Investigating the role of adherence and flow rates on the effectiveness of ceramic water filter interventions using an agent-based model

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Kyle M. Monahan

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Advisor: Dr. Mark Woodin

ABSTRACT

Globally, 1.8 billion people use contaminated water, leading to childhood diarrhea. Ceramic water filters can reduce diarrhea when used consistently and correctly, although adherence can decline over time. These declines have previously been investigated using agent-based models (ABMs) in Limpopo, South Africa. In this thesis, the previous ABM was re-built with minimal field data, and adherence and flow rate preference were incorporated as variables of interest. Additionally, a linear regression model was developed as a traditional comparison. Normalized water contamination matched the previous ABM within 200 days. Altering adherence produced statistically significant ($p<0.0001$) but non-field-relevant declines in diarrhea, while changing flow rate preference produced larger declines ($p<0.0001$). The linear regression model had $R^2 = 0.535$, but contained bias in residuals. I found adherence was less influential than other studies suggest. Nonetheless, ABMs can reproduce water contamination accurately without full access to original data, thus deserving consideration alongside traditional modeling techniques.

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INTRODUCTION

Goal 6 of the United Nation's Sustainable Development Goals (SDG) is to "ensure availability and sustainable management of water and sanitation for all" by 2030.[1] This goal has not yet been reached, as globally an estimated 1.8 billion people use sources of water with fecal contamination.[2] This contamination contributes to 8.5% of child deaths from diarrhea, which is the second leading killer of children under five.[3,4] Household water treatment and safe storage (HWTS) technologies are low-cost interventions which can improve household-level drinking water quality. Further, these interventions can reduce the burden of diarrheal disease until populations can be provided with other infrastructure capable of delivering water free of fecal contamination.[5]

Household water treatment technologies

Current HWTS technologies include a myriad of designs in various settings. Globally, the five most common HWTS options are chlorination, solar disinfection, filtration (biosand filters and ceramic water filters, CWFs), combined filtration and chlorination, and combined flocculation and chlorination.[6] Promotion of HWTS technologies as a targeted intervention strategy has occurred over the past two decades.[7] These technologies have been evaluated with randomized controlled trials, some of which have shown a protective effect against diarrhea as summarized in systematic reviews.[8–10] There have been concerns about exaggerated estimates of effect from observer bias due in part to implementing organizations concurrently administering surveys[5,10,11] and the limited duration of HWTS interventions in the field.[12] These technologies are nonetheless supported by international organizations such as the World Health Organization (WHO) as an interim solution to preventing diarrheal disease.[13,14]

Ceramic water filters (CWFs)

One of the most promising HWTS technologies is the CWF as they are simple and durable items.[15] Filters were first designed and implemented in the 1980's and further developed by Potters for Peace in the late 1990s.[16] As of 2012, filters were manufactured and distributed locally in approximately 50 factories around the world with an estimated 700,000 in use.[17]

Filters consist of a silver-coated ceramic 'pot' filter element suspended in a storage container fitted with a tap for dispensing treated water.[16] A mixture of locally-sourced clay and a burn-out material, such as sawdust or rice husk, is pressed into the filter frustum (pot) shape, allowed to dry, and then fired to approximately 800-900°C. The clay to burn-out material ratio is determined contextually by testing prototype filters for flow rate and microbiological efficacy under local conditions. The antimicrobial properties of silver are well known and used in water treatment.[18,19] Thus, silver is added as a bactericide and it is either applied to fired filters or added to the filter mixture.[16] After production, each filter's flow rate is measured; filters that meet the factory-established acceptable flow rate are packaged for sale or distribution. Filter flow rates are factories' most common quality control criterion.

Efficacy of CWFs

Reductions in diarrheal disease were reported among users of CWFs in field settings,[15,20–22] and CWFs were the only HWTS technology with significant disease reduction over a one year period.[12] Locally produced CWFs were shown to be three to six times more cost-effective, as measured in Disability Adjusted Life Years (DALY), with filters at $47/DALY and centralized piped systems at $141/DALY averted.[23]

Use rates and declines in filter use

Consistent and correct CWF use has yielded promising results within selected study populations; however, usage declines over longer follow-up periods[20] which can impact effectiveness.[12] The use rates of CWFs have been shown to decline by two percent per month after implementation over four years of follow-up in rural Cambodia.[24] This rate of decline has been shown to be up to 13% per month in other HWTS interventions.[25] A summary of these interventions is shown in Table 1.

Both the metric for measuring CWF use and the context of the intervention are important for understanding variability in the rate of decline of use. Determining the use rate of a household water treatment technology in the field can be achieved in many ways. For example, self-reported use can be measured by a written survey or verbal questionnaire. Confirmed use provides data that has been observed and compiled by a researcher, commonly collected simultaneously with self-reported use. Finally, effective use is the percent of targeted households that use microbiologically contaminated water sources which also use the filter to improve water quality to achieve international health standards.[26,27] Self-reported use can sometimes report inflated values due to the previously mentioned observer bias[28] (as shown in Table 1), so confirmed use and effective use are the preferred metrics.[26]

Beyond the anticipated variation in estimated usage rates derived from the different methods for assessment of use, usage is also influenced by the context of interventions. Intervention locations differ according to gender roles, socio-economic status, and household structures.[29] This suggests that understanding both the contextual factors and the methods for assessing usage are important in determining the overall effectiveness of interventions.[30–32]

Table 1 *Measures of adherence from selected CWF field implementations.*

Measure of filter use	**Follow up time**	**Use rate**	**Location**	**Type of use**	**Rate of decline**	**Source**
	Months	*%*	*Country*	*Measurement*	*% per month*	
Survey	0.8	100	Ghana	Self-reported use	-	33
Survey	1	75	India	Self-reported use	-	34
Observation	4	46	Ghana	Confirmed use	-	35
Survey & Observation	6	21	Bangladesh	Confirmed use	13	25
Survey & Observation	9	67	Bolivia	Confirmed use	4	36
Survey & Observation	24	76	Sri Lanka	Confirmed use	-	37
Survey & Observation	42	31	Cambodia	Effective use	2	24

Factors in filter use decline

To achieve the goal of effective use, there is a chain of events by which individuals must consistently be able to purchase the filter, maintain the filter, treat water at an acceptable flow rate, and safely dispense filtered water. Technological, behavioral (psychosocial), and contextual factors can disrupt this chain.[8,38–43] These factors have been synthesized as an Integrated Behavioral Model for Water, Sanitation and Hygiene (IBM-WASH).[29] The IBM-WASH approach attempts to capture the complex nature of interventions in WASH (Water, Sanitation and Hygiene). A systematic review focusing on sustained adoption of WASH technologies has evaluated the IBM-WASH framework.[44] In this review, the limitations of CWFs highlighted technological factors including declining flow rates, risk of breakage, and availability of replacement parts taken together with skilled local technicians to provide repair, as well as behavioral factors such as perceived susceptibility to water-borne disease and filter effectiveness, and contextual factors including seasonality and household income.[44]

As an example, perceived filter flow rate is one of the behavioral factors which influences acceptability of CWF and thus intervention effectiveness.[15] The flow rate of a filter also acts as a technological factor of intervention success. The flow rate of a CWF slowly degrades as the filter surface and internal pore structure are blocked by materials in the water.[45] A filter must provide enough volume of water for household uses at a reasonable rate. If the flow rate is too low, or perceived as too low, an individual may not find the filter practically or socially acceptable continue to use.[21]

The IBM-WASH model suggests that there is a link between the chain of household-level steps for effective filter use and the sustainability of CWFs. The response to a given intervention may be different for each individual within a household. Such differences require an individual-level assessment of filter users. Nevertheless, the relative importance and impact of these individual factors remain unclear. To investigate the comparative importance of these factors in the field, models can be used to simulate CWF interventions among individuals. These individual-level differences can be assessed using agent-based models.

Agent-based models

Agent-based models (ABMs) are a type of model that combine elements of both analytic and computational models. Analytic models often use formal structures and relations to represent a physical or social phenomenon and they can allow for prediction and formulation of generalized outcomes. Computational models use computers to simulate formal structures. This provides a more rapid output of the model than would be possible by hand calculation of the (commonly mathematical) relations.[46]

Agent-based models, sometimes referred to as individual-based models, are a type of computational model containing the formal structure of entities (agents) that are individually represented so that (local) behaviors, agency and interactions can be assessed.[46] Agency can be defined as the ability of an individual to take goal-directed and autonomous actions.[47] Representations of agents can be processed on specialized software platforms such as Netlogo, AnyLogic, Swarm, Mason, and Repast.[48] These models are especially useful for complex systems (also called complex adaptive systems). Commonly, complex adaptive systems are not fully explained through the modeling of individual elements without including agency and interaction.[49] Interaction between agents often go beyond traditional statistical interaction in that they may contain complex feedback loops among both the individual variable(s) and the outcome.[50] These unique benefits of the ABM structure has led to their development and use in many fields.

The history of ABMs spans more than four decades with applications in ecology, social science, economics, and more recently epidemiology. The first work on ABMs included work by Thomas Schelling on community segregation[51] and Robert Axelrod on the Prisoner's Dilemma, in the 1970s. The first known application of ABM to a biological problem was by Craig Reynolds in 1987 with a simulation of bird flocking patterns.[52] In the 1990s many programming languages were developed for agent-based simulations, the Journal of Artificial Societies and Social Simulation was first released, and many applications of ABMs were pursued.[53] Models adapting cognitive characteristics into agent-based social simulations were developed in the mid-2000's[54,55] with further implementation of ABMs into systems pharmacology and health sciences as recently as 2015.[56] Most recently, ABMs have been used as a tool to better understand the transmission of Zika virus in agents with variable *Aedes Aegypti* (vector) control[57] and the individual transmission probability of Ebola virus in Liberia.[58]

The recent use of ABMs in epidemiological studies may help isolate the influence of variables in a network of causes, which may better address the complex, interrelated processes which are resistant to interventions focused on one or two causal effects.[59,60] Researchers in social epidemiology have been moving towards social network analyses and agent-based models within the last decade.[61] Within this time, ABMs have also been designed and built to assess water treatment technologies.

Designing, building and running an ABM

ABMs have also been used to simulate behavior regarding water treatment decision-making.[62] Researchers have used ABMs to investigate water usage in Dutch and US households,[63] and to arrive at HWTS predictors of early childhood diarrhea (ECD) incidence within a community.[62] Some researchers have found the complex interactions in water and sanitation systems are better studied with a systems approach. Since agents contain both internal (e.g. elevated risk for a disease, perception of risk of transmission) and external factors (e.g. transmission of disease, diffusion of information, climate) both must be accounted for to model the system as a whole. This allows investigators to predict outcomes within a population and social environment, given different intervention characteristics. ABMs are well-suited to adopt a systems approach at the individual-level as they can look at multiple HWTS interventions within a community and determine the influence of technological, behavioral and psychosocial factors.[64,65] Therefore, ABMs can complement established randomized controlled trials of HWTS, which commonly look at only one intervention and impact, by looking at multiple possible interventions. Like the IBM-WASH model, ABMs can capture the complex nature of field interventions and interactions between factors predicting success. ABMs can also produce policy-relevant testbeds for alternative interventions.[61] Along with these benefits, the process of designing and using an ABM to investigate health outcomes brings with it important challenges.

Care must be taken when designing, running, and interpreting ABMs. To design an ABM, the individual behaviors of each agent and the interactions with other agents and the environment must be well-defined and justified.[50] As with any model, these must be based on the research question and knowledge of the context within which the agents exist. Design of an ABM model consists of developing a conceptual framework of the agents that describes the relationship of these agents to the broader environment. This conceptual framework can include methods for comparing the interactions of agents and the outputs of the model. This is important, as the conceptual framework of the model directly influences the scope of the model to be built.

Model building consists of translating the conceptual framework of agents and their interactions into computer code which a program can use to create a simulation. This can be done in a "top-down" way, where the conceptual framework and research question are translated directly into computer code, or in a "bottom-up" way, where the research question and computer code are allowed to influence and interact with each other.[50] Most ABMs use the latter process.

Several decisions must be made prior to running ABMs. Decisions such as the number of iterations, the value of parameters to alter, and the amount of time to run the model are elements that must be specified *a priori*. With many iterations, there is a risk of producing statistically significant results that have no practical significance.[66] This suggests the number of iterations should be only as high as required to minimize stochastic variation. The volume of data produced by these iterations within any altered parameters can be called the model "space."

Exploration of the model space is an important part of evaluating the model outcome variability. Specifically, it is important to assess variance within iterations of model runs and the varied parameters. This can be completed through manual methods that consist of using trial-and-error to find the dominant parameter values and sensitivities within the model. A sensitivity analysis can also be completed though query-based model exploration, in which dominant parameters are discovered using specific algorithms.[66] Comparing altered parameter values to a "baseline" model state is another technique used.[50] Commonly, the replication of ABMs is necessary,[67] though few replications of ABMs have been reported.[68] Regardless of the strategy used to identify the dominant parameters, once the dominant parameters are identified, they can be used as "levers" in the real world to shift the system towards a new behavior state.[53] This differs from traditional models in that the results from ABMs are less interpretable for specific agents but more amendable to wide-scale policy implications, making them useful in evaluating water and sanitation interventions. ABMs can look at the individual factors which lead to a change in the overall water use behaviors in an intervention.

CWF interventions and ABMs

Agent-based models are especially appropriate for investigating the importance of factors such as long-term adherence to CWF interventions. This is important as experimental field studies have limited follow-up times due to resource constraints.[5] Using ABMs as a modeling framework also accounts for high heterogeneity within the characteristics of filter users, which has been reported as an issue in HWTS interventions and a source of uncertainty in field results.[5] Heterogeneity in the acceptability of filter attributes and adherence to filter use have been reported.[64] This heterogeneity is accounted for within an ABM since the aggregate outcome is a function of the behaviors of autonomous individuals, shaped within variable rules with stochastic modifiers.

Health interventions to reduce diarrheal disease such as CWFs are complex systems, which display characteristics of emergence in that processes which are observed at the system level not encoded for or measured at the individual level.[50] A well-built ABM would allow researchers to understand the myriad impacts that could be present in a HWTS intervention.[69] For example, the ABM structure is flexible enough to allow for feedback, adaption, and emergent behavior. These characteristics are hard or impossible to replicate using other statistical methods.[70] Furthermore, ABMs can be calibrated with relevant survey data to investigate the sustainability of a specific intervention context.[70,71] This allows for the ABMs to be especially well-suited in dealing with the complexity in CWF interventions, along with other model designs.

Comparing ABMs to other model types

A comparison of traditional statistical models to ABMs is provided in Table 2. Comparing the output of ABMs to other types of models is not straightforward.[46,66,72] A recent paper in the Journal of Land Use Science has suggested it is important to use ABMs alongside other statistical models, such as specifically linking to regression methods.[73] A comparison of these models is also important, as ABMs can model behaviors that vary among individuals and over time, but linear regression may be a simpler option if the effect of these behaviors on the overall system outcome is negligible. Agent-based models also do not require independent samples, and may be useful for outcomes such as diarrhea where the likelihood of having the outcome one day can be predictive of having the outcome the next.[59] A comparison between these two models could be facilitated by joint output analysis through box plots.[66]

***Table 2** A comparison of statistical models relevant to CWF interventions and model characteristics.*

Type of model	Model Name	Iterations required?	Outcomes modeled	Outcome as individual response or mean response	Source
Traditional statistical models	Linear regression	No	Continuous	Mean	74
	Logistic regression	No	Categorical	Mean	74
	Mixed linear model	No	Continuous	Individual/Mean	74
Agent-based models	Intervention ABMs	Yes	Continuous/Categorical	Individual/Mean	50

Limitations of ABMs

Although ABMs are well-suited to some research applications, this modeling technique has limitations. The issues stem from the fact that small changes within agents drive large-scale systematic outputs or results. This leads to issues with verification, calibration, process uncertainty, stochasticity, interpretation and validation.[70,75]

In order to verify an ABM, the mechanism, process, and output must be compared for consistency with the research question. First, the output must be cross-checked with realistic estimates for accuracy, including both external and internal validation. For example, a report on an ABM of tobacco use stated that the model was verified using social network data on smoking cessation outcomes as a source of external validation.[69] However, these verifications may be biased if the sample selected in the network is not representative of the broader population. These results are complemented by a process of internal validation where the internal processes and outputs are compared to expected values. The internal validation process is especially complex due to the common occurrence of emergent phenomena which can change the results.[70] This can be overcome by meticulous cross-checking of model processes in isolation to be sure all components work as expected; however, it is unexpected that testing each element in isolation would produce coherent results due to the emergent properties of the system. Thus, both testing of internal elements along with cross-checking output with realistic estimates must occur.

After verifying the external and internal consistency of the code and model design, there is still a need for calibration. This consists of "tuning" the parameters in the model to fit the actual system being modeled. If data have been collected on the parameters of interest, then quantitative calibration can occur; otherwise, a qualitative estimate can be used.[70] This calibration can be a source of error and a limitation if data are not available.

Even after calibrating the model, there is still uncertainty implicit in the ABM modeling process. The main outputs of the model are a function of the evolution of the system as a whole, and commonly includes random variables. This structure is meant to simulate the portion of agent heterogeneity which is due to random variations of unmeasured variables. To overcome random influences many model iterations are needed. Another limitation of working with ABMs is that the outputs are hard to summarize, as they are dependent on the number of iterations used. Additionally, the number of iterations must be enough to detect a change in the outcome if it exists, but not so many that commonly employed statistical tests lose practical significance.[66] Models often include reproducible randomness, through the use of random number generators to change a process value by a small (seed) amount during multiple model runs.[50] Multiple iterations produce the data from which relevant trends must be extracted.[66]

Finally, interpretation and theoretical validation of the extracted model results requires careful thought, similar to all theoretical models. The ABM output can be compared to empirical data (other than those used as input data e.g. similar comparison populations), qualitative patterns drawn from the literature, an examination of the applicability of the assumptions which underlie the model itself, or an evaluation of the theories behind the assumptions in the model.[70] Standard protocols for describing, testing and presenting ABMs have been suggested in the literature[76,77] and these may help formalize the process of understanding the ABM output.

In cases where agents are not heterogeneous and the individual behaviors are less influential, other statistical models or systems dynamics tools may be simpler and more appropriate to use. For example, the United States Food and Drug Administration has used both simple linear regression models and complex ABM techniques to model the likelihood of smoking given certain policy decisions.[69] They found that the more parsimonious linear regression model adequately predicted the outcome and this suggests that, in some cases, a technique such as linear regression may be able to capture much of the variability in the outcome of interest, without unnecessary complexity. Nonetheless, ABMs may prove to be an important tool for assessing the sustainability of an environmental health intervention when accounting for complex interactions is required, such as found in evaluating CWF interventions.

ABM for CWF intervention in South Africa

Despite the potential utility of ABMs to evaluate CWF interventions, there is only one known ABM that has been developed for this context. It was used to model a CWF intervention in Limpopo, South Africa.[64] The province of Limpopo consists of two communities (Tshapasha and Tshibvumo), with 90% of their population living in impoverished rural areas[78] and diarrhea being the second leading cause of death among resident children.[79] The model structure included two agents: households and children. Households owned characteristics that affected the microbiological quality of water consumed by children within the household. One child was randomly allocated to each household at the start of each model run. Households were selected as agents, although caregivers were the actual water treating entities. The model simulated each day or "tick" (the smallest unit of time within the model) where each household could collect water from one of three sources present in the community. Each household had a preferred primary and secondary water sources as well as the number of days they could wait if their source was not functional. Water source functionality was drawn from survey data (% of time functional). During this waiting time, stored water could be subject to contamination from hands, biofilm layer growth, and water transfer implements (e.g. a cup or ladle). Next, households could treat this water using a CWF if: 1) they had one, 2) they chose to treat their water (adherence), and 3) the filter had not yet broken. At the one-year mark, all households clean their filters, if they have one. A summary of the steps is available in Figure 1. This series of events resulted in an overall water quality (water contamination, WC) value for each household in the model, which carried over to other days and predicted diarrheal rates.[64] The model was run for two years, and thus all model children were under two years of age. This model sought to understand the role of microbiological removal effectiveness, adherence, and filter prevalence on ECD.

Although this model considered many factors influencing CWF effectiveness, some key additions can be made. For example, rather than calculating adherence as the percentage of days using the filter (if present) for all households in the study, varying levels of adherence (always, partial, never adhere) can be used within households to describe individual likelihoods to filter. This incomplete adherence within a household water source has been shown to influence field CWF intervention effectiveness.[80] Additionally, flow rate estimates were not included in the model, although flow rates have been recorded for CWF interventions in Limpopo,[81] and low flow rate has been reported as a reason for CWF disuse.[24] The previous ABM was re-derived from source code ("re-built") to address these key additions.

The goal of this thesis is to address these gaps through the further development of theoretical models. The importance of individual factors such as filter cleaning, flow rate preference, and correct and consistent use (adherence) on the potential long-term effectiveness of CWFs will be assessed using ABMs. Here the ABM will include decision-making "agents" defined as individuals with some autonomy, that operate under behavioral rules in a dynamic environment.[82]

Aims of this study

The overall aim of this study is to evaluate the utility of models in explaining the effectiveness of CWF interventions and to select the most valid model for future field applications. In order to do this, I will:

1. Re-build an established ABM in predicting ECD for a CWF intervention, and compare to previous results.
    a. Build on the previously published ABM to incorporate additional measures of adherence and filter flow rate in four separate experiments.
2. Compare the results of the modified ABM to the results of a simple linear regression model in predicting the number of cases of ECD in a CWF intervention to determine the most valid model.

1 SETUP

- Create **Households** (n = 410)
- Attribute **initial values** to some households (n = 49).
- Create **Children** (n = 410)

2 WATER CONTAMINATION (WC)

- Collect water from **primary source**?
    - Community piped (CP)
    - Surface water (SW)
    - Municipal Tap (MT)
- Source **operational**?
- If **not**, can household wait? If no, use **secondary source**.
- **Calculate** contamination from source to house, regrowth, and cleaning
- **Final** WC

3 CERAMIC WATER FILTER

- Use Final WC from (2)
- Household **has** filter?
    - **Clean** filter today?
    - Do filters **break today?**
        - Can **purchase** new filter?
    - **Is filter flow rate acceptable? Will household adhere?**
    - Is water quality greater than the **threshold** of detection?
- **Use CWF today** if possible.
- **Final** WC

4 ECD CALCULATION

- Use Final WC from (3)
- **Used** CWF today?
- **Boiled** water today?
- Calculate **ECD probabilities** based on CFU / 100 mL water
    - Increase likelihood if **age < 1 year**
- Is child **drinking** water?
- Is child **vaccinated**?
- Is household **washing hands**?
- Calculate final **ECD** probability

KEY VARIABLES: Ticks (time), daily water contamination, primary water source, secondary water source, today's water source, hand-washing contamination, storage container type, days households keep water, boiling frequency, filter cleaning frequency, adherence, flow rate preference, and WTP.

Figure 1 *A simplified flow chart of the ABM, with additional model modifications highlighted in red. A list of key variables is provided. Further information on variables and model steps is provided in the Appendix.*

METHODS

There were three major components of this thesis. First, an ABM which had already been developed and validated in the field was re-built without personally identifiable data from potential filter users. Next, alterations to the ABM structure in adherence to filter use and perception of filter flow rate were performed. Finally, a linear regression model was developed, and the predicted diarrhea rates were compared to the results of the ABM to determine the most valid model.

1. **CWF Agent-based model Investigation**

Model Building

The agent-based model was built using previously published source code.[64] Computer code was extracted from the published source code as a Portable Document Format (.pdf) file using Optical Text Recognition in Microsoft Word (Redmond, VA) and exported in text (.txt) file format.

The resulting text was manually entered into the ABM computer program NetLogo (Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL), which has been used previously to model complex systems.[48,83] Next, model structural validity was confirmed through visual inspection of code, NetLogo complier check, assessment of reasonable values (e.g. positive integers for ECD) and matching of model water contamination and mean cumulative ECD cases to previously published values.

In order to adapt the previously developed model without using personally-identifiable information from study households, an estimation of missing data was needed. This data was not available due to both time constraints and limited access to original, personally-identifiable data. It was assumed that mean values reported for households in previous studies could be adapted using a frequency distribution of random normal or random exponential values around each mean.[50] Additional data required for running the model including the frequency of household source water use, type of household source water use, and frequency of household water treatment were collected by personal communication with the original model author. Randomness is made reproducible using a consistent random-seed value, which draws the randomness from a similar random distribution for each model run. The assumptions for each unknown variable are outlined below.

Water source usage

The individual water source usage frequencies (the types of water source each house uses) for each household were collected from field data and were unavailable at the time of this writing.[64] The frequency of water source use was estimated from a previous study of bacterial regrowth in containers based in Limpopo which showed that 57% of participants received water from the community pipes, 25% received water from the municipal tap, and 17% received water from surface water.[84] It was previously reported that the community piped system in Tshibvomo provides untreated river water to the pipes. The hoses also used the same untreated water as pipes.[64] Thus, it was assumed that 10% of the households using pipes actually use hose water.

Household locations

The global positioning system (GPS) coordinates of each household were originally collected during the 2009 census of Limpopo[84] and were used in the resulting ABMs to define the relative locations of agent households.[62,64] As these data were not available from the original study, the relative GPS coordinates were extracted from a screenshot of the household locations in Figure S3 of the Supporting Information of the original ABM paper[85] using the geo-referencing procedure in qGIS.[86] This provides the same relative position of households, without individually-identifiable GPS coordinates. These are shown in Figure 2.

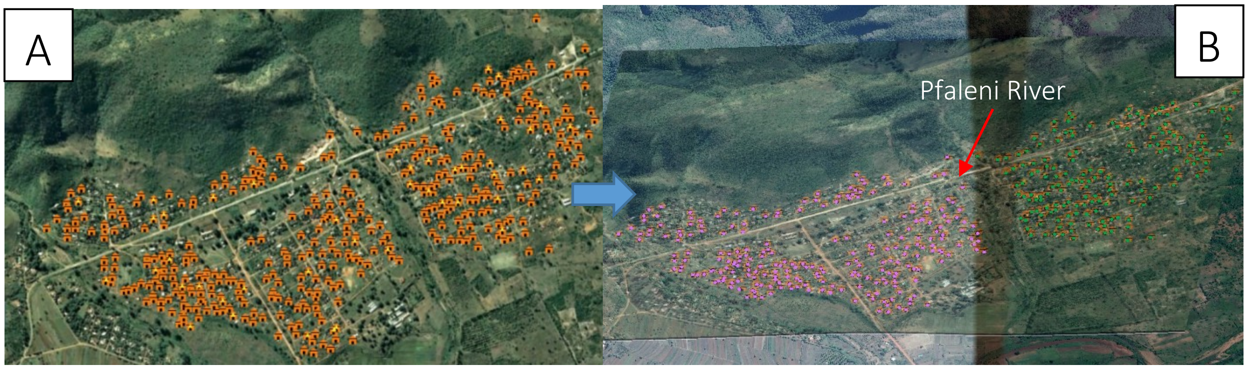

Figure 2 *The original photo which served as the source for the geo-referencing process (A) and the final product (B), showing all households as green (Village 2) and purple (Village 1) dots.*[62,87] *Image A is provided with permission from ASCE. This material may be downloaded for personal use only. Any other use requires prior permission of the American Society of Civil Engineers.*

Household preferred water sources

The individual household preferences for water sources include both primary and secondary preferences. Although data for these were not available, preferred water sources were given on the village level in previous work.[87] Each of the two villages in Limpopo have about 3,000 residents in more than 400 households.[88] Model households were split by village type, using the Pfaleni River as a dividing line. Selected Village 1 households had a relative latitude and longitude of less than 30.453016 and -22.778395, respectively. All other selected households were considered part of Village 2. In the previous study, preferences of water source were assumed and are stated in Table 3.[87] Therefore, a random number of households in each village were asked to set their primary and secondary water sources to a certain type of water at the given frequencies. This is consistent with previously published values of secondary reliance on surface water sources.[88]

Table 3 *The water source preferences for the villages in Limpopo, South Africa.*

Village	**Water source** *type*	**Sand Filter** *%*	**Municipal Tap** *%*	**Surface Water** *%*
1	Primary	82	13	6
1	Secondary	41	16	43
2	Primary	0	34	66
2	Secondary	0	9	91

Household storage containers

The frequency of storage containers used by each household were obtained from personal communication with the model author, reported as approximately 1/3rd open to 2/3rd closed neck. Containers were classified by closed top (1) and open top (2), shown below in Figure 3.[84]

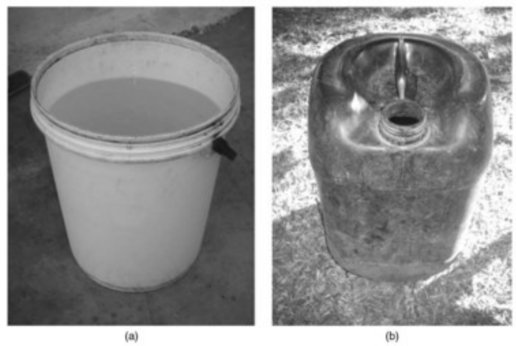

Figure 3 *The types of containers used by households in Limpopo, (a) is open and (b) is closed or narrow neck.*[87] *Images provided with permission of Journal of Artificial Societies and Social Simulation.*

Fecal coliform contamination

The level of fecal coliform present in each storage container and water transfer device (cups) was measured in the field but was not available for the present study. The known frequencies of contamination were given as histograms for total coliform measurements of biofilm on storage containers and biofilm inside of cups as reported in the original ABM (Supplemental Information).[85] These frequencies were visually extracted from each graph and were input manually into Microsoft Excel (Redmond, VA). Then, these values were entered as a matrix into Netlogo. Each household then could randomly select a value from the list of fecal coliform measurements. This same process was also completed for minimum collection interval, maximum collection interval, maximum days a household could wait before getting water, the number of times water was boiled per day, and handwashing frequency. This process is shown in Figure 4.

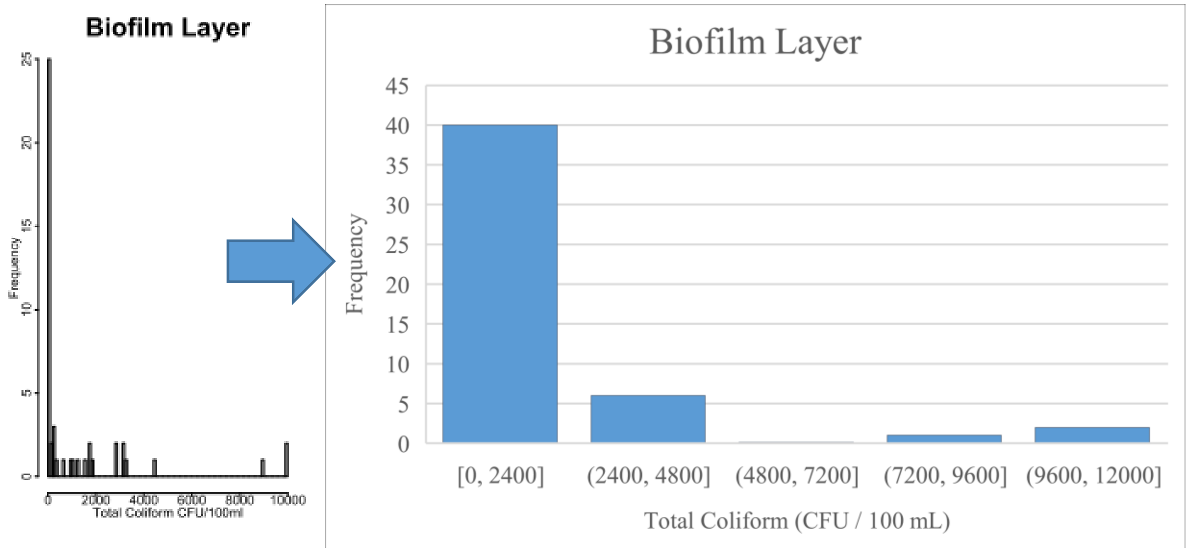

Figure 4 *Values for contamination frequencies at each bin size were extracted from published work*[85] *and converted to known frequency values. These were input as a matrix into Netlogo for the surveyed households (n=49) where the remaining households were randomly assigned the value of the most proximal surveyed household.*

A comparison of the characteristics of the ABM developed herein and models which preceded it are provided in Appendix A. For more detail, Appendix B provides an in-depth comparison of the assumptions used to develop this aggregate ABM. The parameters used in two previous iterations of this model were summarized and used to provide guidance for the aggregate ABM. Values within the baseline model in the originally published work[64] were selected to replicate previous model assumptions. These included: 100% prevalence of CWF, 90% adherence to CWF use, a threshold detection of water contamination, and 730 total days of model time, among other factors (Appendix B). Then, in Appendix C the Overview, Design Concepts and Details + Decision-making framework is adapted to provide a theoretical background, an overview of the modeling process, and information about the steps agents take within the model. Previous researchers have suggested that epidemiologists should develop standardized reporting and best practices for ABMs, I use this framework to do so.[61] The goal of this standardized reporting framework is to provide future investigators adequate information to understand the attribute of the model presented in this thesis. Next, Appendix D provides a flow chart of model design for model setup, water contamination calculation, ceramic water filter intervention, and final ECD calculation.

Statistical analyses

To compare with previously published values, WC is measured as 100 Colony Forming Units (CFU) per 100 mL and ECD is measured as number of events (cases) over 100 iterations. The influence of parameters including drinking water collection level (frequency), boil level (frequency), and municipal tap contamination level (CFU per 100 mL) on ECD cases was compared with previous model output. Results are plotted as box plots and marginal means plots in Stata 13.1. If the mean WC output over a single model run was significantly different from previously published work according to a t-test, the baseline model was reviewed to check for errors. The baseline model was developed to match the baseline characteristics of the previously published model. After any alterations, the model code was reviewed for errors. If errors were found, the model was reviewed again. If no errors were found in the baseline model after twenty review cycles, the model was considered complete.

Model Testing

For each experiment, the model was run for two years (730 days) in accordance with previously published methods.[64] The main model outputs were mean daily WC and total ECD cases of the households. These were automatically exported as means, medians, or total (sums) for each model day over 100 iterations. The averages were compared to previously published ECD values using an analysis of variance (ANOVA) test at equivalent follow-up times in Stata 13.1 (College Station, TX) to ascertain realistic model function. The number of iterations was limited based on maximum file size to import output into Stata.

Model parameters for adherence (amount, decline, and type) and average filter flow rate preference were varied in four separate experiments. Each experiment was completed using the Behavior Space analysis tool in Netlogo. With this tool, all other variables were held constant and the parameter of interest was varied. The mean daily WC and total ECD cases were monitored for each agent. This parameter sweep analysis allowed for the investigation of the influence of a single parameter on many outputs of the ABM system. The specific variables altered in these experiments were: 1) varying adherence (0-100%); 2) declining adherence (0-100% decline in use per month); 3) type of adherence (0-100% split into always, partial and never); and 4) flow rate preference (4.7% decline to adhere to filter use).

Varying adherence

Varying adherence was modeled by randomly selecting 0-100% (in 1% increments) of all model households to adhere to filter use. All other households did not adhere to filter use. Random selection was performed in Netlogo using a random number generator.

Rate of decline in adherence

Declining adherence was modeled by randomly selecting values between 0-100% (in 5% increments) of all model households with filters to stop using the filter at the end of each 30-day time step.

Type of adherence

Type of adherence was modeled by setting each household with a filter as either: 1) always using treated water (children receive only water treated by CWFs if the household is adhering, 100% adherence); 2) partially using treated water (households randomly adhere to treatment from 1-99% of days); or 3) never using treated water (children receive no treated water, 0% adherence) for each day. This provided a household-level adherence estimate with households selecting a random partial adherence each day.

Flow rate preference

Flow rates were modeled by relating the flow rate of filters to acceptability estimates. For a CWF in South Africa, 4.7% of participants found an average flow rate of 3.94 L/hr ± 1.10 L / hour as too slow, and 90.7% found the this flow rate acceptable.[89] To model the impact of flow rates on the intervention, a random selection of 4.7% of total model households with a filter were selected to view the filter as "too slow" (rounded to the nearest household), and were modeled as "never adherent" even if they were previously classified as adherent.

2. CWF Model Selection and Comparison

Model Selection

Due to the structure of the data with random allocation of one child within each household observed over 730 days, a linear regression model was selected. Linear regression may be the most parsimonious model, as household and children's characteristics are randomly allocated between runs which may approximate independent sampling. The regression model was developed using household predictors including daily household WC, primary household water source type, secondary household water source type, current source of water, before hand-washing contamination, storage container type, length of time a household will store water, boiling rate (maximum), filter cleaning frequency (maximum), adherence rate, declines in adherence, acceptable filter flow rate (%), time (days), willingness to pay, and child geographic coordinates (X and Y).

The predictors were used to predict cases of ECD over the course of the baseline model run. Water contamination, another outcome of the previous model, was used only as a predictor in this case. Data for these predictors for each model household and child were extracted from the baseline ABM model in Limpopo, South Africa, and personal communication with the model author, using the methods previously described.[64] Outcome data of predicted episodes of diarrhea were collected for every model day for each child.

A linear regression model was developed in Stata 13.1 (College Station, TX). Any variables which were not significantly predictive of ECD in univariate linear regression analysis ($p > 0.05$) were excluded. Additionally, when a variable increased the R^2 by less than 0.30, it was excluded. Variables were added individually. The beta coefficients, standard error, and p-values for each included predictor variable were recorded for the final regression model. A non-constant linear regression was used as ECD cases are confined at zero. Collinearity was assessed by considering the variance inflation factors and correlation matrix for each model. Interactions between variables were tested based on theoretical justification, and were selected from the included predictors. The distribution of the residuals was examined (Appendix E).

Model Comparison

Significant predictors in the linear regression were listed and compared to dominant predictors previously identified by Behavior Space (sensitivity) analysis in the ABM model. Additionally, the daily predicted cumulative ECD cases for the ABM and the linear model were compared by scatter plot over the model period.

RESULTS

1. CWF Agent-based Model Investigation

Model Building

The structural validity of the source code was ascertained by visual inspection of code, compiler check in Netlogo, and comparison to previously published model characteristics.[62] With each model alteration, the relevant outcomes (water contamination and ECD) were reviewed to ascertain if the value was reasonable (for instance, a positive number). The model was iterated twenty times, and determined to be structurally similar to the previous model.

The current model adequately reproduces the results for WC as generated by the previous ABM (Figure 5). Overall, the current baseline model predicts a mean WC of 256 ± 151 CFU / 100 mL and a mean of 1391 ± 1043 cases of diarrhea over the two-year model period. The WC model has a similar general trend as the previous model with WC increasing over each one-year model run. Specifically, mean WC increases until agents clean the filters at the one-year mark, which decreases the WC to almost baseline (~ 10 CFU / 100 mL for Mellor *et al.* 2014 and ~ 100 CFU / 100 mL for current ABM model). Note that the order of magnitude of the predicted WC is different though the trends are similar. Due to this, the increased mean WC was significantly different from the previous ABM (t_{730}= -34.17, $p < 0.001$). Nevertheless, predicted water contamination fit much better when normalized by the initial predicted values (subtracting 100 CFU / 100 mL from each value), as shown in Figure 5b.

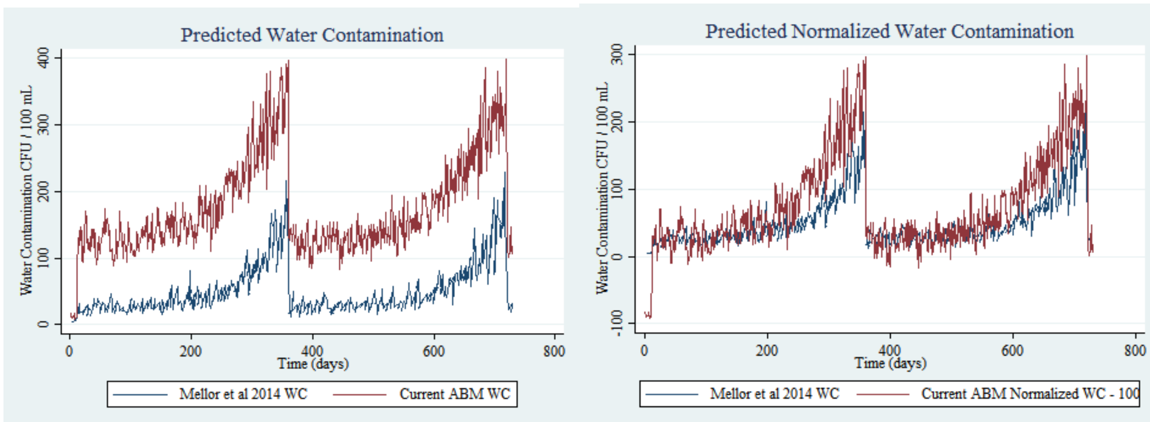

Figure 5 *The water contamination for the baseline model in the current ABM model (red) compared to the previous ABM model (blue) over two simulated years (730 days) (A). After decreasing the current ABM predictions by 100 CFU / 100 mL, predictions were closer (B).*

The model output was compared to the previously published model output (Figure 6). The aggregate model developed herein shows strong over-prediction of median WC by at most 150 CFU / 100 mL compared to the original model.

All parameters show a strong skew and different temporal trends than the previous model, including drinking water collection level, boil level, and municipal tap contamination level. Collection interval and boil interval show an increasing trend in median WC with increasing collection and boil levels compared to the previous model (Figures 6a and 6b). Municipal tap (MT) water contamination also shows an increasing trend in median WC, but becomes static after 200 CFU / 100 mL (Figure 6c).

Nonetheless, a comparison between baseline aggregate model output and the previously published output suggests that the model outcomes are realistic. The mean predicted ECD per household for the two-year model period was 3.4 (s = 2.5, maximum = 7.9) cases, which compares with the previous model mean of 8.49 cases per household and a 2010 survey of children in Africa which reported a mean of 8.45 cases per household.[90]

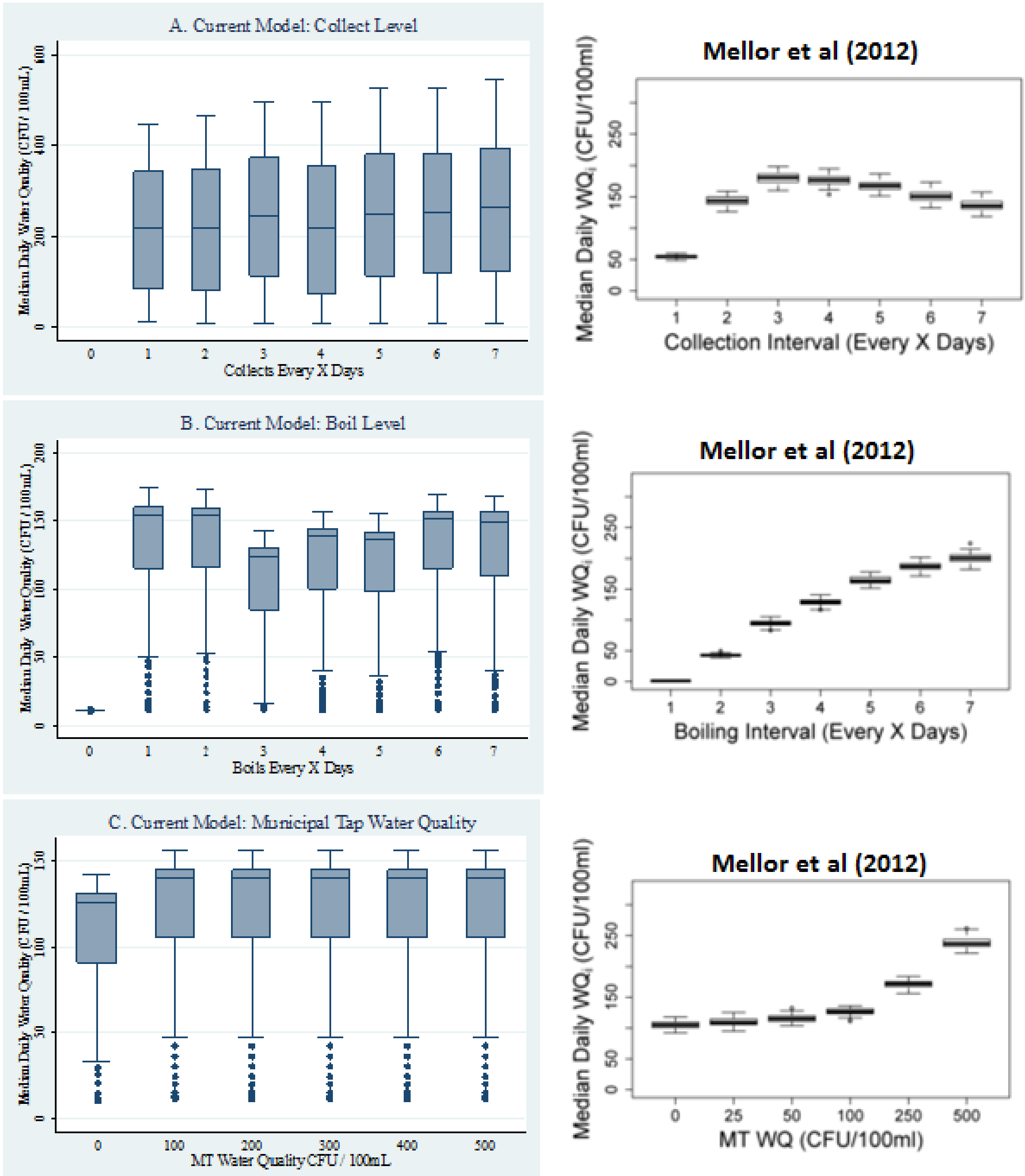

Figure 6 *Box plots of aggregate ABM model output and previously published averages. Models were run under baseline conditions for 100 iterations using the Behavior Space function in Netlogo.*

Model Testing

Parameters for adherence (amount, decline, and type) and average filter flow rate were varied in four separate experiments using the Netlogo BehaviorSpace analysis tool over 100 iterations. Varying adherence from 0-100% over the two-year model period produced a significant variation in mean ECD cases ($F_{10, 804099} = 255.94$, $p < 0.0001$) compared to baseline. The relationship between declines in adherence and ECD was non-linear, as shown Figure 7a. Overall, the predicted mean ECD cases decline from 1145 cases at 20% to 1075 cases at 50-90% adherence to 1050 cases at 90–100% adherence.

Altering the rate of decline in adherence from 0-100% produced a significant variation in ECD ($F_{9, 708033} = 580.54$, $p < 0.0001$) compared to baseline. The relationship between the rate of decline in adherence and ECD was non-linear, though the mean predicted ECD cases was generally lower with higher adherence (Figure 7b).

Similarly, altering the type of adherence (always, partial, never) from 0-100% produced a significant variation in ECD ($F_{10, 804100} = 27.95$, $p < 0.0001$) compared to baseline. As type of adherence varied from 0-90% per month, the expected number of ECD cases was near 2160 though this dropped to 2060 cases with greater than 90% type of adherence (Figure 7c).

Finally, altering the percent of households that found the flow rate acceptable from 0-100% produced a significant variation in ECD ($F_{20, 708033} = 18185.13$, $p < 0.0001$) compared to baseline. As flow rate preference varied from 0-90% per month, the expected number of ECD cases was near 2500 though this dropped to almost zero cases with greater than 90% flow rate preference (Figure 7d).

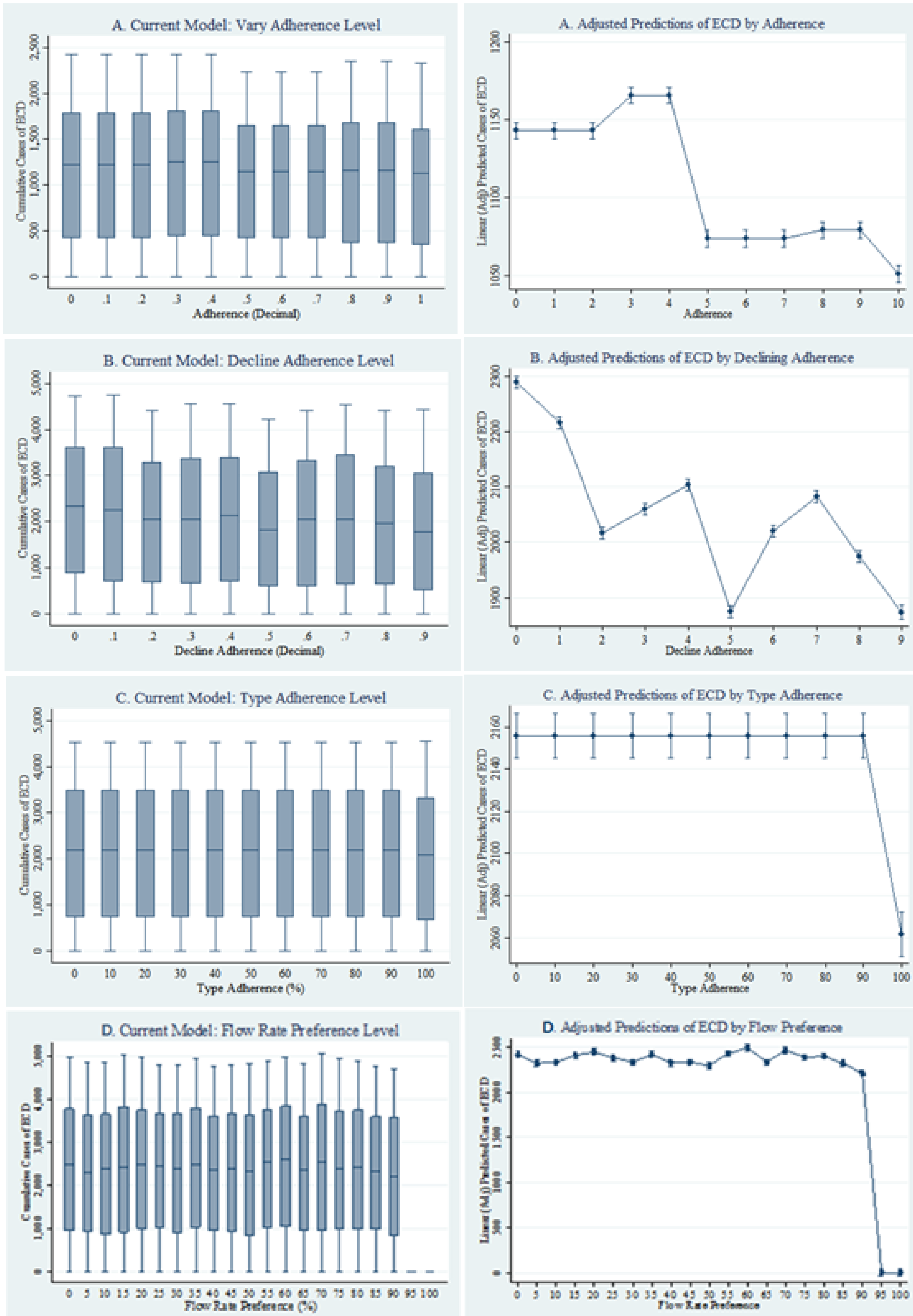

***Figure** 7 Box plots and marginal mean plots for predicted ECD for values of adherence, decline in adherence, type of adherence and flow rate preference experiments. This models 410 households containing 410 children. Whiskers on marginal mean plots are confidence intervals.*

2. CWF Model Selection and Comparison

Model Selection – Linear regression

Variables extracted from the ABM are summarized in Table 4. Variables were considered iteratively in the order listed in Table 4 to generate a linear regression model of the mean daily ECD cases.

Table 4 *Variables which were extracted from the ABM for use in regression analysis.*

Variable		Obs (*n*)	Mean	Std. Dev.	Minimum	Maximum
Ticks (time)	*days*	29971000	365	211.0	0	730
Daily water contamination	*CFU / 100 mL*	29971000	524.8	902.6	11.9	4911.3
Primary Water Source	*River water (RW)*					
2	*Community Piped (CP)*	29971000	0.07	0.25	0	1
3	*Municipal Tap (MT)*	29971000	0.32	0.47	0	1
Secondary water source	*RW*					
2	*CP*	29971000	0.01	0.12	0	1
3	*MT*	29971000	0.12	0.33	0	1
Today's water source	*RW*					
2	*CP*	29971000	0.06	0.24	0	1
3	*MT*	29971000	0.12	0.32	0	1
Before hand-washing contamination	*CFU / 100 mL*	29971000	924.7	2187	0	9000
Storage container type	*1 = wide neck 2 = narrow neck*	29971000	0.58	0.49	0	1
Days household can keep water	*Days*	29971000	0.94	2.0	0	44
Boiling frequency (maximum)	*Boils every X days*	29971000	17.7	12.4	1	30
Filter cleaning frequency (maximum)	*Cleans every X days*	29971000	136.6	142.3	0	492
Adherence	*% of time using the filter*	29971000	33.4	24.0	6.5	89.9
Adherence (overall)	*% yearly sustained*	29971000	90	0	90	90
Flow rate preference	*% of people who dislike the filter*	29971000	4.7	0	4.7	4.7
Willingness to pay	*South African Rand*	29971000	177	155	20	500

Child Longitude	*Degrees*	29971000	-0.76	18.8	-30.42	30.42
Child Latitude	*Degrees*	29971000	15.8	32.1	-60.19	60.36

Variables including ticks, primary and secondary water sources, today's water source, days household can keep water, maximum boiling interval, maximum cleaning interval, adherence (overall), flow rate preference, willingness to pay, child's latitude, and child's longitude showed strong collinearity ($r > 0.30$), were non-significant predictors in linear regression ($p > 0.05$), or increased the R^2 by less than 0.30 and were thus removed from analysis. The variables adherence and hand-washing contamination were added as an interaction term, as households were more likely to adhere with higher threshold contamination levels, which can be then decreased through hand-washing.[64]

The remaining variables were used as independent variables in a linear regression model to predict ECD cases. The theoretical equation for this model of n = 410 children across n = 730 days over n = 100 iterations can be expressed as:

$$ECD_{ij} = \beta_1 \times WC_i + \beta_2 \times BeforeHW_i + \beta_3 \times StorC_i + \beta_4 \times Adhere_i + \beta_5 \times Adh\#BHW_i + \epsilon_{ij}$$

where:

ECD_{ij}	predicted household ECD for each child from the ABM (mean total cases)
WC_i	daily water contamination for each household (CFU / 100 mL)
$BeforeHW_i$	hand-washing contamination (CFU / 100mL)
$StorC_i$	storage container growth and contamination (CFU/ 100mL)
$Adhere_i$	adherence to using the filter (% of time using the filter)
$Adh\#BHW_i$	the interaction between adherence and hand-washing contamination
ϵ_i	unexplained variance in the model (error)

All independent variables were significant predictors of ECD (Table 5). The model explained 53.5% of the variability in mean ECD cases ($p < 0.001$).

Table 5 *The model output for the linear regression model.*

Variable	Coef.	Std. Error	p-value	95% CI	
Daily water contamination	0.594	< 0.001	< 0.001	0.593	0.594
Before handwashing contamination	0.085	< 0.001	< 0.001	0.084	0.085
Adherence	1.55	0.006	< 0.001	1.54	1.57
Storage Container	1260.6	0.451	< 0.001	1260	1261
Adherence and Before HW Interaction (9000 CFU / 100 mL)	-37.3	0.037	< 0.001	-37.4	-37.2
Intercept:	*No constant (intercept) was used in this model.*				

Variance inflation factors for the constant-containing regression were between 1.13 and 1.19 (mean = 1.16). Residuals were distributed as shown in a scatterplot of the standardized residuals (Appendix E) suggesting that there is bias in the linear model, which may be due to unaccounted for interactions. A comparison of the predicted ECD values for the ABM (blue line) and the linear regression model (red line) is provided in Figure 8. Both models predicted increasing cases of ECD over increased time (ticks), with different trends.

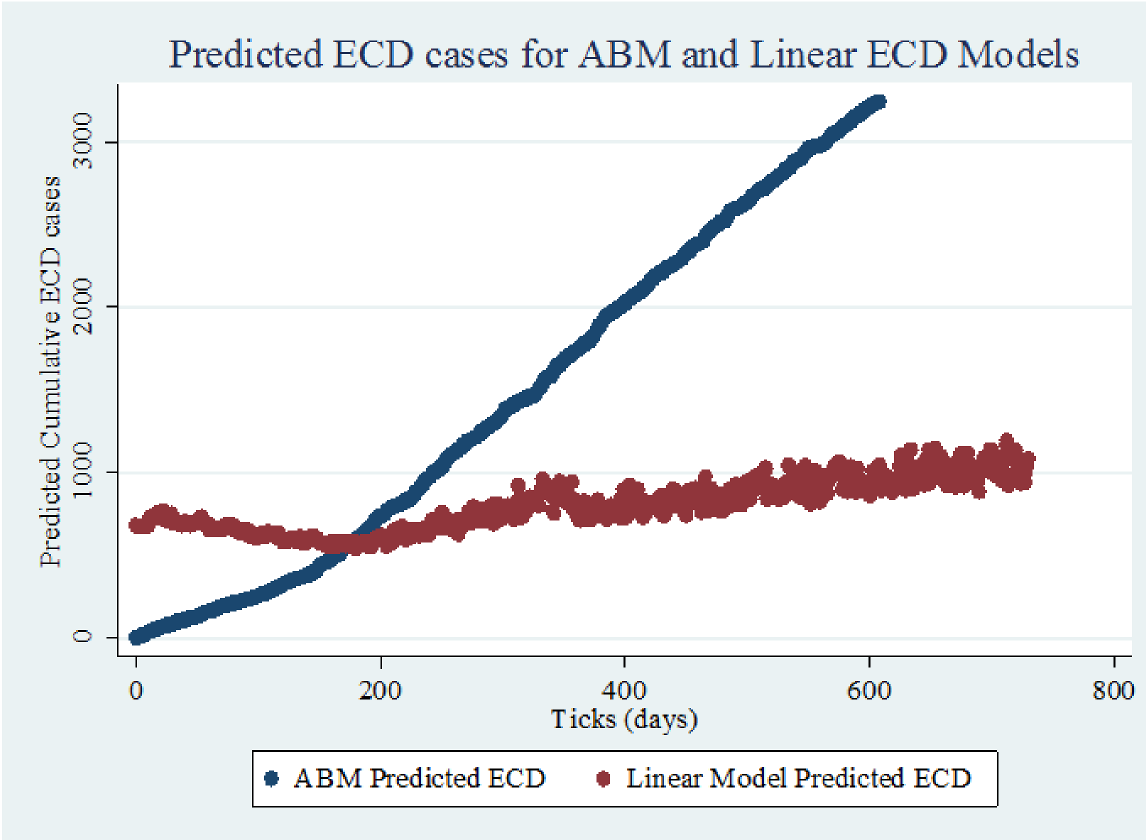

Figure 8 *Predicted cases of ECD over the model period for the ABM (blue) and the linear model (red).*

DISCUSSION

In this thesis, a previously developed ABM predicting ECD in Limpopo, South Africa was reproduced without additional individual-level data. As with the previously developed model, the present ABM suggested that filter adherence and declining adherence are among the most important predictors of ECD rates.[62] Additionally, the ABM was constructed to consider other factors including individuals' perception of filter flow rate. Perception of filter flow rate was a significant predictor of ECD and further supports the theory that high adherence is necessary to sustain reduction in diarrhea cases as a result of CWF interventions.[31] Type of adherence results supported the importance of consistent use, as partial adherence provided reduced ECD declines. This agrees with previous studies that have shown that social and behavioral factors can impact diarrheal disease rates.[91,92] This thesis provides insight into the complex interactions between technological factors (filter flow rates) and behavioral factors (flow rate perception) that influence CWF sustainability and use.

Model Building - Reproducing an Agent-based model

The ABM model presented in this thesis is the first known attempt at replicating a water and sanitation ABM. This reproduction is important to further the use of ABM as a methodology in water and sanitation models. Notably, the original ABM was reproducible even without complete individual-level data. The outputs from both the original and reconstructed model matched in magnitude of predicted contamination, biofilm growth, and in the influence of factors such as the presence and adherence to CWF use. For example, in the original ABM, the predicted biofilm contamination was as high as 1979 CFU/100 mL and the predicted contamination of hands was as high as 1040 CFU/100 mL.[84] In the reconstructed model, the predicted mean biofilm growth was 2187 CFU / 100 mL, and the mean contamination from hands was 925 CFU / 100 mL. These magnitudes match reasonably well and this agreement makes sense since it was previously found that biofilm regrowth was due both to poor handwashing and to contamination from water transfer devices (cups).[84]

Despite the overall agreement in the results from the original and reconstructed models, there was stronger agreement in WC during the first 200 days of the model. The pattern deviated from 200 to 365 days. This is likely due to the use of random distributions based on static, field derived values which may have over-estimated water contamination over time. For example, assumptions about bacteriological regrowth and storage container contamination may have produced higher household WC contamination than the previous model. Previous versions of this model by Jeffrey Demarest et al. have used random-normal distributions to approximate water contamination and child height. This assumption may have limited their overall model accurarcy.[83] In this model, initial water contamination observations were derived from field data in the model code, but stochastic variation within the model framework can lead to deviations over time. These drifts across time series have been reported as a challenge in creating ABMs. Time-series analyses can be applied to reduce the apparent deviation.[66] Further deviation was found between the trends as baseline parameters were changed, including drinking water collection level, boil level, and municipal tap contamination level. Although trends were non-linear, this is not unprecedented, even in disease models.[93] This non-linearity in trends within ABMs has been reported elsewhere, and can be a explained as a result of unanticipated or complex relationships among variables.[94]

It was also found that adherence was less influential in this ABM model than other studies have shown. My model produced declines in ECD up to 8.2% with varied adherence, whereas other studies have reported diarrheal declines up to 96%.[31] Studies of chlorine have also shown significant declines in intervention effectiveness as other measures of adherence (free chlorine residual) decline.[10] A review of multiple household water treatment technologies also found that adherence was a major predictor of intervention effectiveness.[95] This means the current ABM model may underestimate the impact of adherence on intervention effectiveness compared to the previously published literature. Additionally, flow rate preference produced a rapid decline of cases of ECD, to almost zero. However, this was likely a result of the way that this variable was coded. The code asks the households who will adhere (set to 90% at baseline) minus those who do not prefer the filter flow rate, to use the filter. However, this circumvents other portions of the model including ceramic water filter efficiency declines, and may not be realistic. These differences may be addressed in the future by better estimates of the role of perception of ceramic water filter flow rates and subsequent acceptability among households.

Notwithstanding these inconsistencies, important conclusions about the influence of factors on the effectiveness of ceramic water filters in reducing water contamination can be drawn. Median WC was especially influenced by factors such as adherence and the rate of decline in adherence. Increased water collection frequency and boiling frequency were previously reported as decreasing water contamination.[64] This general relationship was replicated by the reconstructed model, though WC was over-predicted in the reconstructed model. The high modeled WC would underestimate the impact of preventative measures, as CWF interventions are less effective at reducing higher levels of fecal coliform contamination to a safe level then at lower levels of contamination. This may not have substantially impacted the overall results as the mean number of diarrhea cases reported in the previous model (8.49 cases per household)[64] are close to the maximum predicted cases of ECD in the present reconstructed model (7.9 cases per household).

In the original (Mellor *et al.* 2012) study, baseline data including water sources and treatment methods from Guatemala and South Africa were used for calibration. Results were different between the Guatemalan and South African models, but contained similar values of ECD.[62] This suggests that the model is transferable to similar contexts, as long as the data can be re-derived in aggregate form.[67,96,97] As shown in this thesis, reconstructing the model with aggregate data is possible. Reconstructing ABMs can overcome logistical, budgetary, and ethical constraints in long-term intervention-controlled trials where individual data may not be available.

Reproducibility of complex system models is an important, yet challenging, practice. Previous work has attempted replication of ABMs and has reported issues in finding statistical equivalence between models.[67] Due to the random behavior and stochasticity between models, replication is challenging if models are drawn from different data or if they have different assumptions.[50]

Implementation of agent interactions can differ if agents have different rules for interaction and the rules are not explicit.[67] This can make the comparison of ABMs with traditional statistical tools equally challenging. In this work, comparisons were completed at the same level of iterations (100) and follow-up time (730 days) for each analysis. These were carefully matched to the previously developed model to produce a structurally similar model. Finally, some individual household parameters were estimated as original data was not available.

In order to correctly estimate household parameters, assumptions were made about preferences (water sources, flow rate, *etc*.) during the design of the model. Values for these variables were drawn from published material and discussions with Dr. Jonathan Mellor.[50] This is an important step for developing an aggregate agent-based model, with reference to the original conceptual framework of how agents and their environment relate. With careful development of assumptions, conceptual design and edited computer code, the replication of a model can be standardized. Similarly, careful application of statistical tests including checking for heteroscedasticity and controlling the number of observations collected can produce comparable results. Finally, internal and external validation checks were especially important during model building and analysis. The use of a main outcome (water contamination, WC) as a validation target was essential for determining proper model function. The ability of ABMs to assess multiple outcomes with joint influences from predictors makes the framework especially useful.[98] Multiple outcomes (WC and ECD) also provide greater opportunities for model comparison.

Even if a reproduced ABM is statistically comparable to the original however, ABMs are still not robust when considering entirely missing data or systems that are not well-characterized at the local level. For example, height-for-age z-scores (HAZ) data on child height stunting, which was included in the original model,[62] was not replicated in this model due to the lack of individual-level data. Obtaining access to individual data in this case would have improved the utility of the ABM.

Comparing modeling methods

The ABM developed for this thesis was able to predict WC trends in Limpopo. This suggests that ABMs can be a useful research tool, depending on the research question of interest. Nevertheless, there is a question of whether this approach is superior to traditional modeling approaches. To address this question, a simple linear model was also developed and compared against the ABM. The linear model predicted 53% of the variability of ECD cases using only five predictor variables, including WC (Table 5). Notably, this linear model did not use child-specific predictors as these were randomly allocated to each household at the start of each model run and would not be expected to predict ECD cases. The random allocation of children to households also meant that a more complex model structure, such as a multilevel model, was not necessary. In real-world systems, children are nested within households so if individual-level data were used, a multilevel model would be more appropriate than a simple linear model.

Although the linear model performed well, the ABM might be better suited to model systems that change with time. The linear model also assessed the interaction between hand-washing contamination and adherence, to see if households that have higher handwashing contamination are more or less likely to adhere. This term was significant ($p < 0.001$), suggesting that there is an interaction between those variables and the behaviors may influence each other over the course of the two-year model period. For example, when comparing modeling strategies to predict demographic transitions due to armed conflict in Nepal, the linear model was more predictive of stable behaviors while the ABM was more predictive of behaviors that changed over time.[96] This makes sense since ABMs can explicitly include time in the simulations whereas linear models cannot. The linear regression developed in this thesis used similar methods to the Nepal model to compare the two models. Both used the predicted outcome over the period of study, drawn from non-random predictors in the linear regression model. Selection and estimation of parameters for individuals was noted as an important challenge, and an area where ABMs may be more suitable than other models such as linear regression.[96] Due to changes in behaviors over time, ABM can be a useful model for prospective intervention studies.

Additionally, ABMs are useful when agent heterogeneity has a strong influence on the model output(s) and when there are multiple interacting technological, environmental, and behavioral factors.[99,100] Depending on the complexity of the interactions, these could still be modeled with traditional approaches. Nevertheless, an ABM could include dynamic sub-models of agent decision-making processes that could be more representative of real-world systems.[50] In practical terms, ABMs are more challenging to run as they take longer, use more storage and processing, and require and use more complex input data. These practical considerations will likely become less important as computational resources and processing power increase.[50] Training of practitioners in the use and interpretation of ABMs would also assist the development of ABMs.

Overall, linear regression modeling was only marginally sufficient to answer the research question posed in this thesis. This is likely due in part to the complexity in the calculation of ECD risk for each level of water contamination over time. A direct relationship was assumed between the exposure to water contamination (CFU / 100 mL) and a resulting likelihood of ECD in the original model.[64] An ABM is more useful in this context as there were more non-linear relationships within the system and interactions between agents and their environment. For example, ABMs are useful for modeling processes which can be influenced by human decisions, such as how water quality can be affected by means of transport from source to storage to use within the household. These non-linear impacts on intervention effectiveness can be linked back to the social, technological and contextual factors as outlined in the IBM-WASH framework.[29] This thesis confirms that social factors such as adherence and flow rate preference can impact the effectiveness of a CWF intervention.

Limitations

Although this study has produced largely comparable results with the original study,[64] there are some limitations to note. First, some limitations were carried over from the original study. For example, since drinking water samples for coliform analysis were only taken monthly, there could be seasonal variation or sampling error.[88] There were also limitations introduced through the reproduction of the ABM. From a theoretical perspective, it may not be reasonable to assume that the population size and birth rate are static over the two-year model period. Additionally, the lack of individual information precluded child-level factors from being included in the model since these characteristics were randomly assigned each iteration. It was also assumed that the underlying data is drawn from a normal distribution, in order to generate the random values. This may have also been incorrect and that would decrease the accuracy of the model. Furthermore, the assumption that a previous case of ECD increases the risk of a future case by 2.05 may not adequately capture the influence of nutrition uptake, breakdown of intestinal cilia, or other factors.[101]

Moving forward, it would be useful for models to account for pathogens other than fecal coliform since that would better approximate real-world conditions. Over 50% of tested municipal tap samples have assimilable organic carbon that could support the growth of cholera and *E. Coli.*[84] Additionally, since CWF do not remove all pathogens with the same level of effectiveness (e.g. CWF do not effectively remove parasites such as *Cryptosporidium*), it would be useful to include contamination by parasites and viruses in the model.[64] Finally, the link between fecal coliform and diarrhea that is used to assign ECD risk (Appendix B) is not strongly supported in the literature. There is a weak link between fecal coliform and diarrhea for highly contaminated water (>1000 CFU / 100 mL) waters,[102] but this model does not approach that level of water contamination. There is a stronger link between *E. Coli* concentration in drinking water and diarrhea,[103] but no data for *E. Coli* in the source water in Limpopo, South Africa was available.

Future suggestions for ABMs

Future studies should use frameworks such as the Overview, Design Concepts and Details + Decision-making (ODD+D) framework to standardize reporting of ABM design and results (Appendix C). The use of this framework will help provide clarity for future replication of results. Ensuring that a more computationally simple method is not sufficient should precede efforts to build ABMs.[67,104] Each ABM should be interpreted carefully based on the context of the study population.

Reflections on sensitivity and replication

The re-built model predicted water contamination and diarrhea (ECD) cases with similar magnitude but different trends than the originally published model. Additionally, when the frequency of water collection, frequency of boiling, and municipal tap frequency were varied, different trends in mean water contamination were recorded. The response of the model to adherence was also more restrained than previous work, and was not consistent with epidemiological literature on adherence.[31,64] Both the previous ABM and current epidemiological literature show a stronger impact of adherence on intervention success than reported herein. This suggests that the previous ABM and this ABM are different in important ways, and the success of the replication should be reviewed.

Other ABM researchers have suggested that there are five components of importance in completing a replication exercise. These include: time, hardware, (computer) languages, toolkits, algorithms and authors.[67] In this work, I replicate a model two years after its original publication, on different hardware, using different toolkits and algorithms, completed by a different author. Only the computer code is consistent between models. Researchers in computer science have noted the importance of a replication standard for comparing simulation models, including both similar outputs (numerical similarity) and distributions (distributional similarity).[105] I find that the replication standard of numerical and distributional similarity did not match between the re-built ABM model and previous model as discussed above, although many replication characteristics were similar. The limited sensitivity analysis completed for the frequency of water collection, frequency of boiling, and municipal tap contamination showed a different magnitude of sensitivity in the re-built ABM model.

This would suggest that the reproduced model developed herein may not adequately represent all interactions present in the original model. This discrepancy must be investigated if a claim of complete reproduction is to be made. Interactions leading to divergent results can be investigated using sensitivity analysis.[50,106] Sensitivity analysis can be defined as a method to understand how results vary across the range of a single parameter or interest (keeping all other values unchanged).[107]

A sensitivity analysis using the Behavior Space platform within Netlogo can be completed. This has been used in previous studies to provide an estimate of the influence of a single variable on overall system outcomes.[64,72] In this thesis, the frequency of water collection and boiling were varied in a rudimentary sensitivity analysis, but further analysis should include all model parameters. However, the researcher would be required to manually develop code routines for testing all possible interactions.[62] This process of incrementally varying single variables is called "one factor at a time" or OFAT, and is the simplest way to conduct a sensitivity analysis when considering relatively few variables. However, this simple approach could lead to user error, and requires long processing times with a greater number of variables of interest. The OFAT approach only functions well for linear models, and a hallmark of agent-based models is their non-linear behavior.[108] Other methods of sensitivity analysis can account for some non-linearity, including model free output variance decomposition (or global/Sobol sensitivity analysis) and model-based output variance decomposition (regression-based sensitivity analysis).[109] Each method of sensitivity analysis has benefits and drawbacks, and have been reviewed previously.[108,110] However, the ability of these methods to compare ABM sensitivities for model reproduction has not been assessed. Such an assessment is a useful next step.

Thus, methods of sensitivity analysis are currently insufficient for investigating the reproduction of complex agent-based model without robust application.[108,110] To address this problem, there has been recent work linking Netlogo and other agent-based modeling programs to more powerful statistical software. These programs can provide a full suite of sensitivity analysis methods. For example, work by Dr. Jan Thiele produced the Netlogo-R-Extension statistical package for the program R.[111] This paper did not suggest any specific sensitivity analysis techniques, but the program R contains many other software routines (commonly called "packages") which can perform these tasks. One example of this is the R package "lhs", which can perform Latin Hypercube Sampling (LHS). This is a method for extracting values from the multidimensional parameter space in order to find the area that obtains the most representative subset of results given a known set of parameters of interest.[112] This has been used alongside sensitivity analysis for agent-based models of social systems.[113] Completing this process of sensitivity analysis using robust statistical programs with the correct methods may clarify the completeness of a model reproduction. For example, the field of economics has begun to use sensitivity analysis (OFAT) to compare models and the assumptions within them.[107] These approaches to estimate model sensitivity may be a better method than visual comparison. I suggest that future studies compare multiple methods of sensitivity analysis to ascertain replication. Other agent-based models must also produce sensitivity estimates, in order to facilitate comparison and future replication. This will better allow researchers to characterize goodness of fit between agent-based models, and provide a method for replication studies.

CONCLUSIONS

An ABM of the water sanitation behavior in Limpopo, South Africa was reconstructed from a previously published model using aggregate data. The reconstructed model over-predicted water contamination and under-estimated the influence of factors such as water collection frequency and boiling interval.[64] The ABM predicted ECD risk well, however. This suggests that replication is possible using aggregate data which means that ABMs could be used to derive additional information about the long term sustainability of interventions where short term field-studies have already been completed. This method has advantages including protecting individual privacy, increased flexibility in model-building, and increased speed and ease in model building. Applying this methodology in the case of Limpopo suggested that the sustainability of CWF interventions is influenced by factors such as perception of flow rates.

Although it was possible to build and use an ABM from aggregate data, ABMs did not clearly perform better than simple linear regression models in predicting ECD cases. Linear regression modeling was a more efficient and more easily interpreted ECD model. Nevertheless, ABMs did characterize individual WC more accurately and this underlines the importance of the choice of an analytical model most appropriate for the research question. The linear model also contained bias according to standardized residuals. Overall, ABMs can provide useful insight into the field of water and health and further research employing ABM methods should be conducted.

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APPENDIX

Appendix A – A comparison of models for the effectiveness of the ceramic water filter (CWF) intervention against early childhood diarrhea. NR = not reported, N/A = not applicable

Model *Citation*	**QMRA** *Brown et al (2012)*	**ABM** *Mellor et al (2012)*	**CWF-ABM** “Basic CWF Routine” *Mellor et al (2014)*	**CWF-ABM** “Additional CWF Routine” *Mellor et al (2014)*	**CWF-ABM** *This paper*
Design	Quantitative Microbial Risk Assessment (QMRA)	Agent-Based Model (ABM)	Agent-Based Model (ABM)	Agent-Based Model (ABM)	Agent-Based Model (ABM)
Health Outcome	Disability-adjusted life years (DALYs)	Early-childhood diarrhea (ECD)	Early-childhood diarrhea (ECD)	Early-childhood diarrhea (ECD)	Early-childhood diarrhea (ECD)
Log Removal (Bacterial removal effectiveness)	“Best case” 3.01 - 6 $\log_{10}$	N/A	Filter log reduction 2.92 $\log_{10}$	Filter log reduction 1 $\log_{10}$	Filter log reduction 2.92 $\log_{10}$
	“Mid-range” 2.01 - 3 $\log_{10}$	N/A	Filter log reduction 1.63 $\log_{10}$		Filter log reduction 1.63 $\log_{10}$
	“Basic level” 1 - 2 $\log_{10}$	N/A	Filter log reduction 0.42 $\log_{10}$	Filter log reduction 5 $\log_{10}$	Filter log reduction 0.42 $\log_{10}$
Adherence	High 91-100%	N/A	Compliance was varied from 80-90% at 10% intervals	Compliance was varied from 0-100% at 10% intervals	Adherence was varied from 0-100% at 1% intervals.
	Medium 71-90%	N/A			
	Low 50-70%	N/A			
Source water	Treated water Untreated water	Surface water (SW)	Varied given experimental mean values	Varied given experimental mean values	Varied given experimental mean values
		Community piped water (CP)			
		Municipal tap (MT)			
Source water contamination	“High risk” 1 CFU / L “Moderate high risk” 0.1 CFU / L “Moderate risk” 0.01 CFU / L “Moderate low risk” 0.001 CFU / L “Low risk”	SW NR	Varied given experimental mean values	Varied given experimental mean values	Varied given experimental mean values
		CP 0 – 5,000 CFU / L			
		MT 0 – 1,000 CFU / L			

	0.0001 CFU / L				
Breakage rate	NR	N/A	20%	N/A	20%
Prevalence of CWFs	NR	N/A	100%	0-100%	100%
Detection of Contamination	NR	N/A	NR	2.05 times as likely to treat if threshold 0 – 2,000 CFU / L	2.05 times as likely to treat if threshold 0 – 2,000 CFU / L, threshold set at 100 CFU / L
Software used	Oracle Crystal Ball, Fusion Edition	Netlogo	NetLogo	NetLogo	Netlogo
Volume Drank	1 – 5 Liters / person / day	N/A	N/A	N/A	N/A
Perception of filter effectiveness	N/A	N/A	N/A	N/A	4.7% less likely to use a filter due to filter perception, range from 0 – 100%

Appendix B – A comparison of the model variables and parameters between the models developed by Dr. Jonathan Mellor[62,64] and this work.

Variable type	**Parameter (units)**	**Model** *Citation*			
		Aggregate ABM *This paper*	**ABM** *Mellor et al (2012)*	**ABM** *Mellor et al (2012) BehaviorSpace Range*	**ABM** *Mellor et al (2014)*
General variables	**Children (n)**	410	410	410	410
	Households (n)	410	410	410	410
	Filter Prevalence	100%	N/A	0-100% by 10%	100%
	Filter Breakage Rate (over two years)	20%	N/A	0-100% by 10%	20%

	Adherence (compliance)	90%	N/A	0-100% by 10%	90%
	Cleaning Interval (Every X days)	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	N/A	0 – 730 by 60 days	No baseline, 0 – 730 days
	Yearly adherence (compliance) decline	Baseline 2%, 0 – 100% from Cambodia CWF Study[15]	N/A	0-100%	No baseline, 0 – 100%
	Breakage Date	10 [day], 0 – 730 days	N/A	0 – 730 by 60 days	No baseline, 0 to 730 days
	Threshold Water contamination	100 CFU / 100mL	N/A	0 – 2000 CFU / 100mL	No baseline, 0 – 2000 CFU / 100mL
	Willingness to Pay	Selects a random value from the list. one-*of [50 100 300 150 30 500 50 20 500 150 70 200 100 100 80 250 500 150 100])*	N/A	20 – 500 Rand	No baseline, 20 – 500 Rand
	Rotavirus vaccine effectiveness	44.1%	44.1%	44.1%	44.1%
	Daily Water contamination	Drawn from source water contamination data for SW, CP, MT and the Water Chain analysis	Drawn from source water contamination data for SW, CP, MT and the Water Chain analysis	0 – 4000 CFU / 100mL	Drawn from source water contamination data for SW, CP, MT and the Water Chain analysis
	Primary water source	SW, CP, MT	SW, CP, MT	SW, CP, MT	SW, CP, MT
	Secondary water source	SW, CP, MT	SW, CP, MT	SW, CP, MT	SW, CP, MT
	Days have kept water	> 0 days	> 0 days	> 0 days	> 0 days
	Maximum days can keep water	Frequencies drawn from histograms in Figure S6 Mellor et al 2012	Values reported by households in surveys Figure S6	1 – 14 days	N/A

	Water collection interval	Frequencies drawn from histograms in Figure S6 Mellor et al 2012	Values reported by households in surveys Figure S6	Every 1 – 10 days	N/A
	Water container cleaning interval	Drawn from a CWF study in the same community[81]	Unclear source	Every 1 – 365 days	N/A
	Water boiling interval	Frequencies drawn from histograms in Figure S7 Mellor et al 2012	Values reported by households in surveys Figure S7	Every 1 – 30 days	N/A
	Daily handwashing interval	Frequencies drawn from histograms in Figure S8 Mellor et al 2012	Values reported by households in surveys Figure S8	0 - 24 days	N/A
	Coliforms associated with hands	Frequencies drawn from histograms in Figure S5 Mellor et al 2012	Values measured within surveyed households in Figure S5	0 – 8615 CFU / 100mL	N/A
	Biofilm layer coliform contribution (HHS)	Frequencies drawn from histograms in Figure S5 Mellor et al 2012	Values measured within surveyed households in Figure S5	0 – 10,000 CFU / 100mL	N/A
	Water transfer device coliform contribution	Frequencies drawn from histograms in Figure S5 Mellor et al 2012	Values measured within surveyed households in Figure S5	0 – 5064 CFU / 100mL	N/A
	Sex	M / F	M / F	N/A	N/A
	Age (days)	0 – 730	0 – 730	0 – 730	N/A
	ECD Status	Single case, Double case, none	Single case, Double case, none	Single case, Double case, none	N/A
	Daily growth increment	-0.198 – -0.176 cm	-0.198 – -0.176 cm	-0.198 – -0.176 cm	N/A
Global variable	**Duration of stunted growth**	240 days	240 days	240 days	N/A
	Single ECD Case HAZ Reduction	-1.50 – 1.47	-1.50 – 1.47	-1.50 – 1.47	N/A
	Double ECD Case HAZ Reduction	-2.18 – 1.93	-2.18 – 1.93	-2.18 – 1.93	N/A
	SW Water contamination	0 – 4120 CFU / 100mL	0 – 4120 CFU / 100mL	0 – 4120 CFU / 100mL	N/A
	CP Water contamination	0 – 1220 CFU / 100mL	0 – 1220 CFU / 100mL	0 – 1220 CFU / 100mL	N/A
	MT Water contamination	0 – 500 CFU / 100mL	0 – 500 CFU / 100mL	0 – 500 CFU / 100mL	N/A
	SW Reliability	N/A	100%	100%	N/A
	CP Reliability	N/A	45.4%	45.43%	N/A
	MT Reliability	N/A	68.4%	68.43%	N/A

	Probability ECD | WC 0 – 1 CFU / 100mL	N/A	0%	0%	N/A
	Probability ECD | WC 1 – 10 CFU / 100mL	N/A	0.75 – 2.00%	0.75 – 2.00%	N/A
	Probability ECD | WC 10 – 100 CFU / 100mL	N/A	0.87 – 3.00%	0.87 – 3.00%	N/A
	Probability ECD | WC 100 – 1000 CFU / 100mL	N/A	0.94 – 3.71%	0.94 – 3.71%	N/A
	Probability ECD | WC > 1000 CFU / 100mL	N/A	1.08 – 3.29%	1.08 – 3.29%	N/A
Single Parameter Behavior Space Analysis	**MT Usage**	The water usage was assumed to be between 0.49 and 0.96 for each day.	0 – 100%	0 – 100%	N/A
	CP Usage	The water usage was assumed to be between 0.49 and 0.96 for each day.	0 – 100%	0 – 100%	N/A
	SW Usage	The water usage was assumed to be between 0.49 and 0.96 for each day.	0 – 100%	0 – 100%	N/A
	“Narrow Neck” Container Use	The water usage was assumed to be between 0.49 and 0.96 for each day.	0 – 100	0 – 100	N/A
	Biofilm Layer Contribution	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	0 – 5000 CFU / 100mL	0 – 5000 CFU / 100mL	N/A
	Water Transfer Device (Cup) Contribution	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	0 – 5000 CFU / 100mL	0 – 5000 CFU / 100mL	N/A
	Slow Sand Filter	ON	ON	ON / OFF	N/A
	SW Reliability (Every X Days)	Frequencies drawn from histograms in Figure S8 Mellor et al 2012	Values reported by households in surveys Figure S8	1 - 7	N/A
	CP Reliability (Every X Days)	45.43%	45.43%	1 - 7	N/A
	MT Reliability (Every X Days)	68.43%	68.43%	1 - 7	N/A

	Collection Interval (Collect Every X Days)	Frequencies drawn from histograms in Figure S6 Mellor et al 2012	Values reported by households in surveys Figure S6	1 - 7	N/A
	Cleaning Interval (Clean every X Days)	Frequencies drawn from histograms in Figure S8 Mellor et al 2012	Values reported by households in surveys Figure S8	1 - 7	N/A
	Hand-washing (Hand-washing events per day)	Frequencies drawn from histograms in Mellor et al 2012	Values reported by households in surveys Figure S5	1 - 32	N/A
	SW Water contamination	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	Values drawn from field measurements	0 – 2500 CFU / 100mL	N/A
	CP Water contamination	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	Values drawn from field measurements	0 – 1000 CFU / 100mL	N/A
	MT Water contamination	Frequencies drawn from histograms in Figure S4 Mellor et al 2012	Values drawn from field measurements	0 - 500 CFU / 100mL	N/A
	Boiling Interval (Every X Days)	Frequencies drawn from histograms in Figure S7 Mellor et al 2012	Values reported by households in surveys Figure S7	1 – 7	N/A
	Storage Container Type	1= Wide or 2 =Narrow	1= Wide or 2 =Narrow	1= Wide or 2 =Narrow	N/A

Appendix C – This was adapted from the template for (Overview, Design Concepts and Details + Decision-making) ODD+D, with the guiding questions and responses relevant to this study meant to formalize the description of agent-based models with a cognitive component. This template is available online and in Muller et al, 2013.[77,114,115]

Outline		Guiding questions	ODD+D Model description
I) Overview	I.i Purpose	I.i.a What is the purpose of the study?	The goal of the agent-based model (ABM) in this study is to understand the effectiveness of established ABM for predicting early childhood diarrhea (ECD) during a CWF intervention, while revising the model to include additional measures of adherence and filter flow rates. This is drawn from the goal of the previous research (to "investigate the role of factors affecting the imperfect use of CWFs in preventing early childhood diarrhea using an extension of an ABM described previously").[62,64]
		I.ii.b For whom is the model designed?	This model has been developed for scientists and researchers. Unique additions to the model include packaging all components (where feasible) into a password protected executable file, to streamline reproducibility while maintaining limited confidentiality. This may allow for the use of the model by others (decision makers, stakeholders). This model was developed without complete individual-level data, as a replication of the original model.
	I.ii Entities, state variables, and scales	I.ii.a What kinds of entities are in the model?	Agents in this model include households and children. Household agents own attributes which relate to their WASH status and available drinking water contamination (WC). Households can provide water to child agents. Children are all under two years of age, consume water in the household, and get sick from consuming poor quality water. There is one child per household in this model. The grid cells in this model correspond to GPS points, which include household locations, and water source locations. These GPS points are measured in decimal format. They do not

			correspond directly to actual household locations due to the geo-referencing process.
		I.ii.b By what attributes (i.e. state variables and parameters) are these entities characterized?	<u>Agents:</u> There are 410 children born to 410 households at "day 0" of the model. Children are at age 0, and grow until age 2 during the course of the model. They are located at the GPS coordinates of the households in Limpopo, South Africa and were subjects of an original series of agent-based models.[62,64] The sex ratio of the children is taken from survey data. The height distribution is taken from the WHO SD heights. Households can own ceramic water filters, and they can use these filters if they decide to. Each household is randomly assigned a filter degradation curve, taken from field measurements. Households who have no information on water source, filter usage, or water storage search radially out until the find a household with survey information, and set their information to match the survey information. More households are simulated in this model then survey data were originally collected for. <u>Spatial units:</u> In Netlogo, the spatial units are aligned on a grid of x and y coordinates. <u>Collectives:</u> Filters collectively break on a given day and children are born on a given day (day 0). More information on agent characteristics can be found in Appendix B.
		I.ii.c What are the exogenous factors / drivers of the model?	The sources of water available to the agents are derived from field measures. In this way, water contamination is driven by the shifts in microbiological contamination among three sources of water. Additionally, the children can be protected from the main outcome (ECD) through vaccination, which is influenced by a myriad of contextual factors.

		I.ii.d If applicable, how is space included in the model?	This is a georeferenced model, with spatial data incorporated into the locations of households. Space is included as the location of households and children.
		I.ii.e What are the temporal and spatial resolutions and extents of the model?	One time step ("*tick*") represents one day in the model time. One grid cell represents one decimal point of GPS coordinate system. Children grow for two years, and the model is run for two years. For the baseline model, each single parameter value was run 100 times (using the Behavior Space Analysis tool in Netlogo).
	I.iii Process overview and scheduling	I.iii.a What entity does what, and in what order?	At the start of the model, children (in code: *children)* are randomly born to households (*households)*, one per house. These are linked within the model conceptually. Each day, each household can collect water (*collect-water*) from various water sources, including a municipal tap system (*mt-WQ*), a local river surface water (*surf-WQ*) and community piped water supply (*pipe-wq*). Each household has a preferred source (*pri-water-source*), and a secondary preferred source (*sec-water-source*), if the primary source is not operational. Each source has a field-derived frequency of which it is operational. If their primary source is not operational, agents wait a number of days (with a frequency drawn from survey data, and applied randomly to all households) until reach their limit of waiting (*hh-days-can-wait)*, and then switch to their secondary source and repeat. After the households collect water, it must be stored in a storage container (*storage-container)* which has some risk of biofilm growth, which can have a narrow or wide neck (*narrow-neck* or *wide-neck)*. Water can be removed with a cup or hand, resulting in contamination (*cup_total or bhw_total)*. This process has been described with a "Water Chain Contamination Model".[84] Households can clean their storage containers, which can improve water quality. The household now has a final water

			quality for each "tick" or day of WQ*i* (Described as WC in thesis, and WQ*i* in code). At this point, if a household has a filter (*has-filter = 1)* they can use the filter to reduce water contamination. Some level of households who have a filter will decline to use the filter according to an adherence (*adherence*) value. Of those that chose to use, those that find their filter too slow (4.7% randomly selected households) will chose to stop filtering their water, even if they would otherwise filter. Finally, the water contamination (*WQi)* after filtering is converted into a potential for ECD given the propensity for drinking water and the probability of getting ECD (*previous-cases, vaccination, hand-wash*). Finally, this probability is converted into predicted cases of early childhood diarrhea (*all-ecd-cases*) among children, which causes growth stunting, recorded as total days stunting (*total-stunt-days)*. In the version of the model used herein, the growth stunting model is not utilized. Model steps are provided in Appendix D.
II) Design Concepts	II.i Theoretical and Empirical Background	II.i.a Which general concepts, theories or hypotheses are underlying the model's design at the system level or at the level(s) of the submodel(s) (apart from the decision model)? What is the link to complexity and the purpose of the model?	The general concept which underlies this model is that although CWFs have been shown to work well in the field, issues with adherence (correct and consistent use) filter breakage, filter flow rate, and bacterial recontamination of water storage vessels has been an issue. This model addresses these concerns for field implementations of CWF in a virtual way, without the expense of long-term field studies. The link to complexity is especially shown with the filter flow rate perception, as the response of households to the performance of the filter has shown strong heterogeneity, and this may influence the effectiveness of CWF interventions.
		II.i.b On what assumptions is/are the	**Decision** | Assumption **Which source of water to use?** | We assume that households can communicate about their water use patterns and that the households surveyed, on

		agents' decision model(s) based?	average, reflect the processes of those around them. It has been noted that the preference for water treatment is influenced by social pressure and previous cultural experiences.[29] **Should I filter this water?** | It has also been shown that in some cases, people are able to perceive shifts in water quality and adapt to these shifts in contamination. We assume that households with a WC above a threshold (100 CFU/100mL) are 2.05 times as likely as those below to filter their water.[37] We assume that the ability of households to detect contamination does not appreciably vary among households **Should I buy another filter?** | After the first batch of 410 CWF are distributed free of charge on day 0, some of these filters may break. When they do, households have an option to replace them, if the current price of ceramic water filters is below their willingness to pay as determined by experimental field data. **Should I wash my hands?** | Hands, in the case that they were used for the transport of water from the storage container, were a possible vector for exposure to pathogens. Therefore, the agent's choice to wash hands is another factor. This choice is drawn from experimental field data, and frequencies for each level of handwashing are applied to all households, randomly.
		II.i.c Why is a/are certain decision model(s) chosen?	Experimental and field-derived decision models were preferred over theoretically derived models. References to other studies were also used.
		II.i.d If the model / a submodel (e.g. the decision model) is based on empirical data, where does the data come from?	The model comes from household surveys, direct observations by previous study staff, statistical census (WHO height values), GIS data collection, and previously published work.

		II.i.e At which level of aggregation were the data available?	Most data are at the household or individual level (each household has one child). The only group level variables would be: the *break-date* for filters, the frequency of water collection (*water-collect-freq*), the GPS locations of the households (*hhb_abm_gps_locations2.txt, ceramic-abs-locations-2.txt, remaining-abm-gps-locations2.txt*), and the water contamination of the sources (*pipe-wq, mq-wq, surf-wq*).
	II.ii Individual Decision Making	II.ii.a What are the subjects and objects of decision-making? On which level of aggregation is decision-making modeled? Are multiple levels of decision making included?	Households without survey data (water source, length of time that agents can wait to use it, and handwashing and water storage behaviors) look to other households nearby that have survey data and match themselves to "fit in" with those results in a radial pattern. Households can also look to the water quality of their sources and decide whether to treat or not to treat.
		II.ii.b What is the basic rationality behind agents' decision-making in the model? Do agents pursue an explicit objective or have other success criteria?	Agent behaviors are mostly drawn from the results of field studies; thus they would be an example of bounded rationality. This may suffer from publication bias, however. Agents do not pursue a specific objective, but rather refer to a set of field and study derived rules.
		II.ii.c How do agents make their decisions?	Decision trees are used to model agent's decision making. The household's decision profiles (e.g. Am I an adherent household or not?) are ascribed randomly.
		II.ii.d Do the agents adapt their behavior to changing endogenous and	Yes. Agents can "perceive" contaminated water and adapt their filtering or treating methods to adjust. This is completed by comparing the household

		exogenous state variables? And if yes, how?	water contamination to a threshold of detection, set at 100 CFU / 10 mL in the baseline model.
		II.ii.e Do social norms or cultural values play a role in the decision-making process?	Partially. Households look to their neighbors and copy them directly. In this way, there is a cultural norm for water source selection.
		II.ii.f Do spatial aspects play a role in the decision process?	Yes. Households who are next to each other are more likely to be similar.
		II.ii.g Do temporal aspects play a role in the decision process?	Yes. Children who have had diarrhea are more likely to have diarrhea again.
		II.ii.h To which extent and how is uncertainty included in the agents' decision rules?	Stochastic elements in agent's decision making and the random allocation of agent characteristics for highlight uncertainty.
	II.iii Learning	II.iii.a Is individual learning included in the decision process? How do individuals change their decision rules over time as consequence of their experience?	Agents do not learn through time.
		II.iii.b Is collective learning	No collective learning (no genetic algorithms or evolution).

		implemented in the model?	
	II.iv Individual Sensing	II.iv.a What endogenous and exogenous state variables are individuals assumed to sense and consider in their decisions? Is the sensing process erroneous?	Agents can directly sense water quality. Household agents can also sense other households who have survey data.
		II.iv.b What state variables of which other individuals can an individual perceive? Is the sensing process erroneous?	None.
		II.iv.c What is the spatial scale of sensing?	Local (sense until you see another survey household, or look for the closest water source).
		II.iv.d Are the mechanisms by which agents obtain information modeled explicitly, or are individuals simply assumed to know these variables?	Sensing is only local. Network-based sensing would be useful, but is not currently implemented.
		II.iv.e Are costs for cognition and costs for gathering information included in the model?	No.

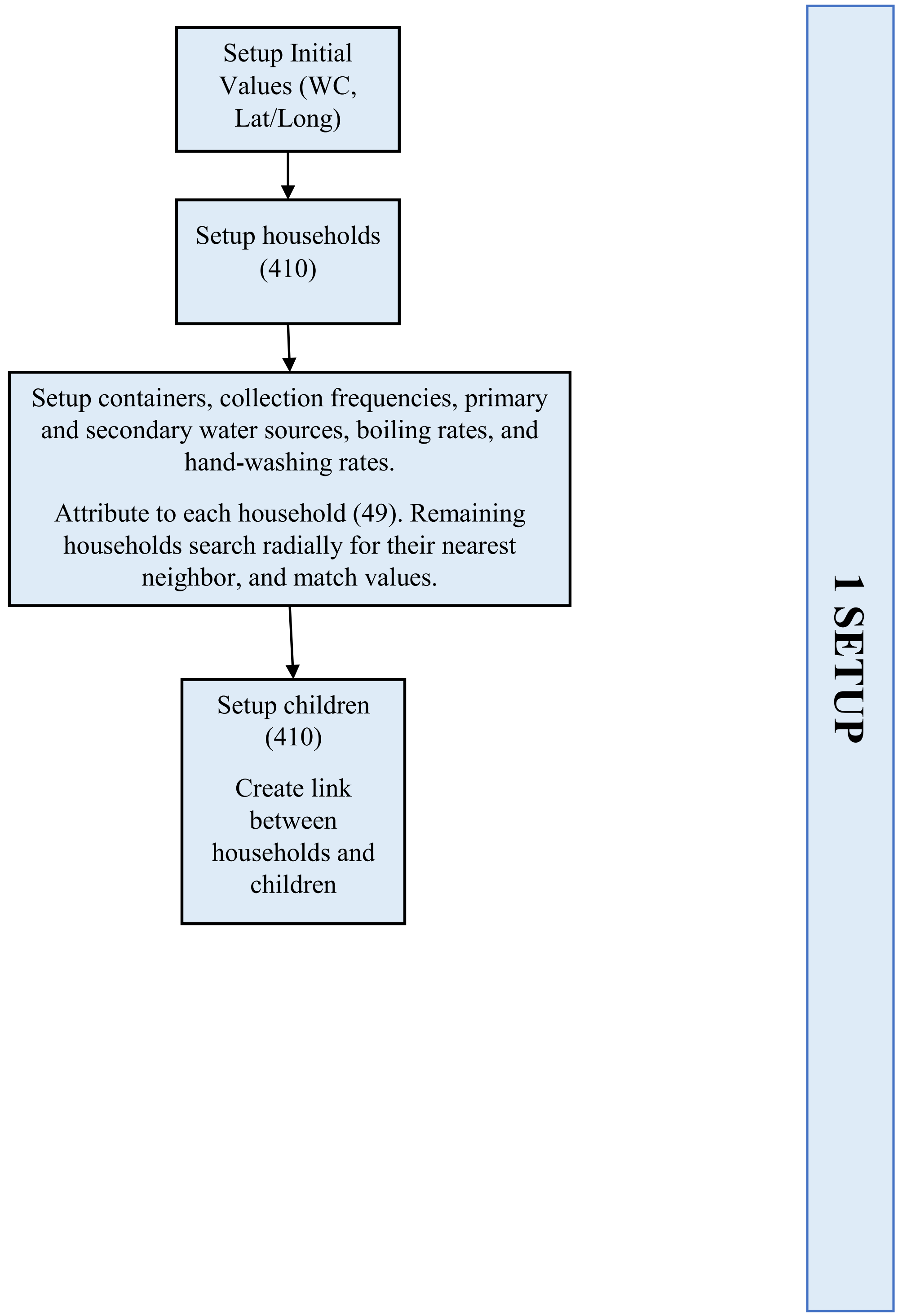
	II.v Individual Prediction	II.v.a Which data uses the agent to predict future conditions?	Spatial observations.
		II.v.b What internal models are agents assumed to use to estimate future conditions or consequences of their decisions?	They do not have internal models. They do have a limit of how long they can keep water and how long they can wait if they cannot access a source of water before they revert to their secondary water source.
		II.v.c Might agents be erroneous in the prediction process, and how is it implemented?	Agents are never wrong – no internal capability was modeled. Nevertheless, the ability of agents to sense the water is a range (uncertain).
	II.vi Interaction	II.vi.a Are interactions among agents and entities assumed as direct or indirect?	Agents are always interacting directly. There is an undirected link from household to child which allows them to transfer information.
		II.vi.b On what do the interactions depend?	Spatial distance (GPS)
		II.vi.c If the interactions involve communication, how are such communications represented?	N/A
		II.vi.d If a coordination network exists, how does it	No coordination network beyond GPS coordinates.

		affect the agent behaviour? Is the structure of the network imposed or emergent?	
	II.vii Collectives	II.vii.a Do the individuals form or belong to aggregations that affect, and are affected by, the individuals? Are these aggregations imposed by the modeller or do they emerge during the simulation?	No social groups or human networks.
		II.vii.b How are collectives represented?	Collectives are not represented in the model.
	II.viii Heterogeneity	II.viii.a Are the agents heterogeneous? If yes, which state variables and/or processes differ between the agents?	Yes. Agents are heterogeneous by source water type, WASH behaviors (handwashing, water storage, etc.), and by GPS location.
		II.viii.b Are the agents heterogeneous in their decision-making? If yes, which decision models or decision objects differ between the agents?	Yes. Agents are randomly allocated to different decision paths.

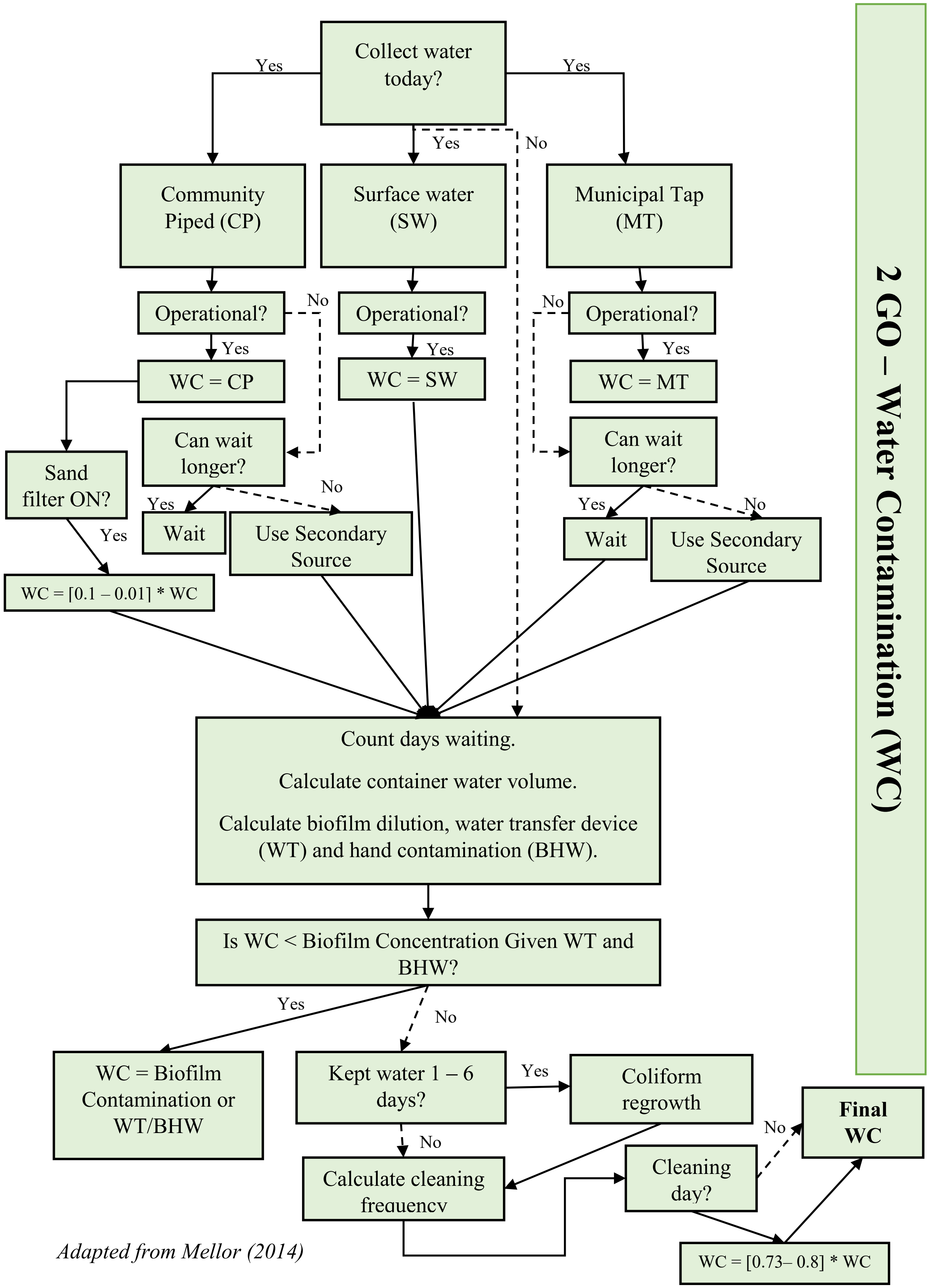
	II.ix Stochasticity	II.ix.a What processes (including initialization) are modeled by assuming they are random or partly random?	Coliform contamination of water sources, filter microbiological removal deterioration rate, and HAZ values are modified by random variables along their distribution.
	II.x Observation	II.x.a What data are collected from the ABM for testing, understanding, and analyzing it, and how and when are they collected?	Two main outcomes are collected: the total number of ECD cases per child (*ecd-cases*) and the total WQi (*WQi, herein WC*) for each household. They are automatically output by Netlogo in .xls format.
		II.x.b What key results, outputs or characteristics of the model are emerging from the individuals? (Emergence)	None.
III) Details	II.i Implementation Details	III.i.a How has the model been implemented?	#1: Windows 10 | i5-3320 Processor | 8 GB RAM #2: Windows 10 | i7-6500 Processor | 16 GB RAM Simulation Platform: Netlogo 5.3 and Netlogo 5.3.1 Runtime: From 10 hours – 32 hours
		III.i.b Is the model accessible and if so where?	Please email kyle.monahan@tufts.edu, permission from Dr. Jonathan Mellor will be requested.
	III.ii Initialization	III.ii.a What is the initial state of the model world, i.e. at time t=0 of a simulation run?	The households are formed without water sources and with one child inside each. All variables other than water quality and location are set to null, or a set containing no data (*[ ]*).
		III.ii.b Is initialization	The initialization is always the same. A random seed value of 22 is used to standardize randomness.

		always the same, or is it allowed to vary among simulations?	
		III.ii.c Are the initial values chosen arbitrarily or based on data?	They are based on data.
	III.iii Input Data	III.iii.a Does the model use input from external sources such as data files or other models to represent processes that change over time?	Yes. Water quality inputs are drawn from field observations.
	III.iv Submodels	III.iv.a What, in detail, are the submodels that represent the processes listed in 'Process overview and scheduling'?	Sub-models would include the Water Source Chain, where the water can be contaminated along the "chain" from source, transport, storage, and ingestion. A simple sub-model of cognition includes the assumption that 4.7% of households do not adhere due to a low perceived flow rate.
		III.iv.b What are the model parameters, their dimensions and reference values?	Model parameters are given in Appendix A and B.
		III.iv.c How were submodels designed or chosen, and how were they parameterized and then tested?	The Water Source Chain sub-models were parameterized by previous authors.[64]

Appendix D – A flow chart for the ABM process, adapted from Supplemental Info for the previous model.[64] This includes: 1) setup, 2) water contamination, 3) ceramic water filter intervention and 4) ECD calculations.

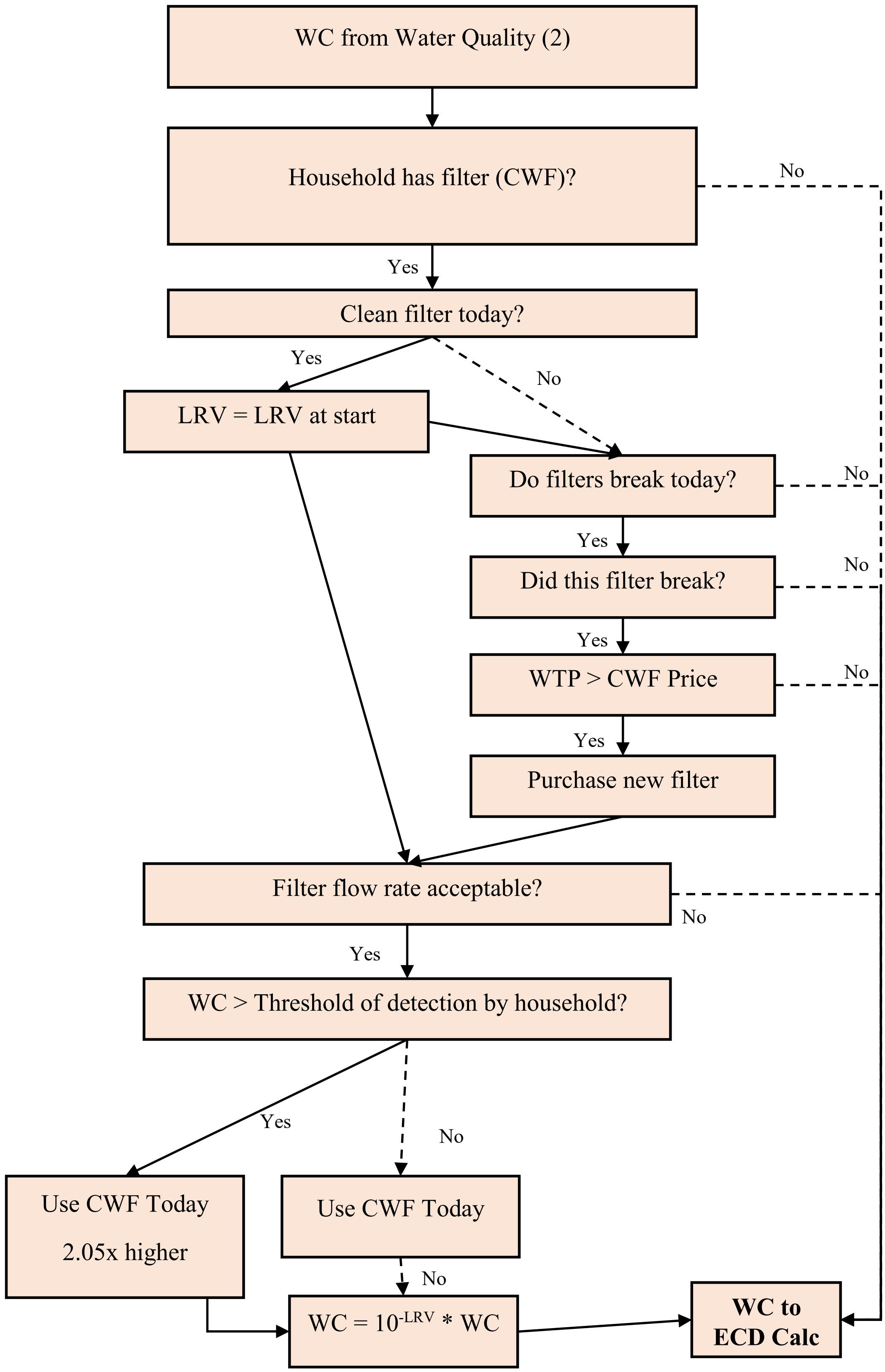


2 GO – Water Contamination (WC)



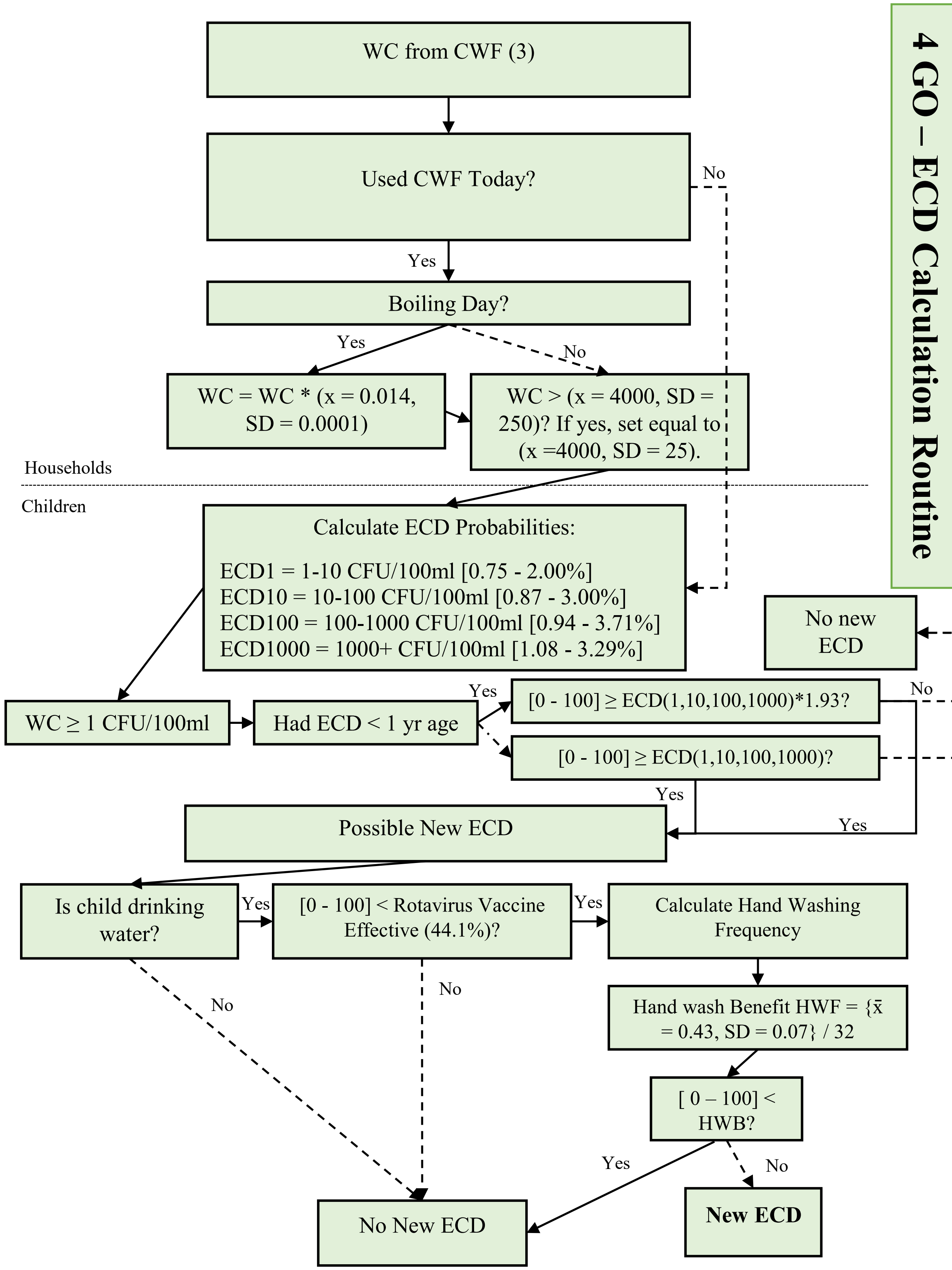
Adapted from Mellor (2014)

3 GO – Ceramic Water Filter Routine



Adapted from Mellor (2014)

4 GO – ECD Calculation Routine



Adapted from Mellor (2014)

Appendix E – The standardized predicted residuals for the linear regression analysis are plotted. There is notable bias within the residual plot, suggesting linear regression may not be appropriate.