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

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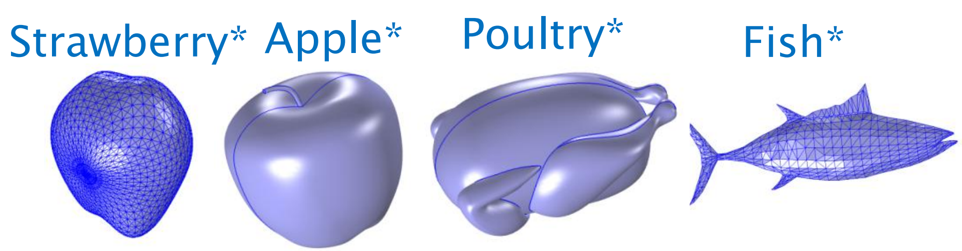
Simulation enhances education through:

- **Active learning**
  - Student can actively dial product, process and microbiological parameters and do “what if” scenarios
- **Reinforcing basic concepts**
  - How do microbiological kinetics depend on temperature (i.e., sterilization happens faster at higher temperature)
- **Exploring more complex and multi-disciplinary situations**
  - Multiphysics
  - Realistic geometries



- **Improving problem-solving skills**
  - When sterilization temperature drops, time need to be extended

*Geometries are freely available from GradCad and GoogleSketchup

Course Goal (Example Module)

What engineers are good at

Heat/ Mass Transfer

+

What bio scientists are good at

Microbiology/

Chemical Kinetics

=

Together they improve at

Food Sterilization Process

But what bio scientists might not be

But what engineers might not be

Basic overview of user experience

COMSOL Model	
Filename:	C:\Users\adw88.CORNELL\Dropbox\Food Safety Software\Can.mph

Enter the Geometry and Time Information Here

Parameter	Expr	Description
Time_Tot	720	Total Process Time, Seconds
Time_Rec	180	Time Step Intervals, Seconds
Prod_R	0.1	Product Radius, m
Prod_H	0.1	Product Height, m
Elem	5	Element Quality, 1 is course, higher is finer

Problem Schematic

Domain Volume, m^3	0.003141593
Sample Density, kg/m^3	802.4276877
Sample Mass, kg	2.520900929

Show Schematic

Initial Conditions

Name	Expr	Description
T10	10	Initial temperature, C
phi	0.9	porosity

Visual Basic Button

Initial Product Composition, wet basis

Get Composition

Select Food Group:	sea food
Select Food:	ABALONE,MXD SP,CKD,FRIED

Name	Expr	Description
wt_Water	60.1	
wt_Prot	19.63	
wt_Fat	6.78	
wt_Ash	1.77	
wt_Carb	11.05	
wt_Fiber	0	
Total % Weight	**99.33**	

Boundary Conditions

Name	Expr	Description
h_top	10	Conv. heat transfer coef on top, W m^-2 K^-1
T_top	20	Top can temperature, C
h_right	10	Conv. heat transfer coef on right, W m^-2 K^-1
T_right	20	Right can temperature, C
h_bottom	10	Conv. heat transfer coef on bottom, W m^-2 K^-1
T_bottom	20	Bottom can temperature, C

Microbial Growth Kinetics

Update Microbe Growth and Inactivation Kinetics

Microbe number 1:	Staphylococcus
Growth Model Type:	First Order

Name	Expr	Description
Rate1	0.0073*T -	Growth rate, log(CFU/ml)/s
Lag1	7.34*T)*(T>=8)*(T<17	lag time, s
N01	3	log(CFU/ml)

Microbe number 2:	Staphylococcus
Growth Model Type:	Sigmoidal

Name	Expr	Description
Rate2	/(1+exp(-(0.554*T^2-	
Lag2	0	
N02	3	log(CFU/ml)

Microbe number 3:	E. coli O157
Growth Model Type:	First Order

Name	Expr	Description
Rate3	(0)*N3/(3600*2.3026)	
Lag3	0	
N03	3	log(CFU/ml)

Inactivation Kinetics

Microbe number 1:	Staphylococcus
Inactivation (Yes/No)	No

Name	Expr	Description
D1	0	
z1	0	
Tref1	0	

Microbe number 2:	Staphylococcus
Inactivation (Yes/No)	No

Name	Expr	Description
D2	0	
z2	0	
Tref2	0	

Microbe number 3:	E. coli O157
Inactivation (Yes/No)	No

Name	Expr	Description
D3	0	
z3	0	
Tref3	0	

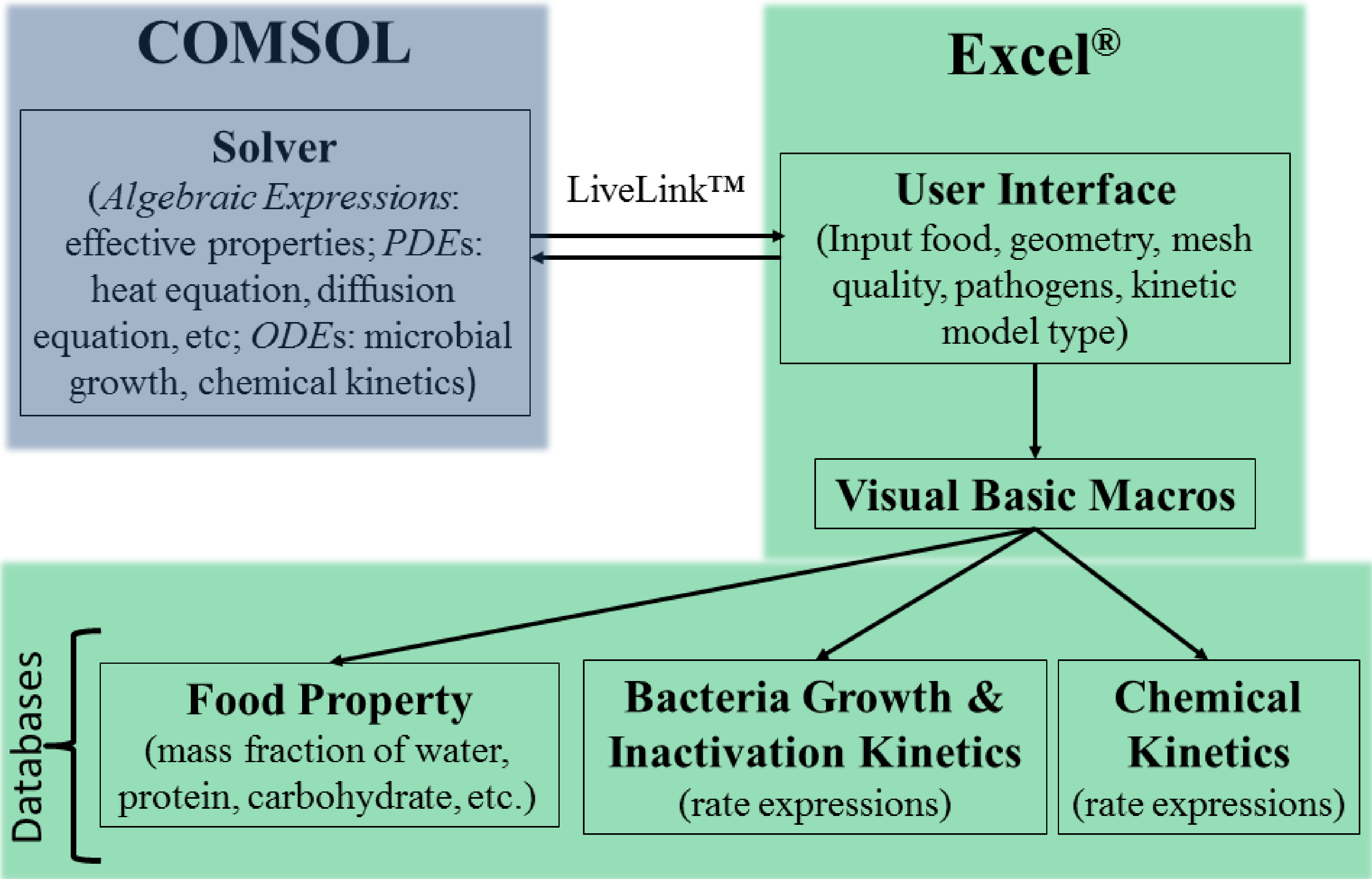
Generation/Degradation of Chemicals

Update Chemical

Chemical:	MeIQx
Formation or Degradation	Formation

Name	Expr	Description
C0	0	
Cmax	5.266	
kg	0.0004*T+0.0378	
kd	0	

General idea of how software works



Functionalities of software

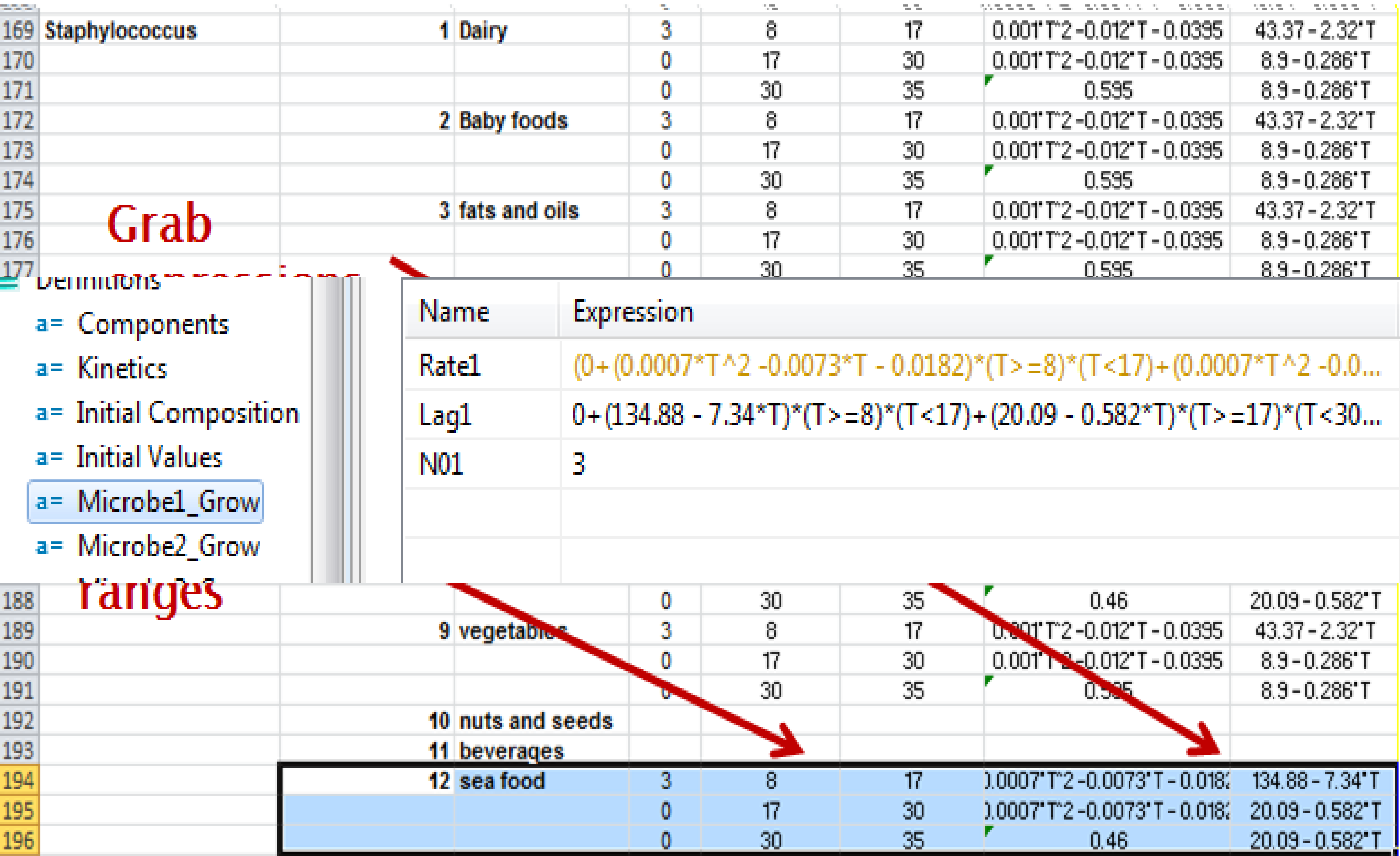
- Built in composition database
- Built in kinetic database for microbes and chemicals
- Meshing is automated
- Students avoid equation and solver inputs
- Post-Processing is set-up ahead of time
- No programming (i.e. Matlab)

Properties and Meshing

Name	Expression
rho_s	tot/(wt_Water/rho_w+wt_Ash/rho_ash+wt_Carb/rho_carb+wt_Fat/rho...
cp_s	(wt_Water*cp_w+wt_Ash*cp_ash+wt_Carb*cp_carb+wt_Fat*cp_fat+wt...
k_s_parallel	tot/(wt_Water/k_w+wt_Ash/k_ash+wt_Carb/k_carb+wt_Fat/k_fat+wt_...
k_s_perp	(wt_Water*k_w+wt_Ash*k_ash+wt_Carb*k_carb+wt_Fat*k_fat+wt_Fibe...
k_s	0.5*(k_s_parallel+k_s_perp)
cp_protein	2008.2+1.2089*T2-.0013129*T2*T2
rho_w	997.18+.0031439*T2-.0037574*T2*T2
rho_ash	2423.8-.28063*T2
cp_carb	1548.8+1.9625*T2-.0059399*T2*T2
cp_fat	1984.2+1.4373*T2-.0048008*T2*T2
k_fibre	0.18331+.0012497*T2-.0000031683*T2*T2
k_w	0.57109+.001762*T2-.0000067036*T2*T2
k_fat	0.18071+.0027604*T2-.00000017749*T2*T2
k_carb	0.20141+.0013874*T2-.0000043312*T2*T2
cp_w	4176.2-.0909*T2+.0054731*T2*T2

Effective properties automatically calculated in COMSOL from composition

Properties and Meshing, ctd.



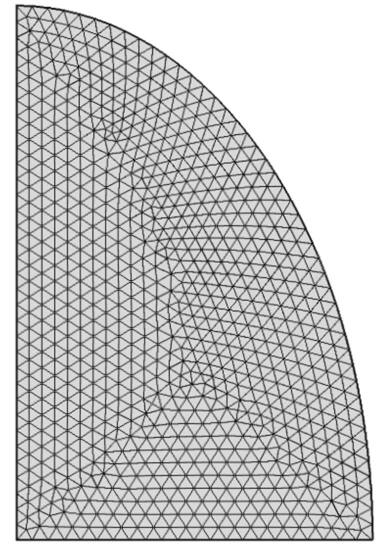
169	Staphylococcus	1	Dairy	3	8	17	0.001*T^2 -0.012*T - 0.0395	43.37 - 2.32*T
170				0	17	30	0.001*T^2 -0.012*T - 0.0395	8.9 - 0.286*T
171				0	30	35	0.595	8.9 - 0.286*T
172		2	Baby foods	3	8	17	0.001*T^2 -0.012*T - 0.0395	43.37 - 2.32*T
173				0	17	30	0.001*T^2 -0.012*T - 0.0395	8.9 - 0.286*T
174				0	30	35	0.595	8.9 - 0.286*T
175		3	fats and oils	3	8	17	0.001*T^2 -0.012*T - 0.0395	43.37 - 2.32*T
176				0	17	30	0.001*T^2 -0.012*T - 0.0395	8.9 - 0.286*T
177				0	30	35	0.595	8.9 - 0.286*T

Name	Expression
Rate1	(0+(0.0007*T^2 -0.0073*T - 0.0182)*(T>=8)*(T<17)+(0.0007*T^2 -0.0...
Lag1	0+(134.88 - 7.34*T)*(T>=8)*(T<17)+(20.09 - 0.582*T)*(T>=17)*(T<30...
N01	3

188				0	30	35	0.46	20.09 - 0.582*T
189		9	vegetables	3	8	17	0.001*T^2 -0.012*T - 0.0395	43.37 - 2.32*T
190				0	17	30	0.001*T^2 -0.012*T - 0.0395	8.9 - 0.286*T
191				0	30	35	0.595	8.9 - 0.286*T
192		10	nuts and seeds					
193		11	beverages					
194		12	sea food	3	8	17	).0007*T^2 -0.0073*T - 0.018	134.88 - 7.34*T
195				0	17	30	).0007*T^2 -0.0073*T - 0.018	20.09 - 0.582*T
196				0	30	35	0.46	20.09 - 0.582*T

Properties and Meshing, ctd.

- **Automatic meshing with logical statements**



Element Size Parameters

☑ Maximum element size:

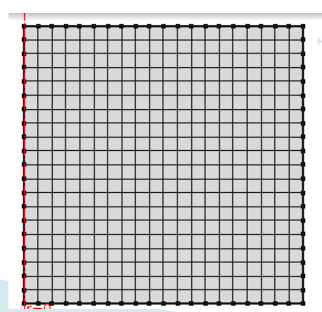
1/Elem*.025*(Prod_H^2+Prod_R^2)^.5 m

☑ Minimum element size:

.5*1/Elem*.025*(Prod_H^2+Prod_R^2)^.5 m

Number of elements:

(Prod_H>=1)*ceil(Prod_H*Elem/.05)+(Prod_H<1)*(Prod_H>=.05)*ceil(Prod_H*Elem/.005)+(Prod_H<.05)*(Prod_H>=.01)*ceil(Prod



Future Plans

- New modules
- Implementing, testing and evaluating in a number of courses at various universities, covering varying background of students and faculty
- Possibly extend to STEM curricula where simulation is not routine

Questions?