Informing water policy using dynamic, process-based system modelling

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EXTENDED ABSTRACT

Stresses on Australian water resources are reaching critical levels, due to growing population; increasingly complex material discharges to sewer; climatic uncertainty; and prolonged drought. Policy responses to water shortages are often high in environmental impact, such as energy-intensive desalination, or dual reticulation, which is high in material consumption.

Water policy needs to be well informed by science, to minimise such environmental impacts while still providing reliable, cost-effective water services. A tool is needed, which can rigorously assess and compare alternative policy scenarios (greenfield or modifications to existing systems), including:

- Process material flows (e.g. water, PO_4^{3-}, Cd^{2+}, TDS, pesticides, hormones, sludge);
- Materials of construction;
- Energy consumption;
- Embodied energy;
- Economic cost; and
- Dynamic environmental performance.

A literature review reveals that none of the current water models fulfils this need. A system engineering model is being developed in MATLAB/Simulink® (MathWorks Inc. 2007), based on fundamental chemistry and physics, dynamic material and energy balances, kinetics and thermodynamics. It covers all five subsystems of the water cycle:

- Nature;
- Urban;
- Heavy industry;
- Agriculture; and
- Water treatment.

Model construction has commenced with an urban subsystem model. The urban model structure and input data are based on Aurora, an innovative Melbourne subdivision of 8500 houses, which has a local sewage treatment plant, a recycled water treatment plant, dual reticulation for potable and recycled water, and onsite stormwater treatment. This paper explains the model construction, and illustrates underlying equations in detail with two unit operations from the urban subsystem.

The results of the dynamic simulation are used to study alternative policy scenarios, including reliability of service, cost and environmental impact. For a chosen scenario, dynamic simulation is also used to predict system response to peak demands and change.

These results are used to inform policy decisions in an iterative manner, whereby alternative scenarios are assessed and compared, the preferred and most robust scenario is selected, and is then further assessed for vulnerabilities and potential improvements.

Further work on the dynamic model will generalise the urban model to apply to any given urban subsystem structure, and construct models for the remaining four water cycle subsystems. An optimisation model will also be developed around the dynamic model, to allow policy to assess all potential scenarios rather than only selected scenarios, based on user-defined criteria and site-specific constraints and objective functions.

1. INTRODUCTION

Australian water resources are under pressure due to: a growing population; increased complexity of material discharges to sewer; climatic uncertainty; and prolonged drought. Policy responses to water shortages are often energy-intensive (e.g. desalination) or high in material consumption (e.g. dual reticulation for recycled water), which results in high environmental impact. Comprehensive data sets and calibrated models are required to thoroughly inform water policy, encompassing:

- Reliability of water services;
- Cost-effectiveness; and
- Environmental impact.

A whole-of-system view is also essential in policy-making harmonising all actors (Van Schaik et al. 2007), as the effects of a modification to one part of the system carry throughout the whole water cycle. Small-scale views often result in a sub-optimised system, with costs and impacts unknowingly 'exported' from one part of the system to another.

A water system model is needed, which provides the information to rigorously assess and compare alternative policy scenarios in a whole-of-system context, and provides the basis for development of frameworks for environment protection, analogous to the European Union Water Framework Directive (EUWFD 2000).

A literature review reveals that very few of the current water models fulfil this need (Van Schaik et al. 2007). Existing dynamic models do not provide the comprehensive data sets required to inform policy, and are at subsystem scale. Van Schaik et al. (2007) built a system model and solved the optimization problem using AMPL® (AMPL 2006), harmonizing industrial, urban, surface, recycling and agricultural water with water treatment plants, end-of-pipe treatment of sludges and metals in metallurgical and energy recovery systems to investigate water policy.

A conceptual representation of the water cycle and its relation with policy is shown in Figure 1, working further on the work by Van Schaik et al. (2007). The water cycle consists of five dynamically interacting subsystems. Into the system, out of the system and between the five subsystems flow four types of streams: materials; energy; environmental impact; and money. Examples of each stream type are listed. These streams entering and exiting the water cycle link up with other material and energy cycles (e.g. cycles of fertiliser production, energy production). Dynamics within the water system are dependent on physics, chemistry, kinetics, thermodynamics, and water pricing, and these place constraints on the maximum achievable system efficiency. Beyond these constraints on efficiency, there are four categories of factors which also influence system performance (Figure 1), three of which are options for policy.

The ideal water system is of minimum cost, minimum environmental impact (including consumption of water and other resources), and is robust and flexible, to provide reliable services during peak demands and system changes. Policies need to be chosen so water systems approach this ideal. The system engineering approach provides a method to inform this process.

The dynamic water system model is being built progressively, beginning with the urban subsystem model, using data from an innovative urban development in Melbourne. This paper explains the system model construction methodology, discusses the urban subsystem model constructed, and selects two unit operations from the urban subsystem to illustrate detail.

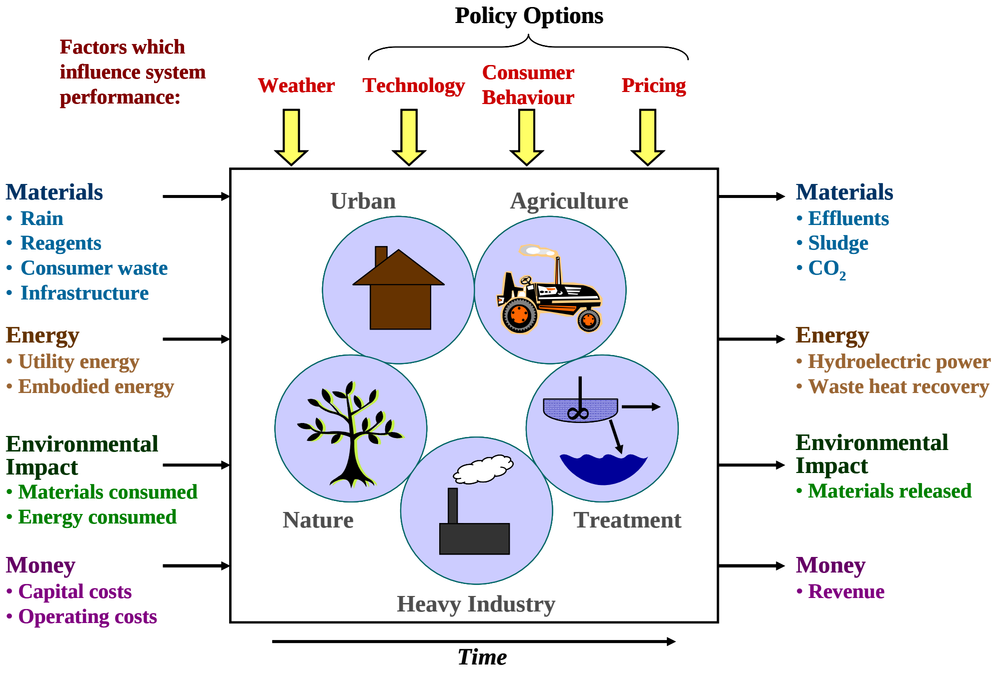

Figure 1. A conceptual representation of the water cycle and the role of policy (Van Schaik et al. 2007).

2. METHOD

2.1. System model

The dynamic system model is based on a process flowsheet of the water system, containing all five subsystems from Figure 1. Water system configurations vary, and a flowsheet of a typical water system (with water recycling) is shown in Figure 2.

The major process steps are displayed in boxes, grouped vertically according to their type (Nature, Consumer, Treatment). Various categories of input and output streams are listed and connected to the relevant process steps. (Some streams types are not connected in this simplified flowsheet, for clarity.) Environmental impact is included but is not listed separately, as all input and output streams contribute to the total impact.

Every stream in the system model is defined by ten signals, shown for the 'Rain' input stream in Figure 2. These signals change in magnitude as they pass through each process step in the flowsheet, according to the material and energy balances for each step. The first six signals (flowrate, concentrations and energy) define the technical performance/reliability of the system, the next two signals define the environmental impact, and the final two signals calculate the cost of the system. Together, these ten signals provide the data required to inform policy.

Signal 1: Flowrate

The flowrate signal quantifies the total volumetric flowrate of a stream including all dissolved species. The equation defining flowrate (Equation 1) is based on a generic unit operation model, containing a time delay, transfer function, stream additions and splits (Figure 3):

$$F_i = k_i\left[\bar{F}_i + L^{-1}\left\{\sum_{i=1}^{n} F'_{0,i}(s)\cdot e^{-\tau_d s}\cdot\frac{k}{\tau s+1}\right\}\right] \qquad (1)$$

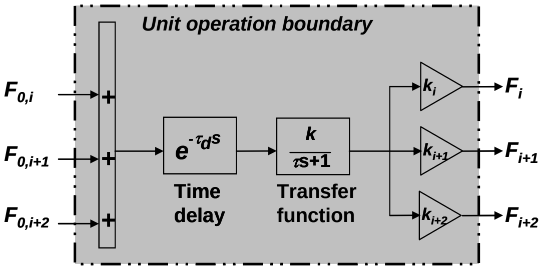

Figure 3. Generic model of a unit operation.

where: F is flowrate (ML/h); k is the steady-state gain (-); τ and τ_d are time constants (h); L^{-1} refers to the inverse Laplace transform; the bar over a variable refers to the average value; and subscripts i and 0 refer to stream number and initial value respectively.

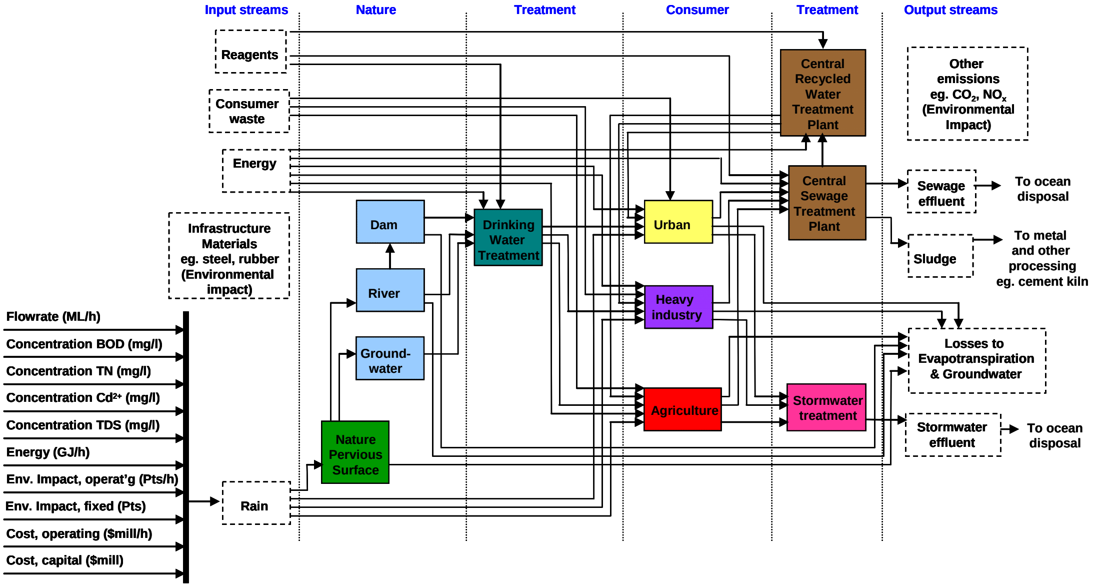

Figure 2. Process flowsheet of a typical water cycle (with water recycling).

Signals 2-5: Concentrations

All four concentration signals are defined by equations of the same type as Equation 1, based on component mass balances rather than total flowrate. Many more than four chemical species are of importance to policy and to environmental impact calculation, so the model is set up for easy replacement of data sets, enabling consecutive simulations for different chemical species.

Signals 6-10: Energy, Environmental Impact and Cost

Energy (signal 6) quantifies the utility energy consumed (which arises from mixing, pumping, compressing and heating) plus any energy that is recovered and utilised (e.g. hydroelectric or waste heat recovery). The total environmental impact is the sum of two components, each of which is a separate signal. Signal 7 is the 'operating' environmental impact, a dynamic signal arising from consumption and release of materials and energy, including changed flow patterns arising from built environments. Signal 8 is the 'fixed' environmental impact, which is associated with the manufacture and construction of infrastructure (including embodied energy), and is constant for a given system. Environmental impact is quantified by the Life-Cycle Assessment-based Eco-Indicator 99 (Goedkoop et al. 2001).

Analogous to the environmental impact signals, the total cost consists of two components, one dynamic and one constant. Signal 9 represents the dynamic operating costs, due to purchase of: chemicals; utilities; maintenance; labour; etc. Signal 10 is the capital cost of infrastructure, and is constant for a given structure.

All these signals are related to the system structure, dynamic flowrate and concentrations by multipliers, including: enthalpy (for energy signal); environmental impact per unit material (obtained from Eco-Indicator 99); and ratios of cost/size (for infrastructure) or cost/volume (for reagents).

2.2. An urban subsystem model

The system model is illustrated using an urban subsystem model, which is entirely contained in the 'Urban' box in Figure 2. The structure of the urban subsystem model and the data used in the model are based on an innovative urban subdivision of 8500 houses in Melbourne, called Aurora. Aurora has a local sewage treatment plant, a recycled water treatment plant, dual reticulation for potable and recycled water (to reduce potable demand), and onsite stormwater treatment. The model is built with process control software MATLAB/Simulink$^{®}$ (MathWorks Inc. 2007), in a layered hierarchical structure (see Figure 4).

As for the process flowsheet (Figure 2), coloured boxes represent one or more unit operations, and the connecting lines are streams, each of which is defined by the same ten signals. The background layer contains the urban water subsystem (Aurora), the middle layer shows the indoor water system of a residential building, and the front layer shows the model of a residential water heater.

Two unit operations from the urban water subsystem model have been selected to illustrate model detail: a residential water heater, based on a dynamic energy balance; and an elevated tank for recycled water delivery, based on a dynamic material balance.

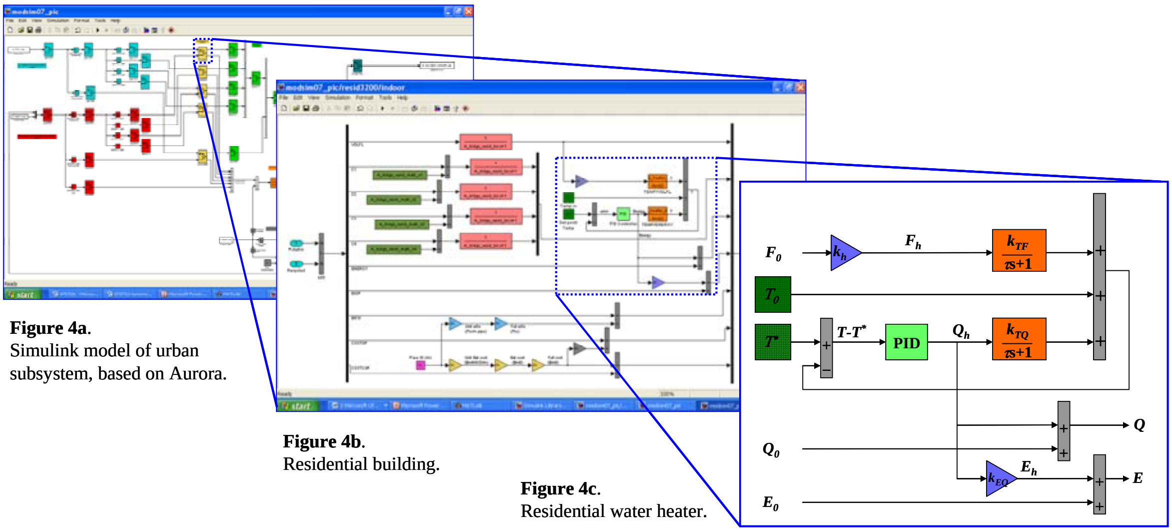

Figure 4a.
Simulink model of urban subsystem, based on Aurora.

Figure 4b.
Residential building.

Figure 4c.
Residential water heater.

Unit operation 1: Residential water heater

Heating water consumes energy, which contributes to environmental impact and costs money. This Simulink subsystem (Figure 4c) calculates the energy demand (Q_h) and the environmental impact (E_h) arising from the heating of water in residential buildings. (The operating and capital costs of the water heater, and the environmental impact from manufacture of the heater lie outside the system boundary. For comparison of alternative household appliances, inclusion of these variables inside the system boundary would be important.) The water heater is modelled as a continuously-stirred tank reactor (CSTR), with an internal heating coil. These further assumptions are made:

- Vessel is well insulated (negligible loss of heat to surroundings);
- Heat input can be varied in magnitude;
- A level controller maintains constant liquid volume in CSTR;
- Temperature is regulated by a feedback loop with proportional control;
- Dynamics of the coil heating, the sensor and controller are negligible; and
- T_0 (initial temperature) is constant.

Not all water heaters will precisely resemble a CSTR with internal heating coil, configured according to the first four assumptions. However, the energy consumption is strongly based on thermodynamics and fluid properties, and varies marginally with heater type or heat source. Therefore the chosen model structure shows reasonable simplification without significant loss in accuracy. The control loops (for level and temperature) are chosen for simplicity, and the high specific heat capacity of water validates the assumption of negligible controller dynamics. The model of the water heater is based on a dynamic energy balance for the CSTR, written in the Laplace domain as required for Simulink (for derivation see eg. Seborg et al. 2004):

$$T'(s) = \frac{k_{TF}}{\tau s+1}F_h'(s) + \frac{k_{TQ}}{\tau s+1}Q_h'(s) \qquad (2)$$

where:

$$k_{TF} = (T_0 - \overline{T})/\overline{F}_h;\ k_{TQ} = 1/(\rho c_p \overline{F}_h);\ \tau = v/\overline{F}_h.$$

$T'(s)$, $F'(s)$, $Q'(s)$ are the temperature, flowrate and energy, ρ is fluid density (kg/ML), c_p is the specific heat capacity of fluid (GJ/kg/ºC), v is the vessel volume (ML), and subscripts *h, TF* and *TQ* refer to the heater, the temperature-flowrate term and the temperature-energy term respectively. The fraction terms in Equation 2 are the transfer functions visible in orange boxes in Figure 4c. The proportional controller gain k_c (GJ/h/ºC) in the PID controller (see Figure 4c) can be shown as (Seborg et al. 2004):

$$k_c = \frac{T^* - T_0 - k_h k_{TF}\overline{F}}{k_{TQ}(T^* - \overline{T})} \qquad (3)$$

where T^* is the controller setpoint temperature. The energy signal exiting the heater subsystem is a sum of the initial energy and the energy used by the heater (Figure 4c).

The operating environmental impact is a function of the energy consumed:

$$E = E_0 + k_{EQ} \cdot Q_h \qquad (4)$$

where E (Pts/h) is the operating environmental impact, and gain k_{EQ} (Pts/GJ) is the operating environmental impact per unit energy consumed.

Unit operation 2: Elevated tank for recycled water storage

After purification in the recycled water treatment plant, recycled water is pumped into an elevated tank, prior to gravity reticulation through the second pipe network. The tank delays the process stream during storage, adds capital cost and fixed environmental impact due to infrastructure, and adds operating cost for maintenance. The tank is modelled as a CSTR, with the following further assumptions:

- No chemical reactions occur in vessel;
- Tank is constructed of steel and concrete;
- Constant density of process fluid; and
- Operating cost is averaged over time, and is a fixed ratio of initial capital cost.

The assumption of a CSTR is not perfect, as there is no agitation. The residence time distribution can be adjusted to reflect poor mixing, if the influence of this unit operation on system performance warrants such detail. The assumption of no chemical reaction is true except for residence times far longer than those under normal operation. The assumption of steel and concrete construction only needs to be modified if other materials of high cost or environmental impact are used. The final assumption uses a constant rate for simplicity, and can be changed to variable if precise cash flow data is required.

Figure 5 shows the Simulink model of the elevated tank, which depicts transfer functions with a mean residence time of τ for the first five signals, based on a dynamic material balance. The fixed environmental impact, operating and capital costs are obtained from the mass of steel (m_s) and volume of concrete (v_c) using various gains.

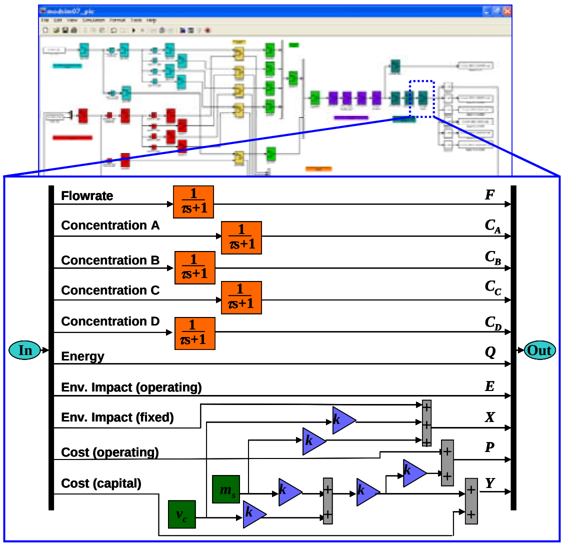

Figure 5. Simulink model of elevated tank for recycled water storage.

3. RESULTS

The dynamic behaviour of alternative policy scenarios can be compared and assessed using the dynamic system model. Figure 6 compares the current urban water use with a potential scenario regarding household washing machines, in which a mandate is placed on minimum washing machine water efficiency, and washing machines are operated using recycled water.

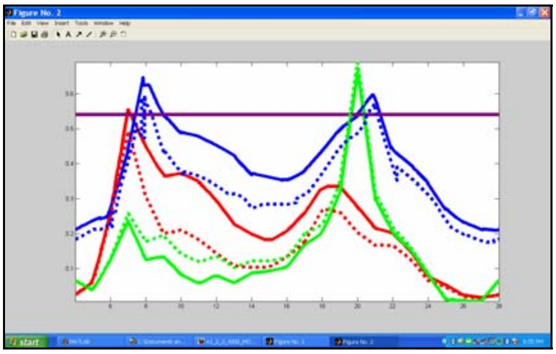

Figure 6. Comparison of current water use (solid lines) with water consumption under a mandate on minimum washing machine water efficiency and use of recycled water in washing machines (dotted lines), showing typical daily dynamic signals of: potable water demand, ML/h (red lines); recycled water demand, ML/h (green lines); energy consumed in heating water, 10^{11}J/h (blue lines); and capital cost of subdivisional reticulation and sewer infrastructure, \$$10^8$ (purple lines).

Figure 7 shows the response of the system to one day of peak water demand (followed by return to average demand), and how fast the system returns to steady state.

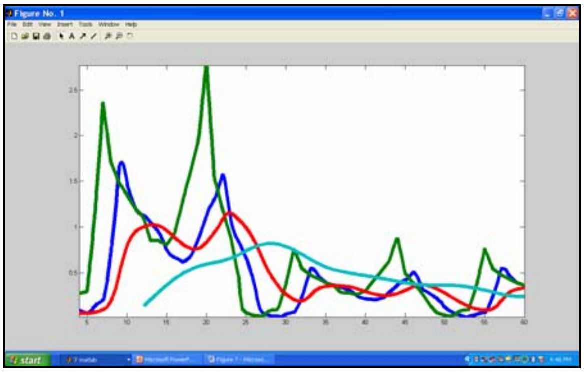

Figure 7. System response to a day of peak demand (followed by return to average demand), at various positions through system (flowrates, ML/h): combined potable and recycled water demand at subsystem entrance (green line); sewage treatment plant inflow (blue line); and flowrate at subsequent locations in sewage treatment plant (red line) and recycled water treatment plant (aqua line).

4. DISCUSSION

These preliminary results of the system model show the type of output, and how results can be applied to informing policy to modify a water system in the direction of its theoretical maximum efficiency. This method is equally applicable to a greenfield site as to a modification to an existing system. The method is iterative, following four steps and utilising results analogous to those shown in Section 3.

1. Assess and compare alternative scenarios (using Figure 6).
2. Select preferred scenario.
3. Assess reliability and (dynamic) robustness of chosen scenario in peak demands and changes (Figure 7).
4. Propose modifications to improve chosen system; repeat above steps.

Further work is developing an optimisation around the dynamic model to replace this iterative process, which will produce the optimum system structure for a set of user-defined criteria and site-specific constraints.

In both Figures 6 and 7, the impacts of changes on only a select number of signals are shown, for clarity. In informing policy, the impacts on all 10 signals across all locations in the system need to be considered. This modelling approach, working from the basic unit operations up to the larger system, provides a way to rigorously simulate, collect and summarise this large amount of data, to support policy.

5. CONCLUSION

The water system is under stress in Australia, and water policy must be selected to provide reliable, cost-effective water services while avoiding large environmental impacts. To achieve this, policy needs to be informed by a science/engineering tool, which models the whole water cycle and system in a comprehensive manner, including: material flows (water, dissolved contaminants, reagents, sludge, etc.); energy consumption; embodied energy; infrastructure materials; cost; and environmental impact. Few current water model fulfil this need, Van Schaik et al (2007) are one of the first to do this on large scale in the Netherlands.

A system engineering model of the urban water system is being developed, in MATLAB/Simulink®, covering all five subsystems of the water cycle: nature; urban; heavy industry; agriculture; and water treatment. Model construction has commenced with an urban subsystem model, using data from an innovative urban development, Aurora.

Dynamic modelling results are used to assess and compare alternative policy scenarios, as well as identify and improve weaknesses for chosen systems. Further work includes: developing a generalised urban subsystem model; extending the model to include the remaining four water cycle subsystems; and development of an integrated optimisation model to allow rigorous assessment and comparison of all potential policy scenarios.

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