

Extending Engineering Simulations to Scientists: Food Safety and Quality Prediction Using COMSOL Multiphysics® and LiveLink™ for Excel®

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Abstract

The objective of this study was to develop an easy to use interface in Excel® that connects to not only the solvers in COMSOL Multiphysics®, but also existing databases of food properties, foodborne pathogenic microorganisms kinetics, and chemical kinetics (see Figure 1), creating a comprehensive simulation software to predict food safety and quality. This study builds on the previous work of Halder et al. (2010) by updating databases and increasing the flexibility and versatility afforded from the LiveLink™ for Excel® available from COMSOL. The food database groups over 8000 foods from the 2012 USDA Natl. Nutrient Database into 14 food groups while including the pathogen and chemical kinetics databases from Halder et al. (2010). The user-interface easily allows the user to select the food, pathogen, and chemical name and then press a visual basic application (VBA) macro button that retrieves the food properties and kinetic equations for the user based on the food. Effective transport properties are then automatically calculated for the user inside COMSOL. The extension of macros significantly improves the data retrieval process, instead of the laborious task of searching through the databases for values and then calculating transport properties.

The main features of the user interface (see Figure 2) are that it includes an easy to use meshing algorithm, seamless data retrieval through VBA macros, easy input for boundary conditions, and post processing plotting already set-up for the user. This easy to use interface has been set up for several food processes with a focus on safety and quality with the main purpose of having the user only deal with the most critical of input parameters for their work, whether it be in industry, extension, or academia.

Reference

A. Halder et al. Development of Associations and Kinetic Models for Microbiological Data to be Used in Comprehensive Food Safety Prediction Software, *Journal of Food Science*, 75(6) R107-R120 (2010)

Figures used in the abstract

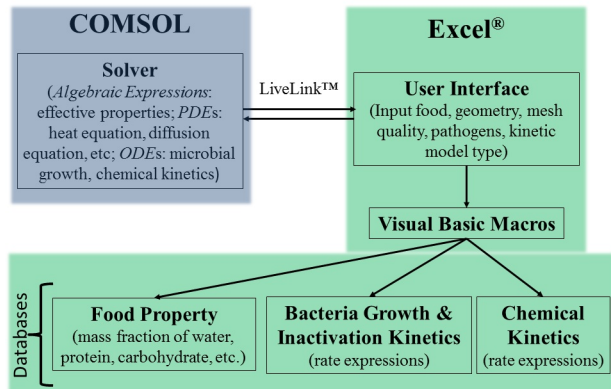


Figure 1: Design of food safety software

COMSOL Model		Excel User Interface	
Parameter	Expr	Problem Schematic	
Enter the Geometry and Time Information Here			
Parameter	Expr	Description	
Prod_W	0.0014	Product Heat W/dB, m	0.00093384
Prod_H	1.12	Product Height, m (downward normal)	401.4735211
Time_Rec	1800	Time steps recorded, seconds	5.116603128
Time_Tot	28800	Total time of recording, seconds	
Time	3		
Initial Conditions			
Name	Expr	Description	
T10		25 Initial temperature, C	
Initial Product Composition, wet basis			
Select Food Group	Expr	Get Composition	
Select Food:	BUTTER_OIL_ANNYDROUS		
Name	Expr	Description	
wc_Water	0.24	mass fraction of water	
wc_Prot	0.28	mass fraction of protein	
wc_Fat	0.48	mass fraction of fat	
wc_Ash	0	mass fraction of ash	
wc_Carb	0	mass fraction of carb	
wc_Fiber	0	mass fraction of fiber	
Total % Weight		100	
Microbial Growth Kinetics			
Microbe number 1:	C_perfrigus		
Growth Model Type:	User Defined		
Name	Expr	Description	
Rate1		Please enter model: Growth Rate, log(CFU/g)/s	
Lag1		Please enter lag: 3.4 g rate, hr	
ND1		2 Initial Load, log(CFU/g)	
Microbe number 2:	C_perfrigus		
Growth Model Type:	User Defined		
Name	Expr	Description	
Rate2		Please enter model: Growth Rate, log(CFU/g)/s	
Lag2		Please enter lag: 3.4 g rate, hr	
ND2		2 Initial Load, log(CFU/g)	
Microbe number 3:	C_perfrigus		
Growth Model Type:	User Defined		
Name	Expr	Description	
Rate3		Please enter model: Growth Rate, log(CFU/g)/s	
Lag3		Please enter lag: 3.4 g rate, hr	
ND3		2 Initial Load, log(CFU/g)	
Chemical Degradation of Chemicals			
Chemical:	None		
Formation or Degradation:	Formation		
Name	Expr	Description	
CS		0 Initial concentration	
CSmax		0 maximum concentration	
kd		0 generation rate, 1/time	
kd		0 degradation rate, 1/time	
Problem Schematic			
Sample Size Thickness	0.10		
Domain Volume, m ³	0.00093384		
Sample Density, kg/m ³	401.4735211		
Sample Mass, kg	5.116603128		
Boundary Conditions			
Name	Expr	Description	
T1b	25	Ambient Temp, C	
h_conv	1000	Convective heat transfer coef, W/m ² K	
Inactivation Kinetics			
Microbe number 1:	C_perfrigus		
Inactivation (Yes/No):	No		
Name	Expr	Description	
D1		D-value, min	
T1d		D-value, delta T, C	
T2d		Reference T, C	
Microbe number 2:	C_perfrigus		
Inactivation (Yes/No):	No		
Name	Expr	Description	
D2		D-value, min	
T2d		D-value, delta T, C	
T3d		Reference T, C	
Microbe number 3:	C_perfrigus		
Inactivation (Yes/No):	No		
Name	Expr	Description	
D3		D-value, min	
T3d		D-value, delta T, C	
T4d		Reference T, C	

Figure 2: Excel User Interface