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ROBUSTNESS OF PROFILE SAMPLING IN DETECTING DISSOLVED LEAD IN HOUSHOLD DRINKING WATER

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Abstract

The norm for dissolved lead in drinking water is lowered in the Netherlands per 2023, from 10 to 5 µg/L. The effect is that: (a) homeowners and the Dutch water utilities want to find problematic lead components and remove them; and (b) the utilities want to know if copper service mains with lead soldering are expected to lead a norm exceedance. This calls for an improved sampling protocol (collected at the tap) to trace dissolved lead.

We help solve this problem using hydraulic and water quality simulations in EPANET. With short time steps, low flow rates, and short pipe lengths, a water quality time step of 1 second is not short enough. As EPANET cannot work with timesteps smaller than 1 second, we devised a work-around to ensure that the numerical solution does not result in a large error.

A household is defined as a system of pipes with various locations where water is used. The water demand patterns at each tap are generated using SIMDEUM. A few (sections of the) pipes are assigned to contain lead wherefrom dissolution occurs. The benchmark scenario involves a two-person household with average Dutch water consumption and with solely the service line containing lead. Next, fourteen scenarios are considered wherein either the geometry of the system, the water consumption, or location/extent of the lead releasing surface(s) are varied individually.

Of the sampling protocols considered, the results show that "profile sampling" is the most promising. In such a protocol, twenty consecutive samples of 300 ml are collected following a minimum of six hours of prolonged stagnation. Irrespective of the scenario (with a lead component), at least one of the twenty samples is guaranteed to possess a high concentration of lead, owing to our choice of a fine sample volume. Just two days of profile sampling can potentially unveil: (1) the location of the lead releasing component, (2) the volume of the lead releasing region, and (3) the saturation concentration of lead dissolution.

The key conclusions (for the current assumptions) are as follows. A lead service line potentially leads to an exceedance of the new norm, necessitating immediate action. The results also provide evidence that one week of proportional sampling is insufficient. Presently, it is considered to be the gold standard for measuring weekly intake of dissolved lead, however, it is susceptible to the stochastic nature of water demand leading to variations exceeding 50%. Lastly, a profile sampling protocol possesses the best opportunity to detect dissolved lead in the household drinking water network in a robust manner. In the future, a bespoke experimental facility ("PilotCity indoor installation") will be used to validate the assumptions surrounding the lead dissolution and advection/diffusion model.

Keywords
Dissolved lead, EPANET water quality prediction, Households, Sampling protocol.

1 INCORPORATING LEAD TEMPORAL VARIABILITY WITH A STOCHASTIC DRINKING WATER DEMAND MODEL

Lead in drinking water has re-emerged as a problem of public interest and policy makers around the world are rushing to orchestrate actions in interest of public health. For example, in the Netherlands, the norm for weekly lead exposure per person is being reduced from 10 to 5 µg/L from 2023. The ultimate desire is to eradicate any lead releasing components, but information about their locations is seldom known. This is even more relevant for components present in premise plumbing, as it lies beyond the jurisdiction of the water utilities. To determine whether a household is exposed to lead in drinking water, sampling plays a crucial role.

Various sampling protocols exist to assess the extent to which lead in drinking water is a problem [1]. The most understudied contributor to lead variability is the impact of water use pattern (see Box 2 in [1]). How water is used has a significant effect on how dissolved lead propagates through the plumbing. The challenge often lies in simulating realistic water demand patterns, which is non-trivial due to its inherent stochasticity.

In this context, we aim to demonstrate how numerical simulations can contribute in estimating lead consumption under realistic water usage scenarios. We account for lead temporal variability by incorporating SIMDEUM [2,3], a stochastic drinking water demand model, in our framework. For this purpose, we perform simulations that are described in Section 2. In premise plumbing, water quality computations are afflicted by the presence of short pipes. To tackle this, in Section 3, we present how the combination of temporal deceleration and demand reduction can improve water quality calculations. In the context of the norm changes to be brought upon in the Netherlands, it is also important to calculate weekly intakes and its sensitivity to various factors (such as geometry of piping, household characteristics and location of lead releasing components). For that purpose, weekly intakes computed from the simulations are used to comment on proportional sampling in Section 4. Thereafter, in Section 5, we discuss the robust performance of profile sampling under varying scenarios. Finally, in Section 6, we summarize our main findings and offer an outlook on how we plan to build up on the present work.

2 SIMULATIONS IN EPANET TO CALCULATE DISSOLVED LEAD CONSUMPTION

While sampling protocols have to be eventually implemented in the real world, in order to design and test the effectiveness of sampling protocols, water quality simulations were deployed on EPANET. The advantages hereof include: perfect control and knowledge of the location of the lead releasing components and lead dissolution behaviour, the ability to control water demand patterns as well as the ability to accurately measure lead exposure. The framework is illustrated in Figure 1, the individual components hereof will be described in the forthcoming sections.

2.1 Framework and components of the numerical simulations

The starting point of the simulations is the definition of an indoor premise plumbing system. For this purpose, the lengths and diameters of the piping as well as the points-of-use need to be defined. We consider a typical Dutch household with water usage spread out over three storeys. The water enters the ground floor via a service line and continues into the indoor plumbing via the water meter. A toilet and kitchen is located on the ground floor, a toilet and shower on the first floor and a washing machine on the second floor. Moreover, on the second floor the boiler serves to supply hot water. Details about this geometry is available elsewhere [4]. The present work appends a service line to the existing plumbing. This service line with a diameter of 32 mm and a length of 1 m is added between the water source and the water meter.

Information about the points-of-use, together with the composition of the household (number of adults and children, attitude towards water consumption) are fed to SIMDEUM [2,3], a stochastic drinking water demand model. This program generates realistic water consumption patterns at each usage point. These generated demand patterns are then added to the EPANET model. The SIMDEUM demand patterns are not normalized (thus, temporal mean is not equal to unity), and thus, the base demand factor in EPANET can be set to unity.

The final aspect of the modelling involves the selection of lead releasing piping/components in the installation. These components are deemed to release dissolved lead into the water according to a lead dissolution model. In EPANET, we make use of a first order saturation growth model for the bulk reaction [5]. The lead dissolution model is described by equation (1).

$$\frac{dC}{dt} = \frac{4M}{DE}(E - C) \tag{1}$$

Here, the increase in dissolved lead concentration, C, in time, t, is governed by the pipe diameter, D, the dissolution rate, M, and equilibrium lead concentration or plumbosolvency, E. The solution to this differential equation is $C = E(1 - e^{-t/T})$, where $T = \frac{DE}{4M}$. The parameter T represents a timescale on how quickly the equilibrium lead concentration is achieved. To be accurate, the lead dissolution model is dependent on the ratio between the surface area and the volume (related to hydraulic diameter). In the case of a cylindrical pipe, this is reduced to $4/D$.

In our simulations, the plumbosolvency is assumed to be 110 μg/l while the lead dissolution rate is assumed to be 0.115 μg/(m^{2}s). These values are known to be dependent on parameters such as water chemistry and temperature. However, these factors are not included in the present study. Moreover, it is assumed that the water from the distribution network contains no lead.

One minor shortcoming of modelling the lead dissolution model as a bulk reaction instead of a wall reaction is that the effect of wall roughness cannot be trivially accounted for. This choice had to be made since the EPANET does not facilitate first order saturation growth models for wall reactions. EPANET has built-in methods to include the effect of wall roughness on the wall reaction rate. While we do not present the results here, we did verify that the EPANET bulk reaction approach gives comparable results with EPANET-MSX with a wall reaction. Since simulations with MSX are much slower, we did not use it further.

Of course, the process of lead dissolution has a lot more intricacies like the slow diffusion of lead from the walls towards the axis [6]. Moreover, the transport of lead is only governed by advection in our simulations. The inclusion of dispersion will influence our results [5]. The inclusion of this phenomenon in future EPANET versions [7] will undoubtedly be useful for reassessing the findings presented herein.

We limit ourselves to the analysis of dissolved lead. It is known that particulate lead can also contribute to lead consumption. However, incorporating the hydraulics of particulate lead goes beyond the scope of the present work. Moreover, we do not consider the additional influence of flow velocity on mechanical degradation of pipe scales which could potentially accelerate mass transfer of dissolved lead [8].

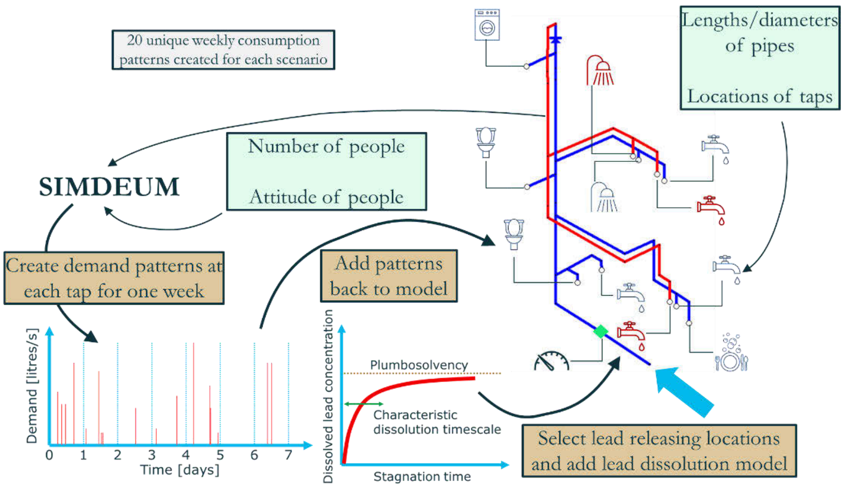


Figure 1: Framework and components of the numerical simulations.

2.2 Temporal deceleration and demand reduction to counteract short pipes

From the perspective of hydraulics, the extended period simulations of EPANET can be seen as a composition of multiple steady state hydraulic simulations. This, however, does not apply to water quality simulations, where a Lagrangian approach is implemented. Thus, it is common practice for the water quality timestep to be much lower than the hydraulic timestep. If the timestep for the water quality calculations exceeds the time needed for water to be advected through a pipe, mass imbalance errors will result in inaccurate water quality predictions [9].

This conundrum is especially relevant for simulations in premise plumbing wherein piping is much shorter than distribution networks, and maximum velocities are comparable to pipe lengths. Inaccurate water quality predictions resulting from mass imbalance errors has been illustrated for EPANET 2.0 [9]. In EPANET 2.2 (released in 2020), mass balance errors are smaller. However, time steps in EPANET may only be long integers and thus cannot be smaller than 1 second [10].

In order to overcome issues that might arise therefrom, a workaround was devised. As a first step, all relevant timescales for the simulations (duration and hydraulic, quality, pattern, report time steps) are increased by a factor of ten. We refer to this as temporal deceleration. The next step is demand reduction wherein the water demand at each usage is reduced by a factor of ten to conserve volumetric intake. The key parameters are summarized in Table 1. Of course, this solution is expected to cause issues in the hydraulics as the Reynolds numbers are varied (variation in velocities but not in pipe diameters). In any case, the purpose of this workaround is to reduce errors that might arise in the water quality simulations.

Table 1: Summary of simulation properties.

Demand pattern generated on SIMDEUM [days]	7 (70 with temporal deceleration)
Duration [days]	140
Hydraulic timestep [s]	10
Quality timestep [s]	1
Report timestep [s]	100
Pattern timestep [s]	100
Base demand factor [-]	0.1
Data used for further analysis	Days 71-140

The inclusion of this workaround also necessitates a corresponding modification in the lead dissolution model. Given that temporal deceleration is a key aspect of the workaround, this must be also applied to the lead dissolution model. Thus, we reduce the parameter T by a factor of ten as well. This ensures dynamic similarity for the lead dissolution model.

The single biggest disadvantage of this workaround is that it leads to a huge rise in computational time. In the present simulations, the chemical reactions in question are relatively simple and can be implemented directly in EPANET. However, if more complex reactions are involved (such as in temperature modelling), the simulations would have to be performed on EPANET-MSX, wherein simulations are slower to begin with.

2.3 Scenarios considered

With the foundation for the simulations set, we now describe the fifteen scenarios we have simulated. These scenarios are shown in Table 2. A benchmark scenario is established, on basis of which variations are brought upon in either the geometry of the premise plumbing, the water consumption patterns, or the location of the lead releasing components. Variations in premise plumbing and location of the lead releasing components was implemented via WNTR [11] whereas changes in the water consumption pattern were implemented using SIMDEUM. Across all these cases, the lead dissolution model constants for plumbosolvency and mass dissolution rates were held constant. However, changes in pipe diameter would affect the characteristic timescale for lead dissolution.

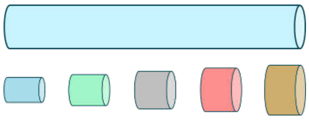
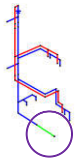
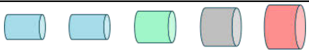
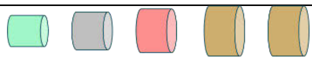
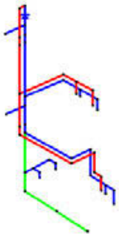
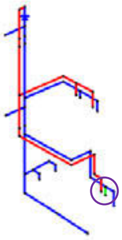
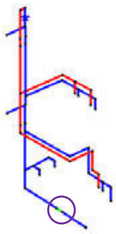
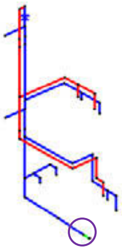
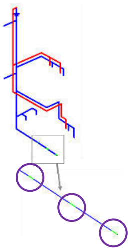
1. Benchmark case: The geometry as defined in Section 2.1 is considered. The water consumption patterns are generated using SIMDEUM with the assumption that it is inhabited by two adults with average water usage characteristics (by Dutch standards). The service line is the sole lead releasing component.
2. Four variations in geometry: The geometry is defined by a system of pipes with attributed lengths and diameters. In two scenarios, all pipes (lead releasing or not) are either shortened or lengthened by 10% each. To vary diameters, the various diameters in the premise plumbing are first inventoried and sorted. Thereafter, to reduce the diameters, the diameter of each pipe was reduced to the next lower possible diameter from the inventory. An exception are pipes with the smallest diameter which are unaffected. A similar approach is used for increasing the pipe diameters, where all pipe diameters are increased to the next possible larger value while the pipes with the largest diameters remain unaffected.
3. Four variations in water consumption patterns: To bring about variations in this category, either the number of inhabitants or their attitude towards water is changed. In this manner, we create water consumption patterns for the house being inhabited by either one adult or two adults with two children. Moreover, we consider the household being inhabited by two adults who either utilize water frugally or extravagantly (either due to habits or appliances) with respect to average Dutch standards. For the high usage, it is assumed that luxurious showers are adopted. For frugal usage, innovative sanitation concepts are applied in addition to efficient showers, washing machines and dishwashers [12].
4. Six variations in location of lead releasing components: First, the system of pipes responsible for lead dissolution is exaggerated. In one case, all pipes from the shutoff valve to the kitchen are responsible for lead dissolution. In another case, all pipes from the shutoff valve to the kitchen tap (excluding the kitchen tap itself) release lead. Then, the length of the lead releasing pipe is reduced to a piece of 20 cm, which is used for three cases - the kitchen tap itself, immediately upstream of the water meter and immediately downstream of the shutoff valve. In the final case, the service line is modified to have a diameter of 25 mm and a length of 3 m. The most upstream, the most downstream, and the central 20 cm of the service line release lead (an exaggerated form of lead soldering).

2.4 Sampling protocols

On top of the generated water demand patterns, sampling protocols were added on using WNTR. For each of the aforementioned fifteen scenarios, the following protocols were simulated:

1. "Proportional Sampling" – no additions/modifications were made to the water consumption patterns. Every moment of water usage at the kitchen tap is treated as a potential sample and no distinction is made whether the water is consumed or not (for example, drinking versus washing hands).
2. Profile sampling – Following a prolonged stagnation of six hours (between 0100-0700), twenty samples of 300 ml are collected consecutively at 0700 on each day of the simulation. These samples are appended as demand (300 mL in 10 seconds). During the prolonged stagnation, any water usage generated in the house by SIMDEUM is annulled.

Table 2: Schematic description of scenarios. Lead releasing locations are shown in green and are encircled.

<table>
<tr><td colspan="2">Benchmark</td><td>
(Pipes of certain lengths and diameters)</td><td>
(Two adults with average Dutch consumption characteristics)</td><td>
(Lead service line)</td></tr>
<tr><td rowspan="2">Variations in geometry</td><td>Length</td><td>
(10% shorter)</td><td colspan="2">
(10% longer)</td></tr>
<tr><td>Diameter</td><td>
(One size smaller)</td><td colspan="2">
(One size larger)</td></tr>
<tr><td rowspan="2">Variations in household consumption characteristics</td><td>Number of people</td><td>
(One adult)</td><td colspan="2">
(Two adults, two children)</td></tr>
<tr><td>Attitude of people</td><td>
(Frugal usage)</td><td colspan="2">
(High usage)</td></tr>
<tr><td colspan="2" rowspan="3">Variations in lead releasing part(s)</td><td>
(Shutoff valve to kitchen)</td><td colspan="2">
(Shutoff valve to kitchen tap)</td></tr>
<tr><td>
(Kitchen tap only)</td><td colspan="2">
(Piece at water meter)</td></tr>
<tr><td>
(Piece at shutoff valve)</td><td colspan="2">
(Lead solder in service line)</td></tr>
</table>

3 EFFECTIVENESS OF TEMPORAL DECELERATION AND DEMAND REDUCTION IN TACKLING SHORT PIPES

The step involving temporal deceleration and demand reduction was specifically devised to tackle short piping and its effect on water quality calculations. In Figure 2(a), it can be seen that in several pipes, the product of maximum velocity and quality time step of 1 second exceeds the pipe length. Pipe lengths vary from 0.1-2 m, whereas maximum velocities vary from 0.29-2.12 m/s. This is a source of numerical errors when advecting plugs of dissolved lead. In order to prove that short piping is an issue and that temporal deceleration + demand reduction are effective, simplified numerical experiments were performed. These numerical experiments entailed water quality calculations using water age, thus bypassing the need for defining reactions.

Since the premise plumbing system shown in Figure 2(a) is quite extensive, a simpler version was created to test the efficacy of temporal deceleration. All points-of-use besides the kitchen tap for cold water were removed. Correspondingly, all plumbing besides the piping between the shutoff valve and the kitchen tap were removed. This is shown in Figure 2(b) as "with short pipes". This route of piping includes segments of shorter lengths as well.

An alternative route is illustrated as "without short pipes" in Figure 2(b). Basically, a straight pipe directly connects the shutoff valve and the kitchen tap. To create this route, the following approach was devised:

1. The system "with short pipes" was skeletonized using the built-in function of WNTR to reduce to a single pipe. This creates one pipe whose diameter is the maximum value from all the pipe diameters before skeletonization (32 mm). The length of the piping equals the sum of all pipe lengths prior to skeletonization (11.89 m).
2. In the process of skeletonization, the total volume of the plumbing between the shutoff valve and the kitchen tap is increased. In order to enable a one-to-one comparison between the two routes, the diameter of the single pipe in "without short pipes" was reduced (20.65 mm) to conserve volume. Conservation of volume is necessitated since the water demands are left untouched.

Hereafter, for each of the two plumbing routes, two simulations are executed. The properties of the two types of simulations are summarized in Table 3. In the post-processing stage, while comparing results, the water age needs to be corrected for the simulations with temporal deceleration. In Figure 2(c), the differences in water ages are compared for the two routes of plumbing. When simulations are performed normally, there are extended periods of several hours wherein the differences (or errors) in the water ages exceeds 100 seconds. This insinuates that shorter pipes are indeed problematic in water quality calculations, especially in the context of premise plumbing. However, it can be seen that the implementation of temporal deceleration + demand reduction does reduce the propensity for errors in water quality calculations. Comparisons between velocities and pressures were performed but are not shown here. In short, velocities were unaffected by temporal deceleration/demand reduction while the pressures were. Since the Reynolds number is not held constant (reduction in velocities but not in diameters), it is unsurprising that the hydraulic calculations are affected. However, these are not expected to affect water quality calculations.

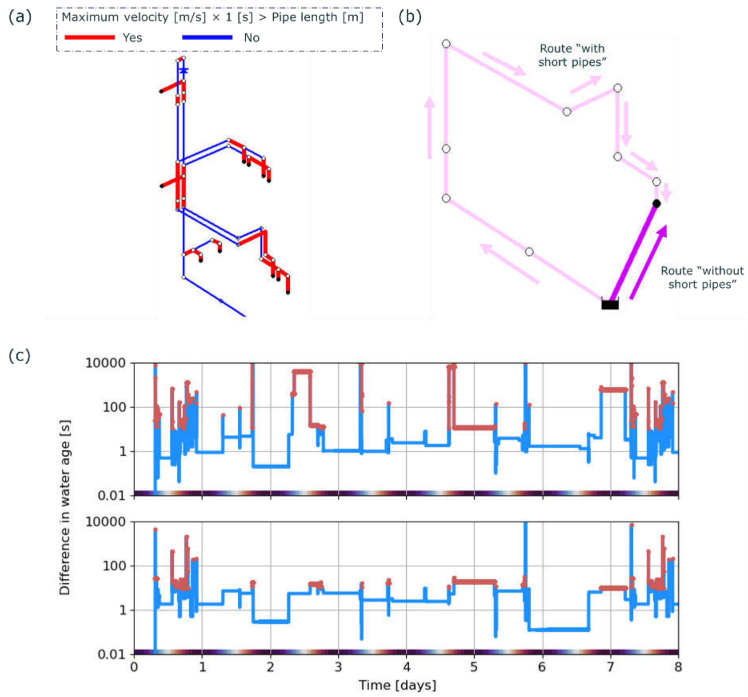


Figure 2: (a) Pipes wherein the product of maximum velocity and quality timestep exceeds pipe length (b) Two routes of plumbing from the shutoff valve to the kitchen tap. (c) Differences in water ages at the kitchen tap between simulations across the two routes, without/with (top/bottom respectively) the implementation of temporal deceleration + demand reduction respectively. Red markers are periods where the difference exceeds 10 seconds.

Table 3: Characteristics of the simulations with(out) temporal deceleration + demand reduction for Figure 2(c).

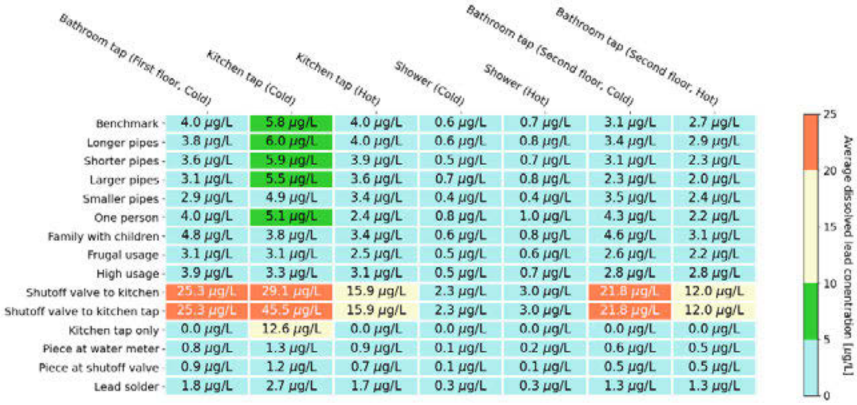
Simulation type → Property ↓	Normal	Temporal deceleration + demand reduction
Factor of deceleration and reduction	1	10
Hydraulic timestep [s]	10	100
Quality timestep [s]	1	1
Duration [days]	8	80
Report timestep [s]	10	100
Pattern timestep [s]	10	100
Base demand factor [-]	1	0.1
Post-processing of data to compare results		
Velocity	No action	×10
Pressure	No action	No action
Water age	No action	÷10

4 WEEKLY INTAKE AND IMPLICATIONS FOR PROPORTIONAL SAMPLING

One of the parameters that needs to be assessed is the weekly lead consumption via drinking water. This is especially of interest to the Dutch water utilities who wish to know whether copper mains with lead soldering can lead to norm exceedance. In this section, we present typical weekly lead consumption trends and how these are affected by the scenarios illustrated in Table 2. To clarify, the simulations considered here do not have any sampling protocol added onto the consumption patterns generated by SIMDEUM.

We consider the lead concentrations encountered at various points-of-use in the household in Figure 3. The key observations are as follows:

1. In the benchmark scenario, the presence of lead service line leads to exceedance of the to-be-sharpened norm at the kitchen tap, but not at the other points of usage. In fact, for the majority of the scenarios, the highest lead concentrations are encountered at the kitchen tap. This implies that the kitchen tap is the best point to perform proportional sampling measurements as it represents the worst-case scenario, next to the fact that most consumption is assumed to take place via the kitchen tap.
2. Variations in the geometry are expected to affect the total volume of lead in the system, propagation towards various nodes, and the timescale at which the equilibrium lead concentration is achieved. All of this leads to minor fluctuations in average consumption, but the conclusion is that a lead service line leads to unsafe conditions and needs immediate action.
3. Variation in household consumption characteristics brings upon reduced lead concentrations than the benchmark scenario. Moreover, in a couple of scenarios the kitchen tap is not the point where the highest lead concentrations are found. This demonstrates the sensitivity of the numerical simulations to water consumption characteristics, and how challenging it would be to generalize average lead consumption without actual measurements.
4. The scenarios wherein extensive lead plumbing is present unsurprisingly leads to norm exceedance. The presence of a small lead component (length 20 cm) can lead to breaches depending on its location relative to the point-of-use. When located at the kitchen tap itself, the norm is breached since the lead cannot be transported elsewhere. However, when these pieces are located further away (for example, in the service line), the lead discharge gets spread out. Our results suggest that the presence of copper service lines with lead solder might not lead to norm exceedance and need not be prioritized by the water utilities.



	Bathroom tap (First floor, Cold)	Kitchen tap (Cold)	Kitchen tap (Hot)	Shower (Cold)	Shower (Hot)	Bathroom tap (Second floor, Cold)	Bathroom tap (Second floor, Hot)
Benchmark	4.0 µg/L	5.8 µg/L	4.0 µg/L	0.6 µg/L	0.7 µg/L	3.1 µg/L	2.7 µg/L
Longer pipes	3.8 µg/L	6.0 µg/L	4.0 µg/L	0.6 µg/L	0.8 µg/L	3.4 µg/L	2.9 µg/L
Shorter pipes	3.6 µg/L	5.9 µg/L	3.9 µg/L	0.5 µg/L	0.7 µg/L	3.1 µg/L	2.3 µg/L
Larger pipes	3.1 µg/L	5.5 µg/L	3.6 µg/L	0.7 µg/L	0.8 µg/L	2.3 µg/L	2.0 µg/L
Smaller pipes	2.9 µg/L	4.9 µg/L	3.4 µg/L	0.4 µg/L	0.4 µg/L	3.5 µg/L	2.4 µg/L
One person	4.0 µg/L	5.1 µg/L	2.4 µg/L	0.8 µg/L	1.0 µg/L	4.3 µg/L	2.2 µg/L
Family with children	4.8 µg/L	3.8 µg/L	3.4 µg/L	0.6 µg/L	0.8 µg/L	4.6 µg/L	3.1 µg/L
Frugal usage	3.1 µg/L	3.1 µg/L	2.5 µg/L	0.5 µg/L	0.6 µg/L	2.6 µg/L	2.2 µg/L
High usage	3.9 µg/L	3.3 µg/L	3.1 µg/L	0.5 µg/L	0.7 µg/L	2.8 µg/L	2.8 µg/L
Shutoff valve to kitchen	25.3 µg/L	29.1 µg/L	15.9 µg/L	2.3 µg/L	3.0 µg/L	21.8 µg/L	12.0 µg/L
Shutoff valve to kitchen tap	25.3 µg/L	45.5 µg/L	15.9 µg/L	2.3 µg/L	3.0 µg/L	21.8 µg/L	12.0 µg/L
Kitchen tap only	0.0 µg/L	12.6 µg/L	0.0 µg/L	0.0 µg/L	0.0 µg/L	0.0 µg/L	0.0 µg/L
Piece at water meter	0.8 µg/L	1.3 µg/L	0.9 µg/L	0.1 µg/L	0.2 µg/L	0.6 µg/L	0.5 µg/L
Piece at shutoff valve	0.9 µg/L	1.2 µg/L	0.7 µg/L	0.1 µg/L	0.1 µg/L	0.5 µg/L	0.5 µg/L
Lead solder	1.8 µg/L	2.7 µg/L	1.7 µg/L	0.3 µg/L	0.3 µg/L	1.3 µg/L	1.3 µg/L

Figure 3: Dissolved lead concentrations at various points-of-use across all scenarios (mean of twenty weeks).

Proportional sampling is rightly perceived as the gold standard as far as measurement of lead consumption at household scales is concerned. However, the sample is typically collected over anywhere between a few days to a week. In Figure 4, we present how week-to-week variations in water consumption affects the dissolved lead concentrations at the kitchen tap across all the scenarios. Note that demand patterns in all scenarios are the same, except when household characteristics are altered. Thus, for a certain week, consumption pattern across the scenarios are correlated (aside from changes in household characteristics) – for example, from week 4 to week 5, increased lead exposure is seen across all scenarios. In the final three columns, the average, minimum, and maximum values across the twenty weeks are shown. In brief, it is irrefutable that week-to-week variations in water consumption patterns trigger variations in dissolved lead concentrations which, in turn, can affect the plan-of-action. Thus, it is recommended to implement proportional sampling over a longer timeframe – for example, five non-consecutive weeks spread out over a year.

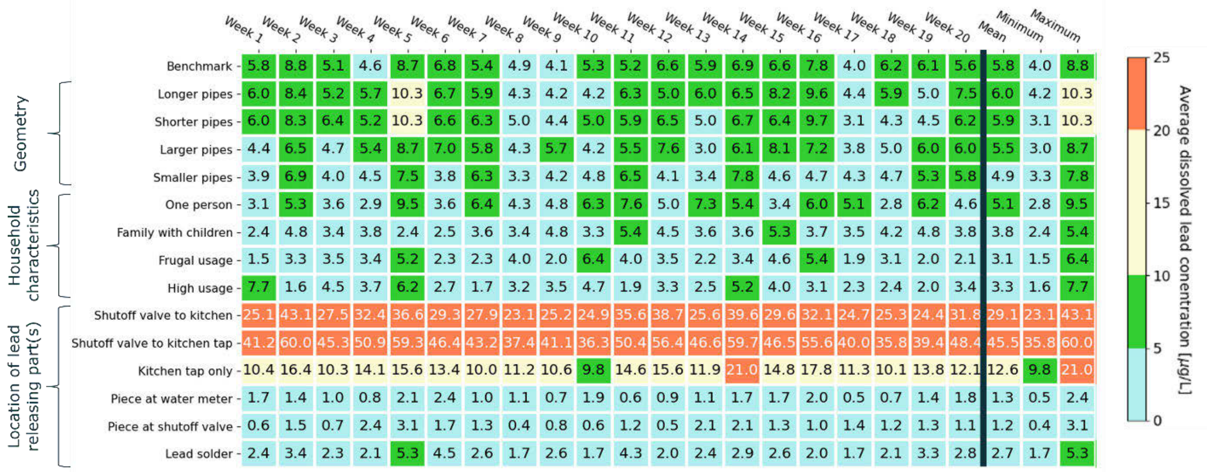


Figure 4: Weekly variations and statistics thereof for dissolved lead concentrations at the kitchen tap.

While judging the results presented in this section, it is important to realize that the absolute values of lead concentration are valid for the assumptions made by us about the lead dissolution model, namely, the values for plumbosolvency and lead dissolution rate. For example, there are numerous factors concerning water chemistry that will lead to variations in lead leaching rates (see Box 1 in [1]). Moreover, the results are specific to this household. An aspect that has not been considered is the layout of the premise itself (for example, the length of the service line or the location of the kitchen in the household). Nevertheless, the results herein show the value of such simulations in assessing lead consumption at household scales.

5 ROBUSTNESS OF PROFILE SAMPLING

Numerous sampling protocols have been devised over the course of history. It is acknowledged that there is no universal protocol that answers all questions (for example, exposure at communal/household scale, presence/location of lead releasing component) and that each protocols answers a specific question [1]. In this section, we specifically consider profile sampling which is capable of localizing the lead releasing component(s).

In our simulations, the measurement protocol is implemented as follows. A prolonged standstill is imposed on each of the 140 days of the simulation between 0100-0700. This means that any water consumption created by SIMDEUM, everywhere in the household, in this timeframe is removed. Immediately following the prolonged standstill, twenty consecutive samples with a volume of 300 ml are collected at the kitchen tap. An example of this collection strategy is shown in Figure 5(a). Please note that the addition of a sampling protocol is intrusive and will affect the numerical values reported in Figure 3 and Figure 4.

The corresponding lead concentrations computed at the kitchen tap are shown in Figure 5(b). The pink line shows what would have been measured by a hypothetical lead concentration sensor inside the tap. From the lead concentrations corresponding to normal usage, it can be seen that there are instances wherein the lead concentration at the tap exceeds the (future) norm of 5 µg/L. This clearly illustrates that the Random Daytime approach (collecting a sample of water at a random time of the day) may be susceptible to these outliers and planning actions on basis thereof is unreliable. In the inset of Figure 5(b), it can also be seen that three of the twenty samples yield strikingly high lead concentrations (close to imposed plumbosolvency).

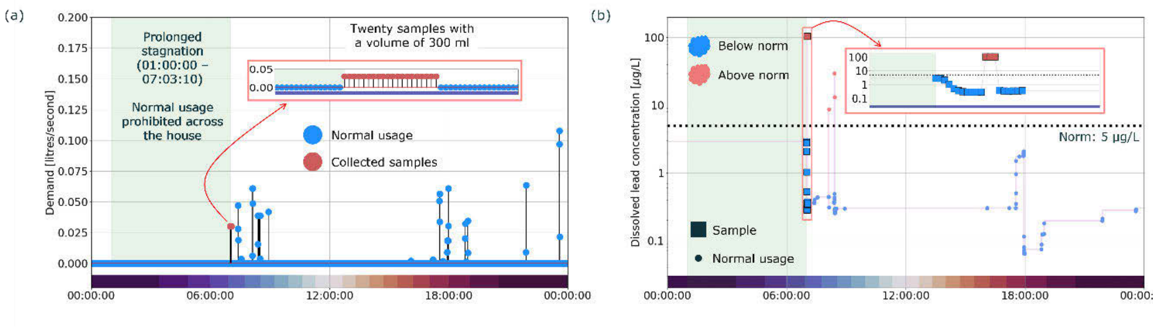


Figure 5: Example of a typical input/output in the simulations over one day at the kitchen tap for (a) water usage and samples for profile sampling (b) dissolved lead concentrations. The gradient colorbar at the bottom is a visual representation of the time of the day.

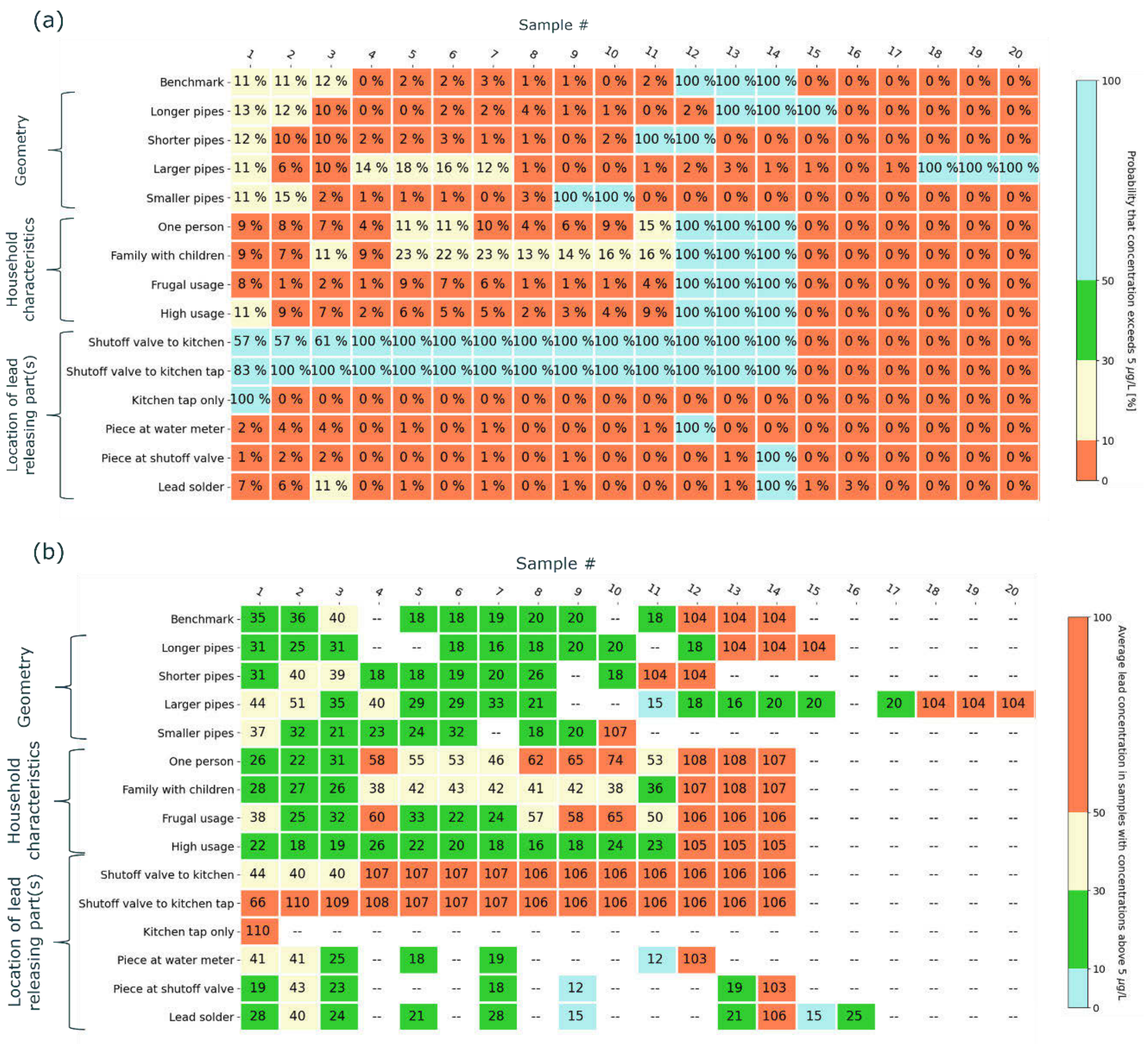


Figure 6: (a) Probability (in percentage) that a sample in a certain scenario contains dissolved lead with concentration above 5 µg/L. (b) Conditionally averaged lead concentrations in all samples wherein the dissolved lead concentration exceeds 5 µg/L.

To investigate the statistics behind the performance of profile sampling, Figure 6 is considered. Basically, in Figure 6(a), for each sample under each scenario, the probability that the lead concentration therein exceeds 5 μg/L is shown.

Samples 1-3 (0.9 litres) in the benchmark case have chances of ~10% to possess concentrations above 5 μg/L. In the Netherlands, the protocol presently used to confirm the presence/absence of lead releasing components involves collecting a one litre sample following a six hour stagnation (corresponding to the average of samples 1-3 in Figure 5/Figure 6). This protocol is recommended by the Dutch National Institute for Public Health and the Environment (RIVM). This suggests that the present approach is inadequate in its goal of detecting the presence/absence of lead releasing components and warrants revisiting.

For the benchmark case, samples 12-14 have a 100% chance of meeting the criterion. From a practical perspective, this is attractive. This means that irrespective of the day/week/month on which this sampling protocol is performed, samples 12-14 are guaranteed to have lead concentration above 5 μg/L. Further reassuring is the fact that irrespective of the scenario, at least one of the twenty samples is guaranteed to possess lead concentrations above 5 μg/L. Even the small components of 20 cm long are picked up by this protocol. This partly demonstrates the robustness of profile sampling under realistic water consumption patterns. It is important to realize that the choice of 20 samples of 300 ml is instrumental. Had sampling been coarser (for example, 10 samples of 600 ml or 5 samples of 1200 ml), samples with high lead concentrations could have gotten diluted, diminishing the robustness of this sampling protocol.

To firmly establish the robustness of profile sampling, Figure 6(b) is considered. The numbers herein are conditionally averaged lead concentrations in samples wherein the concentration exceeds 5 μg/L. For the benchmark case, samples 12-14 have average concentrations above 100 μg/L, while for the other samples, it varies between 20-40 μg/L. In fact, for every sample/scenario combination in Figure 6(a) with 100%, the corresponding conditionally averaged lead concentration is in the vicinity of the plumbosolvency of 110 μg/L. This means that the lead from the lead releasing components will not only invariably end up in the same sample but will also end up in a high concentration, facilitating easy and unambiguous detection.

Figure 7 summarizes the principle behind profile sampling. The plumbing between the distribution network and a single faucet is shown. The water meter is preceded by a service line. The plumbing is partitioned into equal volumes representing the volume of each sample that is to be collected following a prolonged standstill. Based on sample collection over two days, a lot of information can be extracted from the profiles. The first day of measurements returns predictions for potential locations of the lead releasing components. The second day of measurements help classify the true and false positives. For example, in the schematic, sample 5 from day 1 is a false positive since it does not possess high concentrations on day 2. However, samples 12, 13 are true positives and correspond to the lead releasing component. We refer to samples 12, 13 as the peak. Following the peak, the lead is flushed away and there is no chance that a sample will contain any dissolved lead. Based on this peak, the following information can be gathered and can be useful in prioritizing which households need to be investigated first.

1. Location of the peak: If a drawing of the premise plumbing is available, based on the location of the peak and the volume of the individual samples, it should be theoretically possible to estimate where in the plumbing system the lead originates from. The location can be relevant in determining whether it is the responsibility of the premise owner or the water utility. The further away the lead releasing component is from the tap, the better it is for the safety of the inhabitants, since the dissolved lead gets spread out.
2. Breadth of the peak: The total volume of the peak indicates the severity of the problem. Naturally, the narrower the peak, the better it is for the inhabitants.

3. Height of the peak: This contains information about the local level of plumbosolvency which will likely be related to the water chemistry and temperature, specific to the distribution area. The lower the peak, the better it is for the inhabitants.

It is known that each sampling protocol has its own objective. In the case of profile sampling, it is to detect and localize the lead releasing components, and is not expected to provide any insights into the lead consumption by the inhabitants. It would be interesting to see whether an empirical correlation can be established between the above three parameters and the weekly lead consumption. Fully flushing the plumbing prior to stagnation will improve the robustness of the technique by eliminating any false positives. In the present study, not flushing prior to stagnation allows us to assess the performance of the protocol recommended by the Dutch National Institute for Public Health and the Environment (through the first three samples).

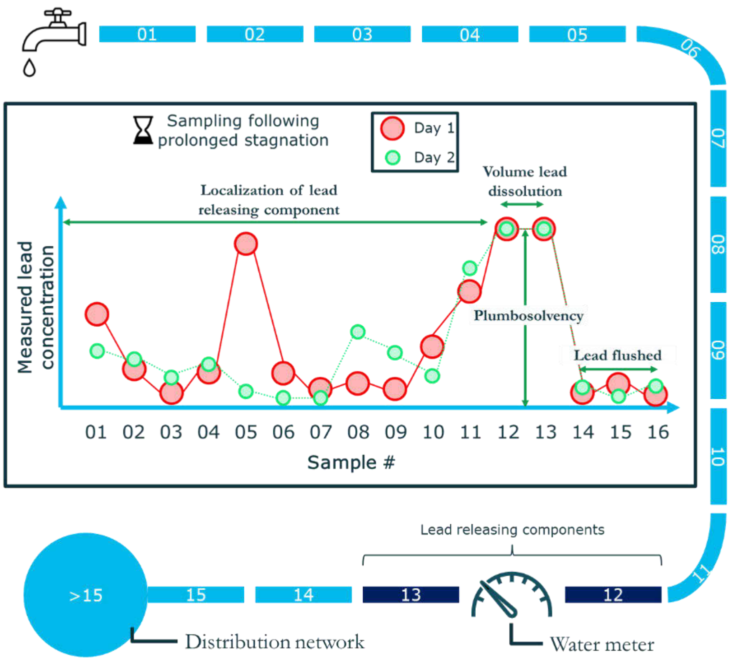


Figure 7: Schematic of the functionality of profile sampling and the information that can be derived therefrom.

Please note that a similar conceptual drawing has been presented elsewhere [13]. However, it primarily illustrates how the slug of high lead concentration is generated and advected over the course of normal use and how it affects the composition of a one litre sample.

Questions can be raised on whether the robustness of profile sampling as demonstrated here can withstand real conditions. Field measurements in Flint [14], showed the value of this protocol in identifying the sources of lead. Similarly, it has been demonstrated [5] that the essence of this protocol can be captured in a laboratory setup (Home Plumbing Simulator of EPA) as well as EPANET based modelling (of the Home Plumbing Simulator). In their comparison, however, the concentration peaks in the experiments were far lower than that seen in their numerical simulations.

Another caveat is that the propagation of dissolved lead in our EPANET simulations are driven by advective forces. In reality, diffusion will also affect the propagation of dissolved lead. The addition of one dimensional mass dispersion to the EPANET framework led to a better match with the profiles obtained in controlled experiments [5]. The addition of this mass dispersion model broadened the concentration peak obtained by profile sampling while also lowering the peak itself. This means that in our simulations, the peak heights are overestimated while the peak widths are underestimated.

6 DISCUSSION: NUMERICAL MODELLING OFFERS AN ADDITIONAL AVENUE TO SUPPORT DECISION-MAKING SURROUNDING LEAD IN DRINKING WATER

The major objective of our work was to demonstrate the added value provided by EPANET hydraulic and water quality simulations in tackling the "lead in drinking water" problem. By leveraging SIMDEUM in generating realistic water usage patterns, we incorporate the understudied aspect of temporal lead variability in premise plumbing. Our numerical simulations combined the geometry of a typical Dutch household, a lead dissolution model (first order saturation growth) and realistic water consumption patterns. Moreover, we studied a total of fifteen scenarios, wherein either the geometry of the piping, household water consumption characteristics, location of lead releasing component was tweaked. For each scenario, 140 days of unique daily water usage patterns were simulated.

A shortcoming of combining EPANET water quality simulations with premise plumbing is that the timescale over which water advects through short pipes is shorter than 1 second, which can lead to numerical errors. To overcome this, and the fact that EPANET cannot work with timesteps shorter than one second, we simultaneously implemented temporal deceleration (increasing timescales of simulations, hydraulic/pattern/report timesteps by a certain factor, ten in our case) and demand reduction (decreasing water demand at each point-of-use by the same factor). This ascertains that the shortcomings caused by short piping is circumvented (reduction in errors).

Establishing a solid framework for our numerical simulations allowed us to estimate average lead exposure via drinking water at several points-of-use. It is seen that the average lead concentrations are highest at the kitchen tap for cold water, for majority of the scenarios. This, in combination with the fact that most consumption is assumed to occur at the kitchen tap, implies that performing proportional sampling should be continued at the kitchen tap itself. Typically, during proportional sampling, the composite sample is collected over one week. Based on our simulations of twenty weeks, we are able to demonstrate how the results of proportional sampling is prone to the week-to-week variations in water usage. Even though we do not make a distinction between the type of water consumption or consider the hot water tap, our results suggest that one week of sampling is insufficient. Thus, to get a better picture of average lead exposure, it is recommended to analyse samples collected over five non-contiguous weeks.

Finally, we demonstrated the strength of profile sampling in localizing the source of dissolved lead. The protocol involves collecting consecutive samples (in our simulations, 20 samples of 300 ml) immediately following a prolonged standstill. Basically, the following three parameters can be derived from the concentration profile across the samples – the location of the lead releasing component (location of the peak), volume of lead release (breadth of the peak), plumbosolvency (height of the peak). In the samples corresponding to the lead releasing location(s), it is expected that the lead concentrations will always exceed 5 µg/l and achieve values close to the plumbosolvency, in contrast to the other samples. This trend is visible across all scenarios, demonstrating the robustness of profile sampling. Flushing the plumbing prior to the prolonged stagnation will likely make the technique more robust (by eliminating any previously stagnated plugs of dissolved lead). It would be interesting to see whether any correlation exists between the above three parameters and the weekly lead consumption.

Our simulations also include several assumptions. Two of the key assumptions are: (i) the parameters for the lead dissolution model (plumbosolvency, mass dissolution rate) have been assumed, (ii) propagation of dissolved lead across the plumbing is driven purely by advection while the influence of diffusion is overlooked. In the future, we intend to utilize a bespoke experimental facility (PilotCity Indoor Installation, whose functionalities resemble the Home Plumbing Simulator of EPA) to probe the extent to which our assumptions are (in)valid.

Accordingly, we can re-do the simulations presented herein with the adjusted assumptions and perform a one-to-one comparison with the results obtained in a controlled laboratory setting.

Nevertheless, the framework presented in this work provides an avenue for future simulations surrounding the topic of dissolved metals in drinking water. Of course, simulations entail assumptions and will always be detached from reality. However, it provides an ideal playing ground to test sampling protocols and prioritize households which need immediate action. We would eventually like to expand our methodology to include locations frequented by children (for example, schools), multi-storeyed housing with common (lead or copper with lead solder) service line. Finally, our approach offers a convenient environment to test sampling protocols that are being proposed by Dutch water utilities, in wake of the stringent norms surrounding lead in drinking water.

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