

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 Dharuri¹ 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 initially 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°C, pH5.5, B) 120°C, pH5.5, C) 100°C, pH6.8 and D) 120°C, pH6.8.

This model corresponds to the model M2 with condition 100°C, pH6.8

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

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To cite BioModels Database, please use [Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. \(2006\) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.](#)

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 m²

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	<input checked="" type="checkbox"/>	

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

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

Nº	Id	Name	Reaction Equation	SBO
1	v1		$\text{DFG} \longrightarrow \text{E1}$	
2	v2		$\text{DFG} \longrightarrow \text{E2}$	
3	v3		$\text{DFG} \longrightarrow \text{Gly} + \text{Cn}$	
4	v4		$\text{E1} \longrightarrow \text{Gly} + \text{_3DG}$	
5	v5		$\text{_3DG} \longrightarrow \text{Cn}$	
6	v6		$\text{_3DG} \longrightarrow \text{FA}$	
7	v7		$\text{E2} \longrightarrow \text{Gly} + \text{_1DG}$	
8	v8		$\text{_1DG} \longrightarrow \text{Cn}$	
9	v9		$\text{_1DG} \longrightarrow \text{AA}$	
10	v10		$\text{E1} \longrightarrow \text{Gly} + \text{Man}$	
11	v11		$\text{E1} \longrightarrow \text{Gly} + \text{Glu}$	
12	v12		$\text{Man} \longrightarrow \text{Glu}$	
13	v13		$\text{Glu} \longrightarrow \text{_3DG}$	
14	v14		$\text{Gly} + \text{Cn} \longrightarrow \text{Mel}$	
15	v15		$\text{Cn} \longrightarrow \text{AA} + \text{FA} + \text{MG}$	
16	v16		$\text{E2} \longrightarrow \text{Gly} + \text{Fru}$	

5.1 Reaction v_1

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

Reaction equation



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

$$v_1 = k_1 \cdot [\text{DFG}] \quad (2)$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.006		<input checked="" type="checkbox"/>

5.2 Reaction v_2

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

Reaction equation



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

$$v_2 = k_2 \cdot [\text{DFG}] \quad (4)$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			0.016		<input checked="" type="checkbox"/>

5.3 Reaction v3

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

Reaction equation



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

$$v_3 = k_3 \cdot [\text{DFG}] \quad (6)$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			0.016		<input checked="" type="checkbox"/>

5.4 Reaction v_4

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

Reaction equation



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

$$v_4 = k_4 \cdot [E1] \quad (8)$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			0.079		<input checked="" type="checkbox"/>

5.5 Reaction v5

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

Reaction equation



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

$$v_5 = k_5 \cdot [_3DG] \quad (10)$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			0.091		<input checked="" type="checkbox"/>

5.6 Reaction v6

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

Reaction equation



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

$$v_6 = k6 \cdot [_3DG] \quad (12)$$

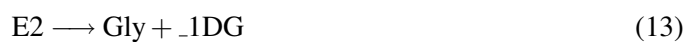
Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			0.027		<input checked="" type="checkbox"/>

5.7 Reaction v7

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

Reaction equation



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

$$v_7 = k_7 \cdot [\text{E2}] \quad (14)$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			0.213		<input checked="" type="checkbox"/>

5.8 Reaction v8

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

Reaction equation



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

$$v_8 = k_8 \cdot [_1DG] \quad (16)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8			0.0		<input checked="" type="checkbox"/>

5.9 Reaction v9

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

Reaction equation



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

$$v_9 = k_9 \cdot [-1DG] \quad (18)$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9			1.909		<input checked="" type="checkbox"/>

5.10 Reaction v10

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

Reaction equation



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

$$v_{10} = k_{10} \cdot [E1] \quad (20)$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k10			0.071		<input checked="" type="checkbox"/>

5.11 Reaction v_{11}

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

Reaction equation



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

$$v_{11} = k_{11} \cdot [E1] \quad (22)$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k11			0.113		<input checked="" type="checkbox"/>

5.12 Reaction v_{12}

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

Reaction equation



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

$$v_{12} = k_{12} \cdot [\text{Man}] \quad (24)$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k12			$8 \cdot 10^{-4}$		<input checked="" type="checkbox"/>

5.13 Reaction v13

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

Reaction equation



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

$$v_{13} = k_{13} \cdot [\text{Glu}] \quad (26)$$

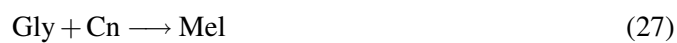
Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13			0.002		<input checked="" type="checkbox"/>

5.14 Reaction v14

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

Reaction equation



Reactants

Table 44: Properties of each reactant.

Id	Name	SBO
Gly		
Cn		

Product

Table 45: Properties of each product.

Id	Name	SBO
Me1		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = k_{14} \cdot [\text{Cn}] \cdot [\text{Gly}] \quad (28)$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k14			0.003		<input checked="" type="checkbox"/>

5.15 Reaction v15

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

Reaction equation



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

$$v_{15} = k_{15} \cdot [\text{Cn}] \quad (30)$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k15			0.016		<input checked="" type="checkbox"/>

5.16 Reaction v_{16}

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

Reaction equation



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

$$v_{16} = k_{16} \cdot [E2] \quad (32)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k16			0.013		<input checked="" type="checkbox"/>

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 $9 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt} \text{DFG} = -v_1 - v_2 - v_3 \quad (33)$$

6.2 Species E1

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

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

$$\frac{d}{dt} \text{E1} = v_1 - v_4 - v_{10} - v_{11} \quad (34)$$

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).

$$\frac{d}{dt}E2 = v_2 - v_7 - v_{16} \quad (35)$$

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).

$$\frac{d}{dt}Cn = v_3 + v_5 + v_8 - v_{14} - v_{15} \quad (36)$$

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).

$$\frac{d}{dt}Gly = v_3 + v_4 + v_7 + v_{10} + v_{11} + v_{16} - v_{14} \quad (37)$$

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).

$$\frac{d}{dt}_3DG = v_4 + v_{13} - v_5 - v_6 \quad (38)$$

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).

$$\frac{d}{dt}FA = v_6 + v_{15} \quad (39)$$

6.8 Species $_1\text{DG}$

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

This species takes part in three reactions (as a reactant in v_8 , v_9 and as a product in v_7).

$$\frac{d}{dt}_1\text{DG} = v_7 - v_8 - v_9 \quad (40)$$

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 v_9 , v_{15}).

$$\frac{d}{dt}\text{AA} = v_9 + v_{15} \quad (41)$$

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 v_{12} and as a product in v_{10}).

$$\frac{d}{dt}\text{Man} = v_{10} - v_{12} \quad (42)$$

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 v_{13} and as a product in v_{11} , v_{12}).

$$\frac{d}{dt}\text{Glu} = v_{11} + v_{12} - v_{13} \quad (43)$$

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 v_{15}).

$$\frac{d}{dt}\text{MG} = v_{15} \quad (44)$$

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 v_{14}).

$$\frac{d}{dt}\text{Mel} = v_{14} \quad (45)$$

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).

$$\frac{d}{dt}\text{Fru} = v_{16} \quad (46)$$

SBML2^ATeX 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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