SBML Model Report

Model name: "Martins2003_AmadoriDegradation"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Harish Dharuri[1] at January 18th 2006 at 6:08 p. m. and last time modified at April fourth 2014 at 12:28 a. m. Table 1 provides 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	14
events	0	constraints	0
reactions	16	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

This a model from the article:
Kinetic modelling of Amadori N-(1-deoxy-D-fructos-1-yl)-glycine degradation pathways. Part II–kinetic analysis.
Martins SI, Van Boekel MA. Carbohydr Res2003 Jul;338(16):1665-78. 12873422,
Abstract:

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A kinetic model for N-(1-deoxy-Image -fructos-1-yl)-glycine (DFG) thermal decomposition was proposed. Two temperatures (100 and 120 C) and two pHs (5.5 and 6.8) were studied. The measured responses were DFG, 3-deoxyosone, 1-deoxyosone, methylglyoxal, acetic acid, formic acid, glucose, fructose, mannose and melanoidins. For each system the model parameters, the rate constants, were estimated by non-linear regression, via multiresponse modelling. The determinant criterion was used as the statistical fit criterion. Model discrimination was performed by both chemical insight and statistical tests (Posterior Probability and Akaike criterion). Kinetic analysis showed that at lower pH DFG 1,2-enolization is favoured whereas with increasing pH 2,3-enolization becomes a more relevant degradation pathway. The lower amount observed of 1-DG is related with its high reactivity. It was shown that acetic acid, a main degradation product from DFG, was mainly formed through 1-DG degradation. Also from the estimated parameters 3-DG was found to be the main precursor in carbohydrate fragments formation, responsible for colour formation. Some indication was given that as the reaction proceeded other compounds besides DFG become reactants themselves with the formation among others of methylglyoxal. The multiresponse kinetic analysis was shown to be both helpful in deriving relevant kinetic parameters as well as in obtaining insight into the reaction mechanism.

Model was intially tested in Jarnac.

The model was recently updated on 9th July 2010. The reference publication has reported two models M1 and M2, where the parameter values are given for conditions A) 100^{o}C, pH5.5, B) 120^{o}C, pH5.5, C) 100^{o}C, pH6.8 and D) 120^{o}C, pH6.8.

This model corresponds to the model M2 with condition 100^{o}C, pH6.8

The model reproduces Figure 6 of the reference publication. The curation figure was recently added

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 micromole (default)

Definition μmol

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 14 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
DFG		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E1		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E2		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Cn		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Gly		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
_3DG		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
FA		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
_1DG		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
AA		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Man		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Glu		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
MG		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Mel		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Fru		compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Reactions

This model contains 16 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	v1		DFG $\longrightarrow$ E1	
2	v2		DFG $\longrightarrow$ E2	
3	v3		DFG $\longrightarrow$ Gly + Cn	
4	v4		E1 $\longrightarrow$ Gly + _3DG	
5	v5		_3DG $\longrightarrow$ Cn	
6	v6		_3DG $\longrightarrow$ FA	
7	v7		E2 $\longrightarrow$ Gly + _1DG	
8	v8		_1DG $\longrightarrow$ Cn	
9	v9		_1DG $\longrightarrow$ AA	
10	v10		E1 $\longrightarrow$ Gly + Man	
11	v11		E1 $\longrightarrow$ Gly + Glu	
12	v12		Man $\longrightarrow$ Glu	
13	v13		Glu $\longrightarrow$ _3DG	
14	v14		Gly + Cn $\longrightarrow$ Mel	
15	v15		Cn $\longrightarrow$ AA + FA + MG	
16	v16		E2 $\longrightarrow$ Gly + Fru	

5.1 Reaction v1

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

Reaction equation

$$\mathrm{DFG} \longrightarrow \mathrm{E1} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
DFG		

Product

Table 6: Properties of each product.

Id	Name	SBO
E1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{k1} \cdot [\mathrm{DFG}] \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.006		☑

5.2 Reaction v2

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

Reaction equation

$$\mathrm{DFG} \longrightarrow \mathrm{E2} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
DFG		

Product

Table 9: Properties of each product.

Id	Name	SBO
E2		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{k2} \cdot [\mathrm{DFG}] \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			0.016		☑

5.3 Reaction v3

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

Reaction equation

$$\mathrm{DFG} \longrightarrow \mathrm{Gly} + \mathrm{Cn} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
DFG		

Products

Table 12: Properties of each product.

Id	Name	SBO
Gly		
Cn		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{k3} \cdot [\mathrm{DFG}] \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			0.016		☑

5.4 Reaction v4

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

Reaction equation

$$\mathrm{E1} \longrightarrow \mathrm{Gly} + \_3\mathrm{DG} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
E1		

Products

Table 15: Properties of each product.

Id	Name	SBO
Gly		

Id	Name	SBO
_3DG		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{k4} \cdot [\mathrm{E1}] \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			0.079		☑

5.5 Reaction v5

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

Reaction equation

$$\_3\mathrm{DG} \longrightarrow \mathrm{Cn} \tag{9}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
_3DG		

Product

Table 18: Properties of each product.

Id	Name	SBO
Cn		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{k5} \cdot [\_3\mathrm{DG}] \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			0.091		☑

5.6 Reaction v6

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

Reaction equation

$$\_3DG \longrightarrow FA \tag{11}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
_3DG		

Product

Table 21: Properties of each product.

Id	Name	SBO
FA		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{k6} \cdot [\_3DG] \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			0.027		☑

5.7 Reaction v7

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

Reaction equation

$$\mathrm{E2} \longrightarrow \mathrm{Gly} + \_1\mathrm{DG} \tag{13}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
E2		

Products

Table 24: Properties of each product.

Id	Name	SBO
Gly		
_1DG		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{k7} \cdot [\mathrm{E2}] \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			0.213		☑

5.8 Reaction v8

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

Reaction equation

$$\_1\mathrm{DG} \longrightarrow \mathrm{Cn} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
_1DG		

Product

Table 27: Properties of each product.

Id	Name	SBO
Cn		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{k8} \cdot [\_1\mathrm{DG}] \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8			0.0		☑

5.9 Reaction v9

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

Reaction equation

$$\_1\mathrm{DG} \longrightarrow \mathrm{AA} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
_1DG		

Product

Table 30: Properties of each product.

Id	Name	SBO
AA		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{k9} \cdot [\_1\mathrm{DG}] \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9			1.909		☑

5.10 Reaction v10

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

Reaction equation

$$\mathrm{E1} \longrightarrow \mathrm{Gly} + \mathrm{Man} \tag{19}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
E1		

Products

Table 33: Properties of each product.

Id	Name	SBO
Gly		
Man		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{k10} \cdot [\mathrm{E1}] \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k10			0.071		☑

5.11 Reaction v11

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

Reaction equation

$$\mathrm{E1} \longrightarrow \mathrm{Gly} + \mathrm{Glu} \tag{21}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
E1		

Products

Table 36: Properties of each product.

Id	Name	SBO
Gly		
Glu		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{k11} \cdot [\mathrm{E1}] \tag{22}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k11			0.113		☑

5.12 Reaction v12

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

Reaction equation

$$\text{Man} \longrightarrow \text{Glu} \tag{23}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
Man		

Product

Table 39: Properties of each product.

Id	Name	SBO
Glu		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{k12} \cdot [\text{Man}] \tag{24}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k12			$8 \cdot 10^{-4}$		☑

5.13 Reaction v13

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

Reaction equation

$$\text{Glu} \longrightarrow \_3\text{DG} \tag{25}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
Glu		

Product

Table 42: Properties of each product.

Id	Name	SBO
_3DG		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{k13} \cdot [\text{Glu}] \tag{26}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13			0.002		☑

5.14 Reaction v14

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

Reaction equation

$$\text{Gly} + \text{Cn} \longrightarrow \text{Mel} \tag{27}$$

Reactants

Table 44: Properties of each reactant.

Id	Name	SBO
Gly		
Cn		

Product

Table 45: Properties of each product.

Id	Name	SBO
Mel		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{k14} \cdot [\mathrm{Cn}] \cdot [\mathrm{Gly}] \tag{28}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k14			0.003		☑

5.15 Reaction v15

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

Reaction equation

$$\mathrm{Cn} \longrightarrow \mathrm{AA} + \mathrm{FA} + \mathrm{MG} \tag{29}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
Cn		

Products

Table 48: Properties of each product.

Id	Name	SBO
AA		
FA		
MG		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{k15} \cdot [\text{Cn}] \tag{30}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k15			0.016		☑

5.16 Reaction v16

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

Reaction equation

$$\text{E2} \longrightarrow \text{Gly} + \text{Fru} \tag{31}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
E2		

Products

Table 51: Properties of each product.

Id	Name	SBO
Gly		

Id	Name	SBO
Fru		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{k16} \cdot [\mathrm{E2}] \tag{32}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k16			0.013		☑

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 DFG

Initial concentration $9\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v1, v2, v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DFG} = -v_1 - v_2 - v_3 \tag{33}$$

6.2 Species E1

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

This species takes part in four reactions (as a reactant in v4, v10, v11 and as a product in v1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E1} = v_1 - v_4 - v_{10} - v_{11} \tag{34}$$

6.3 Species E2

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in v7, v16 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E2} = v_2 - v_7 - v_{16} \tag{35}$$

6.4 Species Cn

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in five reactions (as a reactant in v14, v15 and as a product in v3, v5, v8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cn} = v_3 + v_5 + v_8 - v_{14} - v_{15} \tag{36}$$

6.5 Species Gly

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in seven reactions (as a reactant in v14 and as a product in v3, v4, v7, v10, v11, v16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly} = v_3 + v_4 + v_7 + v_{10} + v_{11} + v_{16} - v_{14} \tag{37}$$

6.6 Species _3DG

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in v5, v6 and as a product in v4, v13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{\_3DG} = v_4 + v_{13} - v_5 - v_6 \tag{38}$$

6.7 Species FA

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a product in v6, v15).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FA} = v_6 + v_{15} \tag{39}$$

6.8 Species _1DG

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in v8, v9 and as a product in v7).

$$\frac{\text{d}}{\text{d}t}\text{\_1DG} = v_7 - v_8 - v_9 \tag{40}$$

6.9 Species AA

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a product in v9, v15).

$$\frac{\text{d}}{\text{d}t}\text{AA} = v_9 + v_{15} \tag{41}$$

6.10 Species Man

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in v12 and as a product in v10).

$$\frac{\text{d}}{\text{d}t}\text{Man} = v_{10} - v_{12} \tag{42}$$

6.11 Species Glu

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in v13 and as a product in v11, v12).

$$\frac{\text{d}}{\text{d}t}\text{Glu} = v_{11} + v_{12} - v_{13} \tag{43}$$

6.12 Species MG

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in one reaction (as a product in v15).

$$\frac{\text{d}}{\text{d}t}\text{MG} = v_{15} \tag{44}$$

6.13 Species Mel

Initial concentration $0\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in one reaction (as a product in v14).

$$\frac{\text{d}}{\text{d}t}\text{Mel} = v_{14} \tag{45}$$

6.14 Species Fru

Initial concentration $0\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in v16).

$$\frac{\text{d}}{\text{d}t}\text{Fru} = v_{16} \tag{46}$$

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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