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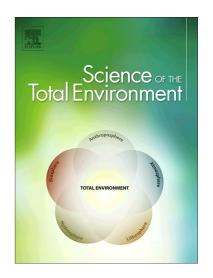
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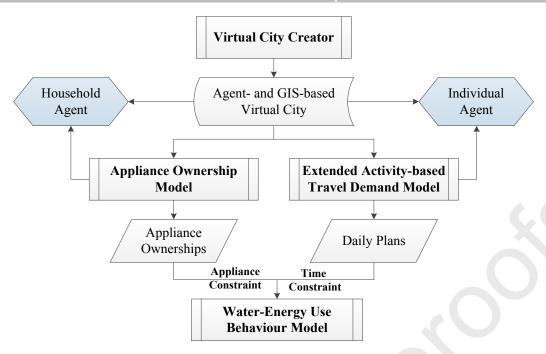
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Graphical Abstract



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Abstract

Water and energy consumptions in the residential sector are highly correlated. A better understanding of the correlation would help save both water and energy, for example, through technological innovations, management and policies. Recently, there is an increasing need for a higher spatiotemporal resolution in the analysis and modelling of water-energy demand, as the results would be more useful for policy analysis and infrastructure planning in both water and energy systems. In response, this paper developed an agent-based spatiotemporal integrated approach to simulate the water-energy consumption of each household or person agent in second throughout a whole day, considering the influences of out-of-home activities (e.g., work and shopping) on in-home activities (e.g., bathing, cooking and cleaning). The integrated approach was tested in the capital of China, Beijing. The temporal results suggested that the 24-hour distributions of water and related energy

consumptions were quite similar, and the water-energy consumptions were highly correlated (with a Pearson correlation coefficient of 0.89); The spatial results suggested that people living in the central districts and the central areas of the outer districts tended to consume more water and related energy, and also the water-energy correlation varies across space. Such spatially and temporally explicit results are expected to be useful for policy making (e.g., time-of-use tariffs) and infrastructure planning and optimization in both water and energy sectors.

Keywords: Nexus of Water and Energy; House Appliances; Consumption Behaviour; Agent-based Modelling; Activity-based Modelling

1 Introduction

1.1 Background

Water plays an important role in economic growth (Distefano and Kelly, 2017). For example, in Chinese history, the so-called shui-li was associated with the shift of key economic areas (Chi, 1936). Energy is required through the whole urban water cycle, primarily involving water extraction, water treatment, water transportation, water distribution, water consumption, wastewater collection and wastewater treatment (Hamiche et al., 2016; Lam et al., 2017; Plappally, 2012; Ren et al., 2016). Among them, water consumption has been found as highly correlated with energy consumption in both residential (Abdallah and Rosenberg, 2012; Escriva-Bou et al., 2015; Jiang et al., 2016) and non-residential (Assaf and Nour, 2015; Gu et al., 2016; Sanders and Webber, 2012) sectors. For example, a recent study in the residential sector suggested that "55% of electricity consumption was coupled with water consumption in Beijing in 2017" (Yu et al., 2018). This paper will be focused on the water and related energy (water-energy) consumptions in the residential sector.

Systematic analyses of water-energy consumptions have recently received substantial attention (Binks et al., 2017; Escriva-Bou et al., 2015; Escriva-Bou et al., 2018; Kenway and Lam, 2016; Mostafavi et al., 2018; Ren et al., 2016), as a better understanding of the correlation between water and energy consumptions could help save both water and energy, for example, through technological

innovations, management and policies, and further could mitigate some global pressing challenges, such as water and energy scarcity and climate change (Chini et al., 2016; Jiang et al., 2016; Ren et al., 2016). At the individual level, several empirical findings suggested that water-energy consumption could be influenced by characteristics and behaviours of occupant (e.g., income, education level, duration and frequency) and availability and features of appliance. Some specific examples are as follows: (Yu et al., 2018) investigated the water-energy use behaviours in bathing, cooking and cleaning and suggested that water-energy consumption was positively correlated with education level, but negatively correlated with household size and age; (Abdallah and Rosenberg, 2012) suggested that households can save both energy and water by using dishwasher instead of using water directly from a faucet; (Kenway et al., 2016) investigated the water-energy consumption in showering and found that the key influential factors included showering duration, showering frequency and number of adults; (Matos et al., 2017) identified two influential factors to the water-energy consumption in bathing, namely the bath temperature and the presence/absence of flow reducer valve; (Jiang et al., 2016) found that the water-energy consumption in Tianjin, China was correlated with both showering frequency and the ratio of hand washing. Therefore, special attention needs to be paid to heterogeneity in analyzing and modelling water-energy consumptions (Abdallah and Rosenberg, 2012).

Urban water and energy systems are commonly recognized as complex adaptive systems (Kanta and Zechman, 2013). Agent-based modelling (Macal and North, 2010), which is a promising bottom-up approach to investigating such systems, has been widely used to simulate both in-home water and energy use behaviours at the micro scale (Kanta and Zechman, 2013), considering the interactions and feedbacks found there. Agent-based modelling has several advantages over traditional approaches (e.g., system dynamics model) (Twomey and Cadman, 2002), such as natural representations, heterogeneity, and easy maintenance and refinement (Zhuge et al., 2018). Furthermore, agent-based models can be easily coupled with Geographic Information System (GIS), resulting in spatially explicit models (Zhuge, 2019). Therefore, agent-based modelling is adopted here as the main approach to simulating the individual water and related energy (water-energy) consumptions at home.

1.2 Pervious Agent-based Models for Water and Energy Consumptions

1.2.1 General Agent-based Models

In general, agent-based water use behaviour models considered household as the core agent type (Athanasiadis and Mitkas, 2005; Galán et al., 2009; House-Peters and Chang, 2011): household agents needed to decide how to use water and purchase water fixtures, considering the potential social influence (Chu et al., 2009; Galán et al., 2009), technologies (Kanta and Zechman, 2013; Schwarz and Ernst, 2009) and regulatory policies (Kanta and Zechman, 2013; Koutiva and Makropoulos, 2016). For example, the work by (Galán et al., 2009) covered all of the potential influential factors above. Specifically, it proposed an agent-based integrated framework for domestic water management in the Valladolid metropolitan area, which incorporated an urban dynamics model, a statistical water consumption model, an opinion diffusion model, and a technological diffusion model. In particular, the opinion diffusion model took social influence (or social network) into account, and the technological diffusion model simulated the adoption of water-related technologies. The integrated model was calibrated based on some similar models in other European cities with no empirical data used, which was a significant limitation of this study. Further, the model was applied into "what-if" scenarios, considering the influence of different polices on water consumption, including immigration and prices of unoccupied dwellings. The simulation results suggested that urban dynamics (e.g., residential relocation) was a very influential factor to water consumption. Some of the water consumption models have also additionally considered the interactions between household agents and other associated agents, such as government agent (Chu et al., 2009; Darbandsari et al., 2017; Kanta and Zechman, 2013) and appliance seller agent (Chu et al., 2009; Yuan et al., 2014). For example, (Chu et al., 2009) developed an agent-based Residential Water Use Model (RWUM) for Beijing, which was capable of simulating the interactions between three agent types, namely regulator, water appliance market agent and household. RWUM also considered several typical influential factors, such as technology adoption and regulatory policies. The model was calibrated primarily using macro-level data from various statistics, planning and surveys. The simulation results suggested that

both regulatory policies (e.g., standard of water device) and technology improvements (e.g., highefficiency devices) were important to water conservation.

Similarly, many agent-based energy use behaviour models have also been developed to simulate how household agents consume energy and purchase energy-related appliances (Natarajan et al., 2011), considering various energy-related technologies (e.g., residential solar photovoltaic) (Jackson, 2010; Lee et al., 2014; Rai and Robinson, 2015; Robinson and Rai, 2015) and policies (e.g., subsides) (Kowalska-Pyzalska et al., 2014; Lee et al., 2014; Yousefi et al., 2011). Two typical examples are as follows: (Lee et al., 2014) proposed an Agent Home Owner Model of Energy (AHOME) driven by empirical findings to analyse various UK policies, such as carbon tax and subsidies. In order to better model the behavioural rules, the data from two discrete choice surveys by the Energy Saving Trust (N= 2019) and the Element Energy (N= 1171) were used to estimate the impact of different factors in a utility function. The AHOME simulations suggested behavioural change could give rise to the uptake of energy-efficient technologies; Another typical example by (Rai and Robinson, 2015) proposed a theoretically-based and empirically-driven solar adoption model. The agent-based adoption model was based on a typical behavioural approach, namely Theory of Planned Behaviour (TPB). It was also coupled with a social network evolution to consider social influence. In order to be behaviourally sound, several datasets were used for model parameterization and validation, including the Austin solar rebate program data, a Longitudinal survey data on PV adopters and light detection and ranging (LIDAR) data. The simulation results suggested that the model could represent the major structural features observed from the historical diffusion curve.

However, these agent-based water or energy models have tended to be only focused on either energy or water, paying little attention to the correlation between water and energy consumptions. To fill this research gap, the agent-based integrated approach proposed in this paper will simulate water and related energy use behaviour, particularly considering the water-energy correlation.

1.2.2 Agent-based Models with High Spatiotemporal Resolutions

Some of the agent-based models reviewed above have somewhat considered spatial or temporal factors, such as the so-called neighbour effect, which could influence the adoption of energy- and water-related technologies (or devices) (Athanasiadis et al., 2005; Athanasiadis and Mitkas, 2005; Chu et al., 2009; Darbandsari et al., 2017). For example, (Rai and Robinson, 2015)'s agent-based energy technology adoption model considered the neighbour effect on the adoption of residential solar photovoltaic (PV) systems in Austin, USA. However, higher spatial and temporal resolutions are needed in the analysis and modelling of water and energy demand, in order to better "assess the resource implications of policy interventions and to design and operate efficient energy and water systems" (Keirstead and Sivakumar, 2012). On the other hand, it has been increasingly recognized that in-home and out-of-home activities are correlated (Ghauche, 2010; Keirstead and Sivakumar, 2012; Meloni et al., 2004; Yu et al., 2011; Yu, 2013): people need to allocate time slots among different in-home and out-of-home activities when they schedule their daily plans for the whole day. For example, (Yu et al., 2011) identified the correlation between in-home and out-of-home activities in Beijing using a questionnaire survey data with 1014 households included, and found that a reduction in energy consumption of in-home activities may lead to an increase in that of out-of-home activities. Therefore, some attempts have been made to simultaneously consider in-home and out-ofhome activities within the extended activity-based travel demand models, in order to estimate the energy consumption in buildings at high spatial and temporal resolutions (Ghauche, 2010; Keirstead and Sivakumar, 2012).

Activity-based travel demand model (Zhuge et al., 2019b), which is a typical bottom-up approach in transport studies, is used to simulate individual daily out-of-home activities (e.g., shopping) and the associated travels. See Rasouli and Timmermans (2014) for a recent review of the activity-based models. The extended activity-based models, which additionally incorporated in-home activities, considered resource and energy demands as a result of performing activities (Chingcuanco and Miller, 2012; Keirstead et al., 2012; Keirstead and Sivakumar, 2012). However, most of the extended activity-based models were used to simulate the domestic energy demand, paying significantly less

attention to the in-home water use behaviour and almost no attention to the correlation between water and energy consumptions. In response, this paper attempts to extend a typical activity-based model, MATSim (Horni et al., 2016), to incorporate in-home activities, so as to simulate water-energy use behaviour with spatiotemporal constraints.

1.3 Research Gaps and Objectives

In summary, agent-based modelling has been widely used to explore urban water and energy systems. However, these agent-based models are limited in the following two aspects: 1) they have tended to investigate water and energy consumptions separately, paying little attention to the correlation between water and energy consumptions; 2) although the interaction between in-home and out-of-home activities has been considered in the studies of domestic energy consumption, it received little attention in the analysis or modelling of the water-energy consumptions. To fill these two research gaps, there is a need for an agent-based spatiotemporal integrated approach to simulate the in-home water-energy use behaviour at the individual level, considering the potential time constraints of out-of-home activities on in-home activities and the interactions between household members. For such a complex model, this paper will start with its conceptual design and will then examine the model performance within a test case of Beijing. The proposed conceptual framework is theory-driven, rather than data-driven. Essentially, the integrated framework incorporates several typical approaches in behavioural studies, such as agent-based model, discrete choice model and activity-based model. In order to make the conceptual model behaviourally sound, some empirical findings about individual behaviours were extracted from two datasets for model development, namely the 2010 Beijing Household Travel Survey data and the survey data on water-energy use behaviour and the ownership of related appliances (collected in 2017). Essentially, the former will help to improve the behavioural rules in the simulation model of out-of-home activities and travels; the latter will help to define the individual behaviours in the simulation model of in-home activities and the associated water-energy consumptions. Some assumptions and simplifications (e.g., the way to assign in-home activities among household members) need also be made in the integrated framework, due to the lack of the relevant empirical findings. The conceptual model could be further improved through the use of more

empirical findings and systematic model uncertainty analyses (e.g., parameter sensitivity analysis and testing model structure, model assumptions and simplifications and future events within various "what-if" scenarios).

The resulting spatially and temporally disaggregate water-energy demand is expected to be useful for policy making and infrastructure planning. More specifically, the temporal distribution of water-energy consumptions could point out the possible peak periods in a day during which consumptions are relatively higher. This information could be useful for shaping policies (e.g., time-of-day tariffs) to shift the peak water-energy demand and thus could benefit the existing water and energy-related infrastructures. More effective policies could be designed, targeting at some specific groups (e.g., people with high income), as heterogeneity is considered in the agent-based integrated approach. The spatial distributions of water-energy consumptions could also suggest, for example, where more water and energy infrastructures may be needed at both disaggregate and aggregate levels. Such information could help local authorities make decisions on infrastructure investment. Furthermore, the spatial distributions are closely associated with land use patterns, and thus such spatially explicit results may also be useful for urban planning that would account for the water and energy conservation.

2 Methodology

2.1 An Agent-based Spatiotemporal Integrated Approach: Overview

The integrated approach (see Figure 1) is composed of four models, namely a virtual city creator, an appliance ownership model, an extended activity-based travel demand model (considering both inhome and out-of-home activities), and a water-energy use behaviour model, which are briefly introduced as follows:

• Virtual City Creator (see Appendix 1.1 in the Supplementary Material for more details): which is a simplified version of the model by (Zhuge et al., 2018), is used here to generate an agent- and Geographic Information System (GIS)-based virtual city comprising a synthetic population and physical environment. A population contains persons and households, as well

as their attributes (e.g., age). The physical environment, where persons perform their daily activities, include facilities and transport network (Zhuge et al., 2018). Here, five typical facility types, namely the facilities for the activities of "home", "work", "shopping", "leisure" and "education", will be modelled (Horni et al., 2016; Zhuge et al., 2018). In the virtual city, each person (or household) is allocated with a residential facility, which is based on a road node (or intersection). This means the model's spatial resolution depends on the road network used for the virtual city creation.

- Appliance Ownership Model (see Appendix 1.2 in the Supplementary Material for more details): is used to predict the appliance ownership for each household in the synthetic population, and thus appliances are also spatially explicit (based on residential facilities). The availability of appliances could influence how individuals perform their in-home activities and further the water-energy use behaviour. The model considers three appliance types, namely bathing, cooking and cleaning appliances (Yu et al., 2018). Both Discrete Choice Model (DCM) and Probabilistic Function (PF) are used for the prediction.
- Extended Activity-Based Travel Demand Model (see Section 2.2): is used to simulate how each individual in the population schedule their daily out-of-home activities (e.g., shopping and work) in second, considering spatial and temporal constraints. The simulation of out-of-home activities here is only used to generate time slots available for in-home activities (e.g., bathing), and the water and energy consumptions of out-of-home activities have not been included. MATSim (Multi-Agent Transport Simulation) (Horni et al., 2016), which is a typical activity-based travel demand model, is used here for the simulation.
- Water-Energy Use Behaviour Model (see Section 2.3): is used to simulate the water energy use behaviour of each individual in the synthetic population in second, with the appliance and time constraints (obtained from the appliance ownership and activity-based models above, respectively), resulting in spatial and temporal distributions of the water-energy demand.

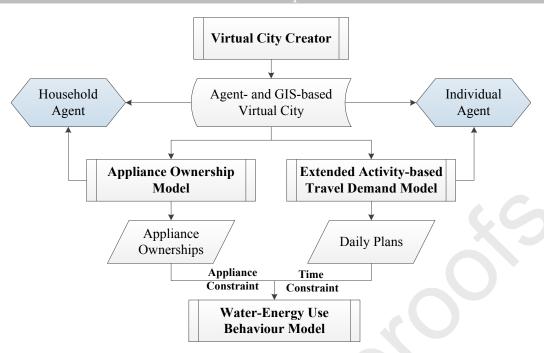


Figure 1 Framework of the Agent-based Integrated Approach

2.2 Extended Activity-based Travel Demand Model (MATSim) for both In-Home and Out-of-Home Activities

Given a synthetic population, an activity-based travel demand model essentially simulates how individual agents schedule their daily plans for a whole day (Zhuge et al., 2019b). A daily plan contains the information on how an agent performs its out-of-home activities (e.g., shopping and work) and how it travels from one place to another using different transport modes (e.g., car). Note that travel is also performed out of home, but is not treated as an out-of-home activity here, as travel is a derived activity, rather than a trip purpose. An example of daily plan is given in Figure 2. Based on daily plans, the time slots available (from 20:00 to 8:00 in this case) for each individual to perform their in-home activities, such as cooking and bathing, can be obtained, so that the spatial and temporal distributions of residential water-energy demand can be further estimated.

Out-of-home activities could influence whether and when in-home activities can be performed. Specifically, some daily activities, such as dining, can be performed either at home or outside, and thus will influence the amounts of water and related energy consumed through these activities. For example, dining outside will influence the water-energy consumption through cooking. Furthermore, due to the constraints of out-of-home activities (e.g., work), people can only perform their in-home

activities at some specific time slots. For example, for full-time workers, they generally can only preform in-home activities (e.g., bathing and cleaning) before they leave for work in the morning or after they get off work in the evening. These could influence the temporal distributions of water-energy consumptions. The two types of constraint above will be simulated within the extended activity-based model.

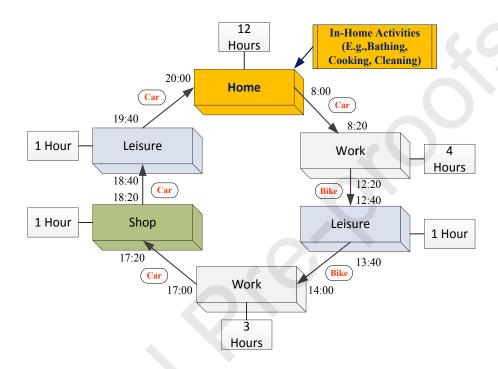


Figure 2 An Example of Daily Plan (Source: adapted from (Zhuge et al., 2018))

This paper extends MATSim, which is a typical activity-based model, to include the water-energy consumption related in-home activities, as MATSim appears to be one of the most-used activity- and agent- based models (Horni et al., 2016). Essentially, MATSim is composed of three modules, namely Execution, Scoring and Replanning (see Figure 3), which run for a specific number of iterations until optimized daily plans are obtained (Horni et al., 2016; Zhuge et al., 2019a; Zhuge and Shao, 2018). These optimized plans can be further used to generate time slots for each person to perform their inhome activities. In other words, the time slots available can be used as the inputs (or constraints) of the water-energy use behaviour model to be introduced in Section 2.3.

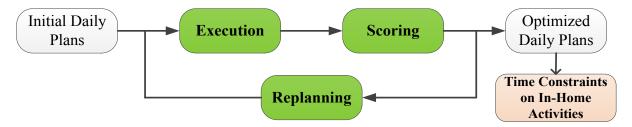


Figure 3 Framework of MATSim (Waraich, 2013; Zhuge and Shao, 2018)

2.3 Water and Related Energy (Water-Energy) Use Behaviour Model

With the constraints on the availability of appliances (obtained from the appliance ownership model) and the time slots available for in-home activities (obtained from the activity-based model, MATSim), the water-energy use behaviour model is further used to simulate how agents schedule their water-energy related activities at home throughout the whole day, considering the potential interactions between household members. According the classification by Yu et al. (2018), the simulation will be focused on three typical types of water-energy use behaviour:

- **Bathing Behaviour:** is involved in showering and foot bathing behaviours;
- Cooking Behaviour: is involved in preparing food, cooking food and washing dishes;
- Cleaning Behaviour: is involved in floor sweeping and mopping, and clothes washing;

Among the behavioural types above, bathing is a person-level behaviour, while cooking and cleaning are viewed as household-level behaviours, as they are associated with all household members. In addition, several Discrete Choice Models (DCMs) will be developed to simulate the decision-making of both person and household agents on water-energy use. Specifically, the DCMs relate individual attributes (e.g., age and household size) to different decisions on water-energy use, such as the frequency of in-home activities and the methods to perform the activities. However, Probabilistic Functions (PFs) will be used instead of DCMs in those cases where there are no statistically significant relationships between individual attributes and choices. In general, both DCMs and PFs can be developed based on empirical findings from a questionnaire survey. For example, in the test case of Beijing (see Section 3), a questionnaire survey (N=1, 000) was conducted from November 2016 to February 2017 to ask about the participants' characteristics (e.g., age) and their decisions on

water-energy use, such as the frequency of cooking (Yu, 2018). This information can be used to develop a DCM or PF which relates their attributes to decisions. This method can be applied to all the three modules below where either a DCM or PF is needed. An example of foot bathing is given in Appendix 2.6 in the Supplementary Material to illustrate how a DCM or PF can be developed based on a questionnaire survey.

Next, the bathing, cooking and cleaning modules will be introduced separately, with a focus on the decision-making process of individual and household agents. More detailed calculation methods (or equations) for water-energy consumptions are given in Appendix 2 of the Supplementary Material.

2.3.1 Bathing Module – Person Agent

The bathing module is used to simulate the bathing behaviour of each person agent in the population, involving in showering and foot bathing.

(1) Showering Module

As shown in Figure 1, the showering module is composed of the following steps (see Figure 4):

Step 1: Each person agent needs to decide whether or not take a shower and if yes, when to do it. Therefore, the decision-making will be linked to the activity-based model that provides the time slots available for showering. A DCM (or PF), which describes the relationships between individual attributes and choices about the showering frequency, will be developed here for the decision-making, based on the empirical survey. Again, either DCM or PF can be developed based on a specific questionnaire survey, as aforementioned.

Step 2: If a person agent decides to take a shower, then it will further choose a showering appliance, considering the availability of appliance, which is obtained from the appliance ownership model. Since showering appliances may differ from each other in the water and energy efficiencies, different technical parameters will be used to estimate the amounts of water and related energy consumed using the equations introduced in Appendix 2.1 of the Supplementary Material.

Step 3: Another DCM (or PF) will be developed to estimate the showering duration (t_{sho}) for each person agent, according to their attributes.

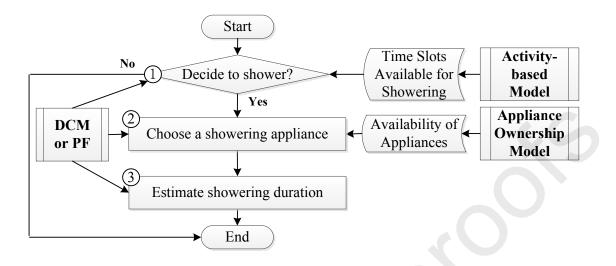


Figure 4 Framework of Showering Module

(2) Foot Bathing Module

Foot bathing is commonly viewed by Chinese people as a way to keep them heathier and thus is a particular type of water-energy consumption behaviour in China. Usually, people do foot bathing with a basin being filled with warm water (Yu et al., 2018). Similar to the showering module, the foot bathing module is composed of the following two steps:

Step 1: A person agent needs to decide whether or not to do foot bathing using a DCM (or a PF), given the time slots available. It is assumed here that an agent would not do foot bathing if it has already taken a shower.

Step 2: If yes in Step 1, then the agent will choose a way to do foot bathing, considering the availability of foot bathing appliances. There are two general ways to bath, namely bathing with a wooden or electronic basin. According to the appliance chosen, the water -energy consumptions can be estimated using the equations appended (see Appendix 2.2 in the Supplementary Material).

2.3.2 Cooking Module – Household Agent

The cooking module is used to simulate how a household agent makes a series of decisions on cooking (see Figure 5):

- **Step 1:** A household agent needs to decide whether or not to cook at breakfast, lunch and supper times, given the time constraints;
- **Step 2:** If yes in Step 1, then the household agent will further decide how many dishes to cook, according to the number of household members currently at home, connecting to the activity-based model;
- **Step 3:** The number of times that food is washed before cooking will be estimated based on a DCM (or a PF);
- **Step 4:** The household agent may choose different appliances to cook using a DCM (or a PF), based on the availability of appliances.
- **Step 5:** Household agents will choose different methods to wash dishes, again considering the availability of appliances. In this paper, there are three washing methods, namely, washing with machine, basin and tap. Agents may consume different amounts of water and related energy using different washing methods.

The equations for calculating the amounts of water and related energy consumed by cooking can be found in Appendix 2.3 of the Supplementary Material.

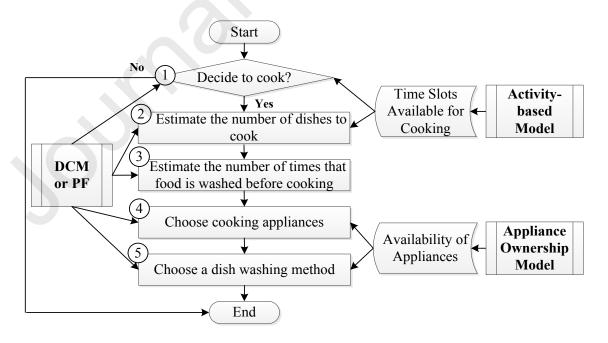


Figure 5 Flowchart of Cooking Module

2.3.3 Cleaning Module – Household Agent

The cleaning module simulates how household agents make decisions on clothes washing and floor sweeping and mopping.

(1) Clothes Washing Module

The clothes washing module is composed of the following steps (see Figure 6):

Step1: Each household agent needs to decide whether or not to wash clothes using a DCM (a PF), considering the time slots available.

Step 2: If the agent decides to wash clothes, it will further choose a washing method, considering the availability of washing machines: If it decides to wash by hand, then another DCM (or PF) will be used to estimate the rinsing times, which will be further used to estimate the water-energy consumptions with the methods introduced in Appendix 2.4 of the Supplementary Material.

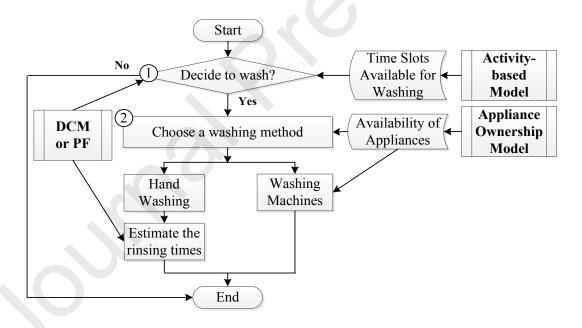


Figure 6 Flowchart of Clothes Washing Module

(2) Floor Sweeping and Mopping Module

Similar to the clothes washing module above, the floor sweeping and mopping module is also composed of two steps below:

Step 1: A household agent needs to firstly decide whether or not to sweep or mop floor using a DCM (or a PF);

Step 2: If yes in Step 1, then the household agent will further decide how to sweep or mop, according to the availability of appliances.

The equations for calculating the amounts of water and related energy consumed by floor sweeping and mopping can be found in Appendix 2.5 of the Supplementary Material.

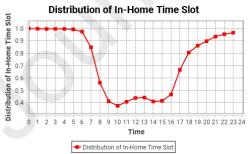
3 Test Case of Beijing, China

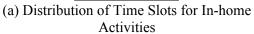
3.1 Description of Test Case

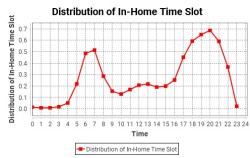
A test case of Beijing was set up here to examine the performance of the proposed integrated approach. As aforementioned, the test case essentially used two datasets, namely the 2010 Beijing Household Travel Survey data (2010 HTS data) and the data on Water-Energy use behaviour and the ownership of related appliances (2017 WE data). HTS is a typical survey in transport studies, and the survey data is generally used to analyse and model travel demand. The 2010 HTS data was collected by asking each household to fill in a questionnaire on the daily out-of-home activities and travels of their household members, which make up a daily plan (see Figure 2 for an example). In addition, the basic characteristics of the household and its members (e.g., age, income and car ownership) were also collected. The 2017 WE data was collected through a face-to-face household survey from November 2016 to February 2017 in Beijing, using both Probability Proportionate to Size sampling and stratified sampling approaches. In total, 1, 000 valid samples were collected. The questionnaire was composed of four parts: 1) water and energy related infrastructures & domestic appliances; 2) water and energy use behaviours (e.g., cooking frequency); 3) personal awareness and willingness regarding water and energy use; 4) individual and household attributes. More details on the survey can be found in the Yu (2018)'s work. One may have noticed that these two datasets were collected in different years, and could not be used straightforwardly for the model test. In response, the 2010 HTS data was firstly used to generate a 2010 virtual Beijing, which was further processed through a

calibrated and validated agent-based land use and transport model, SelfSim (Zhuge et al., 2019c), in order for a 2017 virtual Beijing to match these two datasets. SelfSim here was used to simulate the Beijing urban evolution from 2010 to 2017. Note that this data processing is only required in this specific case due to the lack of input data. The 2017 WE data was used to generate appliance ownerships for each household in the 2017 virtual city and also to calibrate the water-energy use behaviour model (e.g., DCMs and PFs, see Section 2.3). Due to the limited computer data storage (specifically, Random-Access Memory), only 4% of the whole population was used in the simulation, meaning that the simulation results needed to be scaled up accordingly by multiplying the results by 25.

In the resulting 2017 virtual Beijing, most of the agents need to perform out-of-home activities, such as work and shopping, which could generate time constraints on their in-home activities (e.g., cooking). As a result, the distribution of time slots available for different in-home activities can be obtained, as shown by Figure 7-(a). This distribution is an aggregate result considering all of the person agents in the synthetic population (which was 4% of the whole population in Beijing). In order to obtain active in-home activities for each agent, those time slots for overnight sleeping in Figure 7-(a) were excluded using a random method (as detailed in Appendix 3.1 in Supplementary Material), resulting in the distribution of active time slots for in-home activities, as shown by Figure 7-(b). More details on the 2017 virtual Beijing can be found in Appendix 3.1 of the Supplementary Material.







(b) Distribution of Active Time Slots for In-home Activities (Excluding Sleeping)

Figure 7 Distribution of Time Slots for In-home Activities

3.2 Overview of Water and Related Energy (Water-Energy) Consumptions

Table 1 shows the total water-energy consumptions in one particular day in 2017, as well as the consumption per capita per day and the consumption per capita per year. For bathing, cooking and cleaning, the annual water consumptions per capita are 16.5 m³, 7.7 m³ and 8.7 m³, respectively. These are quite similar to the findings of Yu et al. (2018), which are 16.4 m³, 7.5 m³ and 9.2 m³, respectively. The simulation considered two energy types, namely electricity and gas. The annual electricity consumptions per capita are 475.9 kWh, 108.0 kWh, and 63.3 kWh for bathing, cooking and cleaning, respectively. These are also close to the results of Yu et al. (2018), which are 442.3 kWh, 97.5 kWh and 47.1 kWh, respectively. Among the in-home activities (see Figure 8), bathing consumes most water and related energy, with annual consumptions per capita of 15.8 m³ and 613.8 kWh, respectively. It is worth nothing that the annual consumption per capita here is calculated by simply multiplying the consumption per capita per day by 365. This calculation could be improved by simulating the consumption behaviour throughout a whole year, but such a day-to-day simulation could be computationally expensive and needs more input data, for example, on water-energy use behaviour in both weekdays and weekends. More details on the water-energy consumption by appliance type can be found in Appendix 3.2 of the Supplementary Material.

Table 1 Water and Related Energy Consumptions in Beijing in 2017

		Bathing		Cooking			Cleaning	
		Bathing	Foot Bathing	Preparing Food	Cooking Food	Washing Dishes	Washing Clothes	Sweeping & Mopping
Water (m³)	Total Consumption	879249	34953	199429	82587	146404	443657	37660
	Consumption per Capita per Day	0.043	0.002	0.010	0.004	0.007	0.022	0.002
	Consumption per Capita per Year	15.84	0.63	3.59	1.49	2.64	7.99	0.68
Energy (kWh)	Total Consumption	34062739	1276046	2156269	12962238	3314661	3415684	468384
	Consumption per Capita per Day	1.68	0.06	0.11	0.64	0.16	0.17	0.02
	Consumption per Capita per Year	613.83	23.00	38.86	233.59	59.73	61.55	8.44
Electricity (kWh)	Total Consumption	25416955	990248	1611559	1826656	2557211	3043387	468384

	Consumption per Capita per Day	1.23	0.05	0.08	0.09	0.13	0.15	0.02
	Consumption per Capita per Year	458.03	17.84	29.04	32.92	46.08	54.84	8.44
	Total Consumption	866745	28651	54608	1116349	75935	37323	N/A
Gas (m³)	Consumption per Capita per Day	0.043	0.001	0.003	0.055	0.004	0.002	N/A
	Consumption per Capita per Year	15.62	0.52	0.98	20.12	1.37	0.67	N/A

Note: the Gas (m³) to Electricity (kWh) Factor was set to 9.98 in this test case.

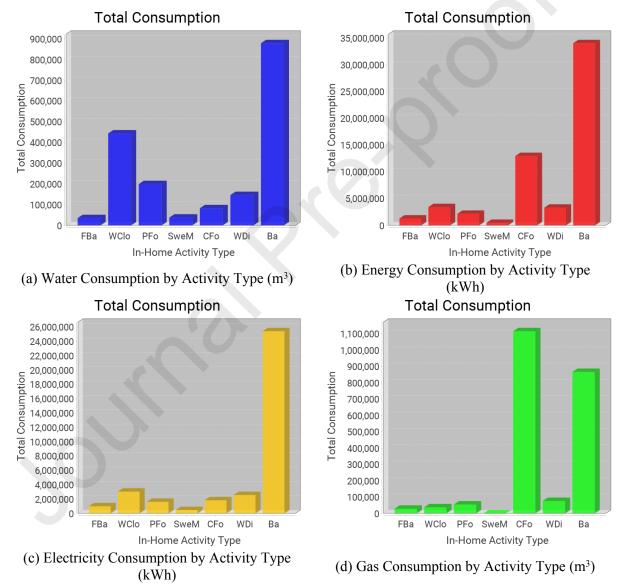


Figure 8 Total Water and Related Energy Consumptions by In-Home Activity Type in One Particular Day

Note: FBa: Foot bathing; WClo: Washing Clothes; PFo: Preparing Food; SweM:Sweeping & Mopping; CFo: Cooking Food; WDi: Washing Dishes; Ba: Bathing

3.3 Temporal Distribution of Water and Related Energy (Water-Energy)

Consumptions

Figure 9 shows the temporal distributions of water-energy consumptions by hour, which are obtained by aggregating the consumptions of around 810, 000 individuals within in around 34, 000 node-based residential facilities (note that a scaling factor was set to 4%, which means one element (e.g., facility) in the simulation represents twenty-five elements in reality). The figure suggests that most of the water and related energy are consumed in the evening. Specifically, there are two significant peak periods in the evening: one is from 5 to 7 PM and the other is from 8 to 11 PM. These two peaks are likely attributed to cooking and bathing, respectively. Another peak occurs in the morning at 6 AM, and this is likely because of cooking for breakfast. In addition, the four temporal distributions in Figure 9 are quite similar, especially in terms of peak hours, suggesting that water consumption may be correlated with energy consumption. In order to quantify this possible correlation, the Pearson correlation coefficient (Benesty et al., 2009), which is a typical measure of the linear correlation between two factors, is used here to explore the relationships between water and energy (waterenergy), water and electricity (water-electricity), and water and gas (water-gas) consumptions. Their Pearson correlation coefficients are 0.89, 0.58 and 0.27, respectively, suggesting that water consumption is highly correlated with energy consumption, especially with electricity consumption, but is weakly correlated with gas consumption. Further, the temporal distribution of the Pearson correlation coefficients is plotted by hour for each of the three correlations, as shown in Figure 10, suggesting that 1) the water-energy and water-electricity have similar trends: specifically, their coefficients tend to level off during the period from 4 AM to 7PM, but start rising after 7 PM. The rise is likely attributed to the activity of bathing, which needs hot water and thus consumes both water and electricity. Note that electricity (around 2.6×10⁷ kWh) is significantly more used for bathing than gas (around 8.5×10⁵ kWh), as shown by Figure 8-(b) and -(c), and thus the Pearson correlation coefficient for water-gas goes down after 7 PM; 2) the coefficient for the water-gas correlation varies throughout the whole day, as probably gas is not the main energy resource for water heating and is only used at times; However, the coefficients at noon tend to be a bit higher, which is likely attributed to cooking

for lunch, as gas is found as the main energy resource for the activity of cooking by comparing Figure 8-(c) and -(d).

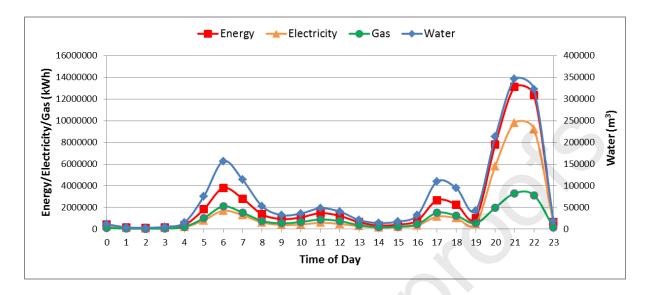


Figure 9 Temporal Distributions of Total Water and Related Energy Consumptions in One Particular

Day

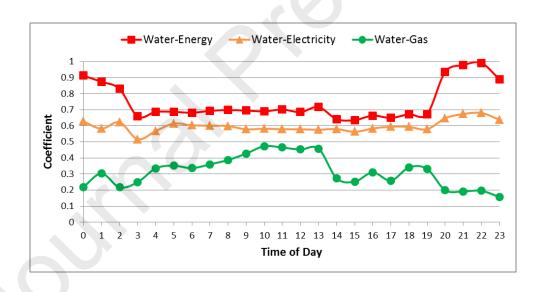


Figure 10 Temporal Distribution of the Pearson Correlation Coefficients

3.4 Spatial Distributions of Water and Related Energy (Water-Energy)

Consumptions

Figure 11 -(a) and Figure 12 -(a) show the spatial distributions of water and related energy consumptions at the facility level, respectively. Note that each dot in the maps represents a residential building where household agents live and perform their in-home activities. The maps suggest that the

residential facilities located in the central districts and central areas of the outer districts tend to have higher water-energy demand (this can also be found at the district level, see Appendices 3.3.1 and 3.3.2 in the Supplementary Material). Here, water-energy consumptions in the maps were grouped with a K-means clustering algorithm (Hartigan and Wong, 1979). In order to further explore how the water and related energy consumptions vary throughout the whole day, Standard Deviation (SD) was used to quantify the variance. Specifically, the individual consumption (either water or energy consumption) was firstly aggregated by hour at the facility level, and the variance of the consumption was further computed with the measure of SD and then mapped, as shown by Figure 11 -(b) and Figure 12 -(b). By comparing the spatial distributions of the consumption and its variance (or SD), it can be found that those residential facilities with higher water-energy demand also tend to have higher variances, meaning that the water-energy consumptions of people living in these facilities vary more significantly throughout the day.

The facility-level results can be further aggregated at the district level, providing spatial information on water-energy consumptions at the macro level. More details on the spatial distributions of water-energy consumptions and consumption per capita at the district level can be found in Appendix 3.3 of the Supplementary Material.

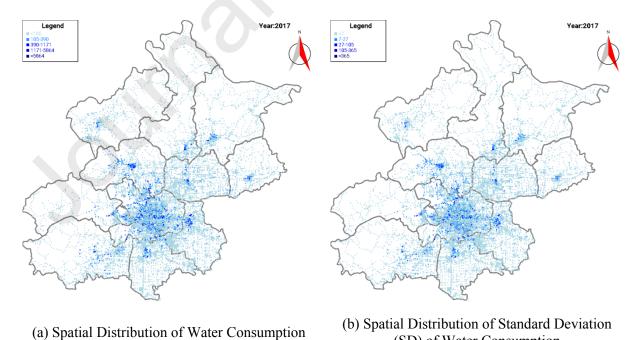


Figure 11 Spatial Distributions of Water Consumption

(SD) of Water Consumption

Figure 11 Spatial Distributions of Water Consumed at the Facility Level in One Particular Day (m³)

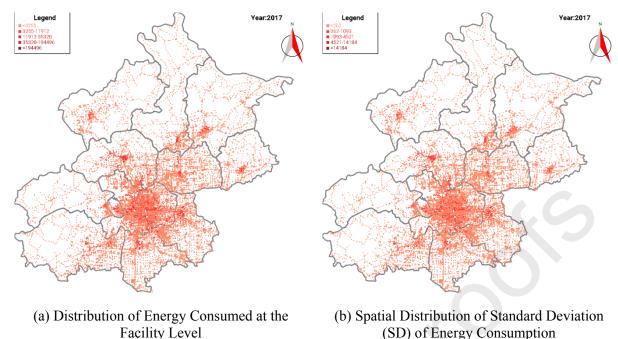
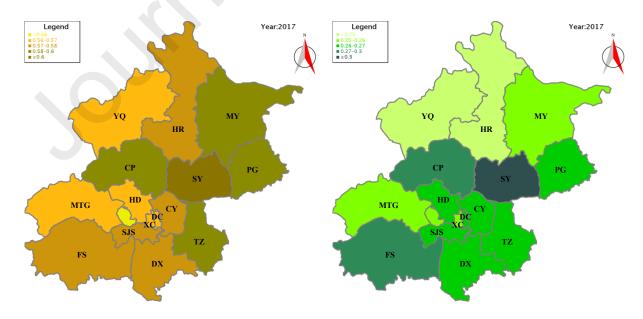


Figure 12 Spatial Distributions of Related Energy Consumed in One Particular Day (kWh)

Figure 13 shows the spatial distributions of (a) water-electricity and (b) water-gas correlations, again using the indicator of Pearson correlation coefficient, suggesting that both of them vary across space at the district level, and have different spatial patterns. For water-electricity, the outer districts (except Yanqing (YQ) and Mentougou (MTG)) tend to have higher correlations than the central districts. In terms of water-gas, the outer districts in the north part of Beijing tend to have smaller correlations and the correlation in the southeast part tends to be at the middle level. Such spatial characterises could be useful for water-energy related infrastructure planning and investment.



(a) Water-Electricity

(b) Water-Gas

Figure 13 Spatial Distributions of Pearson Correlation Coefficients

Note: Mentougou (MTG), Tongzhou (TZ), Shunyi (SY), Huairou (HR), Xicheng (XC), Miyun (MY), Changping (CP), Fangshan (FS), Fengtai (FT), Daxing (DX), Chaoyang (CY), Pinggu (PG), Yanqing (YQ), Haidian (HD), Shijingshan (SJS) and Dongcheng (DC)

3.5 Applying Model Results into Policy Making and Infrastructure Planning

As aforementioned, the spatially and temporally disaggregate water-energy demand obtained from the micro-simulation would be particularly useful for policy-making and infrastructure planning.

Based on the findings from the test case, two specific examples are given as follows:

First, the temporal distributions suggested that there were three peaks in a day: one was in the morning and the other two were in the evening. Among these three peaks, the one occurring from 8 to 11PM tended to be much higher, and was largely attributed to bathing. Since bathing tends to be a more flexible activity, some strategies, such as time-of-use tariffs, could be used to shift the water-energy demand in that peak period. Compared to other in-home activities, bathing also consumes most water and related energy, with annual consumptions per capita of 15.8 m3 and 613.8 kWh, respectively. Therefore, promoting the purchase and use of water-efficient bathing appliances would significantly reduce both water and energy consumptions.

Second, the spatial distributions suggested that those residential buildings in the central districts and central areas of the outer districts tended to have higher water-energy demand, and the water-energy consumptions in these buildings also vary heavier throughout the day. On the supply side, the spatial distributions could help optimize the layout of existing water- and energy-related infrastructures, and could also advise local authorities on infrastructure investment; on the demand side, policies, such as time-of-use tariffs, could also be used here to shift the water-energy demand in those areas with both higher demand and more variances in demand. As a result, the variances would decrease, and the higher demand could be distributed more equally in a day. This could further benefit the existing water- and energy-related infrastructures.

The examples above just present two general ways to apply the model results. However, within a real-world scenario, the model results could not be straightforwardly used for policy making or

infrastructure planning. Instead, the integrated model should be coupled with a policy optimization model or infrastructure optimization model. The results from the integrated model can be used as inputs of the two optimization models which search for optimal solutions. It is worth noting that the extent to which the model results could be useful for policy making and infrastructure planning largely depends on model reliability. The reliability of a model could be influenced by many factors, such as the quality and sufficiency of input data, and model calibration and validation. In this test case, the model was initialised by primarily using two datasets, namely 2010 HTS data and 2017 WE data (see Section 3.1). An additional dataset on scheduling in-home activities would be useful for improving the model reliability in terms of temporal distribution of water-energy consumption.

Although the model appears to work very well at the aggregate level (see Section 3.2), the disaggregate-level results remain to be further validated. Therefore, policy makers and urban planners should bear model reliability in mind when shaping policies and investing in infrastructures based on the findings from the test case.

4 Conclusions

This paper developed an agent-based integrated approach, which was composed of a virtual city creator, an appliance ownership model, an extended activity-based travel demand model and a water and related energy (water-energy) use behaviour model, to simulate how person and household agents consume water and related energy with various appliances, considering three typical types of water-energy use behaviour (namely bathing, cooking and cleaning behaviours), resulting in spatially and temporally disaggregate water-energy demand. In particular, the appliance ownership model and activity-based travel demand model were used to generate appliance and time constraints on performing in-home activities, in order to be behaviourally realistic. The model was tested in Beijing, China, obtaining spatial and temporal distributions of water-energy demand. Some key findings are summarised as follows: 1) bathing consumes most water and related energy than the other in-home activities (e.g., cleaning and cooking); 2) most of the water and related energy are consumed in the evening within two peak periods (5-7 PM and 8-11PM); 3) water consumption is highly correlated

with electricity consumption, but is weakly correlated with gas consumption; 4) the residential facilities located in the central districts and central areas of the outer districts tend to have higher water-energy demand, and the water-energy consumptions of people living in these facilities also vary more significantly throughout the day. Furthermore, ways to apply the model results to policy making and infrastructure planning are discussed.

This study has been limited in some aspects which remain to be further explored in the future work: 1) the empirical findings about scheduling in-home activities: it remains unknown how individuals allocate their in-home time slots among different in-home activities, considering the interactions between household members. Some assumptions have been made in the current version of the model to simplify the allocation behaviour. For example, the activity of cooking can be randomly allocated to any household member aged 18 or above. These sorts of assumptions should be removed when the empirical findings become available. On the other hand, such assumptions indicate what kind of timeuse data needs to be collected in the future work in order to improve the model; 2) currently, the outof-home activities were only used to generate time constraints on in-home activities. The integrated approach can be further extended by additionally considering the water-energy use behaviour associated with out-of-home activities, for example, in commercial and office buildings, so as to capture the interaction between in-home and out-of-home activities in terms of water-energy consumptions; 3) Model uncertainty analysis. The model performance had been examined within a test case of Beijing. However, for such an integrated model with several components included, a systematic uncertainty analysis is needed: first, it would be useful to conduct parameter sensitivity analysis, so as to better understand how the model works and also to identify those important model parameters; In addition, it would be necessary to explore model structure, model assumptions and simplifications and future events within various "what-if" scenarios, so as to provide insights into model uncertainties.

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Highlights

- An agent-based spatiotemporal approach to simulating water-energy consumption
- The influence of out-of-home activities on in-home activities is considered
- The 24-hour distributions of water and related energy consumptions are similar
- The water-energy correlation varies across space

Declaration of Competing Interest

The authors declare no conflicts of interest