upwind discretization of the transport equation is just one of many possibilities of finite-difference approaches to this partial differential equation, see e.g. [Leve1990], [SUP2002], [RBA1993], [RoBo1996]. In particular, [LBV2006a] propose a Lagrangian method as discretization of the transport equation. For this particularly simple advection equations both discretizations yield the same results. However, we used the upwind method in order to incorporate the decay of the containment more easily.

The unknown possible sources $q^j(t)$ are discretized using the variables $q_n^j := q^j(t_n)$. The discretization of the coupling (17) is straight-forward and obtained as

$$c_{n+1}^{i,in} = \frac{q_n^j + \sum\limits_{j\in\delta^+(v,t_n)} A^j |u_n^{i,out}| c_n^{j,out}}{\sum\limits_{j\in\delta^-(v,t_n)} A^j |u_n^{j,in}|}, \quad \forall\, i \in \delta^-(v,t_n). \tag{31}$$

Finally, the objective functional (22) needs to be discretized. To this end, we use the following linear objective function:

$$\sum_{j\in\mathcal{A}_{meas}} \sum_n |c_n^{j,mid} - \overline{c}_n^{j,mid}|\Delta t + \rho \sum_v \theta^v. \tag{32}$$

Here $\theta^v \in \{0, 1\}$ is a binary decision variable indicating whether there is an inflow of containment at node v. This variable is coupled to the inflow via

$$q_n^v \leq M\theta^v, \tag{33}$$

where M is a sufficiently large constant.

5 Computational Results for Water Quality Management

We present computational results on artificial test networks in Section 5.1 to computationally evaluate the complexity of the involved mixed-integer programming problems. In Section 5.2 we show how to find the containment source within a real-world network using the presented approach.

5.1 Simulation and Optimization of Test Networks

Consider the small test net shown in Figure 1. Within this network, the water is always circulating. Every arc has the same length and cross section. We assume that the velocity is a constant function in space and time. As decay rate we select r such that $1 - r\Delta t = 0.98$, that is, after each time step 2% of the containment vanished. At time $t = 0$ we inject the containment at the node marked with q of this network for the 5 next time steps. On the arc marked with m we measure the containment flow and, based on this measured informations, try to estimate the transient inflow profile. The time horizon for the simulation is $T := 100$ time steps. The results are shown in Figure 2. The left picture shows the inflow profile q, the next four picture show the $c^{j,mid}$ values on arcs $1, \ldots, 4$.

The next computational tests aim at a comparison of different algorithms for linear programming. With a branch-and-bound approach for the solution of the MIP models, the integrality condition on the variables is dropped at first. The integrality is then reintroduced via interatively selecting some node $v \in \mathcal{V}$, and creating two subproblems, one with $\theta^v = 0$ and the other with $\theta^v = 1$. For the numerical solution of the resulting linear programs, several algorithms are known. Here we test the primal and the dual simplex, the network simplex, and the barrier

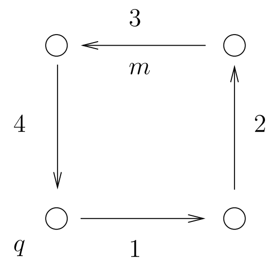

Figure 1: Test network with four arcs $i = 1, 2, 3, 4$.

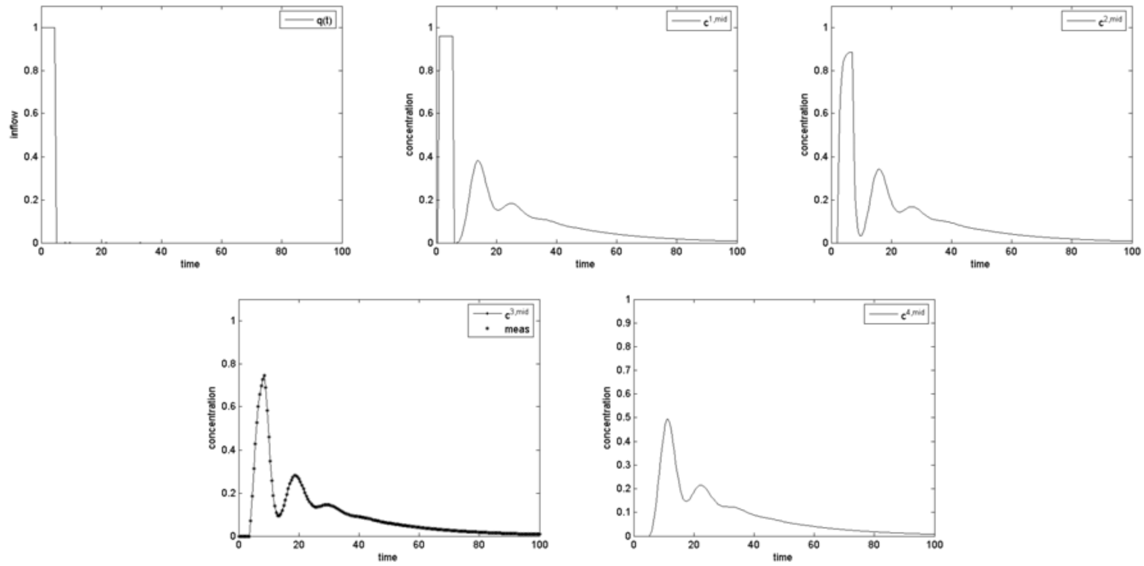

Figure 2: Optimization results for q and arcs $i = 1, 2, 3, 4$ (from left to right).

method (an interior point algorithm), which can all be found within the ILOG Cplex 10 solver suite. Moreover, we want to test the behaviour of these algorithms on instances of different sizes with respect to the number of nodes and the number of time steps. The test networks are rectangular compositions of the network shown in Figure 1 (which in this sense is a 2×2 network). The computational results (solution times in seconds on a standard 2.4 GHz AMD4800X2 personal computer) for a single linear programming relaxation can be found in Table 1.

5.2 Case Study: The Macao Water Supply Network

As a real-world case study we consider the water supply backbone network of the Chinese town Macao, which is inhabited by around half a million people. The network has today a length

size	T	primal	dual	network	barrier
5×5	50	0.1	0.1	0.1	0.1
5×5	100	0.2	0.2	0.2	0.2
5×5	250	0.4	0.4	0.4	0.4
10×10	50	0.7	0.7	0.6	3.7
10×10	100	1.0	0.9	1.0	4.0
10×10	250	2.1	1.8	1.9	5.1
15×15	50	4.1	4.4	6.7	33.5
15×15	100	6.9	6.6	9.8	57.6
15×15	250	9.2	8.9	12.1	59.8
20×20	50	4.3	5.3	8.0	24.5
20×20	100	23.3	37.9	58.4	506.2
20×20	250	27.4	41.6	62.3	401.5

Table 1: Results for various network sizes, time horizons, and LP algorithms.

of about 410 km (for further details see [MACW2006]). The entire backbone network of the three neighbouring cities Macao, Taipa, and Coloane is modeled as a graph that consists of 377 nodes and 601 arcs (see Figure 5). The subnet belonging to Macao is reprensented by a graph having 237 nodes and 407 arcs. The simulation of a contamination is solved on this graph. We now induce a containment in the network at a certain arc, marked with a "q" in Figure 6. On two other arcs, marked with an "m", the containment is measured. The distribution of the containment over the time within the network is shown in Figure 6, which is a magnification of the rectangular region depicted in Figure 5. Each time step in the discrete simulation represents 5 minutes of real time.

We now demonstrate what happens within the branch-and-bound algorithm, when the decision variable θ^v is set to 1 for some arc v. If the inflow originates in this node, then the measured profiles and the resulting concentration profiles on $j \in \mathcal{A}_{meas}$ coincide (see middle and right pictures in Figure 3). The inflow profile of the containment at this node is shown on the left picture in Figure 3.

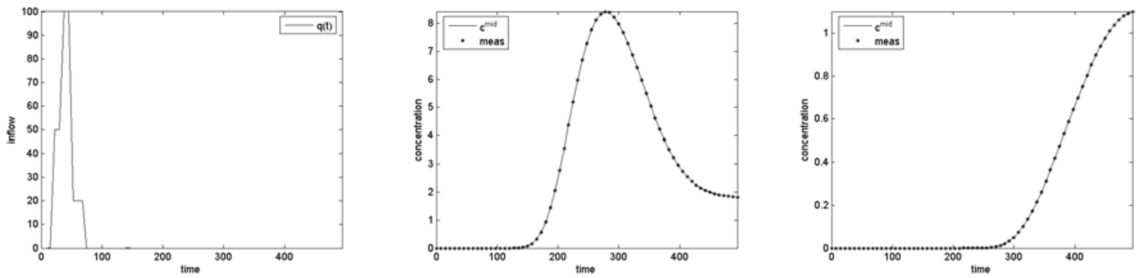

Figure 3: Optimization results for the “right” inflow node

If on the other hand the wrong variable θ^v was selected for branching, then in general we have a gap between the measured and the resulting concentrations (see middle and right picture in Figure 4). This gap leads to a high objective function value, hence the search tree will be pruned as soon as the right node (as above) was found. The inflow profile of the containment of the selected node also has a “strange” appearence (see left picture in Figure 4).

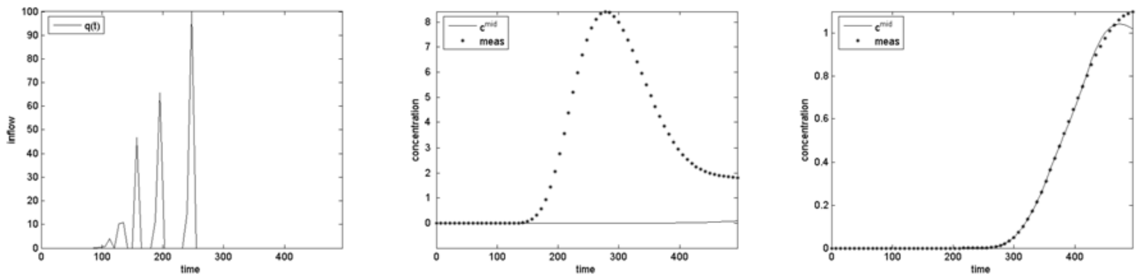

Figure 4: Optimization results for the “wrong” inflow node

6 Other Areas of Application

The applicability of linear mixed-integer programming in continuous PDE optimization is by far not limited to water quality management. In this section we briefly present two other applications where the linear mixed-integer approximation haven been successfully applied in order to simulate and optimize processes on large networks.

6.1 Traffic Flow

The first example is related to traffic flow control for road networks. We briefly summarize the approach and findings of [FHKM2004]. Therein, the starting point has been a continuous model based on partial differential equations for the evolution of traffic flow in networks. The partial differential equation is nonlinear and differs from the one discussed above. Moreover, at each traffic intersection derivation suggestions to drivers are modeled as controls. Then, the detailed model is a coupled system of nonlinear partial differential equations with nonlinear constraints at the road intersections. The task is now to utilize the traffic network in such way, that all cars reach their final destination at the earliest possible time. This determines the derivation suggestions at each single intersection. The difficulty stems from the fact that, due to the partial differential equations which control the dynamics on each arc, a higher utilization of the road yield a lower average traveling speed. Furthermore, for an optimization approach the computational costs for solving the coupled system of equations are too expensive. Therefore, several model reductions have been performed and a simplified dynamics on the roads and at intersections was derived. These can be seen as a coarse-grid discretization of the partial differential equation and an additional averaging for estimating the conditions at intersections. In the next step, all nonlinearities have been approximated by linear equations and binary and real variables. A qualitative comparison showed the applicability of the simplified models and in particular in free flow traffic situations these models perform comparable with the models based on partial differential equations. Moreover, these linear mixed-integer models allowed for optimization of networks of realistic size. For further details we refer to [FHKM2004].

6.2 Production Planning

Production planning in supply chain management has been investigated in relation with continuous and discrete models. In [ADR2006] a completely new access to production planning is introduced. There, a linear partial differential equation for the conservation of goods is derived. This equation is assumed to hold for each supplier. For the modelling of a whole supply network buffering queues are introduced in front of each supplier. Thus, the supply network consists of several suppliers which all have the possibility to store goods. The coupled system of partial and ordinary differential equations describing the supply network allows for simulating large amounts of goods over a long time. In this regard, an optimal control problem is composed of linear (PDE) and nonlinear (queues) constraints. The objective function is also linear and given by maximizing the output and minimizing the amount of goods in all queues. Possible controlling parameters are the distribution rates (used on each vertex where the flux of one supplier is splitted into two new suppliers) or the processing velocities. Similar to the traffic flow control problem we discretize the equations on a coarse grid and substitute the nonlinearity by using binary variables. This leads to a linear mixed-integer programming model. In cases of simple networks where only one supplier is linked to one supplier the continuous model and the MIP model yield same results. A nice poperty of the MIP is the easy extensibility to additional constraints such as the maintenance of suppliers or bounded queues. For further details we refer to [GHK2005], [GHK2006].

7 Conclusions

In this work, we pointed out the relation between continuous models, governed by partial differential equations, and linear mixed-integer programming. This relation is beared on a coarse-grid discretization of the partial differential equation. This technique guarantees the conservation of the original dynamics and also allows for large scale network simulation and optimization. Moreover, the presented way is different from other approaches by Laird, Biegler et al. where non-linear optimization techniques and Lagrangian discretization are applied.

We gave several fields of application where this relation can be used to solve optimal control problems with partial differential equations as constraints. An emphasis was put on the containment source determination in water quality management. In conclusion, we presented a new approach using MIP models, linear programming, and branch-and-bound algorithms for solving continuous optimal control problems.

References

[LBVB2005] Laird, Carl D.; Biegler, Lorenz T.; van Bloemen Waanders, Bart G.; Bartlett, Roscoe A.: Contamination source determination for water networks. In: A.S.C.E. Journal of Water Resources Planning and Management, Vol. 131, No. 2, 2005, pp. 125 – 134.

[LBV2006a] Laird, Carl D.; Biegler, Lorenz T.; van Bloemen Waanders, Bart G.: Real-time, large scale optimization of water network systems using a subdomain approach. To appear in proceedings of the Second CSRI Conference on PDE-Constrained Optimization.

[LBV2006b] Laird, Carl D.; Biegler, Lorenz T.; van Bloemen Waanders, Bart G.: A mixed integer approach for obtaining unique solutions in source inversion of drinking water networks. In: Special Issue on Drinking Water Distribution Systems Security, Journal of Water Resources Planning and Management, Vol. 132, No. 4, 2006, pp. 242 – 251.

[ADR2006] Armbruster, Dieter; Degond, Pierre; Ringhofer, Christian: A Model for the Dynamics of large Queuing Networks and Supply Chains. In: SIAM J. Applied Mathematics, Vol. 66, 2006, pp. 896 – 920.

[FHKM2004] Fügenschuh, Armin; Herty, Michael; Klar, Axel; Martin, Alexander: Combinatorial and Continuous Models for the Optimization of Traffic Flows on Networks. In: SIAM J. Optimization, Vol. 16, No. 4, 2006, pp. 1155 – 1176.

[GHK2005] Göttlich, Simone; Herty, Michael; Klar, Axel: Network models for supply chains. In: Communications in Mathematical Sciences, Vol. 3, No. 4, 2005, pp. 545 – 559.

[GHK2006] Göttlich, Simone; Herty, Michael; Klar, Axel: Modelling and optimization of supply chains on complex networks. In: Communications in Mathematical Sciences, Vol. 4, No. 2, 2006, pp. 315 – 330.

[ILOG2006] ILOG CPLEX Division, 889 Alder Avenue, Suite 200, Incline Village, NV 89451, USA. Information available at URL http://www.cplex.com.

[GuLe2003] Gugat, Martin; Leugering, Günter: Global boundary controllability of the St. Venant equations between steady states. In: Annales des l'Institut Henri Poincaré, Non-linear Analysis, Vol. 20, No. 1, 2003, pp. 1 – 11.

[GLSS2001] Gugat, Martin; Leugering, Günter; Schittkowski, Klaus; Schmidt, E.J.P. Georg: Modelling, stabilization and control of flow in networks of open channels. In: M. Grötschel, S. Krumke, J. Rambau (Eds.): Online optimization of large scale systems. Springer, 2001, pp. 251 – 270.

[GLS2003] Gugat, Martin; Leugering, Günter; Schmidt, E.J.P. Georg: Global controllability between steady supercritical flows in channel networks. In: Mathematical Methods in the Applied Sciences, Vol. 27, No. 7, 2004, pp. 781 – 802.

[Leve1990] LeVeque, Randall J.: Numerical methods for conservation laws. Birkhäuser Verlag, Basel, Boston, Berlin 1990.

[MACW2006] The Macao Water Company. Information available at URL http://www.macaowater.com.

[RBA1993] Rossman, Lewis A.; Boulos, Paul F.; Altman, Tom: Discrete volume-element method for network water-quality models. In: Journal for Water Resource Planing and Management, Vol. 119, No. 5, 1993, pp. 505 – 517.

[RoBo1996] Rossmann, Lewis A.; Boulos, Paul F.: Numerical methods for modeling water quality in distribution systems. In: Journal for Water Resource Planing and Management, Vol. 122, No. 2, 1996, pp. 137 – 146.

[SUP2002] Shang, Feng; Uber James G.; Polycarpou, Marios M.: Particle backtracking algorithm for water distribution systems analysis. In: Journal on Enviromental Engineering, Vol. 128, No. 5, 2002, pp. 441 – 450.

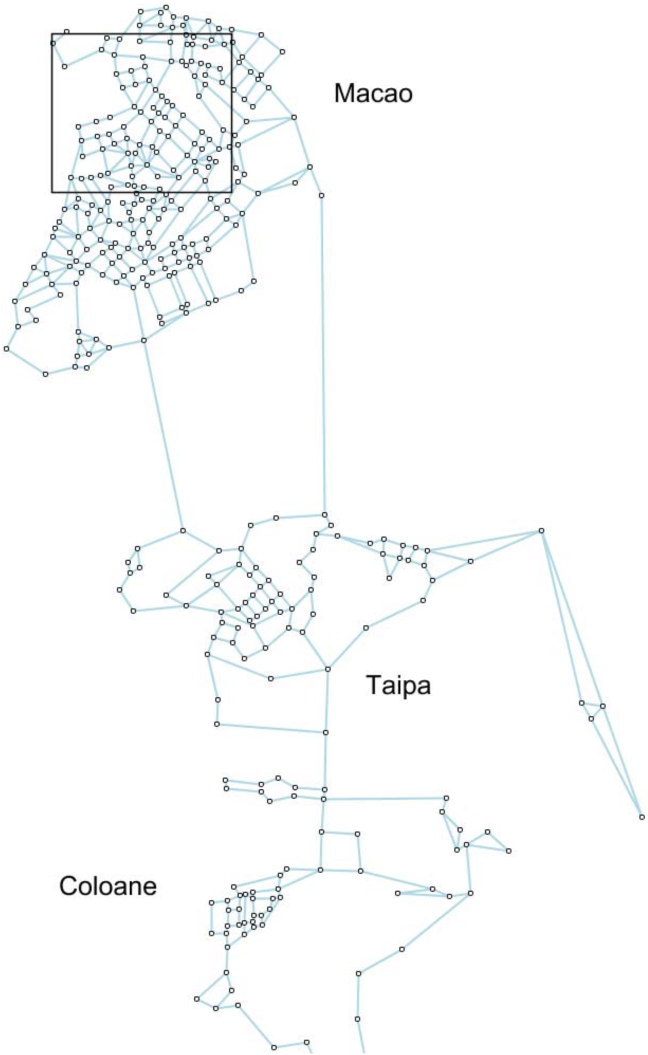

Figure 5: The water supply backbone network of Macao, Taipa, and Coloane.

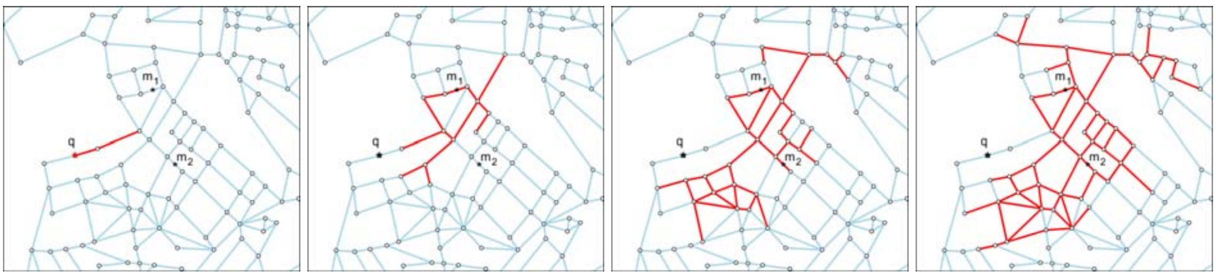

Figure 6: Containment simulation for $t = 9, 28, 47, 66$ (from left to right).