SBML Model Report

Model name: "Radulescu2008_NFkB-_hierarchy_M_39_65_90"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Ovidiu Radulescu² at May 19th 2008 at 2:17 p. m. and last time modified at April eighth 2016 at 4:02 p. 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	2
species types	0	species	60
events	1	constraints	0
reactions	57	function definitions	0
global parameters	88	unit definitions	0
rules	0	initial assignments	0

Model Notes

NFkB model M(39,65,90) - most complex model

This is a model of NFkB pathway functioning from hierarchy of models of decreasing complexity, created to demonstrate application of model reduction methods proposed in

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Robust simplifications of multiscale biochemical networks.

Radulescu O, Gorban A., Zinovyev A., Lilienbaum. A. <u>BMC Syst Biol</u>2008:2:86 18854041, **Abstract:**

BACKGROUND: Cellular processes such as metabolism, decision making in development and differentiation, signalling, etc., can be modeled as large networks of biochemical reactions. In order to understand the functioning of these systems, there is a strong need for general model reduction techniques allowing to simplify models without loosing their main properties. In systems biology we also need to compare models or to couple them as parts of larger models. In these situations reduction to a common level of complexity is needed. RESULTS: We propose a systematic treatment of model reduction of multiscale biochemical networks. First, we consider linear kinetic models, which appear as "pseudo-monomolecular", subsystems of multiscale nonlinear reaction networks. For such linear models, we propose a reduction algorithm which is based on a generalized theory of the limiting step that we have developed in 1. Second, for non-linear systems we develop an algorithm based on dominant solutions of quasi-stationarity equations. For oscillating systems, quasi-stationarity and averaging are combined to eliminate time scales much faster and much slower than the period of the oscillations. In all cases, we obtain robust simplifications and also identify the critical parameters of the model. The methods are demonstrated for simple examples and for a more complex model of NF-kappaB pathway. CONCLUSION: Our approach allows critical parameter identification and produces hierarchies of models. Hierarchical modeling is important in "middle-out,, approaches when there is need to zoom in and out several levels of complexity. Critical parameter identification is an important issue in systems biology withpotential applications to biological control and therapeutics. Our approach also deals naturally with the presence of multiple time scales, which is a general property of systems biology models.

The models are provided in CellDesigner v3.5format. The name of the model M(x,y,z) should be deciphered as following:

x - number of speciesy - number of reactionsz - number of parameters

Simulation protocol: The model can be simulated in CellDesignerdirectly, or in any simulator supporting events. The simulation period should be set up in 40 hours (t=144000 sec). The 'signal' event applies signal to the pathway at the moment t=20 hours=72000 sec. This model reproduces Figure 7c (M(39,65,90)) of the publication.

For additional information please contactAndrei.Zinovyev at curie.fr

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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 which are all predefined by SBML and not mentioned in the model.

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.3 Unit area

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

Definition m^2

2.4 Unit length

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

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default c1	nucleus		3 3	1 1	litre litre	1	default

3.1 Compartment default

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

3.2 Compartment c1

This is a three dimensional compartment with a constant size of one litre, which is surrounded by default.

Name nucleus

4 Species

This model contains 60 species. The boundary condition of 15 of these species is set to true so that these species' amount cannot be changed by any reaction. Section 8 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
s22	FTAx	c1	$\text{mol} \cdot l^{-1}$	\Box	\Box
s36	FTAy	c1	$\text{mol} \cdot 1^{-1}$		
s65	FTAz	c1	$\text{mol} \cdot 1^{-1}$		
s93	IkB_alpha	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s108	csa17_degraded	c1	$\text{mol} \cdot 1^{-1}$		
s109	sa4_degraded	default	$\text{mol} \cdot 1^{-1}$		
s110	p105	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s111	sa438_degraded	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
s112	sa3_degraded	default	$\operatorname{mol} \cdot 1^{-1}$		
s113	mRNAp105	default	$\text{mol} \cdot 1^{-1}$		
s114	p50	default	$\operatorname{mol} \cdot 1^{-1}$		\Box
s117	mRNAp65	default	$\text{mol} \cdot 1^{-1}$		
s118	sa8_degraded	default	$\text{mol} \cdot 1^{-1}$		
s119	p65	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s120	sa9_degraded	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
s122	sa13_degraded	default	$\operatorname{mol} \cdot 1^{-1}$		
s123	IkB_alpha	default	$\text{mol} \cdot 1^{-1}$		
s124	sa12_degraded	default	$\text{mol} \cdot 1^{-1}$		
s126	A20	c1	$\text{mol} \cdot 1^{-1}$		
s127	mRNAA20	default	$\text{mol} \cdot 1^{-1}$		
s128	A20	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		

6	Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
	s129	sa444_degraded	default	$\text{mol} \cdot l^{-1}$		
	s130	IKKi	default	$\operatorname{mol} \cdot 1^{-1}$		
	s131	sa19_degraded	default	$\operatorname{mol} \cdot 1^{-1}$		
	s132	IKKa	default	$\operatorname{mol} \cdot 1^{-1}$		
	s133	IKKn	default	$\operatorname{mol} \cdot 1^{-1}$		\Box
	s134	sa20_degraded	default	$\text{mol} \cdot 1^{-1}$		
	s150	IKK	c1	$\operatorname{mol} \cdot 1^{-1}$		
<u>.</u> .	s153	sa96_degraded	default	$\operatorname{mol} \cdot 1^{-1}$		
Produced by SBML2leTEX	s154	sa97_degraded	default	$\operatorname{mol} \cdot 1^{-1}$		$ \overline{\mathbf{Z}} $
duc	s156	csa21_degraded	default	$\operatorname{mol} \cdot 1^{-1}$	$ \overline{\mathbf{Z}} $	
ed	s157	csa18_degraded	default	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
by	s158	csa9_degraded	c1	$\operatorname{mol} \cdot 1^{-1}$		
88	s160	InactivePRaseonp65	c1	$\operatorname{mol} \cdot 1^{-1}$		
\leq	s165	ActivePRaseonp65	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
Æ	s170	InactivePRaseonp105	c1	$\operatorname{mol} \cdot 1^{-1}$		
\mathbb{Z}	s173	ActivePRaseonp105	c1	$\operatorname{mol} \cdot 1^{-1}$		
	s178	mRNAIKB_alpha	default	$\operatorname{mol} \cdot 1^{-1}$		
	s185	ActivePRaseonIkB_alpha	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
	s188	NFkB:IkB_alpha	default	$\operatorname{mol} \cdot 1^{-1}$		
	s189	NFkB:IKKa:Ikb_alpha	default	$\operatorname{mol} \cdot 1^{-1}$		\Box
	s190	NFkB	default	$\operatorname{mol} \cdot 1^{-1}$		
	s191	IKKa:IKB_alpha	default	$\operatorname{mol} \cdot 1^{-1}$		\Box
	s192	NFkB:IkB_alpha	c1	$\operatorname{mol} \cdot 1^{-1}$		
	s193	Promp65:RNAP2	c1	$\operatorname{mol} \cdot 1^{-1}$		
	s194	Promp65:RNAP2:FTAy	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
	s195	NFkB	c1	$\text{mol} \cdot 1^{-1}$		\Box
	s196	Promp105:RNAP1:p50p65	c1	$\text{mol} \cdot 1^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s197	Promp105:RNAP1:p50p65:IkBa	c1	$\text{mol} \cdot 1^{-1}$		
s198	Promp105:RNAP	c1	$\text{mol} \cdot l^{-1}$		
s199	Promp105:RNAP:FTAX	c1	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s200	Promp105:RNAP1:FTAx:p50p65	c1	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s201	Promp105:RNAP1:FTAx:p50p65:IkBa	c1	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s205	PromIkBa:RNAP3	c1	$\text{mol} \cdot l^{-1}$		\Box
s206	PromIkBa:RNAP3:FTAz	c1	$\text{mol} \cdot l^{-1}$		\Box
s209	InactivePRaseonIkB_alpha	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s212	PromIkBa:RNAP3:p50p65	c1	$\text{mol} \cdot l^{-1}$		\Box
s213	PromIkBa:RNAP3:p50p65:IkBa	c1	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		\Box
s214	IkBa:RNAP3:FTAz:p50p65	c1	$\mathrm{mol}\cdot\mathrm{l}^{-1}$		
s215	PromIkBa:RNAP3:FTAz:p50p65:IkBalpha	c1	$\operatorname{mol} \cdot 1^{-1}$		

5 Parameters

This model contains 88 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1		0.000	
k2		$1.25 \cdot 10^{-4}$	\mathbf{Z}
k3		10^{-5}	
k4		0.100	
k5		0.002	
k6		$1.25 \cdot 10^{-4}$	\square
k7		0.240	
k8		0.100	\square
k9		1.200	\square
k10		0.100	\square
k11		$1.25 \cdot 10^{-4}$	
k12		$2\cdot 10^{-5}$	\mathbf{Z}
kf13		0.500	\mathbf{Z}
kr13		0.000	$\overline{\mathbf{Z}}$
kf14		0.500	
kr14		0.000	\square
kf15		0.003	\square
kr15		$8 \cdot 10^{-5}$	\square
k16		0.500	
k17		$4 \cdot 10^{-4}$	\square
k18		$3 \cdot 10^{-4}$	
k20		$5 \cdot 10^{-7}$	
k19		0.000	
k21		10^{-4}	
k22		0.500	
kf23		0.001	
kr23		$5 \cdot 10^{-4}$	
k25		0.000	
k27		$4 \cdot 10^{-4}$	
kf28		0.010	
kr28		0.000	
kf32		10.000	
kr32		10^{-4}	∠
k42		$5 \cdot 10^{-4}$	\square
k43		0.100	
k33		$5 \cdot 10^{-4}$	
k34		0.100	\mathbf{Z}

Id	Name	SBO	Value	Unit	Constant
k69			0.006		
k70			0.060		
k49			$5 \cdot 10^{-4}$		\square
k50			0.020		$ \overline{\checkmark} $
k61			0.060		
k62			0.600		
k35			0.010		
k36			0.004		
k37			$5 \cdot 10^{-5}$		
k38			$6 \cdot 10^{-5}$		$ \overline{\checkmark} $
k39		1	$1.3 \cdot 10^{-4}$		\mathbf{Z}
k40		($6.4 \cdot 10^{-5}$		
kf41			10.000		$ \overline{\checkmark} $
kr41			10^{-4}		
k44			0.016		\mathbf{Z}
k45			0.005		
k46			$5\cdot 10^{-5}$		$ \overline{\checkmark} $
k47		($5.4 \cdot 10^{-5}$		$ \overline{\checkmark} $
kf48			10.000		
kr48			10^{-4}		\checkmark
k51			0.025		\checkmark
kf52			0.003		\checkmark
kr52			0.001		\mathbf{Z}
k53			$2 \cdot 10^{-4}$		\checkmark
k54			$2 \cdot 10^{-4}$		\mathbf{Z}
kf55			0.620		\mathbf{Z}
kr55		2	$4.8 \cdot 10^{-4}$		\checkmark
kf56			0.620		\square
kr56		4	$4.8 \cdot 10^{-4}$		\checkmark
kf57			18.400		
kr57			0.055		\checkmark
kf58			18.400		
kr58			0.055		\square
kf59			0.004		
kr59			$8 \cdot 10^{-13}$		\checkmark
kf60			0.004		\checkmark
kr60			$8\cdot 10^{-13}$		\checkmark
kf63			0.620		$ \overline{\checkmark} $
kr63		2	$4.8 \cdot 10^{-4}$		
kf64			0.620		$ \overline{\checkmark} $
kr64		2	$4.8 \cdot 10^{-4}$		$ \overline{\checkmark} $
kf65			18.400		$\overline{\mathbf{Z}}$

Id	Name	SBO	Value	Unit	Constant
kr65			0.055		
kf66			18.400		$ \overline{\mathbf{Z}} $
kr66			0.055		
kf67			0.004		$ \overline{\mathbf{Z}} $
kr67			$8 \cdot 10^{-13}$		$ \overline{\mathbf{Z}} $
kf68			0.004		$ \overline{\mathbf{Z}} $
kr68			$8 \cdot 10^{-13}$		$ \overline{\mathbf{Z}} $
k71			$2 \cdot 10^{-4}$		$ \overline{\mathbf{Z}} $
k72			$2 \cdot 10^{-4}$		

6 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

6.1 Event signal

Name signal

Trigger condition	time > 72000	(1)
Delay	0	(2)
Assignment	k1 = 0.0025	(3)

7 Reactions

This model contains 57 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

Nº	Id	Name	Reaction Equation SBC	O
1	re1		$s22 + s198 \longrightarrow s199$	
2	re8		$s199 + s195 \longrightarrow s200$	
3	re14		$s195 + s206 \longrightarrow s214$	
4	re15		$s93 + s212 \longrightarrow s213$	
5	re19		$s195 + s198 \longrightarrow s196$	
6	re20		$s196 + s93 \longrightarrow s197$	
7	re21		$s195 + s205 \longrightarrow s212$	
8	re22		$s200 + s93 \longrightarrow s201$	
9	re23		$s93 + s214 \longrightarrow s215$	
10	re24		$s65 + s205 \longrightarrow s206$	
11	re25		$s197 \longrightarrow s198 + s192$	
12	re26		$s201 \longrightarrow s199 + s192$	
13	re27		$s215 \longrightarrow s206 + s192$	
14	re28		$s213 \longrightarrow s205 + s192$	
15	re29		$s193 + s36 \longrightarrow s194$	
16	re30		$s160 \xrightarrow{s193, s194} s165$	
17	re31		$s170 \xrightarrow{s200, s199, s198, s196} s173$	
18	re32		$s209 \xrightarrow{s214, s212, s205, s206} s185$	
19	re33		$s195 \longrightarrow s108$	
20	re34		$s173 \longrightarrow s113$	
21	re35		$s110 \longrightarrow s109$	
22	re36		$s113 \longrightarrow s112$	

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by
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ALC.

)	No	Id	Name	Reaction Equation	SBO
	23	re37		$s113 \longrightarrow s110 + s113$	
	24	re38		$s110 \longrightarrow s114$	
	25	re39		$s114 \longrightarrow s111$	
	26	re40		$s165 \longrightarrow s117$	
	27	re41		$s117 \longrightarrow s118$	
	28	re42		$s119 \longrightarrow s120$	
	29	re43		$s117 \longrightarrow s119 + s117$	
	30	re44		$s185 \longrightarrow s178$	
	31	re45		$s178 \longrightarrow s124$	
	32	re46		$s123 \longrightarrow s122$	
1	33	re47		$s178 \longrightarrow s123 + s178$	
	34	re48		$s126 \xrightarrow{s195} s127$	
	35	re49		$s133 \longrightarrow s132$	
	36	re52		$s188 \longrightarrow s190$	
	37	re53		$s133 \longrightarrow s131$	
	38	re56		$s132 \longrightarrow s134$	
İ	39	re57		$s191 \longrightarrow s132$	
	40	re58		$s132 + s188 \longrightarrow s189$	
	41	re59		$s189 \longrightarrow s190 + s132$	
	42	re60		$s130 \longrightarrow s129$	
	43	re61		$s127 \longrightarrow s128 + s127$	
	44	re62		$s114 + s119 \longrightarrow s190$	
	45	re63		$s132 \frac{s128}{s130} s130$	
	46	re64		$s150 \longrightarrow s133$	
	47	re65		$s123 + s190 \longrightarrow s188$	
	48	re66		$s123 + s132 \longrightarrow s191$	
	49	re67		$s190 \longrightarrow 5 s195$	
	50	re68		$5 s192 \longrightarrow s188$	

N⁰	Id	Name	Reaction Equation	SBO
51	re69		$s195 + s93 \longrightarrow s192$	
52	re70		$s127 \longrightarrow s153$	
53	re71		$s128 \longrightarrow s154$	
54	re72		$s123 \longrightarrow 5 s93$	
55	re74		$s190 \longrightarrow s156$	
56	re75		$s188 \longrightarrow s157$	
57	re76		$s192 \longrightarrow s158$	

7.1 Reaction re1

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

Reaction equation

$$s22 + s198 \longrightarrow s199 \tag{4}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
s22	FTAx	
s198	Promp105:RNAP	

Product

Table 7: Properties of each product.

	1 1	
Id	Name	SBO
s199	Promp105:RNAP:FTAX	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{kf32} \cdot [\text{s198}] \cdot [\text{s22}] - \text{kr32} \cdot [\text{s199}]$$
 (5)

7.2 Reaction re8

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

Reaction equation

$$s199 + s195 \longrightarrow s200 \tag{6}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
s199	Promp105·RNAP·FTAX	

Id	Name	SBO
s195	NFkB	

Product

Table 9: Properties of each product.

Id	Name	SBO
s200	Promp105:RNAP1:FTAx:p50p65	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = kf64 \cdot [s195] \cdot [s199] - kr64 \cdot [s200] \tag{7}$$

7.3 Reaction re14

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

Reaction equation

$$s195 + s206 \longrightarrow s214 \tag{8}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
s195	NFkB	
s206	PromIkBa:RNAP3:FTAz	

Table 11: Properties of each product.

Id	Name	SBO
s214	IkBa:RNAP3:FTAz:p50p65	

Derived unit contains undeclared units

$$v_3 = \text{kf56} \cdot [\text{s195}] \cdot [\text{s206}] - \text{kr56} \cdot [\text{s214}]$$
 (9)

7.4 Reaction re15

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

Reaction equation

$$s93 + s212 \longrightarrow s213 \tag{10}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
s93	IkB_alpha	
s212	PromIkBa:RNAP3:p50p65	

Product

Table 13: Properties of each product.

Id	Name	SBO
s213	PromIkBa:RNAP3:p50p65:IkBa	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{kf57} \cdot [\text{s93}] \cdot [\text{s212}] - \text{kr57} \cdot [\text{s213}]$$
 (11)

7.5 Reaction re19

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

Reaction equation

$$s195 + s198 \longrightarrow s196 \tag{12}$$

Reactants

Table 14: Properties of each reactant.

	*	
Id	Name	SBO
s195	NFkB	
s198	Promp105:RNAP	

Product

Table 15: Properties of each product.

Id	Name	SBO
s196	Promp105:RNAP1:p50p65	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{kf63} \cdot [\text{s195}] \cdot [\text{s198}] - \text{kr63} \cdot [\text{s196}]$$
 (13)

7.6 Reaction re20

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

Reaction equation

$$s196 + s93 \longrightarrow s197 \tag{14}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
s196 s93	Promp105:RNAP1:p50p65 IkB_alpha	

Table 17: Properties of each product.

Id	Name	SBO
s197	Promp105:RNAP1:p50p65:IkBa	

Derived unit contains undeclared units

$$v_6 = \text{kf65} \cdot [\text{s93}] \cdot [\text{s196}] - \text{kr65} \cdot [\text{s197}]$$
 (15)

7.7 Reaction re21

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

Reaction equation

$$s195 + s205 \longrightarrow s212 \tag{16}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
s195	NFkB	
s205	PromIkBa:RNAP3	

Product

Table 19: Properties of each product.

	1 1	
Id	Name	SBO
s212	PromIkBa:RNAP3:p50p65	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{kf55} \cdot [\text{s195}] \cdot [\text{s205}] - \text{kr55} \cdot [\text{s212}]$$
 (17)

7.8 Reaction re22

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

Reaction equation

$$s200 + s93 \longrightarrow s201$$
 (18)

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
s200 s93	Promp105:RNAP1:FTAx:p50p65 IkB_alpha	

Product

Table 21: Properties of each product.

Id	Name	SBO
s201	Promp105:RNAP1:FTAx:p50p65:IkBa	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{kf66} \cdot [\text{s93}] \cdot [\text{s200}] - \text{kr66} \cdot [\text{s201}]$$
 (19)

7.9 Reaction re23

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

Reaction equation

$$s93 + s214 \longrightarrow s215 \tag{20}$$

Reactants

Table 22: Properties of each reactant.

Id 1	Name	SBO
	IkB_alpha IkBa:RNAP3:FTAz:p50p65	

Product

Table 23: Properties of each product.

Id	Name	SBO
s215	PromIkBa:RNAP3:FTAz:p50p65:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{kf58} \cdot [\text{s93}] \cdot [\text{s214}] - \text{kr58} \cdot [\text{s215}]$$
 (21)

7.10 Reaction re24

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

Reaction equation

$$s65 + s205 \longrightarrow s206$$
 (22)

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
200	FTAz PromIkBa:RNAP3	

Product

Table 25: Properties of each product.

Id	Name	SBO
s206	PromIkBa:RNAP3:FTAz	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = kf48 \cdot [s65] \cdot [s205] - kr48 \cdot [s206]$$
 (23)

7.11 Reaction re25

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

Reaction equation

$$s197 \longrightarrow s198 + s192 \tag{24}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
s197	Promp105:RNAP1:p50p65:IkBa	

Products

Table 27: Properties of each product.

	1	1
Id	Name	SBO
s198 s192	Promp105:RNAP NFkB:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = kf67 \cdot [s197] - kr67 \cdot [s192] \cdot [s198]$$
 (25)

7.12 Reaction re26

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

Reaction equation

$$s201 \longrightarrow s199 + s192 \tag{26}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
s201	Promp105:RNAP1:FTAx:p50p65:IkBa	

Products

Table 29: Properties of each product.

Id	Name	SBO
	Promp105:RNAP:FTAX NFkB:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = kf68 \cdot [s201] - kr68 \cdot [s192] \cdot [s199]$$
 (27)

7.13 Reaction re27

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

Reaction equation

$$s215 \longrightarrow s206 + s192 \tag{28}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
s215	PromIkBa:RNAP3:FTAz:p50p65:IkB_alpha	

Products

Table 31: Properties of each product.

Id	Name	SBO
s206	PromIkBa:RNAP3:FTAz	
s192	NFkB:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = kf60 \cdot [s215] - kr60 \cdot [s192] \cdot [s206]$$
 (29)

7.14 Reaction re28

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

Reaction equation

$$s213 \longrightarrow s205 + s192 \tag{30}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
s213	PromIkBa:RNAP3:p50p65:IkBa	

Products

Table 33: Properties of each product.

Id	Name	SBO
	PromIkBa:RNAP3	
s192	NFkB:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = kf59 \cdot [s213] - kr59 \cdot [s192] \cdot [s205]$$
(31)

7.15 Reaction re29

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

Reaction equation

$$s193 + s36 \longrightarrow s194 \tag{32}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
s193	Promp65:RNAP2	

Id	Name	SBO
s36	FTAy	

Product

Table 35: Properties of each product.

Id	Name	SBO
s194	Promp65:RNAP2:FTAy	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = kf41 \cdot [s36] \cdot [s193] - kr41 \cdot [s194]$$
(33)

7.16 Reaction re30

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$s160 \xrightarrow{s193, s194} s165$$
 (34)

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
s160	InactivePRaseonp65	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
s193	Promp65:RNAP2	
s194	Promp65:RNAP2:FTAy	

Table 38: Properties of each product.

Id	Name	SBO
s165	ActivePRaseonp65	

Derived unit contains undeclared units

$$v_{16} = k42 \cdot [s193] + k43 \cdot [s194] \tag{35}$$

7.17 Reaction re31

This is an irreversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$s170 \xrightarrow{s200, s199, s198, s196} s173$$
 (36)

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
s170	InactivePRaseonp105	

Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
s200	Promp105:RNAP1:FTAx:p50p65	
s199	Promp105:RNAP:FTAX	
s198	Promp105:RNAP	
s196	Promp105:RNAP1:p50p65	

Table 41: Properties of each product.

Id	Name	SBO
s173	ActivePRaseonp105	

Derived unit contains undeclared units

$$v_{17} = k33 \cdot [s198] + k34 \cdot [s199] + k69 \cdot [s196] + k70 \cdot [s200]$$
 (37)

7.18 Reaction re32

This is an irreversible reaction of one reactant forming one product influenced by four modifiers.

Reaction equation

$$s209 \xrightarrow{s214, s212, s205, s206} s185 \tag{38}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
s209	InactivePRaseonIkB_alpha	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
s214	IkBa:RNAP3:FTAz:p50p65	
s212	PromIkBa:RNAP3:p50p65	
s205	PromIkBa:RNAP3	
s206	PromIkBa:RNAP3:FTAz	

Table 44: Properties of each product.

Id	Name	SBO
s185	ActivePRaseonIkB_alpha	

Derived unit contains undeclared units

$$v_{18} = k49 \cdot [s205] + k50 \cdot [s206] + k62 \cdot [s214] + k61 \cdot [s212]$$
 (39)

7.19 Reaction re33

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

Reaction equation

$$s195 \longrightarrow s108$$
 (40)

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
s195	NFkB	

Product

Table 46: Properties of each product.

Id	Name	SBO
s108	csa17_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = k54 \cdot [s195] \tag{41}$$

7.20 Reaction re34

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

Reaction equation

$$s173 \longrightarrow s113$$
 (42)

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
s173	ActivePRaseonp105	

Product

Table 48: Properties of each product.

Id	Name	SBO
s113	mRNAp105	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = k35 \cdot [s173] \tag{43}$$

7.21 Reaction re35

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

Reaction equation

$$s110 \longrightarrow s109$$
 (44)

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
s110	p105	

Table 50: Properties of each product.

Id	Name	SBO
s109	sa4_degraded	

Derived unit contains undeclared units

$$v_{21} = k38 \cdot [s110] \tag{45}$$

7.22 Reaction re36

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

Reaction equation

$$s113 \longrightarrow s112$$
 (46)

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
s113	mRNAp105	

Product

Table 52: Properties of each product.

	1	
Id	Name	SBO
s112	sa3_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = k37 \cdot [s113] \tag{47}$$

7.23 Reaction re37

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

Reaction equation

$$s113 \longrightarrow s110 + s113 \tag{48}$$

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
s113	mRNAp105	

Products

Table 54: Properties of each product.

Id	Name	SBO
s110	p105	
s113	mRNAp105	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = k36 \cdot [s113] \tag{49}$$

7.24 Reaction re38

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

Reaction equation

$$s110 \longrightarrow s114$$
 (50)

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
s110	p105	

Table 56: Properties of each product.

Id	Name	SBO
s114	p50	

Derived unit contains undeclared units

$$v_{24} = k39 \cdot [s110] \tag{51}$$

7.25 Reaction re39

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

Reaction equation

$$s114 \longrightarrow s111$$
 (52)

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
s114	p50	

Product

Table 58: Properties of each product.

-	Id	Name	SBO
-	s111	sa438_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = k40 \cdot [s114] \tag{53}$$

7.26 Reaction re40

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

Reaction equation

$$s165 \longrightarrow s117$$
 (54)

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
s165	ActivePRaseonp65	

Product

Table 60: Properties of each product.

Id	Name	SBO
s117	mRNAp65	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = k44 \cdot [s165] \tag{55}$$

7.27 Reaction re41

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

Reaction equation

$$s117 \longrightarrow s118$$
 (56)

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
s117	mRNAp65	

Table 62: Properties of each product.

Id	Name	SBO
s118	sa8_degraded	

Derived unit contains undeclared units

$$v_{27} = k46 \cdot [s117] \tag{57}$$

7.28 Reaction re42

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

Reaction equation

$$s119 \longrightarrow s120$$
 (58)

Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
s119	p65	

Product

Table 64: Properties of each product.

	1	
Id	Name	SBO
s120	sa9_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = k47 \cdot [s119] \tag{59}$$

7.29 Reaction re43

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

Reaction equation

$$s117 \longrightarrow s119 + s117 \tag{60}$$

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
s117	mRNAp65	

Products

Table 66: Properties of each product.

Id	Name	SBO
s119	p65	
s117	mRNAp65	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = k45 \cdot [s117] \tag{61}$$

7.30 Reaction re44

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

Reaction equation

$$s185 \longrightarrow s178$$
 (62)

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
s185	ActivePRaseonIkB_alpha	

Table 68: Properties of each product

Id	Name	SBO
s178	mRNAIKB_alpha	

Derived unit contains undeclared units

$$v_{30} = k51 \cdot [s185] \tag{63}$$

7.31 Reaction re45

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

Reaction equation

$$s178 \longrightarrow s124$$
 (64)

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
s178	mRNAIKB_alpha	

Product

Table 70: Properties of each product.

Id	Name	SBO
s124	sa12_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = k27 \cdot [s178] \tag{65}$$

7.32 Reaction re46

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

Reaction equation

$$s123 \longrightarrow s122$$
 (66)

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
s123	IkB_alpha	

Product

Table 72: Properties of each product.

Id	Name	SBO
s122	sa13_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = k21 \cdot [s123] \tag{67}$$

7.33 Reaction re47

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

Reaction equation

$$s178 \longrightarrow s123 + s178 \tag{68}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
s178	mRNAIKB_alpha	

Table 74: Properties of each product.

Id	Name	SBO
s123	IkB_alpha	
s178	mRNAIKB_alpha	

Derived unit contains undeclared units

$$v_{33} = k22 \cdot [s178] \tag{69}$$

7.34 Reaction re48

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Reaction equation

$$s126 \xrightarrow{s195} s127$$
 (70)

Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
s126	A20	

Modifier

Table 76: Properties of each modifier.

Id	Name	SBO
s195	NFkB	

Table 77: Properties of each product.

Id	Name	SBO
s127	mRNAA20	

Derived unit contains undeclared units

$$v_{34} = k19 + k20 \cdot [s195] \tag{71}$$

7.35 Reaction re49

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

Reaction equation

$$s133 \longrightarrow s132$$
 (72)

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
s133	IKKn	

Product

Table 79: Properties of each product.

Id	Name	SBO
s132	IKKa	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = k1 \cdot [s133] \tag{73}$$

7.36 Reaction re52

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

Reaction equation

$$s188 \longrightarrow s190$$
 (74)

Reactant

Table 80: Properties of each reactant.

Id	Name	SBO
s188	NFkB:IkB_alpha	

Product

Table 81: Properties of each product.

Id	Name	SBO
s190	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = k12 \cdot [s188] \tag{75}$$

7.37 Reaction re53

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

Reaction equation

$$s133 \longrightarrow s131$$
 (76)

Reactant

Table 82: Properties of each reactant.

Id	Name	SBO
s133	IKKn	

Table 83: Properties of each product.

Id	Name	SBO
s131	sa19_degraded	

Derived unit contains undeclared units

$$v_{37} = k2 \cdot [s133] \tag{77}$$

7.38 Reaction re56

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

Reaction equation

$$s132 \longrightarrow s134$$
 (78)

Reactant

Table 84: Properties of each reactant.

Id	Name	SBO
s132	IKKa	

Product

Table 85: Properties of each product.

Id	Name	SBO
s134	sa20_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = k6 \cdot [s132] \tag{79}$$

7.39 Reaction re57

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

Reaction equation

$$s191 \longrightarrow s132$$
 (80)

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
s191	IKKa:IKB_alpha	

Product

Table 87: Properties of each product.

Id	Name	SBO
s132	IKKa	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = k8 \cdot [s191] \tag{81}$$

7.40 Reaction re58

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

Reaction equation

$$s132 + s188 \longrightarrow s189 \tag{82}$$

Reactants

Table 88: Properties of each reactant.

Id	Name	SBO
s132	IKKa	
s188	NFkB:IkB_alpha	

Table 89: Properties of each product.

Id	Name	SBO
s189	NFkB:IKKa:Ikb_alpha	

Derived unit contains undeclared units

$$v_{40} = k9 \cdot [s132] \cdot [s188] \tag{83}$$

7.41 Reaction re59

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

Reaction equation

$$s189 \longrightarrow s190 + s132 \tag{84}$$

Reactant

Table 90: Properties of each reactant.

Id	Name	SBO
s189	NFkB:IKKa:Ikb_alpha	

Products

Table 91: Properties of each product.

Id	Name	SBO
s190	NFkB	
s132	IKKa	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = k10 \cdot [s189] \tag{85}$$

7.42 Reaction re60

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

Reaction equation

$$s130 \longrightarrow s129$$
 (86)

Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
s130	IKKi	

Product

Table 93: Properties of each product.

Id	Name	SBO
s129	sa444_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = k11 \cdot [s130] \tag{87}$$

7.43 Reaction re61

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

Reaction equation

$$s127 \longrightarrow s128 + s127 \tag{88}$$

Reactant

Table 94: Properties of each reactant.

Id	Name	SBO
s127	mRNAA20	

Table 95: Properties of each product.

Id	Name	SBO
s128	A20	

Id	Name	SBO
s127	mRNAA20	

Derived unit contains undeclared units

$$v_{43} = k16 \cdot [s127] \tag{89}$$

7.44 Reaction re62

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

Reaction equation

$$s114 + s119 \longrightarrow s190 \tag{90}$$

Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
s114	p50	
s119	p65	

Product

Table 97: Properties of each product.

Id	Name	SBO
s190	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = kf52 \cdot [s114] \cdot [s119] - kr52 \cdot [s190]$$
(91)

7.45 Reaction re63

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Reaction equation

$$s132 \xrightarrow{s128} s130$$
 (92)

Reactant

Table 98: Properties of each reactant.

Id	Name	SBO
s132	IKKa	

Modifier

Table 99: Properties of each modifier.

Id	Name	SBO
s128	A20	

Product

Table 100: Properties of each product.

Id	Name	SBO
s130	IKKi	

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = k5 \cdot [s132] + k4 \cdot [s132] \cdot [s128]$$
 (93)

7.46 Reaction re64

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

Reaction equation

$$s150 \longrightarrow s133$$
 (94)

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
s150	IKK	

Product

Table 102: Properties of each product.

Id	Name	SBO
s133	IKKn	

Kinetic Law

Derived unit not available

$$v_{46} = k3$$
 (95)

7.47 Reaction re65

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

Reaction equation

$$s123 + s190 \longrightarrow s188 \tag{96}$$

Reactants

Table 103: Properties of each reactant.

Id	Name	SBO
s123 s190	IkB_alpha NFkB	

Table 104: Properties of each product.

Id	Name	SBO
s188	NFkB:IkB_alpha	

Derived unit contains undeclared units

$$v_{47} = \text{kf13} \cdot [\text{s190}] \cdot [\text{s123}] - \text{kr13} \cdot [\text{s188}]$$
 (97)

7.48 Reaction re66

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

Reaction equation

$$s123 + s132 \longrightarrow s191 \tag{98}$$

Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
s123	IkB_alpha	
s132	IKKa	

Product

Table 106: Properties of each product.

Id	Name	SBO
s191	IKKa:IKB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{48} = k7 \cdot [s132] \cdot [s123] \tag{99}$$

7.49 Reaction re67

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

Reaction equation

$$s190 \longrightarrow 5 s195$$
 (100)

Reactant

Table 107: Properties of each reactant.

Id	Name	SBO
s190	NFkB	

Product

Table 108: Properties of each product.

Id	Name	SBO
s195	NFkB	

Kinetic Law

Derived unit contains undeclared units

$$v_{49} = \text{kf15} \cdot [\text{s190}] - \text{kr15} \cdot [\text{s195}] \tag{101}$$

7.50 Reaction re68

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

Reaction equation

$$5\,\mathrm{s}192 \longrightarrow \mathrm{s}188 \tag{102}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
s192	NFkB:IkB_alpha	

Table 110: Properties of each product.

Id	Name	SBO
s188	NFkB:IkB_alpha	

Derived unit contains undeclared units

$$v_{50} = \text{kf28} \cdot [\text{s192}] - \text{kr28} \cdot [\text{s188}] \tag{103}$$

7.51 Reaction re69

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

Reaction equation

$$s195 + s93 \longrightarrow s192 \tag{104}$$

Reactants

Table 111: Properties of each reactant.

Id	Name	SBO
s195	NFkB	
s93	IkB_alpha	

Product

Table 112: Properties of each product.

Id	Name	SBO
s192	NFkB:IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{51} = kf14 \cdot [s195] \cdot [s93] - kr14 \cdot [s192]$$
(105)

7.52 Reaction re70

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

Reaction equation

$$s127 \longrightarrow s153$$
 (106)

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
s127	mRNAA20	

Product

Table 114: Properties of each product.

Id	Name	SBO
s153	sa96_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{52} = k17 \cdot [s127] \tag{107}$$

7.53 Reaction re71

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

Reaction equation

$$s128 \longrightarrow s154$$
 (108)

Reactant

Table 115: Properties of each reactant.

Id	Name	SBO
s128	A20	

Table 116: Properties of each product.

Id	Name	SBO
s154	sa97_degraded	-

Derived unit contains undeclared units

$$v_{53} = k18 \cdot [s128] \tag{109}$$

7.54 Reaction re72

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

Reaction equation

$$s123 \longrightarrow 5s93$$
 (110)

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
s123	IkB_alpha	

Product

Table 118: Properties of each product.

Id	Name	SBO
s93	IkB_alpha	

Kinetic Law

Derived unit contains undeclared units

$$v_{54} = \text{kf23} \cdot [\text{s123}] - \text{kr23} \cdot [\text{s93}] \tag{111}$$

7.55 Reaction re74

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

Reaction equation

$$s190 \longrightarrow s156$$
 (112)

Reactant

Table 119: Properties of each reactant.

Id	Name	SBO
s190	NFkB	

Product

Table 120: Properties of each product.

Id	Name	SBO
s156	csa21_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{55} = k53 \cdot [s190] \tag{113}$$

7.56 Reaction re75

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

Reaction equation

$$s188 \longrightarrow s157$$
 (114)

Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
s188	NFkB:IkB_alpha	

Table 122: Properties of each product.

Id	Name	SBO
s157	csa18_degraded	

Derived unit contains undeclared units

$$v_{56} = k71 \cdot [s188] \tag{115}$$

7.57 Reaction re76

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

Reaction equation

$$s192 \longrightarrow s158$$
 (116)

Reactant

Table 123: Properties of each reactant.

Id	Name	SBO
s192	NFkB:IkB_alpha	

Product

Table 124: Properties of each product.

Id	Name	SBO
s158	csa9_degraded	

Kinetic Law

Derived unit contains undeclared units

$$v_{57} = k72 \cdot [s192] \tag{117}$$

8 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.

8.1 Species s22

Name FTAx

Charge 0

This species takes part in one reaction (as a reactant in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}22 = -v_1\tag{118}$$

8.2 Species s36

Name FTAy

Charge 0

This species takes part in one reaction (as a reactant in re29).

$$\frac{d}{dt}s36 = -v_{15} \tag{119}$$

8.3 Species s65

Name FTAz

This species takes part in one reaction (as a reactant in re24).

$$\frac{d}{dt}s65 = -v_{10} \tag{120}$$

8.4 Species s93

Name IkB_alpha

Initial amount 0 mol

This species takes part in six reactions (as a reactant in re15, re20, re22, re23, re69 and as a product in re72).

$$\frac{\mathrm{d}}{\mathrm{d}t} s93 = 5 v_{54} - |v_4| - |v_6| - |v_8| - |v_9| - |v_{51}|$$
(121)

8.5 Species s108

Name csa17_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re33), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}108 = 0\tag{122}$$

8.6 Species s109

Name sa4_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re35), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}109 = 0\tag{123}$$

8.7 Species s110

Name p105

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re35, re38 and as a product in re37).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}110 = |v_{23}| - |v_{21}| - |v_{24}| \tag{124}$$

8.8 Species s111

Name sa438_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re39), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}111 = 0\tag{125}$$

8.9 Species s112

Name sa3_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re36), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}112 = 0\tag{126}$$

8.10 Species s113

Name mRNAp105

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re36, re37 and as a product in re34, re37).

$$\frac{\mathrm{d}}{\mathrm{d}t}s113 = |v_{20}| + |v_{23}| - |v_{22}| - |v_{23}| \tag{127}$$

8.11 Species s114

Name p50

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re39, re62 and as a product in re38).

$$\frac{\mathrm{d}}{\mathrm{d}t}s114 = |v_{24}| - |v_{25}| - |v_{44}| \tag{128}$$

8.12 Species s117

Name mRNAp65

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re41, re43 and as a product in re40, re43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s117 = |v_{26}| + |v_{29}| - |v_{27}| - |v_{29}| \tag{129}$$

8.13 Species s118

Name sa8_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re41), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}118 = 0\tag{130}$$

8.14 Species s119

Name p65

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re42, re62 and as a product in re43).

$$\frac{\mathrm{d}}{\mathrm{d}t}s119 = |v_{29}| - |v_{28}| - |v_{44}| \tag{131}$$

8.15 Species s120

Name sa9_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re42), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}120 = 0\tag{132}$$

8.16 Species s122

Name sa13_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re46), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}122 = 0\tag{133}$$

8.17 Species s123

Name IkB_alpha

Initial amount 0 mol

This species takes part in five reactions (as a reactant in re46, re65, re66, re72 and as a product in re47).

$$\frac{\mathrm{d}}{\mathrm{d}t}s123 = |v_{33}| - |v_{32}| - |v_{47}| - |v_{48}| - |v_{54}| \tag{134}$$

8.18 Species s124

Name sa12_degraded

Initial amount 0 mol

This species takes part in one reaction (as a product in re45).

$$\frac{d}{dt}s124 = v_{31} \tag{135}$$

8.19 Species s126

Name A20

Initial amount 0 mol

This species takes part in one reaction (as a reactant in re48).

$$\frac{d}{dt}s126 = -v_{34} \tag{136}$$

8.20 Species s127

Name mRNAA20

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re61, re70 and as a product in re48, re61).

$$\frac{\mathrm{d}}{\mathrm{d}t}s127 = |v_{34}| + |v_{43}| - |v_{43}| - |v_{52}| \tag{137}$$

8.21 Species s128

Name A20

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re71 and as a product in re61 and as a modifier in re63).

$$\frac{d}{dt}s128 = |v_{43}| - |v_{53}| \tag{138}$$

8.22 Species s129

Name sa444_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re60), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}129 = 0\tag{139}$$

8.23 Species s130

Name IKKi

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re60 and as a product in re63).

$$\frac{d}{dt}s130 = |v_{45}| - |v_{42}| \tag{140}$$

8.24 Species s131

Name sa19_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re53), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}131 = 0\tag{141}$$

8.25 Species s132

Name IKKa

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in re56, re58, re63, re66 and as a product in re49, re57, re59).

$$\frac{\mathrm{d}}{\mathrm{d}t}s132 = |v_{35}| + |v_{39}| + |v_{41}| - |v_{38}| - |v_{40}| - |v_{45}| - |v_{48}| \tag{142}$$

8.26 Species s133

Name IKKn

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re49, re53 and as a product in re64).

$$\frac{\mathrm{d}}{\mathrm{d}t}s133 = |v_{46}| - |v_{35}| - |v_{37}| \tag{143}$$

8.27 Species s134

Name sa20_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re56), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}134 = 0\tag{144}$$

8.28 Species s150

Name IKK

Initial amount 0 mol

This species takes part in one reaction (as a reactant in re64).

$$\frac{d}{dt}s150 = -v_{46} \tag{145}$$

8.29 Species s153

Name sa96_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re70), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}153 = 0\tag{146}$$

8.30 Species s154

Name sa97_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re71), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}154 = 0\tag{147}$$

8.31 Species s156

Name csa21_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re74), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}156 = 0\tag{148}$$

8.32 Species s157

Name csa18_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re75), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}157 = 0\tag{149}$$

8.33 Species s158

Name csa9_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re76), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}158 = 0\tag{150}$$

8.34 Species s160

Name InactivePRaseonp65

Initial amount 0 mol

This species takes part in one reaction (as a reactant in re30).

$$\frac{d}{dt}s160 = -v_{16} \tag{151}$$

8.35 Species s165

Name ActivePRaseonp65

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re40 and as a product in re30).

$$\frac{\mathrm{d}}{\mathrm{d}t} s 165 = |v_{16}| - |v_{26}| \tag{152}$$

8.36 Species s170

Name InactivePRaseonp105

Initial amount 0 mol

This species takes part in one reaction (as a reactant in re31).

$$\frac{d}{dt}s170 = -v_{17} \tag{153}$$

8.37 Species s173

Name ActivePRaseonp105

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re34 and as a product in re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}s173 = |v_{17}| - |v_{20}| \tag{154}$$

8.38 Species s178

Name mRNAIKB_alpha

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re45, re47 and as a product in re44, re47).

$$\frac{\mathrm{d}}{\mathrm{d}t}s178 = |v_{30}| + |v_{33}| - |v_{31}| - |v_{33}| \tag{155}$$

8.39 Species s185

Name ActivePRaseonIkB_alpha

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re44 and as a product in re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}s185 = |v_{18}| - |v_{30}| \tag{156}$$

8.40 Species s188

Name NFkB:IkB_alpha

Initial amount 0 mol

Charge 0

This species takes part in five reactions (as a reactant in re52, re58, re75 and as a product in re65, re68).

$$\frac{\mathrm{d}}{\mathrm{d}t}s188 = |v_{47}| + |v_{50}| - |v_{36}| - |v_{40}| - |v_{56}| \tag{157}$$

8.41 Species s189

Name NFkB:IKKa:Ikb_alpha

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re59 and as a product in re58).

$$\frac{\mathrm{d}}{\mathrm{d}t}s189 = |v_{40}| - |v_{41}| \tag{158}$$

8.42 Species s190

Name NFkB

Initial amount 0 mol

This species takes part in six reactions (as a reactant in re65, re67, re74 and as a product in re52, re59, re62).

$$\frac{\mathrm{d}}{\mathrm{d}t}s190 = v_{36} + v_{41} + v_{44} - v_{47} - v_{49} - v_{55} \tag{159}$$

8.43 Species s191

Name IKKa:IKB_alpha

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re57 and as a product in re66).

$$\frac{\mathrm{d}}{\mathrm{d}t} s191 = |v_{48}| - |v_{39}| \tag{160}$$

8.44 Species s192

Name NFkB:IkB_alpha

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in re68, re76 and as a product in re25, re26, re27, re28, re69).

$$\frac{\mathrm{d}}{\mathrm{d}t}s192 = |v_{11}| + |v_{12}| + |v_{13}| + |v_{14}| + |v_{51}| - 5|v_{50}| - |v_{57}|$$
(161)

8.45 Species s193

Name Promp65:RNAP2

Initial amount $6.66666666666667 \cdot 10^{-6} \text{ mol}$

This species takes part in two reactions (as a reactant in re29 and as a modifier in re30).

$$\frac{d}{dt}s193 = -v_{15} \tag{162}$$

8.46 Species s194

Name Promp65:RNAP2:FTAy

Initial amount 0 mol

This species takes part in two reactions (as a product in re29 and as a modifier in re30).

$$\frac{d}{dt}s194 = v_{15} \tag{163}$$

8.47 Species s195

Name NFkB

Initial amount 0 mol

This species takes part in eight reactions (as a reactant in re8, re14, re19, re21, re33, re69 and as a product in re67 and as a modifier in re48).

$$\frac{\mathrm{d}}{\mathrm{d}t}s195 = 5 v_{49} - v_2 - v_3 - v_5 - v_7 - v_{19} - v_{51}$$
 (164)

8.48 Species s196

Name Promp105:RNAP1:p50p65

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re20 and as a product in re19 and as a modifier in re31).

$$\frac{d}{dt}s196 = |v_5| - |v_6| \tag{165}$$

8.49 Species s197

Name Promp105:RNAP1:p50p65:IkBa

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re25 and as a product in re20).

$$\frac{d}{dt}s197 = |v_6| - |v_{11}| \tag{166}$$

8.50 Species s198

Name Promp105:RNAP

Initial amount $6.66666666666667 \cdot 10^{-6} \text{ mol}$

This species takes part in four reactions (as a reactant in re1, re19 and as a product in re25 and as a modifier in re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}s198 = |v_{11}| - |v_1| - |v_5| \tag{167}$$

8.51 Species s199

Name Promp105:RNAP:FTAX

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re8 and as a product in re1, re26 and as a modifier in re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}s199 = |v_1| + |v_{12}| - |v_2| \tag{168}$$

8.52 Species s200

Name Promp105:RNAP1:FTAx:p50p65

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re22 and as a product in re8 and as a modifier in re31).

$$\frac{d}{dt}s200 = |v_2| - |v_8| \tag{169}$$

8.53 Species s201

Name Promp105:RNAP1:FTAx:p50p65:IkBa

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re26 and as a product in re22).

$$\frac{d}{dt}s201 = |v_8| - |v_{12}| \tag{170}$$

8.54 Species s205

Name PromIkBa:RNAP3

Initial amount $6.66666666666667 \cdot 10^{-6} \text{ mol}$

This species takes part in four reactions (as a reactant in re21, re24 and as a product in re28 and as a modifier in re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}s205 = |v_{14}| - |v_7| - |v_{10}| \tag{171}$$

8.55 Species s206

Name PromIkBa:RNAP3:FTAz

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re14 and as a product in re24, re27 and as a modifier in re32).

$$\frac{d}{dt}s206 = |v_{10}| + |v_{13}| - |v_{3}| \tag{172}$$

8.56 Species s209

Name InactivePRaseonIkB_alpha

Initial amount 0 mol

This species takes part in one reaction (as a reactant in re32).

$$\frac{d}{dt}s209 = -v_{18} \tag{173}$$

8.57 Species s212

Name PromIkBa:RNAP3:p50p65

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re15 and as a product in re21 and as a modifier in re32).

$$\frac{d}{dt}s212 = |v_7| - |v_4| \tag{174}$$

8.58 Species s213

Name PromIkBa:RNAP3:p50p65:IkBa

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re28 and as a product in re15).

$$\frac{\mathrm{d}}{\mathrm{d}t}s213 = |v_4| - |v_{14}| \tag{175}$$

8.59 Species s214

Name IkBa:RNAP3:FTAz:p50p65

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re23 and as a product in re14 and as a modifier in re32).

$$\frac{d}{dt}s214 = |v_3| - |v_9| \tag{176}$$

8.60 Species s215

Name PromIkBa:RNAP3:FTAz:p50p65:IkB_alpha

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re27 and as a product in re23).

$$\frac{d}{dt}s215 = |v_9| - |v_{13}| \tag{177}$$

 $\mathfrak{BML2}^{AT}$ EX 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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