

## SBML Model Report

**Model name: “Radulescu2008\_NFkB-  
\_hierarchy\_M\_14\_25\_28\_Lipniacky”**



May 5, 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 Chelliah<sup>1</sup> and Ovidiu Radulescu<sup>2</sup> at February 27<sup>th</sup> 2009 at 4:28 p. m. and last time modified at June third 2014 at 1:55 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	24
events	0	constraints	0
reactions	24	function definitions	0
global parameters	31	unit definitions	0
rules	0	initial assignments	0

### Model Notes

#### NFkB model M(14,25,28) - Lipniacky's NFkB 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

<sup>1</sup>EMBL-EBI, [viji@ebi.ac.uk](mailto:viji@ebi.ac.uk)

<sup>2</sup>IRMAR and IRISA/INRIA, University of Rennes 1, [ovidiu.radulescu@univ-rennes1.fr](mailto:ovidiu.radulescu@univ-rennes1.fr)

This a model from the article:

**Robust simplifications of multiscale biochemical networks.**

Radulescu O, Gorban A., Zinovyev A., Lilienbaum. A. *BMC Syst Biol*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 losing 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 with potential 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.

This model is originally proposed by Lipniacki 2004 (Lipniacki T, Paszek P, Brasier AR, Luxon B, Kimmel M.(2004). Mathematical model of NF-kappaB regulatory module. *J. Theor. Biol.* 228 (2): 195-215. [15094015](#)

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 species y - number of reactions z - number of parameters

**Simulation protocol:**The model can be simulated in CellDesigner directly, or in any simulator supporting events. The simulation period should be set up in 20 hours (t=72000 sec). This model reproduces Figure 3b (M(14,25,28)) of the publication.

For additional information please contact [Andrei.Zinovyev@curie.fr](mailto:Andrei.Zinovyev@curie.fr)

This model originates from BioModels Database: A Database of Annotated Published Models. It is copyright (c) 2005-2009 The BioModels Team.

For more information see the [terms of use](#).

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** l

### 2.3 Unit area

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

**Definition** m<sup>2</sup>

### 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	Size	Unit	Constant	Outside
			Dimensions				
default			3	1	litre	✓	
c2	nucleus		3	1	litre	✓	default

### 3.1 Compartment default

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

### 3.2 Compartment c2

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 24 species. The boundary condition of ten of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 7 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
s121	IKBA	c2	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s122	sa13_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s124	sa12_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s125	mRNAIKBA	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s126	A20	c2	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s127	mRNAA20	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s128	A20	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s129	sa444_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s130	IKKi	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s131	sa19_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s132	IKKa	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s133	IKKn	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s134	sa20_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s135	NFkB:IkB_alpha	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s139	IKKa/IKBa	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s150	IKK	c2	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s152	NFkB/Ikb_alpha/IKKa	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s153	sa96_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s154	sa97_degraded	default	$\text{mol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
s159	NFkB/IkB_alpha	c2	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s160	IkB_alpha	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s161	NFkB	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s164	NFkB	c2	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
s167	IkB_alpha	c2	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

## 5 Parameters

This model contains 31 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.003		<input checked="" type="checkbox"/>
k2			$1.25 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k3			$2.5 \cdot 10^{-6}$		<input type="checkbox"/>
k4			0.100		<input checked="" type="checkbox"/>
k5			0.002		<input checked="" type="checkbox"/>
k6			$1.25 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k7			0.200		<input checked="" type="checkbox"/>
k8			0.100		<input checked="" type="checkbox"/>
k9			1.000		<input checked="" type="checkbox"/>
k10			0.100		<input checked="" type="checkbox"/>
k11			$1.25 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k12			$2 \cdot 10^{-5}$		<input checked="" type="checkbox"/>
kf13			18.400		<input checked="" type="checkbox"/>
kr13			0.000		<input checked="" type="checkbox"/>
kf14			18.400		<input checked="" type="checkbox"/>
kr14			0.000		<input checked="" type="checkbox"/>
kf15			0.003		<input checked="" type="checkbox"/>
kr15			0.000		<input checked="" type="checkbox"/>
k16			0.500		<input checked="" type="checkbox"/>
k17			$4 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k18			$3 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k20			$5 \cdot 10^{-7}$		<input checked="" type="checkbox"/>
k19			0.000		<input checked="" type="checkbox"/>
k21			$10^{-4}$		<input checked="" type="checkbox"/>
k22			0.500		<input checked="" type="checkbox"/>
kf23			0.001		<input checked="" type="checkbox"/>
kr23			$5 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
k27			$4 \cdot 10^{-4}$		<input checked="" type="checkbox"/>
kf28			0.010		<input checked="" type="checkbox"/>
kr28			0.000		<input checked="" type="checkbox"/>
k26			$5 \cdot 10^{-7}$		<input checked="" type="checkbox"/>

## 6 Reactions

This model contains 24 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	SBO
1	re44		$s_{121} \xrightarrow{s_{164}} s_{125}$	
2	re45		$s_{125} \longrightarrow s_{124}$	
3	re46		$s_{160} \longrightarrow s_{122}$	
4	re47		$s_{125} \longrightarrow s_{160} + s_{125}$	
5	re48		$s_{126} \xrightarrow{s_{164}} s_{127}$	
6	re49		$s_{133} \longrightarrow s_{132}$	
7	re52		$s_{135} \xrightarrow{s_{132}} s_{161}$	
8	re53		$s_{133} \longrightarrow s_{131}$	
9	re56		$s_{132} \longrightarrow s_{134}$	
10	re57		$s_{139} \longrightarrow s_{132}$	
11	re58		$s_{132} + s_{135} \longrightarrow s_{152}$	
12	re59		$s_{152} \longrightarrow s_{161} + s_{132}$	
13	re60		$s_{130} \longrightarrow s_{129}$	
14	re61		$s_{127} \longrightarrow s_{128} + s_{127}$	
15	re63		$s_{132} \xrightarrow{s_{128}} s_{130}$	
16	re64		$s_{150} \longrightarrow s_{133}$	
17	re65		$s_{160} + s_{161} \longrightarrow s_{135}$	
18	re66		$s_{160} + s_{132} \longrightarrow s_{139}$	
19	re67		$s_{161} \longrightarrow 5 s_{164}$	
20	re68		$5 s_{159} \longrightarrow s_{135}$	
21	re69		$s_{164} + s_{167} \longrightarrow s_{159}$	



Nº	Id	Name	Reaction Equation	SBO
22	re70		$s_{127} \longrightarrow s_{153}$	
23	re71		$s_{128} \longrightarrow s_{154}$	
24	re72		$s_{160} \longrightarrow 5 s_{167}$	

## 6.1 Reaction re44

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

### Reaction equation



### Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s121	IKBA	

### Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
s164	NFkB	

### Product

Table 8: Properties of each product.

Id	Name	SBO
s125	mRNAIKBA	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = k26 \cdot [s164] \quad (2)$$

## 6.2 Reaction re45

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

### Reaction equation



## Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s125	mRNAIKBA	

## Product

Table 10: Properties of each product.

Id	Name	SBO
s124	sa12_degraded	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = k_{27} \cdot [s125] \quad (4)$$

## 6.3 Reaction re46

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

## Reaction equation



## Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
s160	IkB_alpha	

## Product

Table 12: Properties of each product.

Id	Name	SBO
s122	sa13_degraded	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = k_{21} \cdot [s_{160}] \quad (6)$$

## 6.4 Reaction re47

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

### Reaction equation



### Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
s125	mRNAIKBA	

### Products

Table 14: Properties of each product.

Id	Name	SBO
s160	IkB_alpha	
s125	mRNAIKBA	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = k_{22} \cdot [s_{125}] \quad (8)$$

## 6.5 Reaction re48

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

### Reaction equation



## Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
s126	A20	

## Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
s164	NFkB	

## Product

Table 17: Properties of each product.

Id	Name	SBO
s127	mRNAA20	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = k19 + k20 \cdot [s164] \quad (10)$$

## 6.6 Reaction re49

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

### Reaction equation



## Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
s133	IKKn	

## Product

Table 19: Properties of each product.

Id	Name	SBO
s132	IKKa	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_6 = k1 \cdot [s133] \quad (12)$$

## 6.7 Reaction re52

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

## Reaction equation



## Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
s135	NFkB:IkB_alpha	

## Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
s132	IKKa	

## Product

Table 22: Properties of each product.

Id	Name	SBO
s161	NFkB	

Id	Name	SBO
----	------	-----

### Kinetic Law

**Derived unit** contains undeclared units

$$v_7 = k_{12} \cdot [s_{135}] \quad (14)$$

## 6.8 Reaction re53

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

### Reaction equation



### Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
s133	IKKn	

### Product

Table 24: Properties of each product.

Id	Name	SBO
s131	sa19_degraded	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_8 = k_2 \cdot [s_{133}] \quad (16)$$

## 6.9 Reaction re56

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

### Reaction equation



## Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
s132	IKKa	

## Product

Table 26: Properties of each product.

Id	Name	SBO
s134	sa20_degraded	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_9 = k_6 \cdot [s132] \quad (18)$$

## 6.10 Reaction re57

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

## Reaction equation



## Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
s139	IKKa/IKBa	

## Product

Table 28: Properties of each product.

Id	Name	SBO
s132	IKKa	



### Kinetic Law

**Derived unit** contains undeclared units

$$v_{10} = k_8 \cdot [s_{139}] \quad (20)$$

### 6.11 Reaction re58

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

#### Reaction equation



#### Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
s132	IKKa	
s135	NFkB:IkB_alpha	

#### Product

Table 30: Properties of each product.

Id	Name	SBO
s152	NFkB/IkB_alpha/IKKa	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{11} = k_9 \cdot [s_{132}] \cdot [s_{135}] \quad (22)$$

### 6.12 Reaction re59

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

#### Reaction equation



## Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
s152	NFkB/Ikb_alpha/IKKa	

## Products

Table 32: Properties of each product.

Id	Name	SBO
s161	NFkB	
s132	IKKa	

## Kinetic Law

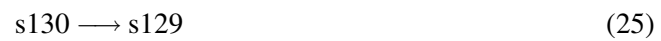
**Derived unit** contains undeclared units

$$v_{12} = k_{10} \cdot [s152] \quad (24)$$

## 6.13 Reaction re60

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

## Reaction equation



## Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
s130	IKKi	

## Product

Table 34: Properties of each product.

Id	Name	SBO
s129	sa444_degraded	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{13} = k_{11} \cdot [s_{130}] \quad (26)$$

### 6.14 Reaction re61

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

#### Reaction equation



### Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
s127	mRNAA20	

### Products

Table 36: Properties of each product.

Id	Name	SBO
s128	A20	
s127	mRNAA20	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{14} = k_{16} \cdot [s_{127}] \quad (28)$$

### 6.15 Reaction re63

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

### Reaction equation



### Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
s132	IKKa	

### Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
s128	A20	

### Product

Table 39: Properties of each product.

Id	Name	SBO
s130	IKKi	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_{15} = k5 \cdot [\text{s132}] + k4 \cdot [\text{s132}] \cdot [\text{s128}] \quad (30)$$

### 6.16 Reaction re64

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

### Reaction equation



### Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
s150	IKK	

## Product

Table 41: Properties of each product.

Id	Name	SBO
s133	IKKn	

## Kinetic Law

**Derived unit** not available

$$v_{16} = k3 \quad (32)$$

## 6.17 Reaction re65

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

## Reaction equation



## Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
s160	IkB_alpha	
s161	NFkB	

## Product

Table 43: Properties of each product.

Id	Name	SBO
s135	NFkB:IkB_alpha	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{17} = k_{f13} \cdot [s161] \cdot [s160] - k_{r13} \cdot [s135] \quad (34)$$

## 6.18 Reaction re66

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

### Reaction equation



### Reactants

Table 44: Properties of each reactant.

Id	Name	SBO
s160	IkB_alpha	
s132	IKKa	

### Product

Table 45: Properties of each product.

Id	Name	SBO
s139	IKKa/IKBa	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{18} = k_7 \cdot [s132] \cdot [s160] \quad (36)$$

## 6.19 Reaction re67

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

### Reaction equation



## Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
s161	NFkB	

## Product

Table 47: Properties of each product.

Id	Name	SBO
s164	NFkB	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{19} = k_{f15} \cdot [s161] - k_{r15} \cdot [s164] \quad (38)$$

## 6.20 Reaction re68

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

## Reaction equation



## Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
s159	NFkB/IkB_alpha	

## Product

Table 49: Properties of each product.

Id	Name	SBO
s135	NFkB:IkB_alpha	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{20} = k_{f28} \cdot [s159] - k_{r28} \cdot [s135] \quad (40)$$

## 6.21 Reaction re69

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

### Reaction equation



### Reactants

Table 50: Properties of each reactant.

Id	Name	SBO
s164	NFkB	
s167	IkB_alpha	

### Product

Table 51: Properties of each product.

Id	Name	SBO
s159	NFkB/IkB_alpha	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{21} = k_{f14} \cdot [s164] \cdot [s167] - k_{r14} \cdot [s159] \quad (42)$$

## 6.22 Reaction re70

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

### Reaction equation





## Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
s127	mRNAA20	

## Product

Table 53: Properties of each product.

Id	Name	SBO
s153	sa96_degraded	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{22} = k_{17} \cdot [s127] \quad (44)$$

## 6.23 Reaction re71

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

## Reaction equation



## Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
s128	A20	

## Product

Table 55: Properties of each product.

Id	Name	SBO
s154	sa97_degraded	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{23} = k_{18} \cdot [s_{128}] \quad (46)$$

## 6.24 Reaction `re72`

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

### Reaction equation



### Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
s160	IkB_alpha	

### Product

Table 57: Properties of each product.

Id	Name	SBO
s167	IkB_alpha	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_{24} = k_{f23} \cdot [s_{160}] - k_{r23} \cdot [s_{167}] \quad (48)$$

## 7 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.

### 7.1 Species `s121`

**Name** IKBA

**Initial amount** 0 mol

**Charge** 0

This species takes part in one reaction (as a reactant in [re44](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{121} = 0 \quad (49)$$

### 7.2 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:

$$\frac{d}{dt}s_{122} = 0 \quad (50)$$

### 7.3 Species `s124`

**Name** `sa12_degraded`

**Initial amount** 0 mol

**Charge** 0

This species takes part in one reaction (as a product in [re45](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{124} = 0 \quad (51)$$

#### 7.4 Species s125

**Name** mRNAIKBA

**Initial amount** 0 mol

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

$$\frac{d}{dt}s_{125} = v_1 + v_4 - v_2 - v_4 \quad (52)$$

#### 7.5 Species s126

**Name** A20

**Initial amount** 0 mol

**Charge** 0

This species takes part in one reaction (as a reactant in [re48](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{126} = 0 \quad (53)$$

#### 7.6 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](#)).

$$\frac{d}{dt}s_{127} = v_5 + v_{14} - v_{14} - v_{22} \quad (54)$$

#### 7.7 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](#)).

$$\frac{d}{dt}s_{128} = v_{14} - v_{23} \quad (55)$$

### 7.8 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:

$$\frac{d}{dt}s_{129} = 0 \quad (56)$$

### 7.9 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](#)).

$$\frac{d}{dt}s_{130} = v_{15} - v_{13} \quad (57)$$

### 7.10 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:

$$\frac{d}{dt}s_{131} = 0 \quad (58)$$

### 7.11 Species s132

**Name** IKKa

**Initial amount** 0 mol

This species takes part in eight reactions (as a reactant in [re56](#), [re58](#), [re63](#), [re66](#) and as a product in [re49](#), [re57](#), [re59](#) and as a modifier in [re52](#)).

$$\frac{d}{dt}s_{132} = v_6 + v_{10} + v_{12} - v_9 - v_{11} - v_{15} - v_{18} \quad (59)$$

### 7.12 Species s133

**Name** IKKn

**Initial amount** 0 mol

**Charge** 0

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

$$\frac{d}{dt}s_{133} = v_{16} - v_6 - v_8 \quad (60)$$

### 7.13 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:

$$\frac{d}{dt}s_{134} = 0 \quad (61)$$

### 7.14 Species s135

**Name** NFkB:IkB\_alpha

**Initial amount** 0.06 mol

**Charge** 0

This species takes part in four reactions (as a reactant in [re52](#), [re58](#) and as a product in [re65](#), [re68](#)).

$$\frac{d}{dt}s_{135} = v_{17} + v_{20} - v_7 - v_{11} \quad (62)$$

### 7.15 Species s139

**Name** IKKa/IKBa

**Initial amount** 0 mol

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

$$\frac{d}{dt}s_{139} = v_{18} - v_{10} \quad (63)$$

### 7.16 Species s150

**Name** IKK

**Initial amount** 0 mol

**Charge** 0

This species takes part in one reaction (as a reactant in [re64](#)), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}s_{150} = 0 \quad (64)$$

### 7.17 Species s152

**Name** NFkB/Ikb\_alpha/IKKa

**Initial amount** 0 mol

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

$$\frac{d}{dt}s_{152} = v_{11} - v_{12} \quad (65)$$

### 7.18 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:

$$\frac{d}{dt}s_{153} = 0 \quad (66)$$

### 7.19 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:

$$\frac{d}{dt}s_{154} = 0 \quad (67)$$

## 7.20 Species s159

**Name** NFkB/IkB\_alpha

**Initial amount** 0 mol

This species takes part in two reactions (as a reactant in [re68](#) and as a product in [re69](#)).

$$\frac{d}{dt}s159 = v_{21} - 5 v_{20} \quad (68)$$

## 7.21 Species s160

**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](#)).

$$\frac{d}{dt}s160 = v_4 - v_3 - v_{17} - v_{18} - v_{24} \quad (69)$$

## 7.22 Species s161

**Name** NFkB

**Initial amount** 0 mol

This species takes part in four reactions (as a reactant in [re65](#), [re67](#) and as a product in [re52](#), [re59](#)).

$$\frac{d}{dt}s161 = v_7 + v_{12} - v_{17} - v_{19} \quad (70)$$

## 7.23 Species s164

**Name** NFkB

**Initial amount** 0 mol

This species takes part in four reactions (as a reactant in [re69](#) and as a product in [re67](#) and as a modifier in [re44](#), [re48](#)).

$$\frac{d}{dt}s164 = 5 v_{19} - v_{21} \quad (71)$$



## 7.24 Species s167

**Name** IkB\_alpha

**Initial amount** 0 mol

This species takes part in two reactions (as a reactant in [re69](#) and as a product in [re72](#)).

$$\frac{d}{dt}s167 = 5 v_{24} - v_{21} \quad (72)$$

SBML2<sup>LaTeX</sup> was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

<sup>a</sup>Center for Bioinformatics Tübingen (ZBIT), Germany

<sup>b</sup>California Institute of Technology, Beckman Institute BNMC, Pasadena, United States

<sup>c</sup>European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

<sup>d</sup>EML Research gGmbH, Heidelberg, Germany