Sequential Estimation of Microbial Inactivation Arrhenius Parameters for Nonisothermal Heating Processes

Dharmendra K. Mishra[1], Kirk D. Dolan[1,2], [1]Dept. of Biosystems & Agricultural Engineering, [2]Dept. of Food science and Human Nutrition Michigan State University.

Abstract

Most thermal food processes are nonisothermal. Better estimates of the kinetic parameters can be made using more realistic nonisothermal data. When the nonisothermal model is used, an inherent difficulty arises in estimation of the Arrhenius parameters (rate constant and activation energy) because of high correlation between them. The objective of this work was to show how to best estimate kinetic parameters for microbial inactivation.

Survival data of *B. Stearothermophilus* spores in canned pea puree, heated at retort temperatures of 104.4, 112.8, and 120.6°C for times 19-305 minutes were used. Temperatures in the pea puree were predicted over time using the solution to the analytical heat conduction equation. The kinetic parameters D_{108C} (89.7 min) and *z* (11.36 °C) were estimated sequentially using an inverse technique with the maximum a posteriori method. The correlation coefficient between the parameters was minimized by iterating over the reference temperature (T_r). Scaled sensitivity coefficients for the two parameters were plotted to determine if any linear dependence existed. Both sequential estimation performance (coming to a constant) and linear independence of the sensitivity coefficients were highly sensitive to choice of the reference temperature. The impact of the results is that researchers using Arrhenius models should determine and use the optimum reference temperature to ensure that parameters can be estimated with low correlation and no convergence difficulties.

Objectives

- To determine the appropriateness of the nonisothermal model by estimating parameters sequentially (updating parameters with addition of each datum).
- To minimize the correlation between the Arrhenius parameters and to minimize the error in their estimation .

Estimation of Kinetic Parameters

$$N(t)/N_0 = 2\iint 10^{\frac{-1}{D_r}\int_0^t 10^{\left(\frac{T(r,z,t)-T_r}{z}\right)} dt}\ r\,dr\,dz$$

For each can $Y(t) = \log(N(t)/N_0)$ = log(survival ratio)

$N(t)$ = microbial count at time t, N_0 =intial count

- Estimate D_r and *z* sequentially using maximum a posteriori
- Minimize D_r and z correlation by iteration to estimate optimum T_r
- Plot the scaled sensitivity coefficients

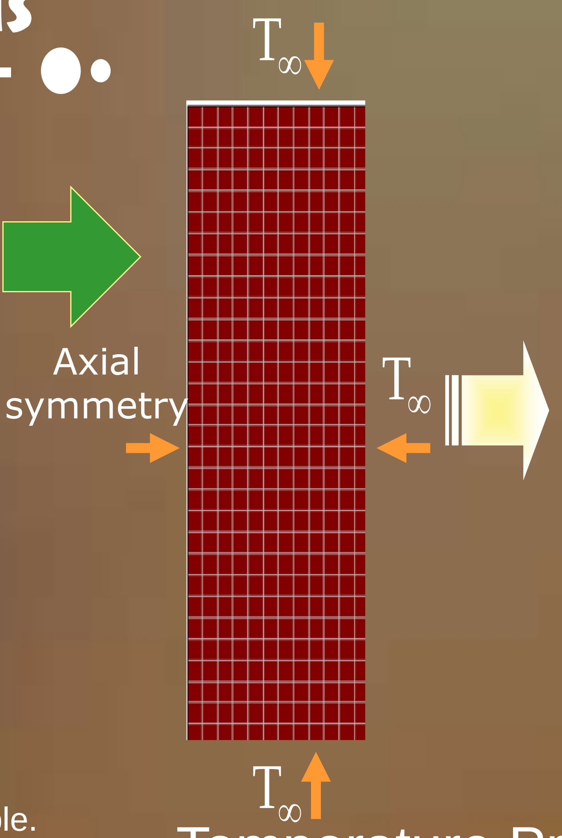
Sensitivity Coefficients

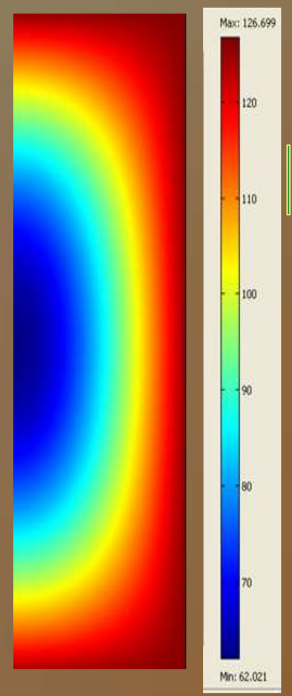
Sensitivity coefficient (*X*) is the first derivative of the function involving the parameter p_i, with respect to p_i. *X´* is the scaled *X* having the same units as Y. ($\delta b = p_i$*.0001)

Finite difference method $$X'_{p_i} \equiv p_i \frac{y(p_i+\delta b) - y(p_i)}{\delta b}$$

Materials & Methods

Pea puree sealed in can with thermocouple. Cans heated in steam at 104.4C, 112.8C, and 120.6C





Temperature Profile of the can

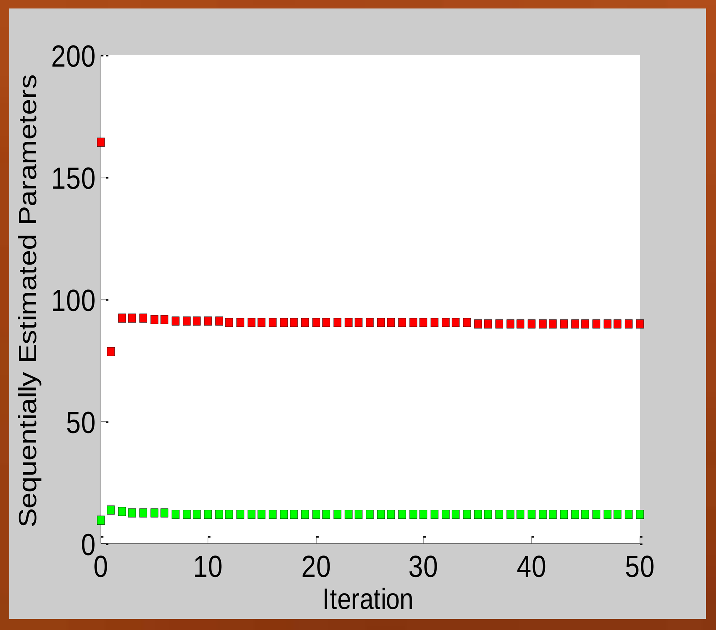
Pea puree inoculated with 9x10[5] cfu/ml B. stearothermophilus spores. k = 0.4 W/mK, Cp = 3850 J/kg K

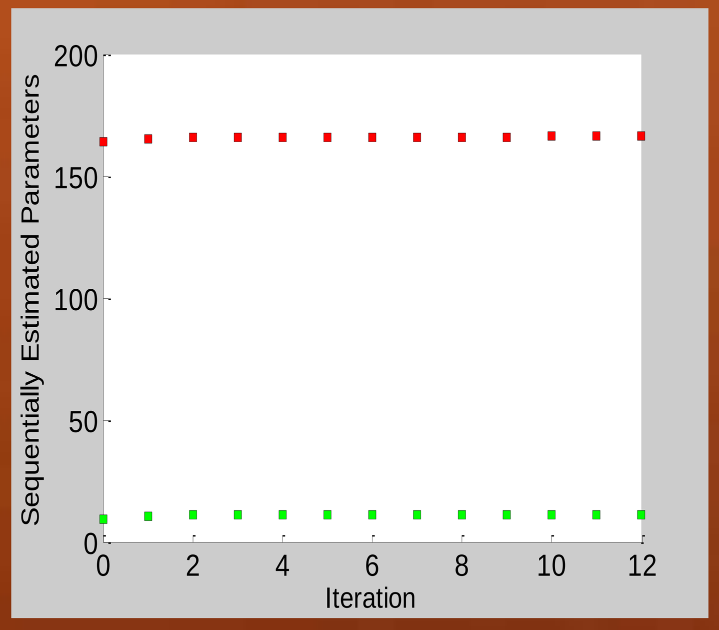
Beck, J.V., Arnold, K.J. (1977). Parameter estimation in engineering and science Wiley, NY.

Welt, B. A. (1996). Kinetic parameter estimation in prepackaged foods subjected to dynamic thermal treatments, Ph.D. thesis, University of Florida, Gainesville, FL.

Table 1. Retort temperature, heating time, and measured survival ratios for 24 heated cans (Welt, 1996).

Can number	Retort Temp-erature (°C)	Heating time (min)	Measured Survival ratios, N/N_o
1	n/a	0	0.891
2	n/a	0	1.109
3	104.4	50	0.689
4	104.4	50	0.769
5	104.4	90	0.656
6	104.4	90	0.744
7	104.4	180	0.387
8	104.4	180	0.476
9	104.4	180	0.279
10	104.4	180	0.266
11	104.4	240	0.0755
12	104.4	240	0.0697
13	104.4	240	0.0703
14	104.4	240	0.0667
15	104.4	275	0.0418
16	104.4	275	0.0401
17	104.4	305	0.00725
18	104.4	305	0.00855
19	112.8	27.5	0.642
20	112.8	32.5	0.433
21	112.8	44	0.159
22	120.6	19	0.500
23	120.6	24	0.266
24	120.6	27.5	0.093





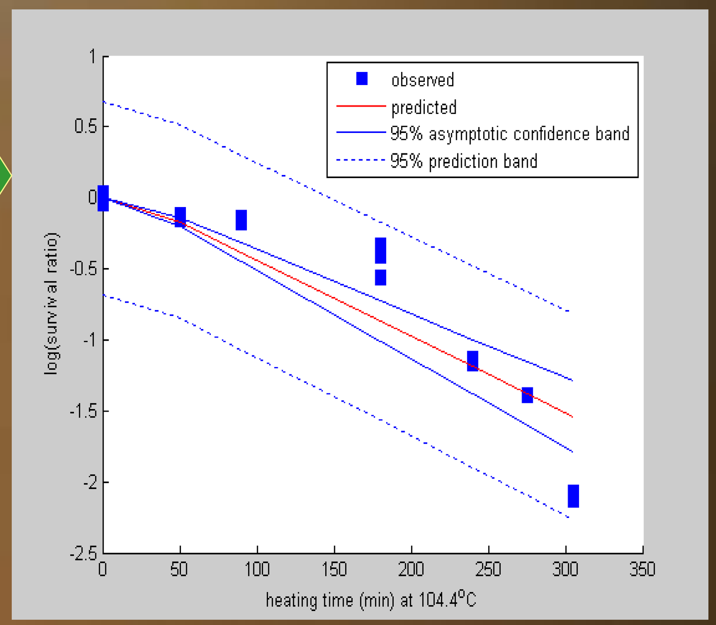
Sequentially estimated parameters Dr and z for Tr = 108C (left) and optimum Tr = 104.95C (right).

Confidence intervals (CI) of D and z vs. Tr

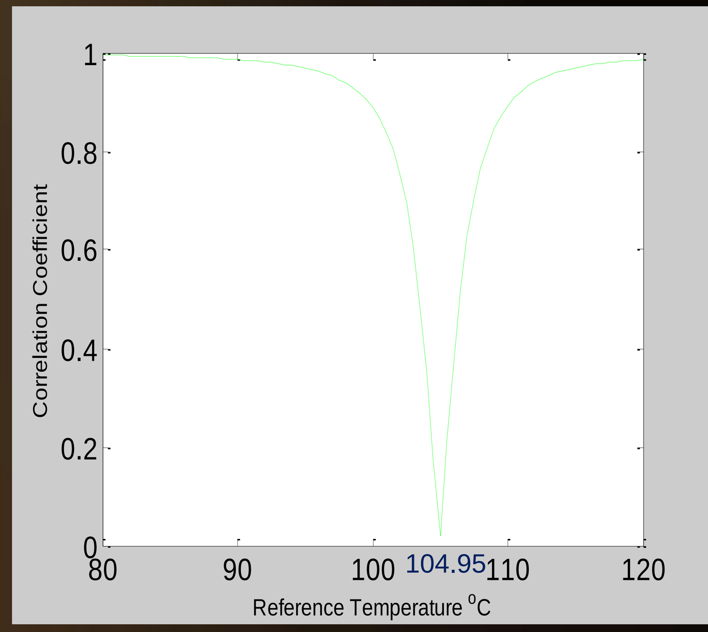
Tr (C)	D121	DCIlower	DCIupp	DCIwidth	z	zCIwidth
120	6.28	1.63	10.94	9.31	11.35	5.43
108	6.28	5.07	7.49	2.42	11.35	5.43
104.95	6.28	5.50	7.06	1.56	11.35	5.43
95	6.28	3.15	9.42	6.27	11.35	5.43
75	6.28	-2.89	15.45	18.34	11.35	5.43

Minimum CI width

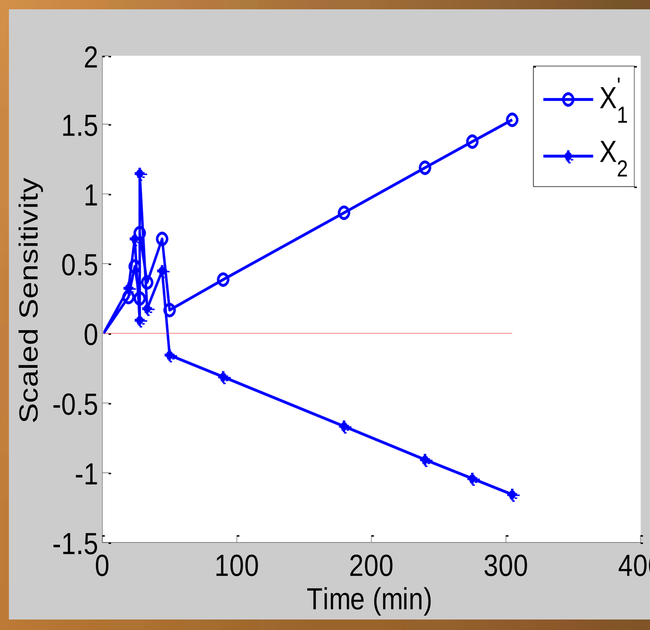
Results



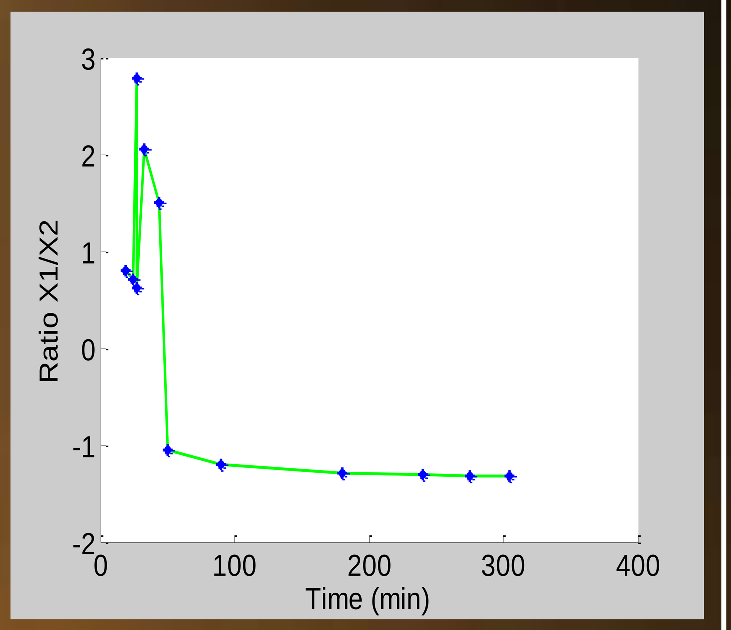
Predicted log survival based on estimated parameters D_{108C} = 89.7 min, z = 11.4C



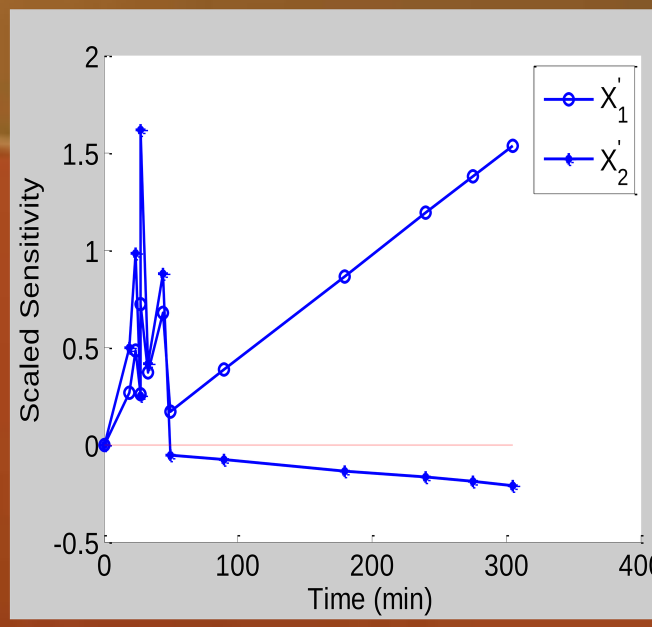
Correlation coefficient between Dr and z as a function of reference temperature Tr



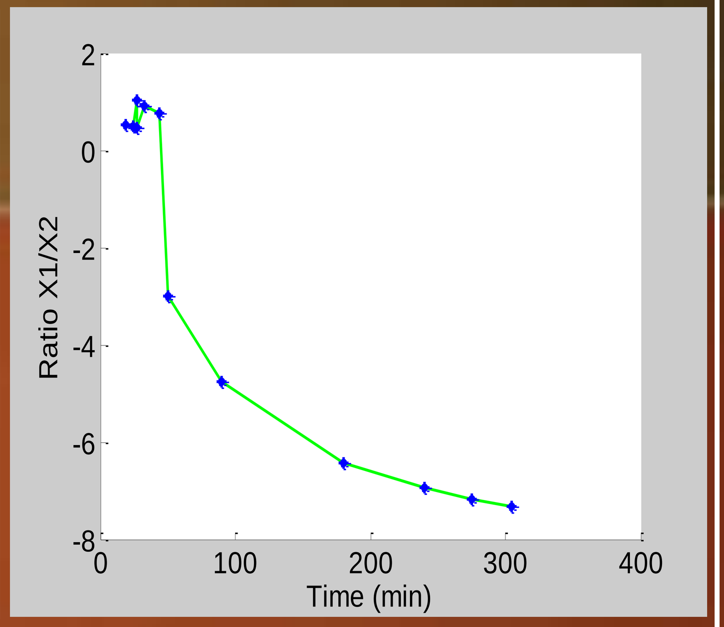
Scaled sensitivity coefficients of parameters Tr = 108C



Ratio of sens coefficients at Tr = 108C shows linear correlation at heating time >= 50 min.



Scaled sensitivity coefficient s for optimum Tr = 104.95C



Ratio of sens coefficients at Tr = 104.95C shows linear independence for all times

Conclusions

- Sequential estimation was faster for optimum Arrhenius Tr than for other Tr
- Sensitivity coefficients were large and uncorrelated only at the optimum Tr; at other Tr's, they were linearly correlated for all heating times > 50 min.
- Confidence interval and standard error for Dr was smallest at optimum Tr.
- Therefore, researchers using the Arrhenius model should minimize correlation coefficient between the parameters.