The Arrhenius Equation as Means to Simulate *E. coli* Survival in Waters

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Background

- *E. coli* is an important microorganism indicator used to show the potential presence of pathogens and possible fecal contamination in waters.
- Knowing *E. coli* survival rates is important in evaluating microbial contamination and making appropriate management decisions.
- *E. coli* survival rates are known to be functions of temperature. To express this dependence, an approximation of the Arrhenius equation is used in the form:

(1) $$k(T) = k(20)\theta^{(T-20)}$$ → *k(T)* is the inactivation rate constant in Chick's equation rewritten to the decimal base seen in equation (2).

(2) $$c = c_0 10^{-k(T)(t-t_0)}$$ → c is the concentration on the time t, c_0 is the concentration at the moment t_0 after which the equation (2) is valid, *T* is temperature in °C, *k(20)* is the inactivation rate constant at 20 °C, and ϑ is the temperature-dependence parameter.

- The suggestion to use the Arrhenius equation to express the dependence of *E. coli* survival on temperature was made 34 years ago based on limited literature on 20 datasets, and the value of ϑ=1.07 was proposed to be used in all computations.
- A large number of *E. coli* survival studies have been performed since then, but the accuracy of the original model has yet to be revisited.
- The objective of this study was to evaluate the accuracy of the Arrhenius equation as a model for the dependence of *E. coli* survival rates on temperatures in various sources of water by using a large selection of recent published data.

The Database/ Determining Survival Rates

- Using Surfer8 and Sigma-Plot software, we assembled a database consisting of 450 digitized survival curves from 70 peer-reviewed papers on *E. coli* inactivation in water.
- We focused on 200 survival curves taken from experiments that were performed in laboratories under dark conditions to exclude the effects of sunlight and other field factors.
- There were several different ways that the survival curves were generally shaped; five occurrences were distinguished. (Fig. 2)

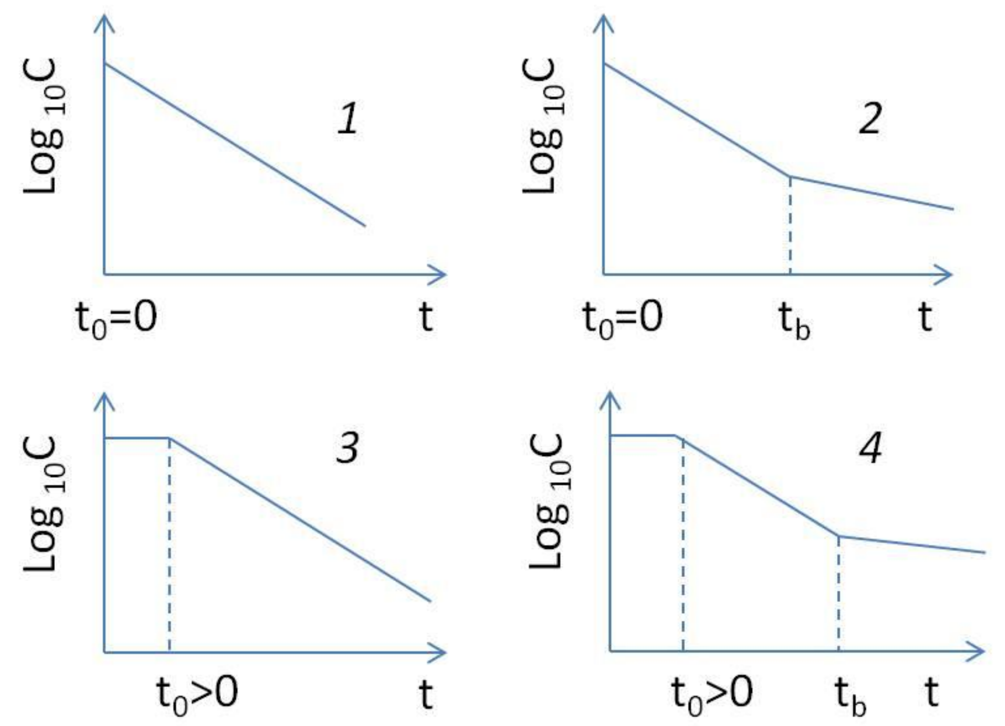

Fig. 2.
Types of trends found in *E. coli* survival curves

- *Type 2* of the survival curves was found most often, in 46 %of all cases; *Type 1* and *Type 3* were encountered in 26% and 21% of all cases, respectively; *Type 2W* was found in 4% of all cases; and *Type 4* was found in 3% of all cases.
- All points of observation on each curve could rarely be fitted with the approximated equation, so the first-order inactivation rate constants were calculated from the linear sections of all curves.
- The sequential linear fitting method was applied. Specifically, to find the breakpoint t_b, the coefficient of determination (R^2) between log C and t was computed for the first three experimental points, then for four points, then for five, etc. The set of points with the highest R^2 value was used to find *k* as an absolute value of the regression slope.
- An example of the application of this algorithm is shown in Fig. 3 and in Table 1.

Experimental Point	Time, Days	log C	R^2
1	0	6.3	n/a
2	1	5.9	n/a
3	2	3.7	0.835
4	4	2.9	0.888
5	**7**	**0.9**	**0.939**
6	14	0.7	0.647
7	28	0.5	0.212
8	42	0.2	0.041

Table 1.
The maximum coefficient of determination is achieved when computed between logC and time for points from 1 through 5.

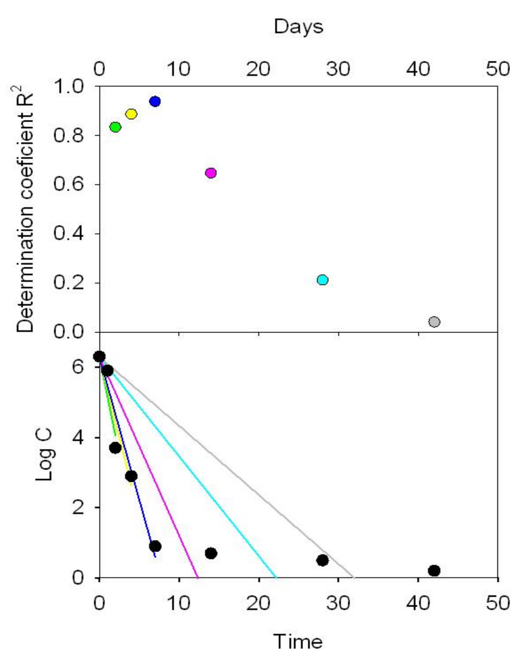

Fig. 3.
Graph illustrating the performance of the method for data in Table 1.

Results

- The determination coefficients from the linear fits of the approximately linear sections of *Types 2, 3,* and *4* datasets provided better accuracy than all points in observations of those datasets. The R^2 values were 0.901 and 0.628, respectively.
- The data was categorized into groups containing waters of agricultural origin (runoff, effluent ponds, catfish ponds), pristine water sources (caves, springs), groundwater and wells, lakes and reservoirs, rivers and streams, estuaries and sea water, and wastewater (Fig. 4)

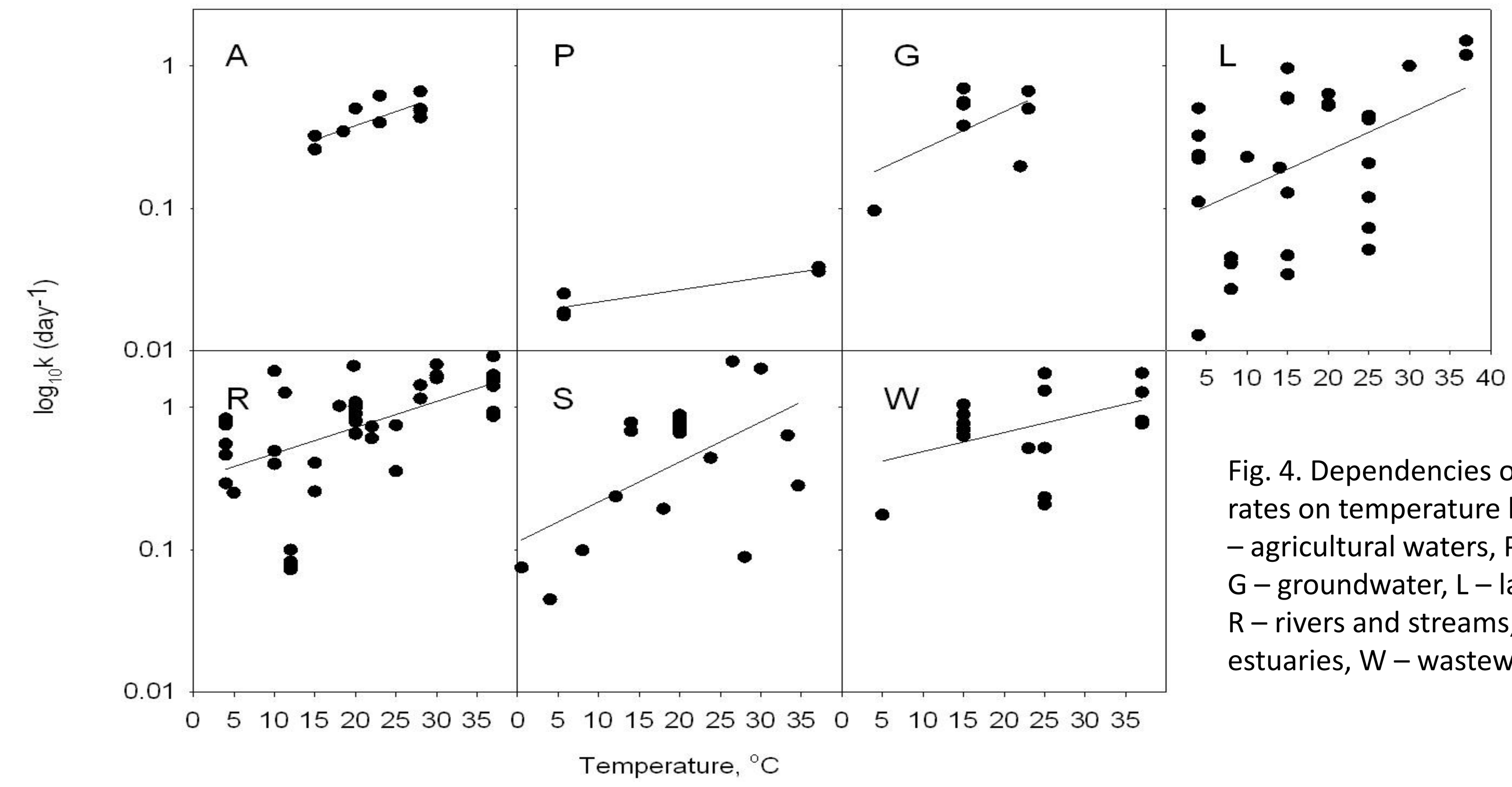

Fig. 4. Dependencies of *E. coli* inactivation rates on temperature by water sources; A – agricultural waters, P – pristine waters, G – groundwater, L – lakes and reservoirs, R – rivers and streams, S – seawater and estuaries, W – wastewater.

- The slope of the regression equation $\log k = \log k(20) + \log\theta(T-20)$ gave the value of θ, and the intercept gave the log of the inactivation constant at 20 deg C.

Water Source	θ	K(20) day $^{-1}$	R^2
A	1.047±0.012	0.380±0.025	0.643
P	1.058±0.014	0.049±0.008	0.858
G	1.062±0.039	0.477±0.121	0.309
L	1.062±0.023	0.253±0.058	0.214
R	1.043±0.011	0.721±0.077	0.278
S	1.067±0.026	0.413±0.093	0.304
W	1.031±0.018	0.665±0.114	0.159

Table 2.
Coefficients of regression lines shown in Fig. 4 for different types of waters.

- Site-specific applications of the Arrhenius equation are shown in Fig. 5.

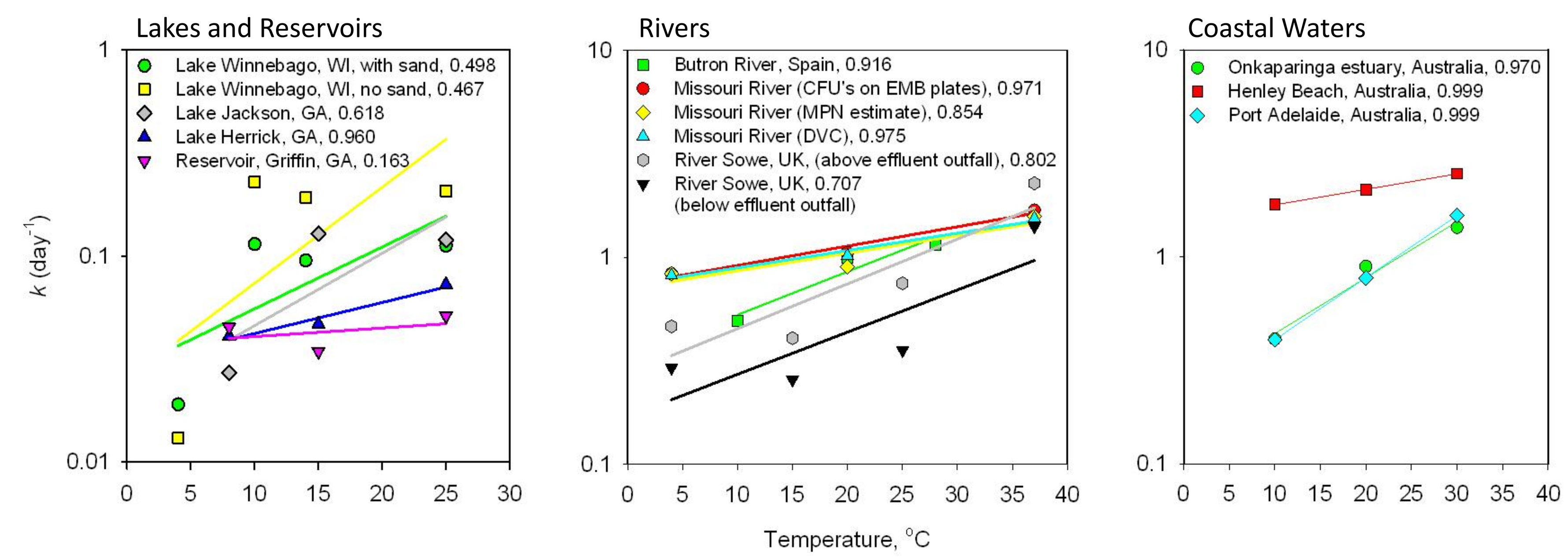

Fig. 5. Change in inactivation rates from three or more temperatures at specific sites. R^2 values of the linear regression lines are listed next to each site name.

Summary

- The approximation of the Arrhenius equation is used to model the dependence of *E. coli* inactivation rates on temperatures in various sources of water when applied to data from the approximately linear sections of inactivation.
- Although the variability of *E. coli* survival rates within groups of water sources is very high, substantial differences between groups can be observed.
- Inactivation rate constants are very small in pristine waters, are moderate in agricultural waters and groundwater, are moderate to large in lakes and reservoirs, and are large in river water, estuaries, and wastewater.
- The Q_{10} equation, $k(T) = k(20)Q_{10}^{(T-20)/10}$, is equivalent to the equation (1) of this work. This model, another approximation Arrhenius equation, is routinely used to express temperature dependence of biological rates.
- This study will be extended to data on *E. coli* inactivation in soils and organic waste as well as data on *Salmonella* and enterococci, to provide guidance in calibration of pathogen fate and transport modeling systems that are used to make environmental management decisions.