Supporting Information for Modeling the Complexities of Water, Hygiene, and Health in Limpopo Province, South Africa

Jonathan E. Mellor,[†] James A. Smith,[*,†,‖] Gerard P. Learmonth,[‡] Vhonani O. Netshandama,[¶] and Rebecca A. Dillingham[§]

Department of Civil and Environmental Engineering - The University of Virginia, Department of Systems Engineering - The University of Virginia, Advanced Nursing Sciences - The University of Venda, and Center for Global Health, School of Medicine - The University of Virginia

E-mail: jsmith@virginia.edu

This Supporting Information section is 27 pages long and contains 16 Figures and 5 tables.

[†]Department of Civil and Environmental Engineering - The University of Virginia
[‡]Department of Systems Engineering - The University of Virginia
[¶]Advanced Nursing Sciences - The University of Venda
[§]Center for Global Health, School of Medicine - The University of Virginia
[‖]P.O. Box 40072, Charlottesville, VA 22904-4742

Supporting Figures and Tables

Table S1: Variables 'owned' by the two agent types: households and children. 1 - variables that can change daily. 2 - variables that are stochastically varied between minimum and maximum reported values. All values based on data collected in the communities for individual households or children. Households not surveyed take on values of their nearest neighbor. SW - surface water, CP - community piped, MT - municipal tap, WQ_i daily water quality of ith household.

Households		Children	
Variable	Range	Variable	Range
Primary water source	SW,CP,MT	Sex	M/F
Secondary water source	SW,CP,MT	Age^1	0 - 730 d
Daily water quality (WQ_i)^1	0-4000 cfu/100ml	ECD Status^1	single/double case
Days have kept water^1	0+ d	Daily growth^1 increment	-0.198 - 0.176 cm
Maximum days can keep water	1 - 14 d	Height^1	0+ cm
Water collection interval^2	every 1 - 10 d		
Water container cleaning interval^2	every 1 - 365 d		
Water boiling interval^2	every 1 - 30 d		
Daily hand-washing interval^2	0 - 24 #/d		
Coliforms associated with hands	0 - 8,615 cfu/100ml		
Biofilm layer coliform contribution (HHS_i)	0 - 10,000 cfu/100ml		
Water transfer device coliform contribution	0 - 5,064 cfu/100ml		

Table S2: Global variables used in model. All variables ranges gathered from field data. ECD - early childhood diarrhea. HAZ - number of standard deviations above or below world health organization normal values. SW - surface water, CP - community piped, MT - municipal tap

Variable	Value or Range
Duration of Stunted Growth	240 d
Single ECD Case HAZ Reduction	-1.50 - 1.47
Double ECD Case HAZ Reduction	-2.18 - 1.93
SW Water Quality	0 - 4120 cfu/100ml
CP Water Quality	0 - 1220 cfu/100ml
MT Water Quality	0 - 500 cfu/100ml
SW Reliability	100.00%
CP Reliability	45.43%
MT Reliability	68.43%

Table S3: Daily probabilities of getting early childhood diarrhea (ECD) based on household water quality (WQ_i). Values based on literature values for *E. Coli* and correspond to WHO guidelines on risk associated with the consumption of various water qualities.

WQ_i	Probability of Getting ECD
0 - 1 cfu/100ml	0%
1 - 10 cfu/100ml	0.75 - 2.00%
10 - 100 cfu/100ml	0.87 - 3.00%
100 - 1000 cfu/100ml	0.94 - 3.71%
1000+ cfu/100ml	1.08 - 3.29%

Table S4: Parameters and their values used in the single-parameter behavior space analysis. All parameters and value ranges used were based field measurements. For the single-parameter behavior-space experiments, each parameter was varied over those respective ranges. Results are summarized in Figure 2 of the main text and in Figure S15 and Figure S16. SW - surface water, CP - community piped, MT - municipal tap

Parameter	Single Parameter Values
MT Useage	0 - 100%
CP Useage	0 - 100%
SW Useage	0 - 100%
‘Narrow Neck’ Container Use	0-100
Biofilm Layer Contribution (cfu/100ml)	0, 100, 200, 300, 400, 500, 1000, 2000, 3000, 4000, 5000
Water Transfer Device Contribution (cfu/100ml)	0, 100, 200, 300, 400, 500, 1000, 2000, 3000, 4000, 5000
Slow Sand Filter	ON, OFF
SW Reliability (Operational every X Days)	1 - 7
CP Reliability (Operational every X Days)	1 - 7
MT Reliability (Operational every X Days)	1 - 7
Collection Interval (Collect every X Days)	1 - 7
Cleaning Interval (Clean every X Days)	1 - 7
Hand-Washing (Hand-washing events per day)	1 - 32
SW Water Quality (cfu/100ml)	0, 250, 500, 1000, 2500
CP Water Quality (cfu/100ml)	0, 50, 100, 250, 500, 1000
MT Water Quality (cfu/100ml)	0, 25, 50, 100, 250, 500
Boiling Interval (Every X Days)	1-7

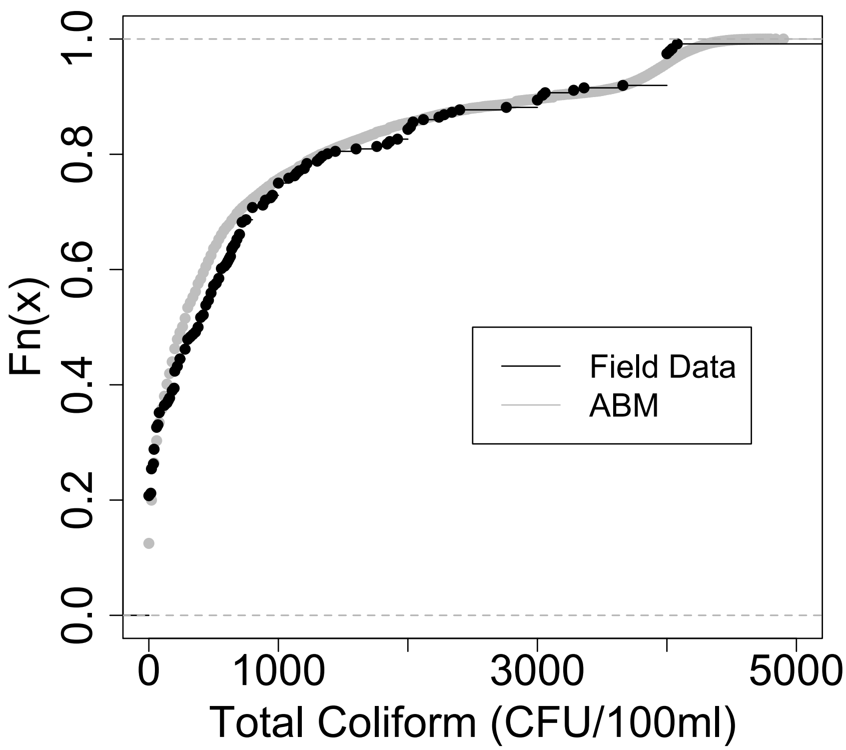

Figure S1: Cumulative distribution function (Fn(x)) of 8 months of household water quality field measurements compared to discretized ABM simulated values.

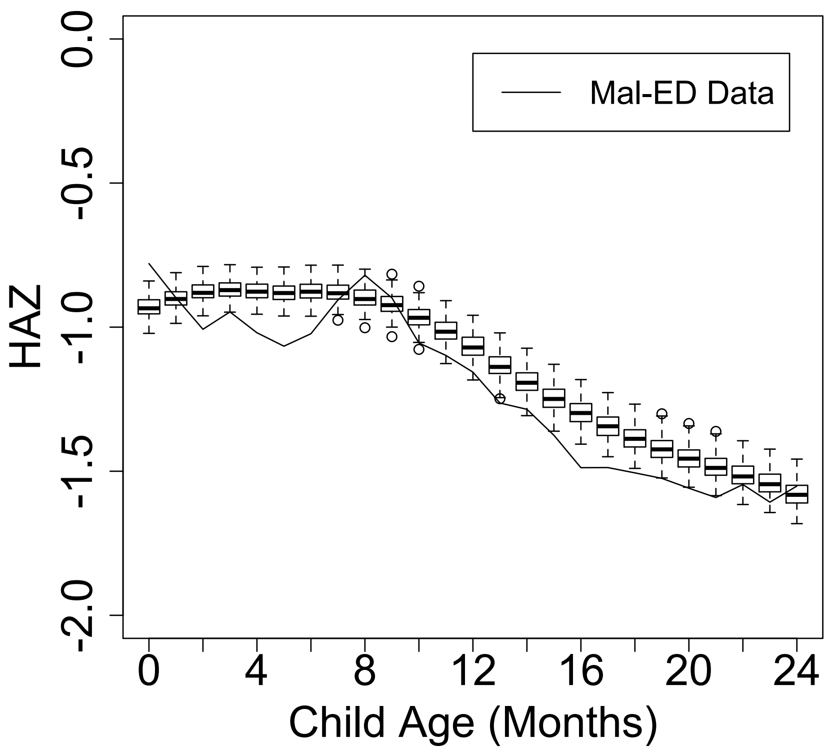

Figure S2: A plot of HAZ scores vs child age. The ABM results are shown with box plots, while the average monthly Mal-ED data is given with the solid line. One sample t-tests shown in Table S5 indicate that the model is accurate for 22 of the 25 months. HAZ - number of standard deviations above or below world health organization normal values.

Table S5: P-values for t-test comparing simulated and field values for child height. These p-values indicate that the model reasonably replicates field data for 22 of the 25 months.

Month	p-value
0	0.014
1	0.971
2	0.068
3	0.286
4	0.054
5	0.019
6	0.053
7	0.735
8	0.381
9	0.776
10	0.329
11	0.331
12	0.344
13	0.133
14	0.301
15	0.201
16	0.049
17	0.135
18	0.285
19	0.363
20	0.403
21	0.382
22	0.813
23	0.653
24	0.850

Model Development

The model was developed using Netlogo with data obtained from community surveys. The first sections of this supplement will describe the setup routines used to initialize the model along with the community survey questions from where the input data was generated. Next are flowcharts describing in detail the model's important subroutines. Finally, expanded sensitivity and behavior space analyses are presented.

Setup

Households

The first setup routine, overlays the 410 households onto a Google Maps®satellite image of the communities. Household placement is based on GPS coordinates recorded and are verified by visual inspection of the Google Map overlay. This arrangement can be seen in Figure S3.

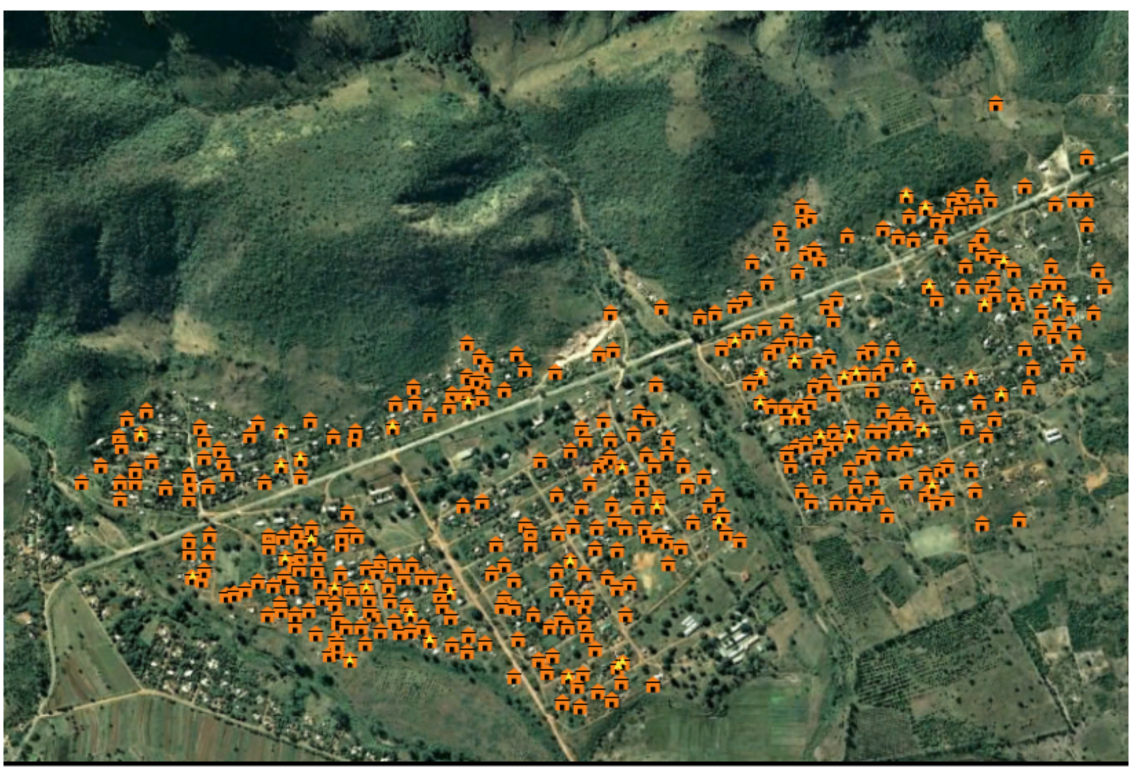

Figure S3: Graphical interface of the ABM in Netlogo. Households locations shown.

Water Sources

The communities rely on three main water sources described in the main text: surface water (SW), community piped (CP) and municipal tap (MT). Each source's quality was measured during 8 months of testing as reported in previous work (1). These data are stored in the model and accessed during the child-drink subroutine below. Histograms of the water quality data for all three sources is given in Figure S4.

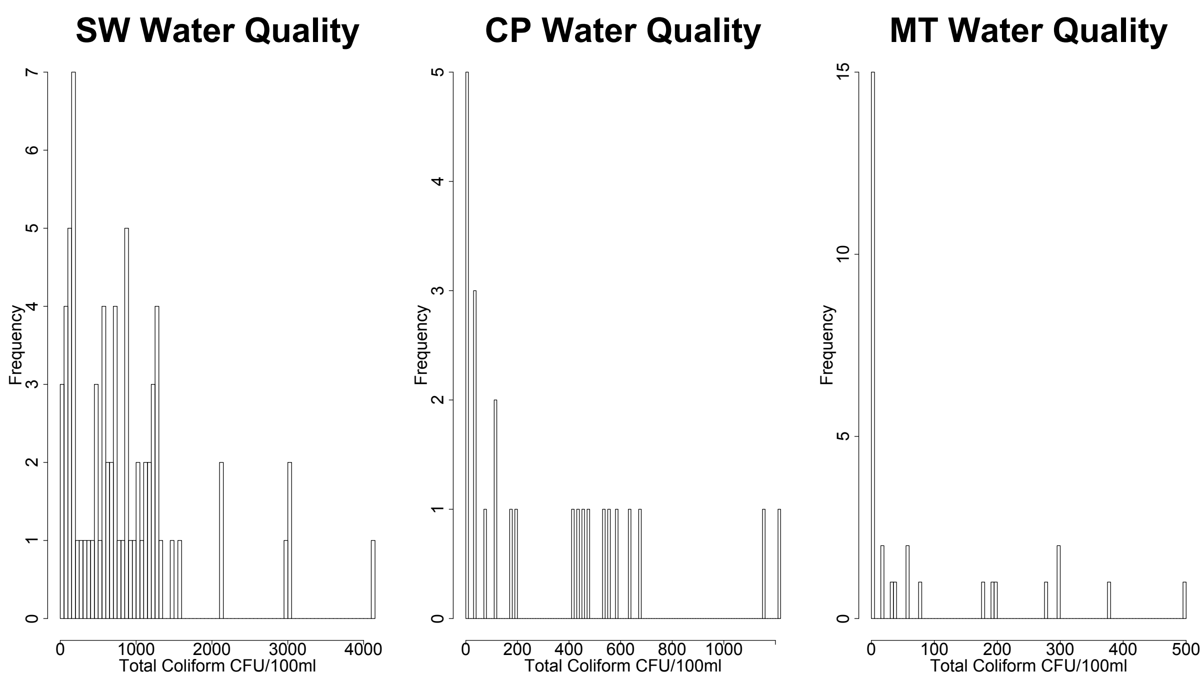

Figure S4: Histograms of water quality measurements used in the ABM for the three main water sources: surface water (SW), community piped (CP) and municipal tap (MT). Data indicate large inter and intra-monthly variability in all three sources.

Water Storage Containers

Biological testing of household water storage containers was reported on previously (1). Residents typically used two different storage container types 'narrow neck' and 'wide neck'. Each storage container has an associated biofilm layer contribution as discussed in the main text. Houses with 'wide neck' style containers must insert their hands and scoop water out which will contaminate the water. The characteristics of surveyed households are then shared to surrounding households by having each surrounding household seek out surveyed households in a progressively larger radius until they find a household with the relevant values. Histograms of these contributions is shown in Figure S5.

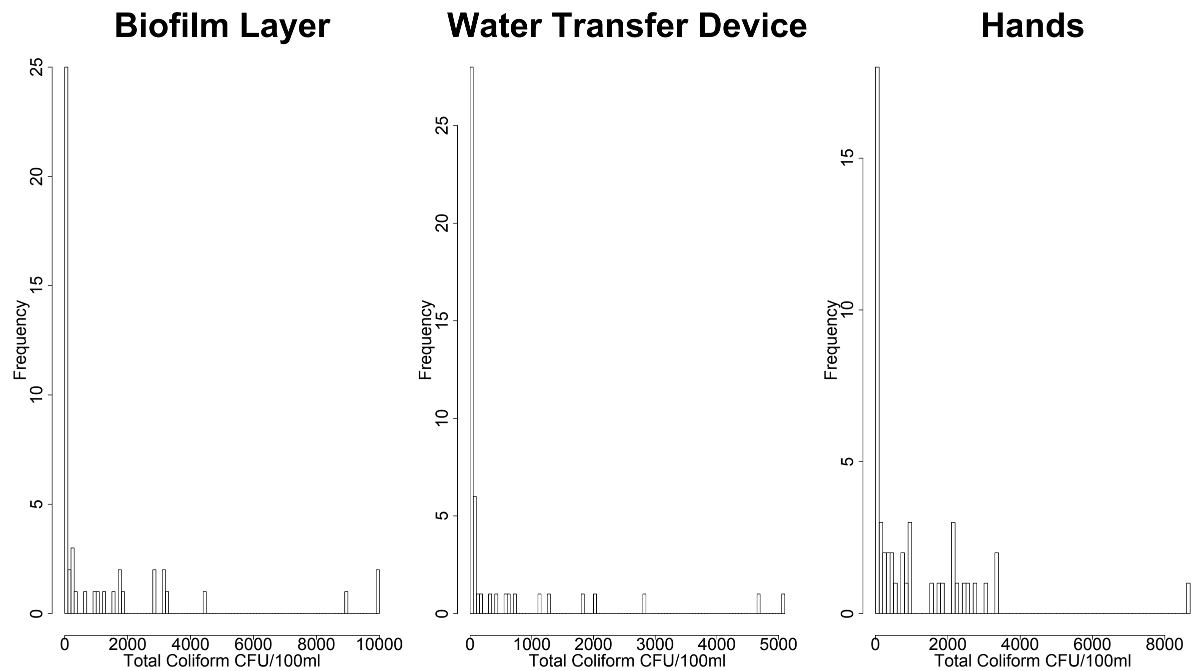

Figure S5: Histograms of biofilm layer (HHS_i), water transfer device and hand contributions to water contamination. All three show large heterogeneity and strong potential as large contributors to household water quality deterioration. Water transfer device and hand contributions have the potential to contaminate 'wide neck' storage containers, but not 'narrow neck' ones.

Water Collection Intervals

Residents were queried several different ways about their water collection habits. First, they were asked what their primary and secondary water sources were. They were then asked the basic question "How often do you collect water?" on two different occasions. Next, they were asked to keep a daily log for 4 weeks detailing each time they collected water. These data were then converted into collection intervals. The lowest and highest reported values are used in the ABM. Finally they were asked "How many days can you wait until you need to use secondary source?" which is used as the maximum number of days households will take before they revert to secondary water sources. As with the other metrics, households that were not surveyed take on the characteristics of nearby households. Histograms of collection frequency are shown in Figure S6.

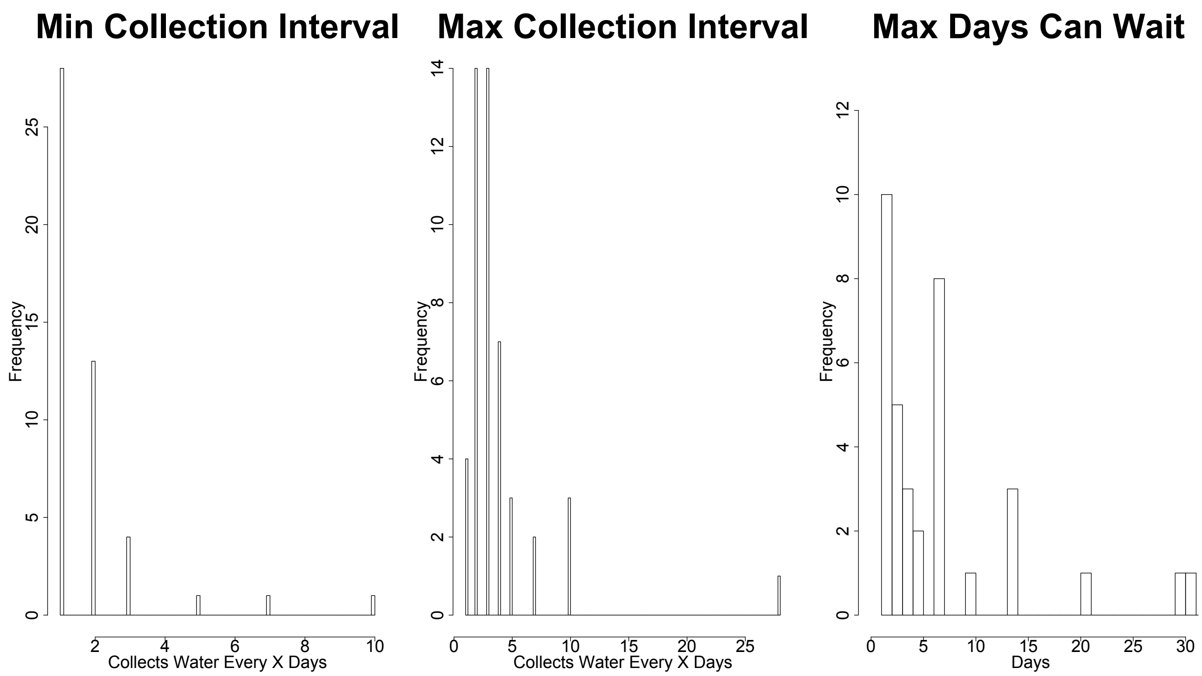

Figure S6: Histograms of collection frequency. Minimum and maximum collection intervals based on the minimum and maximum values reported by households during surveying. Maximum days can wait based on community survey.

Boiling Frequency

Residents reported that they occasionally boil their drinking water to treat it, other treatment methods such as chlorination are not common. Several questions were asked to ascertain resident's boiling frequency including "When did you last treat your water?", "In a given week, how many times do you treat your water?", "In a given day, how many times do you treat your water?", "How frequently do you drink water that has not been treated?". In addition, participants filled out a daily log of their practices. These metrics were all converted to boiling intervals and the minimum and maximum values for each household were used for the ABM. Households not surveyed obtained the boiling intervals of nearby households. Histograms of boiling intervals are shown in Figure S7.

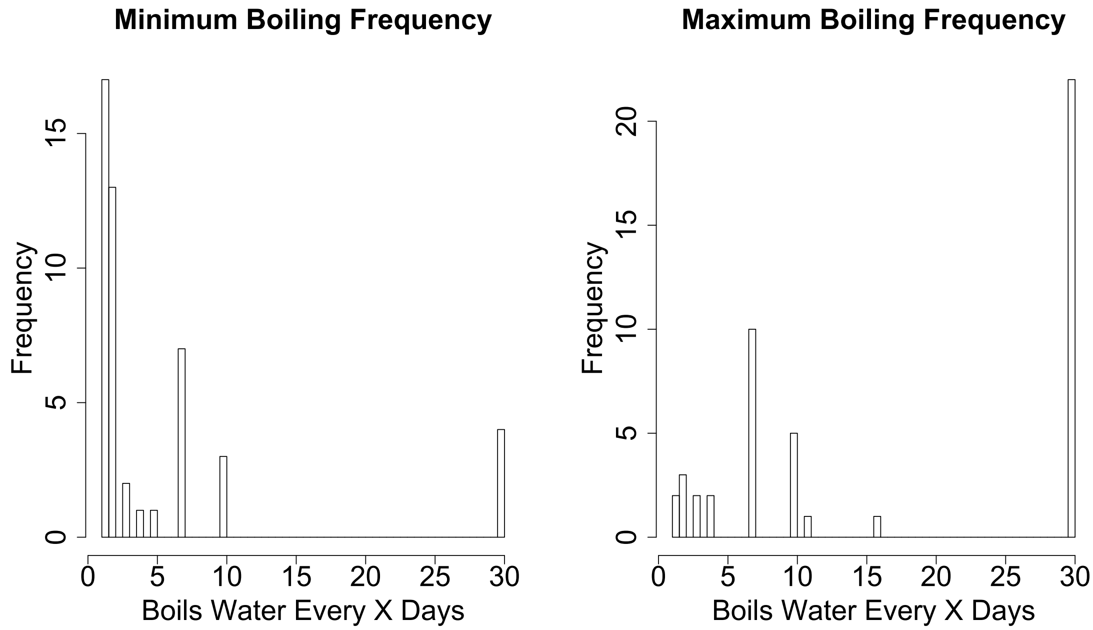

Figure S7: Histograms of boiling frequency. Minimum and maximum boiling intervals based on the minimum and maximum values reported by households during surveys.

Hand-Washing Frequency

Similar to the other metrics, hand-washing was measured in the communities using several questions. These include the questions "In the last 24 hours when did you last wash your hands?", "In the last 24 hours, how many times did you wash your hands?" Participants were also asked to fill out daily logs of hand-washing activities. The minimum and maximum responses were used for the ABM. Households not surveyed took on frequencies of nearby households. Histograms of hand-washing frequency are shown in Figure S8.

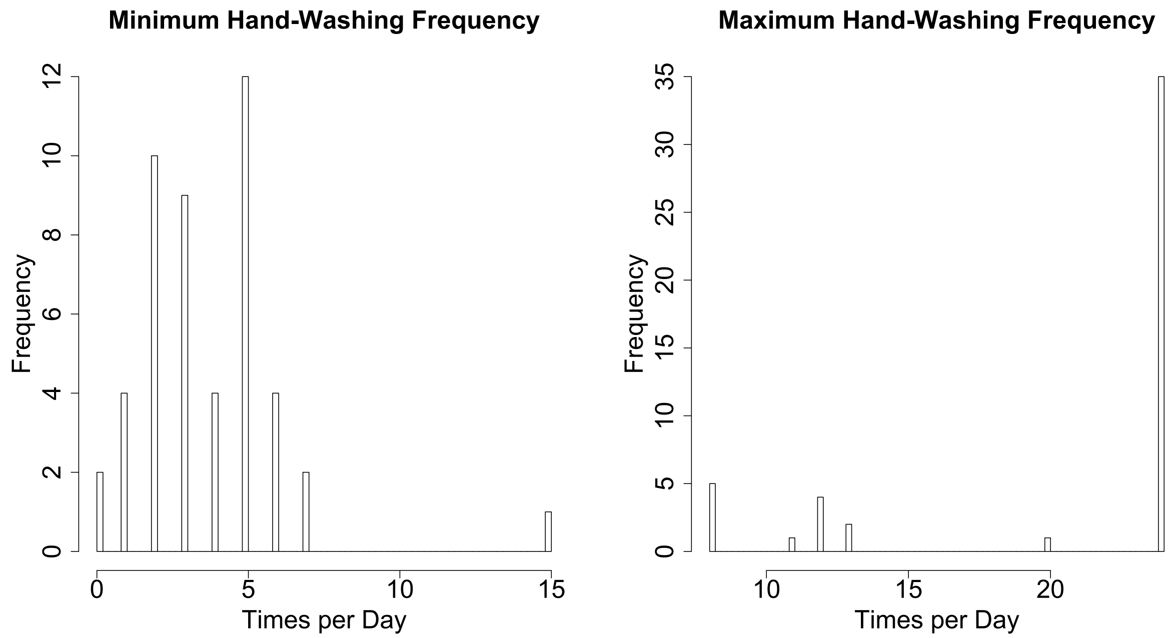

Figure S8: Histograms of hand-washing frequency in terms of the number of times per day. Frequencies based on minimum and maximum values reported by households during surveys.

HAZ

As described in the main text, HAZ scores were calculated by taking the HAZ difference between four months before and four months after an ECD case. Likewise, the calculation was also performed for those with two or more ECD cases during that 8-month period. The ages and HAZ differences are input into the model. When a ABM child gets ECD, they are then assigned a HAZ reduction score of the individual child closest in age to themselves.

Model Overview

Collect Water

The first sub-routine for the model details the water collection, bacteria regrowth, biofilm layer contribution and container cleaning. Residents of the two communities were asked what sources they used and how frequently those sources worked. Results indicate that CP works 45.4% of the time while MT works 68.4% of the time. A flow-chart describing the process is shown in Figure S9.

The experimental protocol reported previously (1) involved introducing 500 mL of sterilized water into empty water storage containers, swirling vigorously and then testing the water to determine the coliform bacteria concentration (HHS_i) (1). This approximates the ability of the biofilm-layer bacteria to contaminate water. However, the ability of a given water container to contaminate a larger volume of water is uncertain. To approximate this process the volume of water in a given water container (V_i) is calculated stochastically between 0.5 and 20 L, which is the range of volumes measured in the community. HHS_i is then diluted according to the following formula where v_i is a stochastic variable between 0.5 L (amount of water used in the experiment) and V_i.

$$hhs_i = HHS_i \times \frac{0.5L}{v_i} \tag{1}$$

This dilution factor ranges in value from 0.025 to 1. WQ_i is not allowed to go below hhs_i during storage.

Water transfer devices are typically cups or ladles used to scoop water from the 'wide neck' storage containers used by approximately half of the households. There is also a significant amount of coliform bacteria associated with a person's hands. If a household has a 'wide neck' storage container then WQ_i is not allowed to go below the sum of these two contamination sources diluted by a factor of $\frac{0.5L}{V_i}$ since those experiments were likewise carried out in 0.5 L of water. Those with 'narrow neck' containers have no such contamination sources.

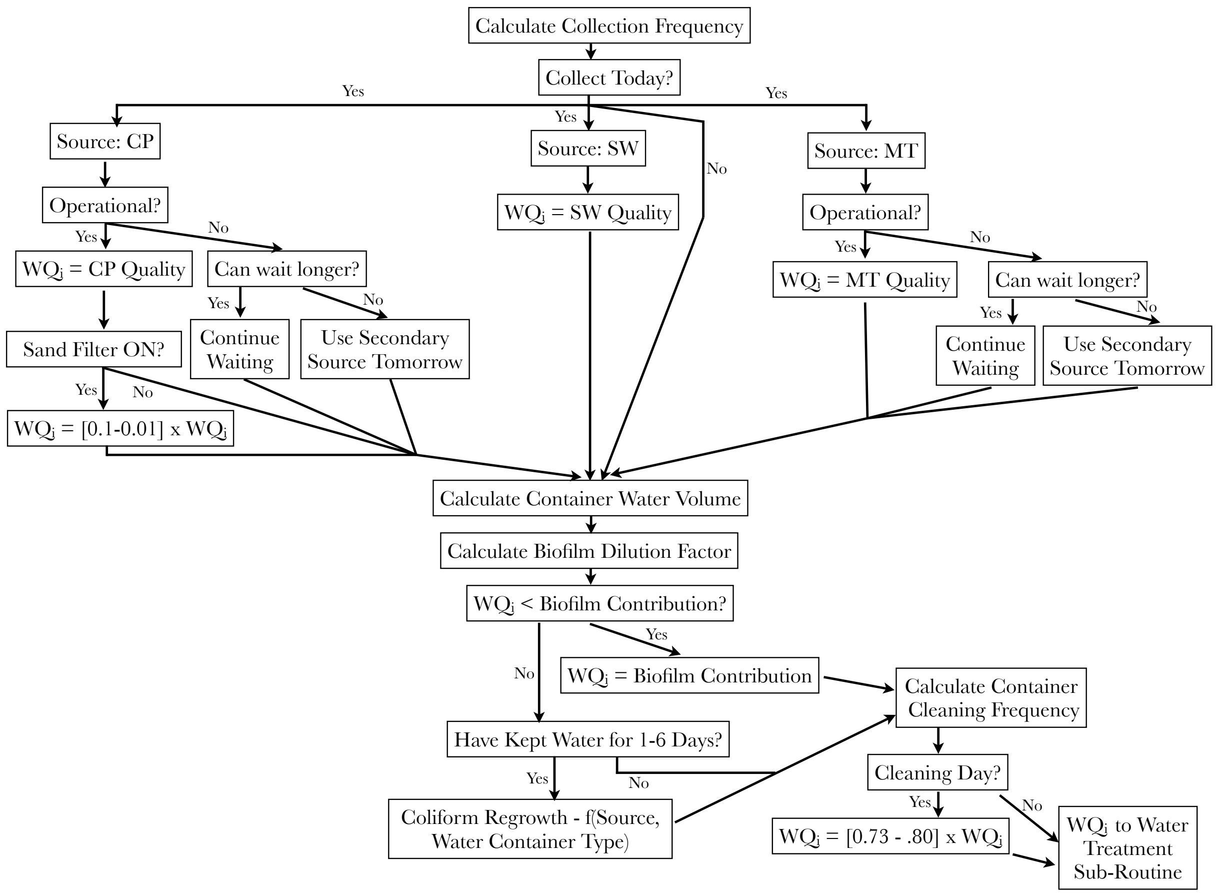

Figure S9: Flow chart of Collect Water Sub-Routine. This flow chart is repeated for each household for each day of the simulation. Square brackets indicate values that are stochastically varied between minimum and maximum values. SW - surface water, CP - community piped, MT - municipal tap, WQ_i daily water quality of ith household.

Treat and Drink Water

The next sub-routine involves the treatment and drinking of water and is summarized in Figure S10.

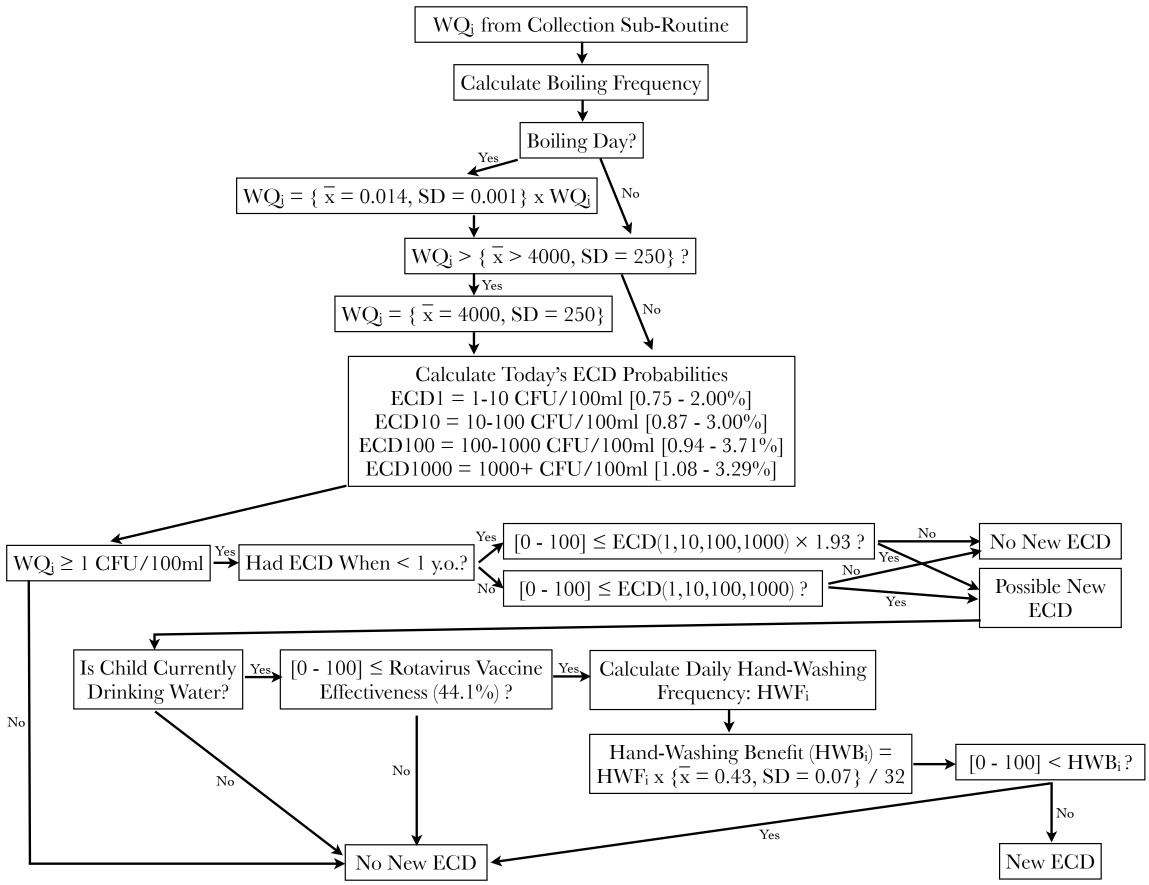

Figure S10: Flow chart of Water Treatment and ECD Calculations. The treatment portion occurs for each household each day. The ECD Calculation portion occurs for each child each day. Curly brackets indicate a variable that is stochastically varied according to a normal distribution with mean and standard deviations idicated. Square brackets indicate values that are stochastically varied between minimum and maximum values. Parentheses indicate a functional relationship, i.e. the probability of getting ECD is a function of WQ_i.

Calculate Height

Finally, children grow according to the sub-routine shown in Figure S11 and detailed below.

The HAZ data are incorporated into the model by using data for the individual Mal-ED child closest in age to the individual ABM model child. This can account for possible HAZ reduction age differences. The daily child growth increment ΔH is calculated considering that the daily HAZ difference (±4 month HAZ reduction values divided by 8 months), ΔHAZ, is as follows in Equation 2:

$$\Delta HAZ = \frac{H_{age} - H^S_{age}}{SD_{age}} - \frac{H_{age+1} - H^S_{age+1}}{SD_{age+1}} \tag{2}$$

In this equation, H is the height, the subscript *age* is the current child age, SD is the age standard deviation (2), the superscript S indicates the WHO standard median values and the $+1$ indicates the subsequent day. Rearranging and introducing the daily growth increment $\Delta H = H_{age+1} - H_{age}$ for children with ECD:

$$\Delta H = H^S_{age+1} - SD_{age+1}\left(\Delta HAZ - \frac{H_{age} - H^S_{age}}{SD_{age}}\right) - H_{age} \tag{3}$$

An ABM child with a 'single' ECD case then grows according to Equation 3 which is a function of the ΔHAZ of the Mal-ED child of the most similar age who had a 'single' case of ECD. If a child has a 'double' ECD case they similarly grow at the ΔHAZ of the most similar age Mal-ED child who had a 'double' ECD case.

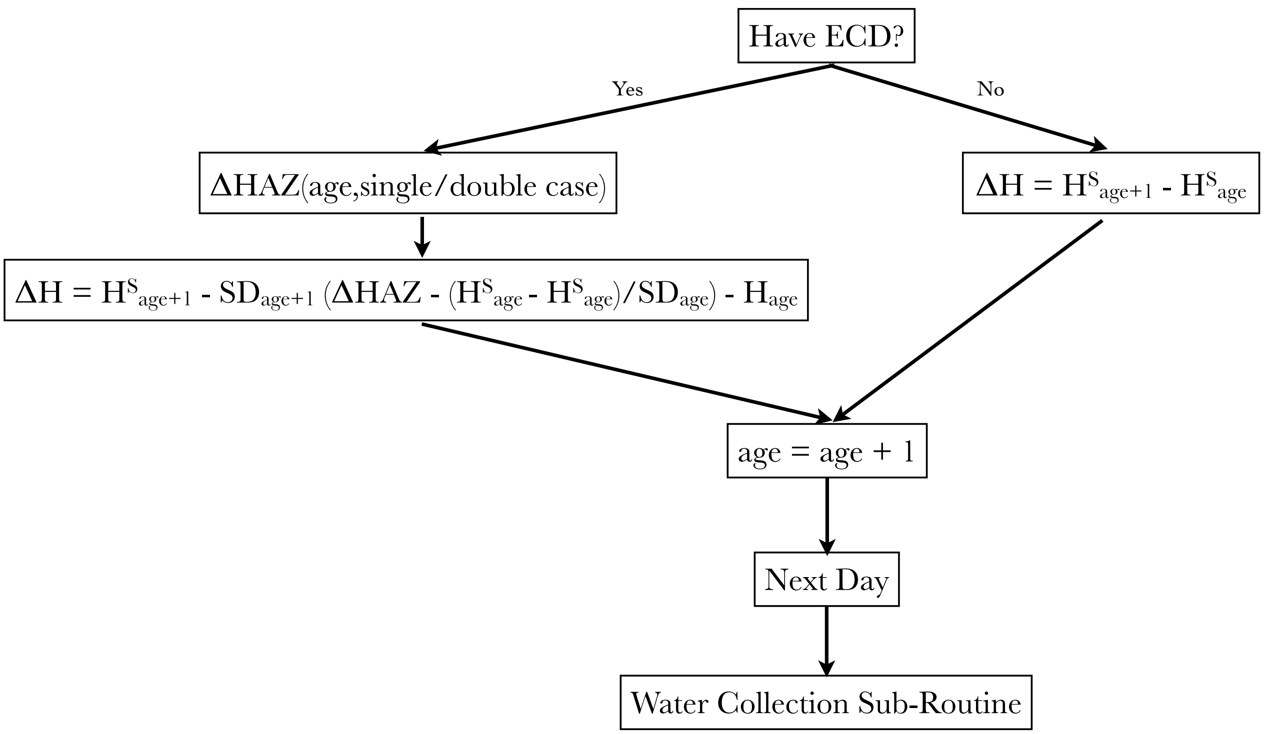

Figure S11: Flow chart of Height Calculations. This sub-routine is performed for each child each day.

Sensitivity Analysis

The sensitivity of the model to two parameters was tested. These parameters include the length of growth-stunting (set at 8 months) and the dose-response relation between coliform bacteria and ECD incidences summarized in Table S3.

For the growth-stunting analysis, the growth-stunting period was varied between 120 and 360 days. Over this interval, mean HAZ_2 values varied between -1.41 and -1.61 as can be seen in Figure S12 indicating a moderate variation over those growth stunting periods. However, since the growth stunting period is based on field measurements using data from the Mal-ED project, this variation is acceptable.

The second analysis introduced multiplicative factors between 0.5 and 1.5 of the stochastically varied dose-response relationship shown in Table S3. These factors did vary ECD rates from 3.8 to 13.3 mean cases and HAZ_2 values from -1.23 to -1.74 as can be seen in Figure S13. Despite this sensitivity, the overall qualitative conclusions seen in, for instance, boiling frequency, remain identical as is seen in Figure S14. In all five factors tested, boiling frequency must be preformed daily to be effective.

Additional Single Parameter Behavior Space Tests

The single parameter behavior space analysis was conducted for the four scenarios in the main text. In addition, eleven other major parameters were tested and are included here for reference.

Figure S15 summarizes results from five different analyses related to water storage, cleaning, biological regrowth and hand-washing. The percent of the community with 'narrow neck' water containers has an effect on median daily water quality ($F = 16,872$, $p < 0.001$), mean total ECD cases ($F = 2176.9$, $p < 0.001$) and HAZ_2 ($F = 233.84$, $p < 0.001$). The effects on WQ_i are significant over this range, but the effects on mean total ECD cases and HAZ_2 are not great. However, it is notable that the multiple scenario analysis found the percent 'narrow neck' was a strongly linked to optimal HAZ_2 values. Residents who use 'narrow neck' containers do not need to use water

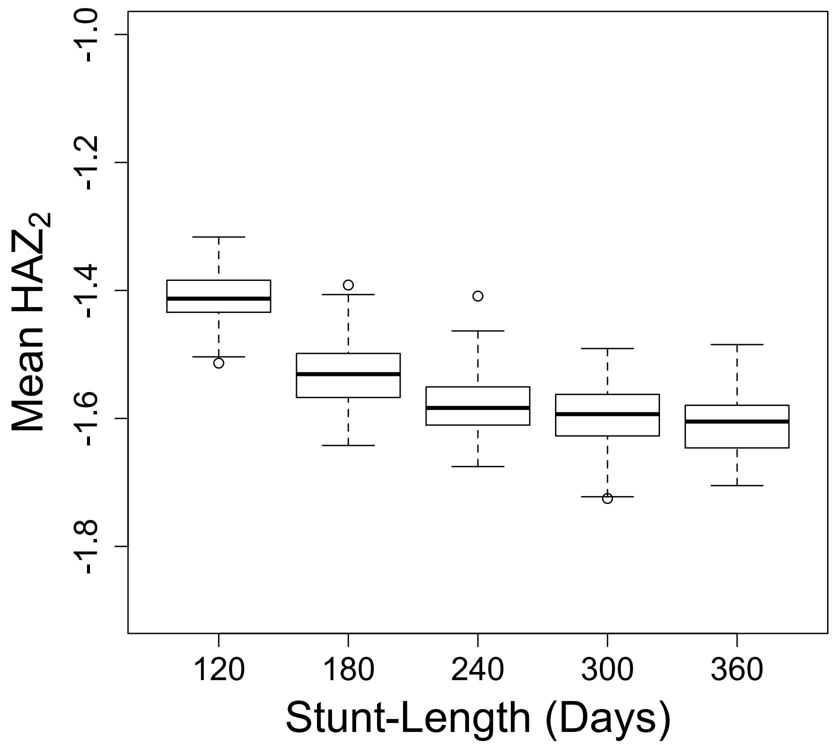

Figure S12: Sensitivity analysis of stunt-length variable. Data indicate a moderate associate between the duration of growth stunting and final HAZ_2 scores.

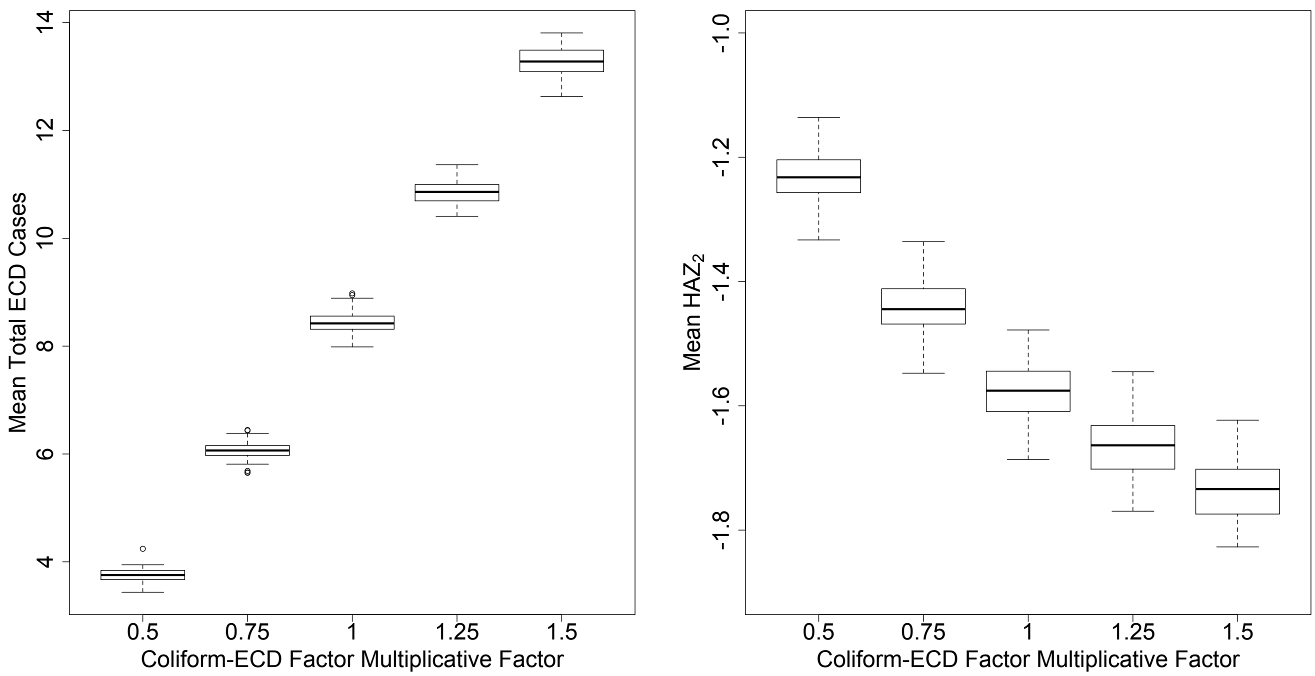

Figure S13: Mean EDC cases and HAZ_2 scores for coliform-ECD factor sensitivity analysis. Results indicate that multiplying the stochastically varied dose-response functions do change both ECD cases and HAZ_2 scores.

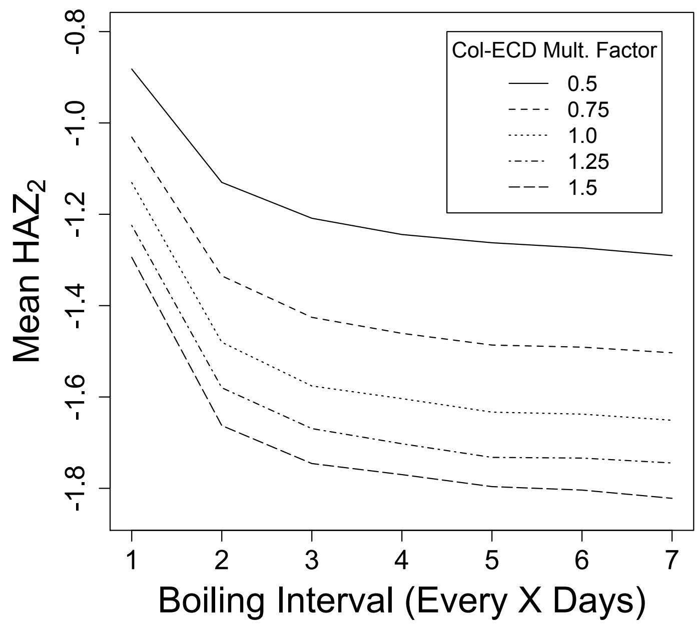

Figure S14: Mean HAZ_2 scores versus boiling frequency for five different coliform-ECD dose response function multiplicative factors. Results indicate that although HAZ_2 is sensitive to the multiplicative factor, the overall conclusions of the model would be identical regardless of that factor's value.

transfer devices and their hands to not contaminate the water when they drink it. Furthermore, biological regrowth is less in such containers.

The water transfer device contribution had an effect on household water quality and child health. Variation statistical significance is as follows: median WQ_i (F = 9251.5, p $<$ 0.001), mean total ECD cases (F = 161.37, p $<$ 0.001), and HAZ_2 (F = 23.644, p $<$ 0.001). Although a rather large difference is seen in terms of WQ_i, there were small differences in mean ECD cases and HAZ_2 indicating that the water transfer device contribution is relatively small. This may be due to the fact that only about 50% of residents use the 'wide' mouth containers that require water transfer devices.

Coliform regrowth was also a statistically significant contributor to median WQ_i (t = 159.7604, p $<$ 0.001), mean total ECD cases (t = 12.8521, p $<$ 0.001) and HAZ_2 (t = -2.2125, p = 0.028). Coliform regrowth has a large impact WQ_i and a smaller impact on mean total ECD cases and HAZ_2. Despite the relatively small differences seen here, coliform regrowth does play a larger role for the collection frequency experiments and is higher in 'wide neck' containers.

Cleaning frequency statistically affected median WQ_i (F = 1329.9, p $<$ 0.001) and mean total ECD cases (F = 63.508, p $<$ 0.001), but not HAZ_2 (F = 2.8892, p = 0.090). Cleaning everyday has a small effect on median WQ_i, but little effect on either mean total ECD cases and no effect on HAZ_2. This is likely because the cleaning effectiveness as measured in the communities is very low. If community members cleaned their storage containers vigorously this metric would likely be far more important.

Hand-washing does not statistically affect median WQ_i (F = 2.241, p = 0.1350) but it does affect mean total ECD cases (F = 42,371, p $<$ 0.001) and HAZ_2 (F = 1546.8, p $<$ 0.001). Since hand-washing is not directly linked to the water chain, there was no variation in WQ_i. The other two outcome variables, mean total ECD incidences and HAZ_2 showed significant declines.

CP water quality statistically affects median WQ_i (F = 3607.1, p $<$ 0.001), mean total ECD cases (F = 405.4, p $<$ 0.001) and HAZ_2 (F = 135.10, p $<$ 0.001). WQ_i deteriorated significantly with CP water quality. This sensitivity of WQ_i to source water is somewhat surprising given previous results (3). Mean total ECD cases and mean HAZ_2 scores only changed by large amounts when CP water quality is optimal.

SW water quality statistically affects median WQ_i (F = 243.25, $p < 0.001$), mean total ECD cases (F = 44.413, $p < 0.001$) and HAZ_2 (F = 11.406, p = 0.001). Surface water is generally a secondary water source for most community members, therefore although it is statistically significant it is not strongly correlated to WQ_i and therefore mean ECD cases and HAZ_2 in this scenario.

The percent coverage of the CP and MT water systems was varied from 0 to 100% to study the potential effects of community members switching to more desirable water sources. In both cases the remainder of the households use an equal distribution of other sources. The results indicate that WQ_i varies (F = 480.03, $p < 0.001$) as do mean total ECD cases (F = 496.74, $p < 0.001$) and HAZ_2 (F = 162.87, $p < 0.001$) in both cases. These results are consistent with the CP and MT results that show that improved source water quality can improve WQ_i.

CP operational frequency statistically affected median WQ_i (F = 2258.1, $p < 0.001$), mean total ECD cases (F = 27.830, $p < 0.001$) but not HAZ_2 (F = 2.6968, p = 0.101). Despite the statistical significance, CP operational frequency is not strongly correlated to WQ_i, mean total ECD cases or HAZ_2. This is especially surprising given the trends seen in the collection frequency experiment. This is likely due to the fact that after the first 72 hours, biological regrowth levels off and so water storage time is less important after this initial period (1). This, coupled with the fact that residents usually only want to collect water every several days is likely the reason for the relative insensitivity of the model to this parameter.

MT operational frequency also showed statistical variation of median WQ_i (F = 515.17, $p < 0.001$) but not mean total ECD cases (F = 2.5888 p = 0.108) or HAZ_2 (F = 0.1143 p = 0.735). These results are largely similar to the CP results above with similar reasoning.

SSF status led to statistical variation of median WQ_i (t = -74.3327, $p < 0.001$), mean total ECD cases (t = -10.6801, $p < 0.001$), and HAZ_2 (t = 3.3165, p = 0.001). WQ_i did vary significantly, but there was less absolute variation in either mean total ECD cases or HAZ_2 scores.

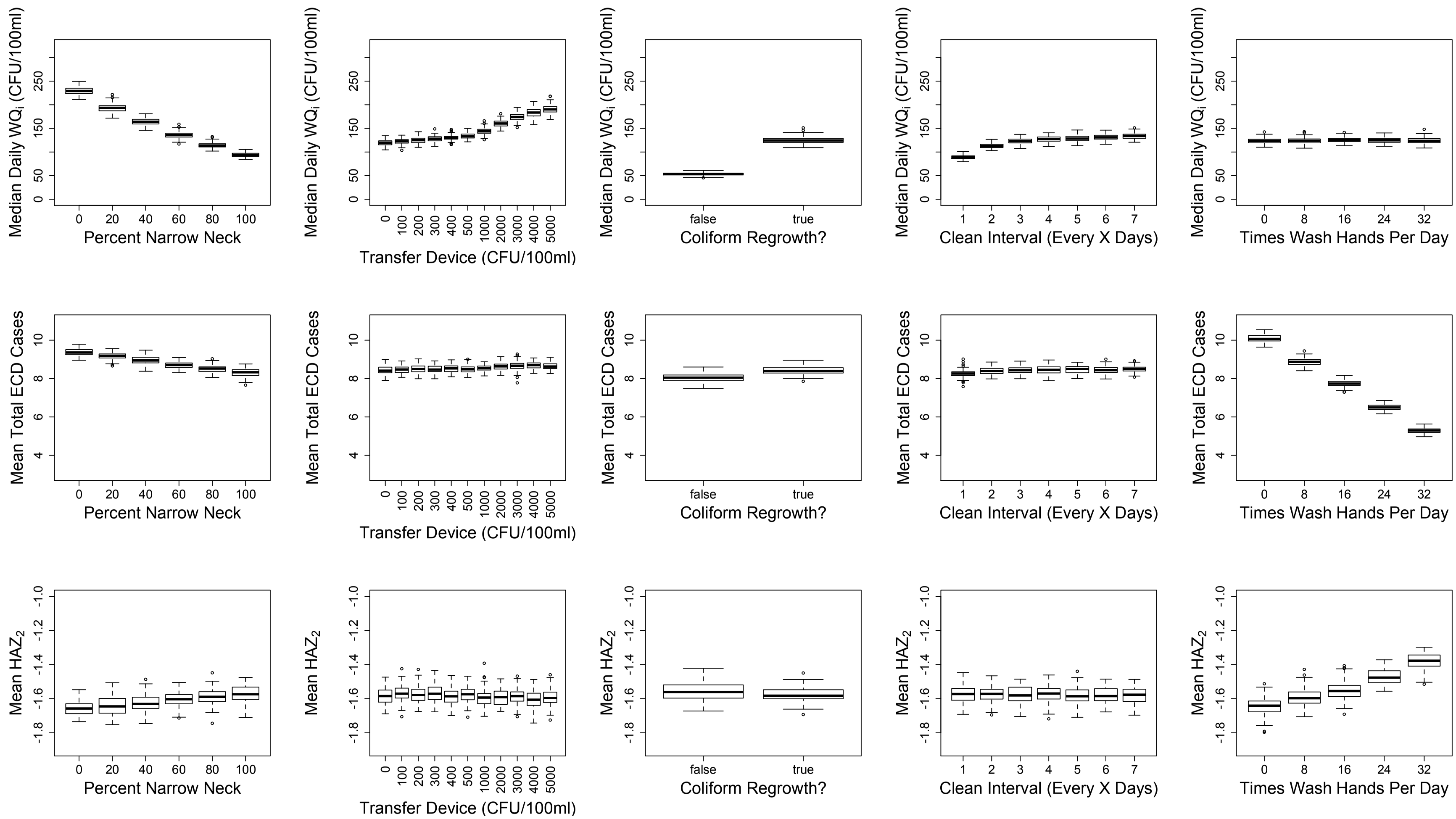

Figure S15: Behavior space analyses for five different important model parameters. Results summarized in terms of median daily WQ_i, mean total ECD cases, and mean HAZ_2. Percent narrow neck, refers to percentage of the community that has ‘narrow neck’ water storage containers as opposed to the ‘wide neck’ variety. Transfer device refers to coliform contamination from water transfer devices, which are typically cups or ladles. Note the non-linear x-axis which is representative of field measurements. The coliform regrowth experiment showed the effects of biological regrowth in water storage containers. The cleaning interval refers to the interval in which households clean their water storage containers, with that effectiveness being determined by field measurements. The times wash hand per day varies from 0 to 32, with 32 times per day being considered optimal. Median daily WQ_i varies for most experiments, but these variations do not lead to large variations in ECD cases or mean HAZ_2. Exceptions include the percent ‘narrow neck’ and hand-washing frequency, but of which showed some improvement with improved behaviors.

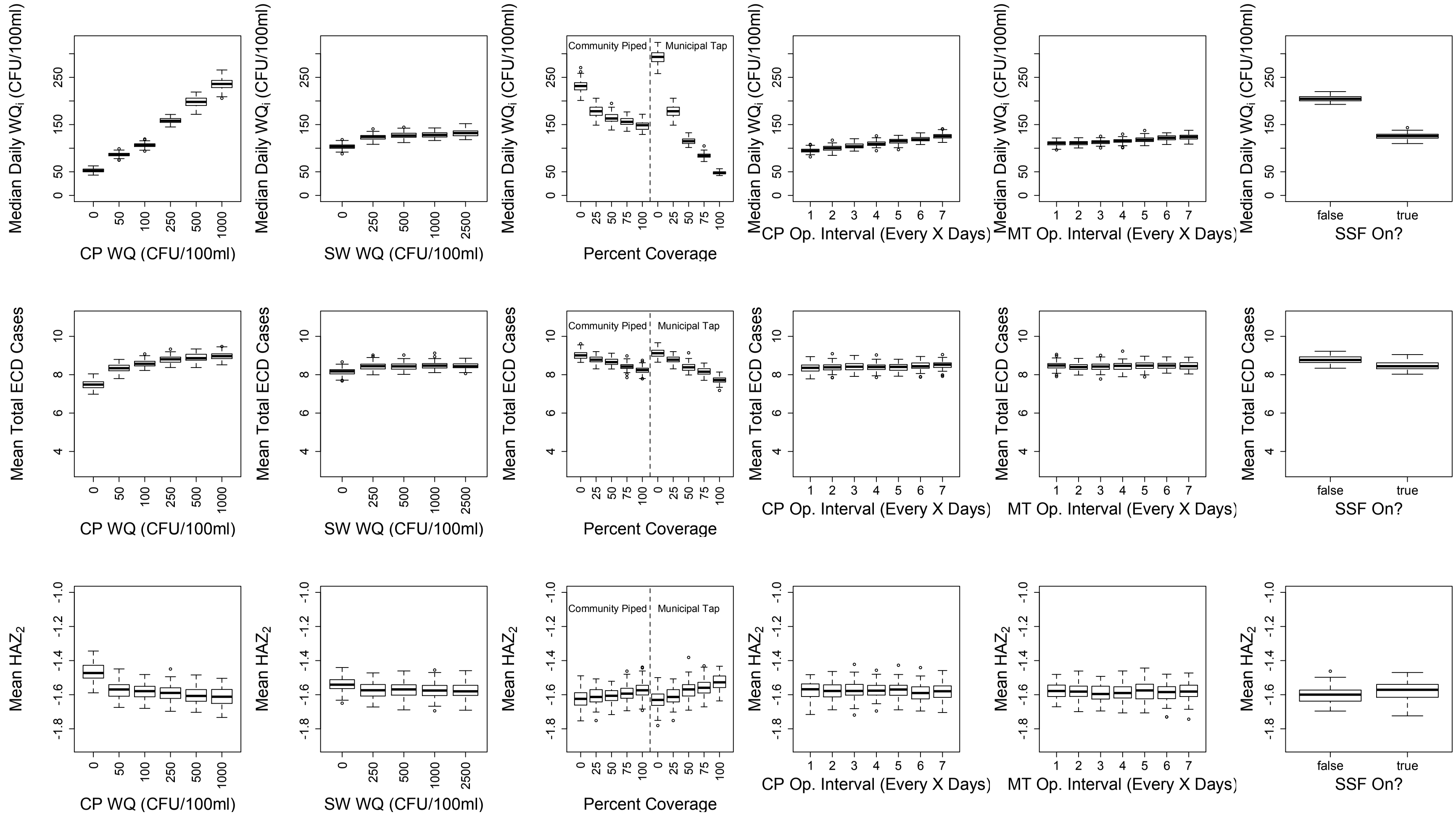

Figure S16: Sensitivity analysis for six additional important model parameters. Results summarized in terms of median daily WQ_i, mean total ECD cases, and mean HAZ_2. CP WQ and SW WQ refer to the source water quality of the community piped water system and surface water respectively. The non-linear x-axes are representative of field measurements. Percent coverage refers to two experiments that varied CP and MT water system reliance with the remaining houses depending on other water sources. CP and MT op. interval refer to the operational interval of those water sources. SSF refers to the operation of the community slow sand filter which is part of the CP water system. Results indicate median WQ_i variation in most cases, but this translated into large changes in ECD rates and HAZ_2 scores for only CP WQ and the percent coverage of MT and CP.

References

(1) Mellor, J.; Smith, J.; Dillingham, R. Pathogen Sources and Mechanisms for Regrowth in Household Drinking Water in Limpopo, South Africa. *61st ASTMH Meeting, Atlanta, GA, November 11-15; American Society of Tropical Medicine and Hygiene, Deerfield, IL* **2012**, *LB-185*.

(2) De Onis, M. *WHO Child Growth Standards: length/height-for-age, weight-for-age, weight-for-length, weight-for-height and body mass index-for-age*; WHO, 2006.

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