Importance of demand modelling in network water quality models: a review

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Abstract

Today, there is a growing interest in network water quality modelling. The water quality issues of interest relate to both dissolved and particulate substances, with the main interest in residual chlorine and (microbiological) contaminant propagation, respectively in sediment leading to discolouration. There is a strong influence of flows and velocities on transport, mixing, production and decay of these substances in the network. This imposes a different approach to demand modelling which is reviewed in this article.

For transport systems the current hydraulic models suffice; for the more detailed distribution system a network water quality model is needed that is based on short time scale demands that considers the effect of dispersion and transients. Demand models that provide stochastic residential demands per individual home and on a one-second time scale are available. A stochastic demands based network water quality model needs to be developed and validated with field measurements. Such a model will be probabilistic in nature and will offer a new perspective for assessing water quality in the DWDS.

1 Introduction

The goal of drinking water companies is to supply their customers with good quality drinking water 24 h per day. With respect to water quality, the focus has for many years been on the drinking water treatment. Recently, interest in water quality in the drinking water distribution system (DWDS) has been growing. On the one hand, this is driven by customers who expect the water company to ensure the best water quality by preventing such obvious deficiencies in water quality as discolouration and (in some countries) by assuring a sufficient level of chlorine residual. On the other hand, since “9/11” there is a growing interest in the detection of (deliberate) contaminations in the DWDS. Consequently, there is an interest in the behaviour of both particulate and dissolved substances throughout the DWDS (Powell et al., 2004).
In modelling water quality in the DWDS the essential aspects are transport, mixing, production and decay, and thus velocities and flows are important elements. Sediment behaviour, and thus discolouration risk, in a DWDS is strongly related to hydraulics (Slaats et al., 2003; Vreeburg, 2007). Also, the spread of dissolved contaminants through the DWDS is strongly related to the flows through the network (Grayman et al., 2006). This means that water quality models are not only important on the level of transport mains but also on the level of distribution mains (Fig. 1).

Here, transport mains are defined as pipes that typically do not supply customers directly; customer connections are attached to distribution mains only. Transport mains have relatively large diameters and supply to distribution mains. As a result, transport mains have only few demand nodes, with demands that show a high cross correlation (i.e. show a similar demand profile over the day), the flows are turbulent and relatively constant (a high auto correlation) and thus there is a low discolouration risk in transport mains. A transport network therefore results in a simple hydraulic model (e.g. EPANET) which can be constructed from information of pipes (diameters, lengths and pipe material) and strongly correlated demand profiles are applied to demand nodes. The model is typically calibrated with pressure measurements (Kapelan, 2002).

Distribution mains have many demand nodes and the demands show little auto and cross correlation (Filion et al., 2006). A distribution network is usually designed on fire flow demands, that typically are much higher than domestic demand (Vreeburg, 2007). Therefore the maximum velocities can be very low (smaller than 1 cm/s) and change rapidly from one second to the next. Flow directions may reverse and travel times may be as long as 100 h due to stagnation (Buchberger et al., 2003; Blokker et al., 2006). In the distribution network sediment does settle and resuspend (Blokker et al., 2007; Vreeburg, 2007). This means a distribution mains model has demands with a low cross correlation and therefore asks for a much more complex structure of demand allocation.

Thus, the key element to a water quality model for a DWDS is a detailed hydraulic model and therefore knowledge of demands is essential. This paper reviews the in-
fluence of (stochastic) demands on water quality models and the consequential constraints on demand modelling. Following first, is a review of water quality modelling of dissolved matter and its relation with demands. Next, water quality modelling of particulate matter and the relation with hydraulic conditions is described. Thirdly, the characteristics of demands in hydraulic network models and in network water quality models are discussed. After that some demand models are being considered.

2 Water quality modelling – dissolved matter

With increasing computational power, hydraulic network models are used more and more for water quality related subjects, such as determining residual chlorine (Propato and Uber, 2004; Bowden et al., 2006) and disinfection by-products in the DWDS (under the US EPA Stage 2 Disinfection By-Products Rule; US EPA, 2006), optimum sensor placement for detection of biological and chemical contaminations (Berry et al., 2005; Nilsson et al., 2005) and source location inversion after a contaminant is detected (McKenna et al., 2005).

Water quality in a network model can be described with the Advection-Dispersion-Reaction (ADR) equation:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} - f(C)$$

where $C$ is the concentration (the water quality parameter), $t$ is the time, $u$ is the flow velocity, $x$ is the direction of the flow, $D$ is a dispersion coefficient and $f(C)$ is a reaction function. The left-hand term of this equation depicts the advection and mainly depends on the water's hydraulic movement, the first term on the right-hand side depicts the dispersion and the last term represents the reaction; both terms depend on the type and nature of the considered substance. The reaction function is very diverse for different substances, e.g. for chlorine decay $f(C) = -KC$ with $K$ the reaction constant. The reaction function can include a production term.
The hydraulic network solver EPANET (Rossman, 2000) comes with a water quality module, as do many commercially available network analysis programs. The water quality module enables the user to calculate travel times and to model the migration of a tracer (both conservative and non-conservative, determined by the value of $K$) through a network. It models advection and reaction with the pipe wall and the bulk of the water, but it does not take dispersion into account (i.e. neglects the first term of the right-hand side of the ADR equation). EPANET can handle many different time scales (i.e. time intervals over which demands are time-averaged). A time scale of one hour is commonly used, but EPANET also supports time scales as low as one second. The solver assumes that the network is well defined (known pipe diameter, pipe roughness and network layout), that demands are known, and that water quality reactions (under influence of residence times and interaction with the pipe wall) are known. Furthermore, EPANET assumes perfect mixing at junctions, and because it is a static (or semi-dynamic) model it disregards transients. The accuracy of the calculated results depend on the validity of these assumptions.

To progress the water quality models, research is done on several of the assumptions in the models. In this review the focus is on model deficiencies with respect to flows and velocities.

With respect to advection the equation shows that time, and thus travel time, is an important factor as is the velocity of the water. Several authors (Pasha and Lansey, 2005; Filion et al., 2005; McKenna et al., 2005) have shown the importance of uncertainty in demands in water quality models. When looking at smaller time steps a steady state assumption may not be valid. Karney et al. (2006) investigated the modelling of unsteadiness in flow conditions with several mathematical models such as extended period approaches (like EPANET does), a rigid water column model that includes inertia effects, and a water hammer model that includes small compressibility effects. The time scale of boundary and flow adjustments relative to the water hammer time scale were found to be important for characterizing the system response and judging the unsteadiness in a system.
Advection is also related to mixing. The assumption of perfect mixing at crosses is being studied with measurements and Computational Fluid Dynamics modelling (Ho et al., 2007; Austin et al., 2007). The studies showed that at T-junctions that are at least a few pipe diameters apart perfect mixing can be assumed, but in cross junctions less than 10% mixing may occur. In fact, at cross junctions the rate of mixture in the two outgoing arms depends on the occurring Reynolds numbers (and thus the flow rates) in the two incoming arms.

The influence of dispersion in water quality modelling was tested with (two-dimensional) ADR models (Tzatchkov et al., 2002; Li, 2006). Li (2006) showed that dispersion is of importance in case of laminar flows and thus especially in the parts of DWDS that have pipe diameters designed for fire flows but with small normal flows. Dispersion is not directly affected by flow pattern or time scale. Flow pattern and time scale do, however, affect the probability of stagnation, laminar and turbulent flows, and thus indirectly do have an effect on dispersion. When the reaction term increases, dispersion is less important.

Powell et al. (2004) have established that there is a need to further investigate the reaction parameters for e.g. chlorine decay, the forming of disinfectant by-products and bacterial regrowth. Where the reaction constant $K$ involves a reaction with the pipe wall the stagnation time is of importance. Flow velocities are important as they affect chlorine decay rates (Menaia et al., 2003).

## 3 Water quality modelling – particulate matter

For particulate matter the ADR model also applies; the reaction function for sediment also includes a velocity term. Under normal flow conditions, sediment coming from the water treatment plant or originating from corrosion of the pipe wall settles and accumulates in the DWDS. During a hydraulic incident (e.g. opening a fire hydrant) the sediment is resuspended and can thus lead to discoloured water (Fig. 2). Vreeburg (2007) has shown that the discolouration risk can be reduced with three types of
measures: the first is to prevent sediment from entering the DWDS by optimizing the water treatment; the second is to prevent sediment from accumulating in the DWDS by designing self-cleaning networks (Vreeburg et al., 2008); and the third is to prevent sediment from resuspension by cleaning (flushing) the DWDS in a timely manner. Although these three steps have proven to reduce the discolouration risk the exact relation between the hydraulics and sediment behaviour (under what conditions does it settle and resuspend) is still unknown. More insight into the hydraulic conditions can further support the second and third step.

Self-cleaning distribution networks (step 2) are effective because of a regularly occurring velocity that prevents sediment from accumulating in the network. The design velocity for self-cleaning DWDS is set to 0.4 m/s. Lab tests in the Netherlands (Slaats et al., 2003) have shown that sediment is partly resuspended at velocities of 0.1 to 0.15 m/s and fully resuspended at velocities of 0.15 to 0.25 m/s. In Australia, Grainger et al. (2003) have researched settlement and resuspension velocities. Settlement was found at 0.21 m/s (at which it could take several hours to a few days before all sediment was settled) and resuspension was found at 0.3 m/s. Field measurements in the Netherlands in 2006 have shown that the self-cleaning concept does work (Blokker et al., 2007; Vreeburg, 2007). The study suggests that the assumed design velocity of 0.4 m/s might be a conservative value and a regular (i.e. a few times per week) occurring velocity of 0.2 m/s or less may be enough. The field measurements also showed that the current method to calculate the maximum flow (the so called $q \sqrt{n}$ method) leads to an overestimate of the regular occurring flow, meaning that the regular flow for which the DWDS is designed (almost) never takes place. Since sediment behaviour is related to instantaneous (peak) flows, modelling of sediment in the network requires time scales of less than one minute.

The self-cleaning design principles have mainly been applied to the peripheral zones of the distribution system which can be laid out as branched networks (sections of up

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to 250 residential connections). In order to scale up the self-cleaning principles to the rest of the (looped) network it is important to look deeper into the relation between hydraulics and sediment resuspension and into the hydraulics at a larger scale.

To determine which part of the DWDS needs cleaning (step 3) several measurement techniques are available to determine where in the DWDS the discolouration risk is the highest (Vreeburg and Boxall, 2007); one example is the Resuspension Potential Method (Vreeburg et al., 2004). Also, some models are being developed for this purpose. Boxall and Saul (2005) have developed a “predictor of discolouration events in distribution systems” (PODDS). This model is based on the assumption that normal hydraulics forces (i.e. maximum daily shear stress) condition the sediment layer strength and hence control the discolouration potential (or discolouration risk).

4 Demands in hydraulic network models

Demand modelling is done on different temporal and spatial aggregation levels, depending on the model’s purpose. Based on the correlation of the demand three different levels of demand modelling and consequently network modelling can be distinguished. The highest level is for planning the operation of the treatment plant, for which it is important to model the demand per day and for the total supply area of a pumping station. The second level is modelling on transport level or to the level to which the assumption of cross correlation is still sufficient while for water quality modelling on a distribution level (the third level) a time scale of less than one minute may be important (Li and Buchberger, 2004; Blokker et al., 2006).

Temporal and spatial aggregation of demands is related to cross and auto correlation of flows. A high cross correlation means that demand patterns at different nodes are similar (flows are proportional to each other). A high auto correlation means that flows patterns change gradually. Cross and auto correlation thus have an effect on maximum flow rates and the stagnation time. This does not only influence water quality; the amount of cross correlation is important with respect to the reliability of a DWDS (Filion
et al., 2005) and thus the cost (Babayan et al., 2005); auto correlation is important with respect to the resilience of a DWDS, i.e. the time to restore service after a break (Filion et al., 2005). Several authors (Moughton et al., 2006; Filion et al., 2006; Li and Buchberger, 2007) have looked at the effect of temporal and spatial aggregation of demands on cross and auto correlation. They have shown that the longer the time scale and the higher the aggregation level, the higher the (cross) correlation. When looking at time scales of 1 h and demand nodes that represent 10 or more connections the assumption of cross correlation is valid.

In a preliminary study Tzatchkov and Buchberger (2006) have examined the influence of transients and showed that the operation of a single water appliance inside a home is almost imperceptible in water mains and larger distribution network pipes and thus the sum of all residential demands of a single home can be used to define demands in a hydraulic model. They also showed that the (instantaneous) demand pulses deform in their path from the demand point to the upstream pipes. Thus, the assumption that demands can be aggregated by taking the sum of the downstream demand pulses is not always justified. (McInnis and Karney, 1995) calculated transients in a complex model from several pressure events using different models of demand aggregation. The model results could be improved (compared to available field data) by artificially damping the residual pressure waves and by increasing instantaneous orifice demands. This means that in transient models insight into demands is very important. Skeletonization also has an impact on hydraulic transient models (Jung et al., 2007), especially in modelling the smaller parts of the distribution network (as opposed to the larger diameter pipes or transport network).

The flow variance and scale of fluctuation, the probability of stagnation and the flow regime (laminar or turbulent flow) are affected by the time scale that is used in a water quality model (McKenna et al., 2003; Li, 2006). In a model, the probability of stagnation decreases with increasing time scale. The probability of turbulent and transitional flow increases with increasing time scale in the case that the average Reynolds number exceeds 4000 or 2000 respectively for turbulent and transitional flow; and it decreases
with increasing time scale when the average Reynolds number is lower than 4000 or 2000. The scale of fluctuation is also affected by the demands, especially by the mean and variance of the duration of the different demand pulses (Li, 2006).

It can be concluded that a transport network can be accurately modelled with a hydraulic model (such as EPANET) with a one hour time step and allocating demands with a “top-down” approach, i.e. assigning the demand pattern of the pumping station to all nodes, proportional to the nodal demand, thus using strongly correlated demands. The model can be calibrated with pressure measurements. An advection-reaction (AR) model suffices for the transport model. Dispersion can be neglected where turbulent flows dominate (Li, 2006).

Water quality modelling requires a detailed model of a distribution system. Demands must be known on a relatively small temporal (less than 15 min) and spatial (mains in a street) aggregation level and should be constructed by a “bottom-up” approach from demands of single homes. Since not every home can be modelled individually a stochastic approach is required. In water quality modelling dispersion must be taken into account in an Advection-Dispersion-Reaction (ADR) model (Tzatchkov et al., 2002; Li, 2006). The effect of unsteadiness in flows may also be important in water quality modelling.

5 Demand modelling

For a water quality network model a stochastic demand model per (household) connection on a per second or per minute basis is needed. Today, two types of demand models are available that fulfil this requirement: the Poisson Rectangular Pulse model and the End Use Model.

Buchberger and Wu (1995) have shown that residential water demand is built up of rectangular pulses with a certain intensity (flow) and duration arriving at different times on a day. The frequency of residential water use follows a Poisson arrival process with a time dependent rate parameter. When two pulses overlap in time the
result is the sum of the two pulses (see Fig. 3). From extensive measurements it is possible to estimate the parameters to constitute a Poisson Rectangular Pulse (PRP) model (Buchberger and Wells, 1996). Measurements were collected in the USA (Ohio; Buchberger et al., 2003), Italy (Guercio et al., 2001), Spain (García et al., 2004) and Mexico (Alcocer-Yamanaka et al., 2006) and for each area the PRP parameters were determined. To estimate intensity and duration different probability distributions are applicable for different data sets, such as log-normal, exponential and Weibull distributions. Alvisi et al. (2003) use an analogous model based on a Neyman-Scott stochastic process (NSRP model) for which the parameters are also found from measurements. The PRP model is the basis for the demand generator PRPsym (Nilsson et al., 2005).

Obtaining the PRP parameters requires many (expensive) measurements (e.g. the parameters of Milford, Ohio (Buchberger et al., 2003) were obtained from 30 days of measurements of 21 homes on a per second basis). It is difficult to correlate the parameters retrieved from these measurements with e.g. the population size, age, and installed water using appliances. As a consequence, the parameters for the PRP model are not easily transferable to other networks. Also, the retrieved PRP parameters lead to mainly short pulses of 1 min or less. This means that showering (ca. 10 to 15 min) is almost never simulated accurately. Another issue is that it is difficult to determine how well the simulation performs compared to the measurements, since the simulation parameters were derived from the same or similar measurements.

Another type of stochastic demand model is based on statistical information of end uses (Blokker and Vreeburg, 2005). The demand generator is called SIMDEUM® (SIMulation of water Demand, an End Use Model). SIMDEUM simulates each end use as a rectangular pulse from probability distribution functions for the intensity, duration and frequency of use and a given probability of use over the day (related to presence at home and sleep-wake rhythm of residents, see Fig. 3). The probability distribution functions are derived from statistics of possession of water using appliance, their (water) use and population data (census data with respect to age and household size). The total simulated demand is the sum of all the end uses. SIMDEUM makes use of
measurement data for validation only. An end use model requires only a few demand measurements for validation. On the other hand, it requires statistical data that are probably related to cultural differences and thus are nation specific. Because SIMDEUM is based on statistical information on in-home installation and residents, the influence of an aging population or replacement of old appliances with new ones can be determined easily and the model can easily be transferred to other networks. SIMDEUM was applied and tested with good results in the Netherlands (Blokker and Vreeburg, 2005; Blokker et al., 2006); it still is unproven in other countries. However, with statistical data from Milford, Ohio, it should be possible to generate demand patterns with SIMDEUM that can be validated with the extensive measurements that are available (Buchberger et al., 2003).

6 Discussion

Network water quality models on the distribution level require demands with low auto and cross correlation. This means that these models call for demand allocation via a bottom-up approach, i.e. allocating stochastic demand profiles with short time scales and small spatial aggregation level.

Pressure measurements do not suffice for calibrating a network water quality model. Calibrating hydraulic models on pressure measurements typically means adjusting pipe roughness. This only affects pressures and not flows. Adjusting flows from pressure measurements is too inaccurate. An accuracy of 0.5 m in two pressure measurements leads potentially to an uncertainty of 1 m in head loss on a total head loss of only 5 m or a 20% imprecision in pressure and thus a 10% imprecision in flow. Calibrating a network water quality model requires demand or travel time measurements, e.g. through tracer studies.

Both the PRPSym and SIMDEUM demand models have been combined with hydraulic models in preliminary studies (McKenna et al., 2005; Blokker et al., 2006). So far, little water quality measurements were done to validate the model results. Li (2006)
has applied PRPSym in combination with EPANET and an ADR-model to compare the model to measurements of fluoride and chlorine concentrations in a network. The ADR-model with the stochastic demand patterns gave good results with the conservative fluoride and reasonable results with decaying chlorine. More network water quality models with stochastic demand should be tested with field data. This will reveal the shortcomings of the models and will indicate where improvement is to be gained.

With the use of stochastic demands in a network model the question arises if a probabilistic approach on network modeling is required and how to interpret network simulations. Nilsson et al. (2005) demonstrated that Monte Carlo techniques are a useful tool for simulating the dynamic performance of a municipal drinking-water supply system, provided that a calibrated model of realistic network operations is available. A probabilistic approach in modelling and interpreting results is a significant departure from prevailing practice and it can be used to complement rather than replace current modelling techniques.

7 Summary and conclusions

Today, there is a growing interest in network water quality modelling. The water quality issues of interest relate to both particulate and dissolved substances, with the main interest in sediment leading to discolouration, respectively in residual chlorine and contaminant propagation. There is a strong influence of flows and velocities on transport, mixing, production and decay of these substances in the network which imposes a different approach to demand modelling. For transport systems the current hydraulic (AR) models suffice; for the more detailed distribution system a network water quality model is needed that is based on short time scale demands that considers the effect of dispersion (ADR) and transients. Demand models that provide trustworthy stochastic residential demands per individual home and on a one-second time scale are available.

The contribution of dispersion in network water quality modelling is significant. The contribution of transients in network water quality modelling still needs to be estab-
lished. A hydraulics based, or rather a stochastic demands based, network water quality model needs to be developed and validated with field measurements. Such a model will be probabilistic in nature and will lead to a whole new way of assessing water quality in the DWDS.

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Importance of demand modelling in network water quality models

E. J. M. Blokker et al.
and relatively constant (a high auto-correlation) and thus there is a low discolouration risk in transport mains. A transport network therefore results in a simple hydraulic model (e.g. EPANET) which can be constructed from information of pipes (diameters, lengths and pipe material) and strongly correlated demand profiles are applied to demand nodes. The model is typically calibrated with pressure measurements (Kapelan, 2002).

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In the distribution network sediment does settle and resuspend (Blokker et al., 2007; Vreeburg, 2007). This means a distribution mains model has demands with a low cross correlation and therefore asks for a much more complex structure of demand allocation.

Thus, the key element to a water quality model for a DWDS is a detailed hydraulic model and therefore knowledge of demands is essential. This paper reviews the influence of (stochastic) demands on water quality models and the consequential constraints on demand modelling. Following first, is a review of water quality modelling of dissolved matter and its relation with demands. Next, water quality modelling of particulate matter and the relation with hydraulic conditions is described. Thirdly, the characteristics of demands in hydraulic network models and in network water quality models are discussed. After that some demand models are being considered.

Water quality modelling – dissolved matter

With increasing computational power, hydraulic network models are used more and more for water quality related subjects, such as determining residual chlorine (Propato and Uber, 2004; Bowden et al., 2006) and disinfection by-products in the DWDS (under the US EPA Stage 2 Disinfection By-Products Rule; US EPA, 2006), optimum sensor placement for detection of biological and chemical contaminations.

Fig. 1. Part of a distribution network. The line color and thickness represent the diameter of the pipes, the blue circles are demand nodes, open circles are nodes with zero demand. The thick yellow, orange and red lines are typically mains with a transport function (i.e. large diameters and very few demand nodes that are directly connected to it); the thin blue and green lines are mains with a distribution function (i.e. supply to customers with small auto and cross correlation).
Powell et al. (2004) have established that there is a need to further investigate the reaction parameters for e.g. chlorine decay, the forming of disinfectant by-products and bacterial regrowth. Where the reaction constant $K$ involves a reaction with the pipe wall the stagnation time is of importance. Flow velocities are important as they affect chlorine decay rates (Menaia et al., 2003).

Water quality modelling – particulate matter

For particulate matter the ADR model also applies; the reaction function for sediment also includes a velocity term. Under normal flow conditions, sediment coming from the water treatment plant or originating from corrosion of the pipe wall settles and accumulates in the DWDS. During a hydraulic incident (e.g. opening a fire hydrant) the sediment is resuspended and can thus lead to discoloured water (Figure 2). Vreeburg (2007) has shown that the discolouration risk can be reduced with three types of measures: the first is to prevent sediment from entering the DWDS by optimizing the water treatment; the second is to prevent sediment from accumulating in the DWDS by designing self-cleaning networks (Vreeburg et al., in prep.); and the third is to prevent sediment from resuspension by cleaning (flushing) the DWDS in a timely manner. Although these three steps have proven to reduce the discolouration risk the exact relation between the hydraulics and sediment behaviour (under what conditions does it settle and resuspend) is still unknown. More insight into the hydraulic conditions can further support the second and third step.

Fig. 2. Processes related to particles in the distribution network.
An end use model requires only a few demand measurements for validation. On the other hand, it requires statistical data that are probably related to cultural differences and thus are nation specific. Because SIMDEUM is based on statistical information on in-home installation and residents, the influence of an aging population or replacement of old appliances with new ones can be determined easily and the model can easily be transferred to other networks. SIMDEUM was applied and tested with good results in the Netherlands (Blokker and Vreeburg, 2005; Blokker et al., 2006); it still is unproven in other countries. However, with statistical data from Milford, Ohio, it should be possible to generate demand patterns with SIMDEUM that can be validated with the extensive measurements that are available (Buchberger et al., 2003).

**PRP model:**
- Demands arrive randomly as a Poisson Process
- A rectangular pulse with random independent intensity and duration is associated with each arrival
- The total demand at any time is the sum of all active pulses

**End use model:**
- End uses demands arrive depending on users daily schedule and frequency of use
- A rectangular pulse with random intensity and duration depending on the end use is associated with each arrival
- The total demand at any time is the sum of all active pulses

**Fig. 3.** Schematic of the PRP and end use demand models. In the PRP model the Poisson arrival rate, intensity and duration are based on the measurements of pulses (like the lower diagram). In the end use model the arrival rate, intensity and duration are based on statistical information of end uses (toilet flushing, showering, washing clothes, doing the dishes, etc.)