SBML Model Report

Model name: "Mellor2012_LipooxygenasePathway"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Nathan Mellor[2] at April tenth 2012 at 1:24 p. m. and last time modified at May 22^{nd} 2014 at 7:03 p. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	10
events	0	constraints	0
reactions	5	function definitions	1
global parameters	9	unit definitions	3
rules	1	initial assignments	0

Model Notes

This model is from the article:
Reduction of off-flavor generation in soybean homogenates: a mathematical model.
Mellor N , Bligh F , Chandler I , Hodgman C J. Food Sci.2010 Sep; 75(7): R131-8; PMID: 2153556,

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Abstract:
The generation of off-flavors in soybean homogenates such as n-hexanal via the lipoxygenase (LOX) pathway can be a problem in the processed food industry. Previous studies have examined the effect of using soybean varieties missing one or more of the 3 LOX isozymes on n-hexanal generation. A dynamic mathematical model of the soybean LOX pathway using ordinary differential equations was constructed using parameters estimated from existing data with the aim of predicting how n-hexanal generation could be reduced. Time-course simulations of LOX-null beans were run and compared with experimental results. Model L(2), L(3), and L(12) beans were within the range relative to the wild type found experimentally, with L(13) and L(23) beans close to the experimental range. Model L(1) beans produced much more n-hexanal relative to the wild type than those in experiments. Sensitivity analysis indicates that reducing the estimated K(m) parameter for LOX isozyme 3 (L-3) would improve the fit between model predictions and experimental results found in the literature. The model also predicts that increasing L-3 or reducing L-2 levels within beans may reduce n-hexanal generation. PRACTICAL APPLICATION: This work describes the use of mathematics to attempt to quantify the enzyme-catalyzed conversions of compounds in soybean homogenates into undesirable flavors, primarily from the compound n-hexanal. The effect of different soybean genotypes and enzyme kinetic constants was also studied, leading to recommendations on which combinations might minimize off-flavor levels and what further work might be carried out to substantiate these conclusions.

2 Unit Definitions

This is an overview of five unit definitions of which two are predefined by SBML and not mentioned in the model.

2.1 Unit `volume`

Name volume

Definition ml

2.2 Unit `time`

Name time

Definition 60 s

2.3 Unit `substance`

Name substance

Definition mmol

2.4 Unit `area`

Notes Square metre is the predefined SBML unit for `area` since SBML Level 2 Version 1.

Definition m^2

2.5 Unit `length`

Notes Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`compartment_1`	compartment	0000290	3	1000	ml	☑	

3.1 Compartment `compartment_1`

This is a three dimensional compartment with a constant size of 1000 ml.

Name compartment

SBO:0000290 physical compartment

4 Species

This model contains ten species. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
species_1	LA	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_7	13HOD-S(Z,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_8	13HOD-R(Z,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_9	13HOD-S(E,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_10	13HOD-R(E,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_11	9HOD-S(Z,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_12	9HOD-R(Z,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_13	9HOD-S(E,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_14	9HOD-R(E,E)	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_15	nHexanal	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟

5 Parameters

This model contains nine global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_1	Km(L1)		0.490		☑
parameter_2	Vm(L1)		0.008		☑
parameter_3	Km(L2)		0.490		☑
parameter_4	Vm(L2)		0.039		☑
parameter_5	Km(L3)		0.490		☑
parameter_6	Vm(L3)		0.003		☑
parameter_7	Km(HPL)		0.050		☑
parameter_8	Vm(HPL-SZE)		0.285		☑
parameter_9	Vm(HPL-RZE)		0.038		☐

6 Function definition

This is an overview of one function definition.

6.1 Function definition `function_1`

Name Henri-Michaelis-Menten (irreversible)

Arguments substrate, Km, V

Mathematical Expression

$$\frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{1}$$

7 Rule

This is an overview of one rule.

7.1 Rule `parameter_9`

Rule `parameter_9` is an assignment rule for parameter `parameter_9`:

$$\mathrm{parameter\_9} = 0.135 \cdot \mathrm{parameter\_8} \tag{2}$$

8 Reactions

This model contains five reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	`reaction_1`	LOX1	$\text{species\_1} \longrightarrow 0 \cdot 574\,\text{species\_7} + 0 \cdot 144\,\text{species\_8} + 0 \cdot 05\,\text{species\_9} + 0 \cdot 012\,\text{species\_10} + 0 \cdot 162\,\text{species\_11} + 0 \cdot 04\,\text{species\_12} + 0 \cdot 014\,\text{species\_13} + 0 \cdot 0040\,\text{species\_14}$	
2	`reaction_2`	LOX2	$\text{species\_1} \longrightarrow 0 \cdot 751\,\text{species\_7} + 0 \cdot 023\,\text{species\_8} + 0 \cdot 025\,\text{species\_9} + 0 \cdot 015\,\text{species\_10} + 0 \cdot 127\,\text{species\_11} + 0 \cdot 026\,\text{species\_12} + 0 \cdot 018\,\text{species\_13} + 0 \cdot 016\,\text{species\_14}$	
3	`reaction_3`	LOX3	$\text{species\_1} \longrightarrow 0 \cdot 068\,\text{species\_7} + 0 \cdot 059\,\text{species\_8} + 0 \cdot 136\,\text{species\_9} + 0 \cdot 107\,\text{species\_10} + 0 \cdot 218\,\text{species\_11} + 0 \cdot 218\,\text{species\_12} + 0 \cdot 098\,\text{species\_13} + 0 \cdot 097\,\text{species\_14}$	
4	`reaction_4`	HPL	$\text{species\_7} \longrightarrow \text{species\_15}$	
5	`reaction_5`	HPL(RZE)	$\text{species\_8} \longrightarrow \text{species\_15}$	

8.1 Reaction reaction_1

This is an irreversible reaction of one reactant forming eight products.

Name LOX1

Reaction equation

$$\text{species\_1} \longrightarrow 0.574\,\text{species\_7} + 0.144\,\text{species\_8} + 0.05\,\text{species\_9} + 0.012\,\text{species\_10} + 0.162\,\text{species\_11} + 0.04\,\text{spec} \tag{3}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
species_1	LA	

Products

Table 7: Properties of each product.

Id	Name	SBO
species_7	13HOD-S(Z,E)	
species_8	13HOD-R(Z,E)	
species_9	13HOD-S(E,E)	
species_10	13HOD-R(E,E)	
species_11	9HOD-S(Z,E)	
species_12	9HOD-R(Z,E)	
species_13	9HOD-S(E,E)	
species_14	9HOD-R(E,E)	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{compartment\_1}) \cdot \text{function\_1}\,([\text{species\_1}], \text{parameter\_1}, \text{parameter\_2}) \tag{4}$$

$$\text{function\_1}\,(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{5}$$

$$\text{function\_1}\,(\text{substrate}, \text{Km}, \text{V}) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{6}$$

8.2 Reaction reaction_2

This is an irreversible reaction of one reactant forming eight products.

Name LOX2

Reaction equation

$$\text{species\_1} \longrightarrow 0\cdot751\,\text{species\_7} + 0\cdot023\,\text{species\_8} + 0\cdot025\,\text{species\_9} + 0\cdot015\,\text{species\_10} + 0\cdot127\,\text{species\_11} + 0\cdot026\,\text{sp} \tag{7}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
species_1	LA	

Products

Table 9: Properties of each product.

Id	Name	SBO
species_7	13HOD-S(Z,E)	
species_8	13HOD-R(Z,E)	
species_9	13HOD-S(E,E)	
species_10	13HOD-R(E,E)	
species_11	9HOD-S(Z,E)	
species_12	9HOD-R(Z,E)	
species_13	9HOD-S(E,E)	
species_14	9HOD-R(E,E)	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left([\mathrm{species\_1}], \mathrm{parameter\_3}, \mathrm{parameter\_4}\right) \tag{8}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{9}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{10}$$

8.3 Reaction `reaction_3`

This is an irreversible reaction of one reactant forming eight products.

Name LOX3

Reaction equation

$$\text{species\_1} \longrightarrow 0.068\,\text{species\_7} + 0.059\,\text{species\_8} + 0.136\,\text{species\_9} + 0.107\,\text{species\_10} + 0.218\,\text{species\_11} + 0.218\,\text{sp} \tag{11}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
`species_1`	LA	

Products

Table 11: Properties of each product.

Id	Name	SBO
`species_7`	13HOD-S(Z,E)	
`species_8`	13HOD-R(Z,E)	
`species_9`	13HOD-S(E,E)	
`species_10`	13HOD-R(E,E)	
`species_11`	9HOD-S(Z,E)	
`species_12`	9HOD-R(Z,E)	
`species_13`	9HOD-S(E,E)	
`species_14`	9HOD-R(E,E)	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_1}\left([\text{species\_1}], \text{parameter\_5}, \text{parameter\_6}\right) \tag{12}$$

$$\text{function\_1}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{13}$$

$$\text{function\_1}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{14}$$

8.4 Reaction `reaction_4`

This is an irreversible reaction of one reactant forming one product.

Name HPL

Reaction equation

$$\text{species\_7} \longrightarrow \text{species\_15} \tag{15}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
`species_7`	13HOD-S(Z,E)	

Product

Table 13: Properties of each product.

Id	Name	SBO
`species_15`	nHexanal	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_1}\left(\left[\text{species\_7}\right], \text{parameter\_7}, \text{parameter\_8}\right) \tag{16}$$

$$\text{function\_1}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{17}$$

$$\text{function\_1}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{18}$$

8.5 Reaction `reaction_5`

This is an irreversible reaction of one reactant forming one product.

Name HPL(RZE)

Reaction equation

$$\text{species\_8} \longrightarrow \text{species\_15} \tag{19}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_8	13HOD-R(Z,E)	

Product

Table 15: Properties of each product.

Id	Name	SBO
species_15	nHexanal	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_1}\left(\left[\mathrm{species\_8}\right], \mathrm{parameter\_7}, \mathrm{parameter\_9}\right) \tag{20}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{21}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{22}$$

9 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`>0 for certain species.

9.1 Species species_1

Name LA

SBO:0000247 simple chemical

Initial concentration $6.69999967735732 \cdot 10^{-5}$ mmol · ml^{-1}

This species takes part in three reactions (as a reactant in reaction_1, reaction_2, reaction_3).

$$\frac{d}{dt}\text{species\_1} = -v_1 - v_2 - v_3 \tag{23}$$

9.2 Species species_7

Name 13HOD-S(Z,E)

SBO:0000247 simple chemical

Initial concentration 0 mmol · ml^{-1}

This species takes part in four reactions (as a reactant in reaction_4 and as a product in reaction_1, reaction_2, reaction_3).

$$\frac{d}{dt}\text{species\_7} = 0.574\, v_1 + 0.751\, v_2 + 0.068\, v_3 - v_4 \tag{24}$$

9.3 Species species_8

Name 13HOD-R(Z,E)

SBO:0000247 simple chemical

Initial concentration 0 mmol · ml^{-1}

This species takes part in four reactions (as a reactant in reaction_5 and as a product in reaction_1, reaction_2, reaction_3).

$$\frac{d}{dt}\text{species\_8} = 0.144\, v_1 + 0.023\, v_2 + 0.059\, v_3 - v_5 \tag{25}$$

9.4 Species species_9

Name 13HOD-S(E,E)

SBO:0000247 simple chemical

Initial concentration 0 mmol · ml^{-1}

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{d}{dt}\text{species\_9} = 0.05\, v_1 + 0.025\, v_2 + 0.136\, v_3 \tag{26}$$

9.5 Species species_10

Name 13HOD-R(E,E)

SBO:0000247 simple chemical

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_10} = 0.012\, v_1 + 0.015\, v_2 + 0.107\, v_3 \tag{27}$$

9.6 Species species_11

Name 9HOD-S(Z,E)

SBO:0000247 simple chemical

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_11} = 0.162\, v_1 + 0.127\, v_2 + 0.218\, v_3 \tag{28}$$

9.7 Species species_12

Name 9HOD-R(Z,E)

SBO:0000247 simple chemical

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_12} = 0.04\, v_1 + 0.026\, v_2 + 0.218\, v_3 \tag{29}$$

9.8 Species species_13

Name 9HOD-S(E,E)

SBO:0000247 simple chemical

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_13} = 0.014\, v_1 + 0.018\, v_2 + 0.098\, v_3 \tag{30}$$

9.9 Species species_14

Name 9HOD-R(E,E)

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in three reactions (as a product in reaction_1, reaction_2, reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_14} = 0.0040\, v_1 + 0.016\, v_2 + 0.097\, v_3 \tag{31}$$

9.10 Species species_15

Name nHexanal

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in two reactions (as a product in reaction_4, reaction_5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_15} = v_4 + v_5 \tag{32}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000247 **simple chemical:** Simple, non-repetitive chemical entity

SBO:0000290 **physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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