SBML Model Report

Model name: "Brands2002 - Monosaccharide-casein systems"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at January 25th 2006 at ten o' clock in the afternoon. and last time modified at April fourth 2014 at 12:30 a. m. Table 1 gives 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	11
events	0	constraints	0
reactions	11	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

Brands2002 - Monosaccharide-casein systems

A kinetic model of the Maillard reaction occurring in heated monosaccharide-casein system.

This model is described in the article:Kinetic modeling of reactions in heated monosaccharide-casein systems.Brands CM, van Boekel MAJournal of Agricultural and Food Chemistry. 2002, 50(23):6725-6739

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Abstract:

In the present study, a kinetic model of the Maillard reaction occurring in heated monosaccharide-casein systems was proposed. Its parameters, the reaction rate constants, were estimated via multiresponse modeling. The determinant criterion was used as the statistical fit criterion instead of the familiar least squares to avoid statistical problems. The kinetic model was extensively tested by varying the reaction conditions. Different sugars (glucose, fructose, galactose, and tagatose) were studied regarding their effect on the reaction kinetics. This study has shown the power of multiresponse modeling for the unraveling of complicated reaction routes as occur in the Maillard reaction. The iterative process of proposing a model, confronting it with experiments, and criticizing the model was passed through four times to arrive at a model that was largely consistent with all results obtained. A striking difference was found between aldose and ketose sugars as suggested by the modeling results: not the ketoses themselves but only their reaction products were found to be reactive in the Maillard reaction.

2 Unit Definitions

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

2.1 Unit `substance`

Name millimole (default)

Definition mmol

2.2 Unit `time`

Name minute (default)

Definition 60 s

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

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			3	1	litre	☑	

3.1 Compartment compartment

This is a three dimensional compartment with a constant size of one litre.

4 Species

This model contains eleven species. Section 6 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
Glu		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Fru		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Formic_acid		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Triose		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetic_acid		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cn		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Amadori		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AMP		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C5		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
lys_R		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Melanoidin		compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Reactions

This model contains eleven 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	_J1		Glu $\longrightarrow$ Fru	
2	_J2		Fru $\longrightarrow$ Glu	
3	_J3		Glu $\longrightarrow$ C5 + Formic_acid	
4	_J4		Fru $\longrightarrow$ C5 + Formic_acid	
5	_J5		Fru $\longrightarrow$ 2 Triose	
6	_J6		Triose $\longrightarrow$ Cn + Acetic_acid	
7	_J7		lys_R + Glu $\longrightarrow$ Amadori	
8	_J8		Amadori $\longrightarrow$ Acetic_acid + lys_R	
9	_J9		Amadori $\longrightarrow$ AMP	
10	_J10		lys_R + Fru $\longrightarrow$ AMP	
11	_J11		AMP $\longrightarrow$ Melanoidin	

5.1 Reaction _J1

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

Reaction equation

$$\text{Glu} \longrightarrow \text{Fru} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Glu		

Product

Table 6: Properties of each product.

Id	Name	SBO
Fru		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{K1} \cdot [\text{Glu}] \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K1			0.01		☑

5.2 Reaction _J2

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

Reaction equation

$$\text{Fru} \longrightarrow \text{Glu} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Fru		

Product

Table 9: Properties of each product.

Id	Name	SBO
Glu		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{K2} \cdot [\mathrm{Fru}] \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K2			0.005		☑

5.3 Reaction _J3

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

Reaction equation

$$\mathrm{Glu} \longrightarrow \mathrm{C5} + \mathrm{Formic\_acid} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
Glu		

Products

Table 12: Properties of each product.

Id	Name	SBO
C5		
Formic_acid		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{K3} \cdot [\mathrm{Glu}] \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K3			$4.7 \cdot 10^{-4}$		☑

5.4 Reaction _J4

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

Reaction equation

$$\mathrm{Fru} \longrightarrow \mathrm{C5} + \mathrm{Formic\_acid} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Fru		

Products

Table 15: Properties of each product.

Id	Name	SBO
C5		

Id	Name	SBO
Formic_acid		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{K4} \cdot [\mathrm{Fru}] \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K4			0.001		☑

5.5 Reaction _J5

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

Reaction equation

$$\mathrm{Fru} \longrightarrow 2\,\mathrm{Triose} \tag{9}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Fru		

Product

Table 18: Properties of each product.

Id	Name	SBO
Triose		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{K5} \cdot [\mathrm{Fru}] \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K5			0.007		☑

5.6 Reaction _J6

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

Reaction equation

$$\text{Triose} \longrightarrow \text{Cn} + \text{Acetic\_acid} \tag{11}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Triose		

Products

Table 21: Properties of each product.

Id	Name	SBO
Cn		
Acetic_acid		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{K6} \cdot [\text{Triose}] \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K6			0.004		☑

5.7 Reaction _J7

This is an irreversible reaction of two reactants forming one product.

Reaction equation

$$\text{lys\_R} + \text{Glu} \longrightarrow \text{Amadori} \tag{13}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
lys_R		
Glu		

Product

Table 24: Properties of each product.

Id	Name	SBO
Amadori		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{K7} \cdot [\text{Glu}] \cdot [\text{lys\_R}] \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K7			$1.8 \cdot 10^{-4}$		☑

5.8 Reaction _J8

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

Reaction equation

$$\text{Amadori} \longrightarrow \text{Acetic\_acid} + \text{lys\_R} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Amadori		

Products

Table 27: Properties of each product.

Id	Name	SBO
Acetic_acid		
lys_R		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{K8} \cdot [\mathrm{Amadori}] \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K8			0.111		☑

5.9 Reaction _J9

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

Reaction equation

$$\mathrm{Amadori} \longrightarrow \mathrm{AMP} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
Amadori		

Product

Table 30: Properties of each product.

Id	Name	SBO
AMP		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{K9} \cdot [\mathrm{Amadori}] \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K9			0.144		☑

5.10 Reaction _J10

This is an irreversible reaction of two reactants forming one product.

Reaction equation

$$\mathrm{lys\_R} + \mathrm{Fru} \longrightarrow \mathrm{AMP} \tag{19}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
lys_R		
Fru		

Product

Table 33: Properties of each product.

Id	Name	SBO
AMP		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{K10} \cdot [\mathrm{Fru}] \cdot [\mathrm{lys\_R}] \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K10			$1.5 \cdot 10^{-4}$		☑

5.11 Reaction _J11

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

Reaction equation

$$\mathrm{AMP} \longrightarrow \mathrm{Melanoidin} \tag{21}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
AMP		

Product

Table 36: Properties of each product.

Id	Name	SBO
Melanoidin		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{K11} \cdot [\mathrm{AMP}] \tag{22}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K11			0.125		☑

6 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.

6.1 Species Glu

Initial concentration $160\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in _J1, _J3, _J7 and as a product in _J2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu} = v_2 - v_1 - v_3 - v_7 \tag{23}$$

6.2 Species Fru

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

This species takes part in five reactions (as a reactant in _J2, _J4, _J5, _J10 and as a product in _J1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru} = v_1 - v_2 - v_4 - v_5 - v_{10} \tag{24}$$

6.3 Species Formic_acid

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

This species takes part in two reactions (as a product in _J3, _J4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Formic\_acid} = v_3 + v_4 \tag{25}$$

6.4 Species Triose

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

This species takes part in two reactions (as a reactant in _J6 and as a product in _J5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Triose} = 2\,v_5 - v_6 \tag{26}$$

6.5 Species Acetic_acid

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

This species takes part in two reactions (as a product in _J6, _J8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetic\_acid} = v_6 + v_8 \tag{27}$$

6.6 Species Cn

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

This species takes part in one reaction (as a product in _J6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cn} = v_6 \tag{28}$$

6.7 Species Amadori

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

This species takes part in three reactions (as a reactant in _J8, _J9 and as a product in _J7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Amadori} = v_7 - v_8 - v_9 \tag{29}$$

6.8 Species AMP

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

This species takes part in three reactions (as a reactant in _J11 and as a product in _J9, _J10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_9 + v_{10} - v_{11} \tag{30}$$

6.9 Species C5

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

This species takes part in two reactions (as a product in _J3, _J4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C5} = v_3 + v_4 \tag{31}$$

6.10 Species lys_R

Initial concentration $15\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in _J7, _J10 and as a product in _J8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{lys\_R} = v_8 - v_7 - v_{10} \tag{32}$$

6.11 Species Melanoidin

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

This species takes part in one reaction (as a product in _J11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Melanoidin} = v_{11} \tag{33}$$

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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