SBML Model Report

Model name: "ODea2007_IkappaB"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Harish Dharuri¹ and Hoffman Alexander² at September fourth 2007 at 10:35 a.m. and last time modified at May 26th 2014 at 11:05 p.m. Table 1 shows 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 | 51 | function definitions | 0 |
| global parameters | 3 | unit definitions | 4 |
| rules | 3 | initial assignments | 0 |

Model Notes

O'Dea, E.L., Barken, D., Peralta, R.Q., Tran K.T., Werner, S.L., Kearns, J.D., Levchenko, A., Hoffmann, A. A homeostatic model of IkB metabolism to control constitutive activity. Molecular Systems Biology, 3:111, pp. 1-7. 2007

Questions concerning the paper should be addressed to the corresponding author. Alexander Hoffmann (ahoffmann@ucsd.edu)

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The original model was written and simulated within MathWorks MatLab 2006a using the ode15s (stiff/NDF) solver. It is highly recommended that those wanting to model this system use the MatLab version which we will freely provide upon request. As always, simulation results vary according to the numerical solver used.

Translation to SBML Level 2.1 was performed via reconstruction of the model within Math-Works SimBiology Desktop (version 2.1) followed by an Export to SBML. Please address questions about this SBML model to Jeff Kearns (jkearns@ucsd.edu).

BioModels DB curation: The model reproduces the values of diffferent species depicted in Fig 3A and 3B (wt) of the paper corresponding to Model1.1. To depict the total IkB alpha, beta epsilon species, three additional parameters and their corresponding assignment rules have been introduced in this model by the creator. Model successfully tested on MathSBML.

This model originates from BioModels Database: A Database of Annotated Published Models. It is copyright (c) 2005-2010 The BioModels Team.

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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 eight unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit substance

Name micromole

Definition µmol

2.2 Unit uM_per_min

Name uM_per_min

Definition $\mu \text{mol} \cdot (60 \text{ s})^{-1} \cdot l^{-1}$

2.3 Unit per_min

Name per_min

Definition $(60 \text{ s})^{-1}$

2.4 Unit per_uM_per_min

Name per_uM_per_min

Definition $\mu mol^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$

2.5 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.6 Unit area

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

Definition m^2

2.7 Unit length

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

Definition m

2.8 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 |
|----------------------|----------------------|-----|--------------------|------|----------------|----------|---------|
| cytoplasm nucleus | cytoplasm nucleus | | 3 3 | 1 | litre litre | 1 | |

3.1 Compartment cytoplasm

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

Name cytoplasm

3.2 Compartment nucleus

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

Name nucleus

4 Species

This model contains 24 species. 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 |
|-------------------------|-------------|-------------------|-------------------------------|----------|----------------------------|
| IkBa_mRNA | IkBat | nucleus | μ mol·l ⁻¹ | | |
| IkBa_cytoplasm | IkBa | cytoplasm | $\mu \text{mol} \cdot 1^{-1}$ | | |
| IkBa_nucleus | IkBan | nucleus | μ mol·l ⁻¹ | | |
| IkBaIKK | IkBaIKK | cytoplasm | $\mu \text{mol} \cdot l^{-1}$ | | |
| IkBaNFkB- _cytoplasm | IkBaNFkB | cytoplasm | $\mu \text{mol} \cdot 1^{-1}$ | | |
| IkBaNFkB_nucleus | IkBaNFkBn | nucleus | $\mu mol \cdot l^{-1}$ | | |
| IkBaIKKNFkB | IkBaIKKNFkB | cytoplasm | μ mol·l ⁻¹ | | |
| $NFkB_cytoplasm$ | NFkB | cytoplasm | μ mol·l ⁻¹ | | |
| IKK | IKK | cytoplasm | μ mol·l ⁻¹ | | |
| NFkB_nucleus | NFkBn | nucleus | $\mu mol \cdot l^{-1}$ | | |
| IkBbIKK | IkBbIKK | cytoplasm | $\mu mol \cdot l^{-1}$ | | |
| IkBbIKKNFkB | IkBbIKKNFkB | cytoplasm | $\mu mol \cdot l^{-1}$ | | |
| IkBbNFkB_nucleus | IkBbNFkBn | nucleus | $\mu mol \cdot l^{-1}$ | | |
| IkBbNFkB- | IkBbNFkB | ${\tt cytoplasm}$ | $\mu mol \cdot l^{-1}$ | | |
| $_\mathtt{cytoplasm}$ | | | | | |
| IkBb_nucleus | IkBbn | nucleus | μ mol·l ⁻¹ | | |
| ${\tt IkBb_cytoplasm}$ | IkBb | ${	t cytoplasm}$ | $\mu \text{mol} \cdot l^{-1}$ | \Box | |
| IkBb_mRNA | IkBbt | nucleus | μ mol · l ⁻¹ | | |
| IkBe_mRNA | IkBet | nucleus | $\mu mol \cdot l^{-1}$ | | \Box |
| ${\tt IkBe_cytoplasm}$ | IkBe | ${	t cytoplasm}$ | $\mu mol \cdot l^{-1}$ | | |
| IkBe_nucleus | IkBen | nucleus | $\mu mol \cdot l^{-1}$ | | |

| Id | Name | Compartment | Derived Unit | Constant | Boundary Condi- |
|-------------------------|-------------|-------------|-------------------------------|----------|--------------------|
| | | | | | tion |
| IkBeNFkB- _cytoplasm | IkBeNFkB | cytoplasm | $\mu \text{mol} \cdot l^{-1}$ | В | В |
| IkBeNFkB_nucleus | IkBeNFkBn | nucleus | $\mu mol \cdot l^{-1}$ | | \Box |
| IkBeIKKNFkB | IkBeIKKNFkB | cytoplasm | $\mu mol \cdot l^{-1}$ | | \Box |
| IkBeIKK | IkBeIKK | cytoplasm | $\mu mol \cdot l^{-1}$ | | |

5 Parameters

This model contains three global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|-----------------------|----------------|----------------|----------|
| Total- _IkBalpha | Total_IkBalpha | 0.0 | В |
| Total- _IkBbeta | Total_IkBbeta | 0.0 | |
| ${\tt Total_IkBeps}$ | Total_IkBeps | 0.0 | |

6 Rules

This is an overview of three rules.

6.1 Rule Total_IkBalpha

Rule Total_IkBalpha is an assignment rule for parameter Total_IkBalpha:

$$Total_IkBalpha = [IkBa_cytoplasm] + [IkBa_nucleus] + [IkBaIKK] + [IkBaIKKNFkB] \\ + [IkBaNFkB_cytoplasm] + [IkBaNFkB_nucleus]$$
 (1)

Derived unit $\mu mol \cdot l^{-1}$

6.2 Rule Total_IkBbeta

Rule Total_IkBbeta is an assignment rule for parameter Total_IkBbeta:

Derived unit $\mu mol \cdot l^{-1}$

6.3 Rule Total_IkBeps

Rule Total_IkBeps is an assignment rule for parameter Total_IkBeps:

$$Total_IkBeps = [IkBe_cytoplasm] + [IkBe_nucleus] + [IkBeIKK] + [IkBeIKKNFkB] + [IkBeNFkB_cytoplasm] + [IkBeNFkB_nucleus]$$

$$(3)$$

Derived unit $\mu mol \cdot l^{-1}$

7 Reactions

This model contains 51 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 | txn_a | txn_a | $\emptyset \longrightarrow IkBa_mRNA$ |
| 2 | ${\tt mdeg_a}$ | mdeg_a | $IkBa_mRNA \longrightarrow \emptyset$ |
| 3 | tsl_a | tsl_a | $IkBa_mRNA \longrightarrow IkBa_mRNA + IkBa_cytoplasm$ |
| 4 | $\mathtt{int}_{\mathtt{-}}\mathtt{ai}$ | int_ai | $IkBa_cytoplasm + IKK \Longrightarrow IkBaIKK$ |
| 5 | $\mathtt{int}_{\mathtt{-}}\mathtt{an}$ | int_an | $IkBa_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBaNFkB_cytoplasm$ |
| 6 | int_an_n | int_an_n | $IkBa_nucleus + NFkB_nucleus \Longrightarrow IkBaNFkB_nucleus$ |
| 7 | int_2ani | int_2ani | $IkBaNFkB_cytoplasm + IKK \Longrightarrow IkBaIKKNFkB$ |
| 8 | int_2ain | int_2ain | $IkBaIKK + NFkB_cytoplasm \Longrightarrow IkBaIKKNFkB$ |
| 9 | \deg_{-a} | deg_a | $IkBa_cytoplasm \longrightarrow \emptyset$ |
| 10 | ${\tt deg_a_n}$ | deg_a_n | IkBa_nucleus $\longrightarrow \emptyset$ |
| 11 | deg_an_n | deg_an_n | IkBaNFkB_nucleus → NFkB_nucleus |
| 12 | $\mathtt{deg}_{\mathtt{-}}\mathtt{an}$ | deg_an | $IkBaNFkB_cytoplasm \longrightarrow NFkB_cytoplasm$ |
| 13 | $\mathtt{deg}_{\mathtt{-}}\mathtt{ai}$ | deg_ai | $IkBaIKK \longrightarrow IKK$ |
| 14 | $\mathtt{deg_ain}$ | deg_ain | $IkBaIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$ |
| 15 | loc_a | loc_a | IkBa_cytoplasm ← IkBa_nucleus |
| 16 | loc_an | loc_an | $IkBaNFkB_nucleus \longrightarrow IkBaNFkB_cytoplasm$ |
| 17 | loc_bn | loc_bn | $IkBbNFkB_nucleus \longrightarrow IkBbNFkB_cytoplasm$ |
| 18 | loc_b | loc_b | IkBb_cytoplasm |
| 19 | $\mathtt{deg_bin}$ | deg_bin | $IkBbIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$ |
| 20 | deg_bi | deg_bi | $IkBbIKK \longrightarrow IKK$ |
| 21 | deg_bn | deg_bn | $IkBbNFkB_cytoplasm \longrightarrow NFkB_cytoplasm$ |
| 22 | deg_bn_n | deg_bn_n | $IkBbNFkB_nucleus \longrightarrow NFkB_nucleus$ |
| 23 | ${\tt deg_b_n}$ | deg_b_n | IkBb_nucleus $\longrightarrow \emptyset$ |

| N₀ | Id | Name | Reaction Equation SBO | |
|----|-----------------|----------|---|----|
| 24 | deg_b | deg_b | IkBb_cytoplasm $\longrightarrow \emptyset$ | |
| 25 | int_2bin | int_2bin | IkBbIKK+NFkB_cytoplasm ⇒ IkBbIKKNFkB | |
| 26 | int_2bni | int_2bni | IkBbNFkB_cytoplasm+IKK ⇒ IkBbIKKNFkB | |
| 27 | int_bn_n | int_bn_n | IkBb_nucleus + NFkB_nucleus | |
| 28 | int_bn | int_bn | $IkBb_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBbNFkB_cytoplasm$ | sm |
| 29 | ${\tt int_bi}$ | int_bi | $IkBb_cytoplasm + IKK \Longrightarrow IkBbIKK$ | |
| 30 | tsl_b | tsl_b | $IkBb_mRNA \longrightarrow IkBb_mRNA + IkBb_cytoplasm$ | |
| 31 | $mdeg_b$ | mdeg_b | $IkBb_mRNA \longrightarrow \emptyset$ | |
| 32 | txn_b | txn_b | $\emptyset \longrightarrow IkBb_mRNA$ | |
| 33 | loc_n | loc_n | NFkB_cytoplasm | |
| 34 | txn_e | txn_e | $\emptyset \longrightarrow IkBe_mRNA$ | |
| 35 | $mdeg_e$ | mdeg_e | $IkBe_mRNA \longrightarrow \emptyset$ | |
| 36 | tsl_e | tsl_e | $IkBe_mRNA \longrightarrow IkBe_mRNA + IkBe_cytoplasm$ | |
| 37 | ${\tt int_ei}$ | int_ei | $IkBe_cytoplasm + IKK \Longrightarrow IkBeIKK$ | |
| 38 | int_en | int_en | $IkBe_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBeNFkB_cytoplasm$ | sm |
| 39 | int_en_n | int_en_n | IkBe_nucleus + NFkB_nucleus | |
| 40 | int_2eni | int_2eni | $IkBeNFkB_cytoplasm + IKK \Longrightarrow IkBeIKKNFkB$ | |
| 41 | int_2ein | int_2ein | $IkBeIKK + NFkB_cytoplasm \Longrightarrow IkBeIKKNFkB$ | |
| 42 | deg_e | deg_e | $IkBe_cytoplasm \longrightarrow \emptyset$ | |
| 43 | deg_e_n | deg_e_n | IkBe_nucleus $\longrightarrow \emptyset$ | |
| 44 | deg_en_n | deg_en_n | $IkBeNFkB_nucleus \longrightarrow NFkB_nucleus$ | |
| 45 | deg_en | deg_en | IkBeNFkB_cytoplasm → NFkB_cytoplasm | |
| 46 | deg_ei | deg_ei | IkBeIKK → IKK | |
| 47 | deg_ein | deg_ein | $IkBeIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$ | |
| 48 | loc_e | loc_e | IkBe_cytoplasm | |
| 49 | loc_en | loc_en | IkBeNFkB_nucleus → IkBeNFkB_cytoplasm | |
| 50 | IKK_deg | IKK_deg | $IKK \longrightarrow \emptyset$ | |
| 51 | itxn_a | itxn_a | $\emptyset \xrightarrow{NFkB_nucleus} IkBa_mRNA$ | |

7.1 Reaction txn_a

This is an irreversible reaction of no reactant forming one product.

Name txn_a

Reaction equation

$$\emptyset \longrightarrow IkBa_mRNA$$
 (4)

Product

Table 6: Properties of each product.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBa_mRNA | IkBat | |

Kinetic Law

Derived unit $\mu mol \cdot (60 \text{ s})^{-1}$

$$v_1 = \text{vol}(\text{nucleus}) \cdot \text{tr}2a$$
 (5)

Table 7: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------|------|-----|-----------------------|--|----------|
| tr2a | tr2a | | $1.848 \cdot 10^{-4}$ | $\mu mol \cdot (60 \text{ s})^{-1} \cdot l^{-1}$ | |

7.2 Reaction mdeg_a

This is an irreversible reaction of one reactant forming no product.

Name mdeg_a

Reaction equation

$$IkBa_mRNA \longrightarrow \emptyset$$
 (6)

Reactant

Table 8: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBa_mRNA | IkBat | |

Kinetic Law

Derived unit $\left(60\,s\right)^{-1} \cdot \mu mol$

$$v_2 = \text{vol}(\text{nucleus}) \cdot \text{tr3a} \cdot [\text{IkBa_mRNA}]$$
 (7)

Table 9: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|-----------|
| tr3a | tr3a | 0.017 | $(60 \text{ s})^{-1}$ | \square |

7.3 Reaction tsl_a

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

Name tsl_a

Reaction equation

$$IkBa_mRNA \longrightarrow IkBa_mRNA + IkBa_cytoplasm \tag{8}$$

Reactant

Table 10: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBa_mRNA | IkBat | |

Products

Table 11: Properties of each product.

| Id | Name | SBO |
|-------------------------|-------|-----|
| IkBa_mRNA | IkBat | |
| ${\tt IkBa_cytoplasm}$ | IkBa | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_3 = \text{vol}(\text{nucleus}) \cdot \text{tr1a} \cdot [\text{IkBa_mRNA}]$$
 (9)

Table 12: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|----------|
| tr1a | tr1a | 0.245 | $(60 \text{ s})^{-1}$ | |

7.4 Reaction int_ai

This is a reversible reaction of two reactants forming one product.

Name int_ai

Reaction equation

$$IkBa_cytoplasm + IKK \rightleftharpoons IkBaIKK$$
 (10)

Reactants

Table 13: Properties of each reactant.

| Id | Name | SBO |
|-----------------------|-------------|-----|
| IkBa_cytoplasm IKK | IkBa IKK | |

Product

Table 14: Properties of each product.

| Id | Name | SBO |
|---------|---------|-----|
| IkBaIKK | IkBaIKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_4 = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a1} \cdot [\text{IkBa_cytoplasm}] \cdot [\text{IKK}] - \text{d1_1} \cdot [\text{IkBaIKK}]\right)$$
 (11)

Table 15: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------------|------------|-----------|---|----------|
| a1 d1_1 | a1 d1_1 | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | Z |

7.5 Reaction int_an

This is a reversible reaction of two reactants forming one product.

Name int_an

Reaction equation

$$IkBa_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBaNFkB_cytoplasm$$
 (12)

Reactants

Table 16: Properties of each reactant.

| Id | Name | SBO |
|----------------------------------|------|-----|
| IkBa_cytoplasm NFkB_cytoplasm | | |

Product

Table 17: Properties of each product.

| Id | Name | SBO |
|-----------------------------|----------|-----|
| ${\tt IkBaNFkB_cytoplasm}$ | IkBaNFkB | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$\begin{array}{l} v_5 = vol \left(cytoplasm \right) \\ \cdot \left(a4_1 \cdot \left[IkBa_cytoplasm \right] \cdot \left[NFkB_cytoplasm \right] - d4_1 \cdot \left[IkBaNFkB_cytoplasm \right]) \end{array}$$

Table 18: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------------|--------------|-----|-------|--|----------|
| a4_1 d4_1 | a4_1 d4_1 | | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1 $ $(60 \text{ s})^{-1}$ | ✓ |

7.6 Reaction int_an_n

This is a reversible reaction of two reactants forming one product.

Name int_an_n

Reaction equation

$$IkBa_nucleus + NFkB_nucleus \Longrightarrow IkBaNFkB_nucleus$$
 (14)

Reactants

Table 19: Properties of each reactant.

| Id | Name | SBO |
|------------------------------|------|-----|
| IkBa_nucleus NFkB_nucleus | | |

Product

Table 20: Properties of each product.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBaNFkB_nucleus | IkBaNFkBn | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

 $v_6 = vol\left(nucleus\right) \cdot \left(a4_2 \cdot [IkBa_nucleus] \cdot [NFkB_nucleus] - d4_2 \cdot [IkBaNFkB_nucleus]\right) \quad (15)$

Table 21: Properties of each parameter.

| Id | Name | SBO Valu | ue Unit | Constant |
|--------------|--------------|----------|---|----------|
| a4_2 d4_2 | a4_2 d4_2 | | 00 $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1}$ 0-5 $(60 \text{ s})^{-1}$ | ¹·1 |

7.7 Reaction int_2ani

This is a reversible reaction of two reactants forming one product.

Name int_2ani

Reaction equation

$$IkBaNFkB_cytoplasm + IKK \rightleftharpoons IkBaIKKNFkB$$
 (16)

Reactants

Table 22: Properties of each reactant.

| Id | Name | SBO |
|---------------------------|-----------------|-----|
| IkBaNFkB_cytoplasm IKK | IkBaNFkB IKK | |

Product

Table 23: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBaIKKNFkB | IkBaIKKNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_7 = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a7} \cdot \left[\text{IkBaNFkB_cytoplasm}\right] \cdot \left[\text{IKK}\right] - \text{d1_2} \cdot \left[\text{IkBaIKKNFkB}\right]\right)$$
 (17)

Table 24: Properties of each parameter.

| Id | Name | SBO Valu | e Unit | Constant |
|------------|------------|----------|--|-------------|
| a7 d1_2 | a7 d1_2 | | 00 $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1}$ 75 $(60 \text{ s})^{-1}$ | ·1 Z |

7.8 Reaction int_2ain

This is a reversible reaction of two reactants forming one product.

Name int_2ain

Reaction equation

$$IkBaIKK + NFkB_cytoplasm \Longrightarrow IkBaIKKNFkB$$
 (18)

Reactants

Table 25: Properties of each reactant.

| Id | Name | SBO |
|----------------|---------|-----|
| IkBaIKK | IkBaIKK | |
| NFkB_cytoplasm | NFkB | |

Product

Table 26: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBaIKKNFkB | IkBaIKKNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_8 = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a4_3} \cdot \left[\text{IkBaIKK}\right] \cdot \left[\text{NFkB_cytoplasm}\right] - \text{d4_3} \cdot \left[\text{IkBaIKKNFkB}\right]\right)$$
 (19)

Table 27: Properties of each parameter.

| Id | Name | SBO Valu | ue Unit | Constant |
|--------------|--------------|----------|---|---------------------------------------|
| a4_3 d4_3 | a4_3 d4_3 | | $\begin{array}{ccc} 000 & \mu \text{mol}^{-1} \cdot (60 \text{ s}) \\ 0^{-5} & (60 \text{ s})^{-1} \end{array}$ | $(s)^{-1} \cdot 1$ $(s)^{-1} \cdot 1$ |

7.9 Reaction deg_a

This is an irreversible reaction of one reactant forming no product.

Name deg_a

Reaction equation

$$IkBa_cytoplasm \longrightarrow \emptyset$$
 (20)

Reactant

Table 28: Properties of each reactant.

| Id | Name | |
|----------------|------|--|
| IkBa_cytoplasm | IkBa | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_9 = \text{vol}\left(\text{cytoplasm}\right) \cdot \text{deg1_c} \cdot \left[\text{IkBa_cytoplasm}\right]$$
 (21)

Table 29: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|--------|--------|-----------------------------|----------|
| deg1_c | deg1_c | $0.12 (60 \text{ s})^{-1}$ | Ø |

7.10 Reaction deg_a_n

This is an irreversible reaction of one reactant forming no product.

Name deg_a_n

Reaction equation

IkBa_nucleus
$$\longrightarrow \emptyset$$
 (22)

Reactant

Table 30: Properties of each reactant.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBa_nucleus | IkBan | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{10} = \text{vol}\left(\text{nucleus}\right) \cdot \text{deg1_n} \cdot \left[\text{IkBa_nucleus}\right]$$
 (23)

Table 31: Properties of each parameter.

| Id | Name | SBO Value U | Jnit Constant |
|--------|--------|-------------|-----------------------|
| deg1_n | deg1_n | 0.12 (| $(60 \text{ s})^{-1}$ |

7.11 Reaction deg_an_n

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

Name deg_an_n

Reaction equation

$$IkBaNFkB_nucleus \longrightarrow NFkB_nucleus$$
 (24)

Reactant

Table 32: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBaNFkB_nucleus | IkBaNFkBn | |

Product

Table 33: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| NFkB_nucleus | NFkBn | |

Kinetic Law

Derived unit $\left(60\,s\right)^{-1} \cdot \mu mol$

$$v_{11} = \text{vol} (\text{nucleus}) \cdot \text{deg4_n} \cdot [\text{IkBaNFkB_nucleus}]$$
 (25)

Table 34: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|-------------------|-----------------------|----------|
| deg4_n | deg4_n | 6 | $5 \cdot 10^{-5}$ | $(60 \text{ s})^{-1}$ | |

7.12 Reaction deg_an

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

Name deg_an

Reaction equation

$$IkBaNFkB_cytoplasm \longrightarrow NFkB_cytoplasm \tag{26}$$

Reactant

Table 35: Properties of each reactant.

| Id | Name | SBO |
|-----------------------------|----------|-----|
| ${\tt IkBaNFkB_cytoplasm}$ | IkBaNFkB | |

Product

Table 36: Properties of each product.

| Id | Name | SBO |
|----------------|------|-----|
| NFkB_cytoplasm | NFkB | |

Kinetic Law

 $\textbf{Derived unit} \ \left(60 \ s\right)^{-1} \cdot \mu mol$

$$v_{12} = \text{vol}(\text{cytoplasm}) \cdot \text{deg4_c} \cdot [\text{IkBaNFkB_cytoplasm}]$$
 (27)

Table 37: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|------------------|-----------------------|----------------|
| deg4_c | deg4_c | | $6\cdot 10^{-5}$ | $(60 \text{ s})^{-1}$ | \overline{Z} |

7.13 Reaction deg_ai

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

Name deg_ai

Reaction equation

$$IkBaIKK \longrightarrow IKK \tag{28}$$

Reactant

Table 38: Properties of each reactant.

| Id | Name | SBO |
|---------|---------|-----|
| IkBaIKK | IkBaIKK | |

Product

Table 39: Properties of each product.

| Id | Name | SBO |
|-----|------|-----|
| IKK | IKK | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{13} = \text{vol}(\text{cytoplasm}) \cdot \text{r1} \cdot [\text{IkBaIKK}]$$
 (29)

Table 40: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|----|------|-----------|-----------------------|----------------|
| r1 | r1 | 0.072 | $(60 \text{ s})^{-1}$ | \overline{Z} |

7.14 Reaction deg_ain

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

Name deg_ain

Reaction equation

$$IkBaIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$$
 (30)

Reactant

Table 41: Properties of each reactant.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBaIKKNFkB | IkBaIKKNFkB | |

Products

Table 42: Properties of each product.

| | · · · · · I | |
|-----------------------|-------------|-----|
| Id | Name | SBO |
| NFkB_cytoplasm IKK | NFkB IKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{14} = \text{vol}(\text{cytoplasm}) \cdot \text{r4} \cdot [\text{IkBaIKKNFkB}]$$
 (31)

Table 43: Properties of each parameter.

| Id | Name | SBO V | value | Unit | Constant |
|----|------|-------|-------|-----------------------|----------|
| r4 | r4 | C | 0.36 | $(60 \text{ s})^{-1}$ | |

7.15 Reaction loc_a

This is a reversible reaction of one reactant forming one product.

Name loc_a

Reaction equation

$$IkBa_cytoplasm \Longrightarrow IkBa_nucleus$$
 (32)

Reactant

Table 44: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBa_cytoplasm | IkBa | |

Product

Table 45: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBa_nucleus | IkBan | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

 $v_{15} = vol(cytoplasm) \cdot tp1a \cdot [IkBa_cytoplasm] - vol(nucleus) \cdot tp2a \cdot [IkBa_nucleus]$ (33)

Table 46: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|------|------|------------------------------|----------|
| tp1a | tp1a | $0.018 (60 \text{ s})^{-1}$ | |
| tp2a | tp2a | $0.012 (60 \text{ s})^{-1}$ | |

7.16 Reaction loc_an

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

Name loc_an

Reaction equation

$$IkBaNFkB_nucleus \longrightarrow IkBaNFkB_cytoplasm \tag{34}$$

Reactant

Table 47: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBaNFkB_nucleus | IkBaNFkBn | |

Product

Table 48: Properties of each product.

| | 1 | |
|--------------------|----------|-----|
| Id | Name | SBO |
| IkBaNFkB_cytoplasm | IkBaNFkB | |

Kinetic Law

Derived unit $\left(60\,s\right)^{-1} \cdot \mu mol$

$$v_{16} = \text{vol}(\text{nucleus}) \cdot \text{k2_a} \cdot [\text{IkBaNFkB_nucleus}]$$
 (35)

Table 49: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|----------|
| k2_a | k2_a | 0.828 | $(60 \text{ s})^{-1}$ | |

7.17 Reaction loc_bn

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

Name loc_bn

Reaction equation

$$IkBbNFkB_nucleus \longrightarrow IkBbNFkB_cytoplasm$$
 (36)

Reactant

Table 50: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBbNFkB_nucleus | IkBbNFkBn | |

Product

Table 51: Properties of each product.

| Id | Name | SBO |
|-----------------------------|----------|-----|
| ${\tt IkBbNFkB_cytoplasm}$ | IkBbNFkB | |

Kinetic Law

Derived unit $\left(60\,s\right)^{-1} \cdot \mu mol$

$$v_{17} = \text{vol}(\text{nucleus}) \cdot \text{k2_b} \cdot [\text{IkBbNFkB_nucleus}]$$
 (37)

Table 52: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|------|------|------------------------------|----------|
| k2_b | k2_b | $0.414 (60 \text{ s})^{-1}$ | |

7.18 Reaction loc_b

This is a reversible reaction of one reactant forming one product.

Name loc_b

Reaction equation

$$IkBb_cytoplasm \Longrightarrow IkBb_nucleus$$
 (38)

Reactant

Table 53: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBb_cytoplasm | IkBb | |

Product

Table 54: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBb_nucleus | IkBbn | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{18} = vol(cytoplasm) \cdot tp1b \cdot [IkBb_cytoplasm] - vol(nucleus) \cdot tp2b \cdot [IkBb_nucleus]$$
 (39)

Table 55: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|------|------|------------------------------|----------|
| tp1b | tp1b | $0.018 (60 \text{ s})^{-1}$ | |
| tp2b | tp2b | $0.012 (60 \text{ s})^{-1}$ | |

7.19 Reaction deg_bin

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

Name deg_bin

Reaction equation

$$IkBbIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$$
 (40)

Reactant

Table 56: Properties of each reactant.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBbIKKNFkB | IkBbIKKNFkB | |

Products

Table 57: Properties of each product.

| I | 1 | |
|-----------------------|-------------|-----|
| Id | Name | SBO |
| NFkB_cytoplasm IKK | NFkB IKK | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{19} = \text{vol}(\text{cytoplasm}) \cdot \text{r5} \cdot [\text{IkBbIKKNFkB}]$$
 (41)

Table 58: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|----|------|-----|-------|-----------------------|----------------|
| r5 | r5 | | 0.12 | $(60 \text{ s})^{-1}$ | \overline{Z} |

7.20 Reaction deg_bi

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

Name deg_bi

Reaction equation

$$IkBbIKK \longrightarrow IKK \tag{42}$$

Reactant

Table 59: Properties of each reactant.

| Id | Name | SBO |
|---------|---------|-----|
| IkBbIKK | IkBbIKK | |

Product

Table 60: Properties of each product.

| Id | Name | SBO |
|-----|------|-----|
| IKK | IKK | |

Kinetic Law

 $\textbf{Derived unit} \ \left(60 \ s\right)^{-1} \cdot \mu mol$

$$v_{20} = \text{vol}\left(\text{cytoplasm}\right) \cdot \text{r2} \cdot [\text{IkBbIKK}]$$
 (43)

Table 61: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|----|------|-----------|-----------------------|----------------|
| r2 | r2 | 0.024 | $(60 \text{ s})^{-1}$ | $ \mathbf{Z} $ |

7.21 Reaction deg_bn

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

Name deg_bn

Reaction equation

$$IkBbNFkB_cytoplasm \longrightarrow NFkB_cytoplasm$$
 (44)

Reactant

Table 62: Properties of each reactant.

| Id | Name | SBO |
|--------------------|----------|-----|
| IkBbNFkB_cytoplasm | IkBbNFkB | |

Product

Table 63: Properties of each product.

| Id | Name | SBO |
|------------------|------|-----|
| $NFkB_cytoplasm$ | NFkB | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{21} = \text{vol}(\text{cytoplasm}) \cdot \text{deg5_c} \cdot [\text{IkBbNFkB_cytoplasm}]$$
 (45)

Table 64: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|-------------------|-----------------------|----------|
| deg5_c | deg5_c | | $6 \cdot 10^{-5}$ | $(60 \text{ s})^{-1}$ | |

7.22 Reaction deg_bn_n

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

Name deg_bn_n

Reaction equation

$$IkBbNFkB_nucleus \longrightarrow NFkB_nucleus$$
 (46)

Reactant

Table 65: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBbNFkB_nucleus | IkBbNFkBn | |

Product

Table 66: Properties of each product.

| | | <u> </u> |
|--------------|-------|----------|
| Id | Name | SBO |
| NFkB_nucleus | NFkBn | |

Kinetic Law

 $\textbf{Derived unit} \ \left(60 \ s\right)^{-1} \cdot \mu mol$

$$v_{22} = \text{vol}(\text{nucleus}) \cdot \text{deg5}_{-\text{n}} \cdot [\text{IkBbNFkB}_{-\text{nucleus}}]$$
 (47)

Table 67: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|--------|--------|--|----------|
| deg5_n | deg5_n | $6 \cdot 10^{-5} (60 \text{ s})^{-1}$ | |

7.23 Reaction deg_b_n

This is an irreversible reaction of one reactant forming no product.

Name deg_b_n

Reaction equation

$$IkBb_nucleus \longrightarrow \emptyset$$
 (48)

Reactant

Table 68: Properties of each reactant.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBb_nucleus | IkBbn | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{23} = \text{vol}(\text{nucleus}) \cdot \text{deg2_n} \cdot [\text{IkBb_nucleus}]$$
 (49)

Table 69: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|--------|--------|-----------|-----------------------|----------|
| deg2_n | deg2_n | 0.18 | $(60 \text{ s})^{-1}$ | |

7.24 Reaction deg_b

This is an irreversible reaction of one reactant forming no product.

Name deg_b

Reaction equation

$$IkBb_cytoplasm \longrightarrow \emptyset$$
 (50)

Reactant

Table 70: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBb_cytoplasm | IkBb | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{24} = \text{vol}(\text{cytoplasm}) \cdot \text{deg}2_\text{c} \cdot [\text{IkBb_cytoplasm}]$$
 (51)

Table 71: Properties of each parameter.

| Id | Name | SBO Value Uni | t Constant |
|--------|--------|---------------|------------|
| deg2_c | deg2_c | 0.18 (60 | $(s)^{-1}$ |

7.25 Reaction int_2bin

This is a reversible reaction of two reactants forming one product.

Name int_2bin

Reaction equation

$$IkBbIKK + NFkB_cytoplasm \Longrightarrow IkBbIKKNFkB$$
 (52)

Reactants

Table 72: Properties of each reactant.

| rable 72: 1 repetites of each reactant. | | | |
|---|---------|-----|--|
| Id | Name | SBO | |
| IkBbIKK | IkBbIKK | | |
| $NFkB_cytoplasm$ | NFkB | | |

Product

Table 73: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBbIKKNFkB | IkBbIKKNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{25} = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a5_3} \cdot [\text{IkBbIKK}] \cdot [\text{NFkB_cytoplasm}] - \text{d5_3} \cdot [\text{IkBbIKKNFkB}]\right)$$
 (53)

Table 74: Properties of each parameter.

| Id | Name | SBO Va | alue Unit | Constant |
|--------------|--------------|--------|--|------------------------------|
| a5_3 d5_3 | a5_3 d5_3 | | $\begin{array}{ccc} 0.000 & \mu \text{mol}^{-1} \cdot (600) \\ 10^{-5} & (600)^{-1} \end{array}$ | $(0 \text{ s})^{-1} \cdot 1$ |

7.26 Reaction int_2bni

This is a reversible reaction of two reactants forming one product.

Name int_2bni

Reaction equation

$$IkBbNFkB_cytoplasm + IKK \Longrightarrow IkBbIKKNFkB$$
 (54)

Reactants

Table 75: Properties of each reactant.

| Id | Name | SBO |
|---------------------------|-----------------|-----|
| IkBbNFkB_cytoplasm IKK | IkBbNFkB IKK | |

Product

Table 76: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBbIKKNFkB | IkBbIKKNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{26} = \text{vol}(\text{cytoplasm}) \cdot (\text{a8} \cdot [\text{IkBbNFkB_cytoplasm}] \cdot [\text{IKK}] - \text{d2.2} \cdot [\text{IkBbIKKNFkB}])$$
 (55)

Table 77: Properties of each parameter.

| | | • | | | |
|--------|--------|--------|--------|---|----------|
| Id | Name | SBO Va | alue U | Unit | Constant |
| a8 | a8 | | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ | |
| $d2_2$ | $d2_2$ | 0. | 105 (| $(60 \text{ s})^{-1}$ | |

7.27 Reaction int_bn_n

This is a reversible reaction of two reactants forming one product.

Name int_bn_n

Reaction equation

$$IkBb_nucleus + NFkB_nucleus \Longrightarrow IkBbNFkB_nucleus$$
 (56)

Reactants

Table 78: Properties of each reactant.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBb_nucleus | | |
| NFkB_nucleus | NFkBn | |

Product

Table 79: Properties of each product.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBbNFkB_nucleus | IkBbNFkBn | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

 $v_{27} = vol\left(nucleus\right) \cdot \left(a5_2 \cdot [IkBb_nucleus] \cdot [NFkB_nucleus] - d5_2 \cdot [IkBbNFkB_nucleus]\right) \quad (57)$

Table 80: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|--------------|--------------|-----------|---|----------|
| a5_2 d5_2 | a5_2 d5_2 | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | 1 |

7.28 Reaction int_bn

This is a reversible reaction of two reactants forming one product.

Name int_bn

Reaction equation

$$IkBb_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBbNFkB_cytoplasm$$
 (58)

Reactants

Table 81: Properties of each reactant.

| Id | Name | SBO |
|----------------------------------|------|-----|
| IkBb_cytoplasm NFkB_cytoplasm | | |

Product

Table 82: Properties of each product.

| Id | Name | SBO |
|--------------------|----------|-----|
| IkBbNFkB_cytoplasm | IkBbNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{28} = \text{vol}(\text{cytoplasm}) \\ \cdot (\text{a5_1} \cdot [\text{IkBb_cytoplasm}] \cdot [\text{NFkB_cytoplasm}] - \text{d5_1} \cdot [\text{IkBbNFkB_cytoplasm}])$$
 (59)

Table 83: Properties of each parameter.

| Id | Name | SBO Valu | e Unit | Constant |
|--------------|--------------|----------|---|--------------|
| a5_1 d5_1 | a5_1 d5_1 | | $\begin{array}{ccc} 00 & \mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \\ -5 & (60 \text{ s})^{-1} \end{array}$ | $-1 \cdot 1$ |

7.29 Reaction int_bi

This is a reversible reaction of two reactants forming one product.

Name int_bi

Reaction equation

$$IkBb_cytoplasm + IKK \Longrightarrow IkBbIKK$$
 (60)

Reactants

Table 84: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBb_cytoplasm | IkBb | |
| IKK | IKK | |

Product

Table 85: Properties of each product.

| Id | Name | SBO |
|---------|---------|-----|
| IkBbIKK | IkBbIKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{29} = \text{vol}(\text{cytoplasm}) \cdot (\text{a2} \cdot [\text{IkBb_cytoplasm}] \cdot [\text{IKK}] - \text{d2_1} \cdot [\text{IkBbIKK}])$$
 (61)

Table 86: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------------|------------|-----|-------|---|----------|
| a2 d2_1 | a2 d2_1 | | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | |

7.30 Reaction tsl_b

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

Name tsl_b

Reaction equation

$$IkBb_mRNA \longrightarrow IkBb_mRNA + IkBb_cytoplasm$$
 (62)

Reactant

Table 87: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBb_mRNA | IkBbt | |

Products

Table 88: Properties of each product.

| Id | Name | SBO |
|-------------------------|-------|-----|
| IkBb_mRNA | IkBbt | |
| ${\tt IkBb_cytoplasm}$ | IkBb | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{30} = \text{vol}(\text{nucleus}) \cdot \text{tr1b} \cdot [\text{IkBb_mRNA}]$$
 (63)

Table 89: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|----------|
| tr1b | tr1b | 0.245 | $(60 \text{ s})^{-1}$ | |

7.31 Reaction mdeg_b

This is an irreversible reaction of one reactant forming no product.

Name mdeg_b

Reaction equation

$$IkBb_mRNA \longrightarrow \emptyset$$
 (64)

Reactant

Table 90: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBb_mRNA | IkBbt | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{31} = \text{vol}(\text{nucleus}) \cdot \text{tr}3\text{b} \cdot [\text{IkBb_mRNA}]$$
 (65)

Table 91: Properties of each parameter.

| Id | Name | SBO Value Un | nit Constant |
|------|------|--------------|--------------|
| tr3b | tr3b | 0.017 (60 | $(Os)^{-1}$ |

7.32 Reaction txn_b

This is an irreversible reaction of no reactant forming one product.

Name txn_b

Reaction equation

$$\emptyset \longrightarrow IkBb_mRNA$$
 (66)

Product

Table 92: Properties of each product.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBb_mRNA | IkBbt | |

Kinetic Law

Derived unit $\mu mol \cdot (60 \text{ s})^{-1}$

$$v_{32} = \text{vol}(\text{nucleus}) \cdot \text{tr}2b \tag{67}$$

Table 93: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------|------|-----|-----------------------|---|-----------|
| tr2b | tr2b | | $4.272 \cdot 10^{-5}$ | $\mu \text{mol} \cdot (60 \text{ s})^{-1} \cdot l^{-1}$ | \square |

7.33 Reaction loc_n

This is a reversible reaction of one reactant forming one product.

Name loc_n

Reaction equation

$$NFkB_cytoplasm \Longrightarrow NFkB_nucleus$$
 (68)

Reactant

Table 94: Properties of each reactant.

| ruere > rreperues | 01 040011 1 | |
|-------------------|-------------|-----|
| Id | Name | SBO |
| $NFkB_cytoplasm$ | NFkB | |

Product

Table 95: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| NFkB_nucleus | NFkBn | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{33} = \text{vol}(\text{cytoplasm}) \cdot \text{k1_2} \cdot [\text{NFkB_cytoplasm}] - \text{vol}(\text{nucleus}) \cdot \text{k1_1} \cdot [\text{NFkB_nucleus}]$$
 (69)

Table 96: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|------|------|------------------------------|----------|
| k1_2 | k1_2 | $5.400 (60 \text{ s})^{-1}$ | Ø |
| k1_1 | k1_1 | $0.005 (60 \text{ s})^{-1}$ | |

7.34 Reaction txn_e

This is an irreversible reaction of no reactant forming one product.

Name txn_e

Reaction equation

$$\emptyset \longrightarrow IkBe_mRNA$$
 (70)

Product

Table 97: Properties of each product.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBe_mRNA | IkBet | |

Kinetic Law

Derived unit $\mu mol \cdot (60 \text{ s})^{-1}$

$$v_{34} = \text{vol} (\text{nucleus}) \cdot \text{tr} 2e$$
 (71)

Table 98: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------|------|-----|-----------------------|--|----------|
| tr2e | tr2e | | $3.048 \cdot 10^{-5}$ | $\mu mol \cdot (60 \text{ s})^{-1} \cdot l^{-1}$ | |

7.35 Reaction mdeg_e

This is an irreversible reaction of one reactant forming no product.

Name mdeg_e

Reaction equation

$$IkBe_mRNA \longrightarrow \emptyset$$
 (72)

Reactant

Table 99: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBe_mRNA | IkBet | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{35} = \text{vol}(\text{nucleus}) \cdot \text{tr3e} \cdot [\text{IkBe_mRNA}]$$
 (73)

Table 100: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|----------|
| tr3e | tr3e | 0.017 | $(60 \text{ s})^{-1}$ | |

7.36 Reaction tsl_e

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

Name tsl_e

Reaction equation

$$IkBe_mRNA \longrightarrow IkBe_mRNA + IkBe_cytoplasm$$
 (74)

Reactant

Table 101: Properties of each reactant.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBe_mRNA | IkBet | |

Products

Table 102: Properties of each product.

| Id | Name | SBO |
|-------------------------|-------|-----|
| IkBe_mRNA | IkBet | |
| ${\tt IkBe_cytoplasm}$ | IkBe | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{36} = \text{vol}(\text{nucleus}) \cdot \text{tr1e} \cdot [\text{IkBe_mRNA}]$$
 (75)

Table 103: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------|------|-----------|-----------------------|----------|
| tr1e | tr1e | 0.245 | $(60 \text{ s})^{-1}$ | |

7.37 Reaction int_ei

This is a reversible reaction of two reactants forming one product.

Name int_ei

Reaction equation

$$IkBe_cytoplasm + IKK \Longrightarrow IkBeIKK$$
 (76)

Reactants

Table 104: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBe_cytoplasm | | |
| IKK | IKK | |

Product

Table 105: Properties of each product.

| Id | Name | SBO |
|---------|---------|-----|
| IkBeIKK | IkBeIKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{37} = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a3} \cdot \left[\text{IkBe_cytoplasm}\right] \cdot \left[\text{IKK}\right] - \text{d3_1} \cdot \left[\text{IkBeIKK}\right]\right)$$
 (77)

Table 106: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------------|------------|-----|-------|---|----------|
| a3 d3_1 | a3 d3_1 | | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | I |

7.38 Reaction int_en

This is a reversible reaction of two reactants forming one product.

Name int_en

Reaction equation

$$IkBe_cytoplasm + NFkB_cytoplasm \Longrightarrow IkBeNFkB_cytoplasm$$
 (78)

Reactants

Table 107: Properties of each reactant.

| Id | Name | SBO |
|------------|--------------|-----|
| $J \sim 1$ | IkBe NFkB | |

Product

Table 108: Properties of each product.

| Id | Name | SBO |
|--------------------|----------|-----|
| IkBeNFkB_cytoplasm | IkBeNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{38} = \text{vol} (\text{cytoplasm}) \cdot (\text{a6_1} \cdot [\text{IkBe_cytoplasm}] \cdot [\text{NFkB_cytoplasm}] - \text{d6_1} \cdot [\text{IkBeNFkB_cytoplasm}])$$
 (79)

Table 109: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|--------------|--------------|-----------|---|----------|
| a6_1 d6_1 | a6_1 d6_1 | | $\frac{0 \mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1}}{5 (60 \text{ s})^{-1}}$ | ·1 🗹 |

7.39 Reaction int_en_n

This is a reversible reaction of two reactants forming one product.

Name int_en_n

Reaction equation

$$IkBe_nucleus + NFkB_nucleus \Longrightarrow IkBeNFkB_nucleus$$
 (80)

Reactants

Table 110: Properties of each reactant.

| Id | Name | SBO |
|------------------------------|------|-----|
| IkBe_nucleus NFkB_nucleus | | |

Product

Table 111: Properties of each product.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBeNFkB_nucleus | IkBeNFkBn | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

 $v_{39} = \text{vol} (\text{nucleus}) \cdot (\text{a6-2} \cdot [\text{IkBe_nucleus}] \cdot [\text{NFkB_nucleus}] - \text{d6-2} \cdot [\text{IkBeNFkB_nucleus}])$ (81)

Table 112: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|--------------|--------------|-----------|---|----------|
| a6_2 d6_2 | a6_2 d6_2 | | $0 \mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $5 (60 \text{ s})^{-1}$ | |

7.40 Reaction int_2eni

This is a reversible reaction of two reactants forming one product.

Name int_2eni

Reaction equation

$$IkBeNFkB_cytoplasm + IKK \rightleftharpoons IkBeIKKNFkB \qquad (82)$$

Reactants

Table 113: Properties of each reactant.

| Id | Name | SBO |
|---------------------------|-----------------|-----|
| IkBeNFkB_cytoplasm IKK | IkBeNFkB IKK | |

Product

Table 114: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBeIKKNFkB | IkBeIKKNFkB | - |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{40} = \text{vol}\left(\text{cytoplasm}\right) \cdot \left(\text{a9} \cdot \left[\text{IkBeNFkB_cytoplasm}\right] \cdot \left[\text{IKK}\right] - \text{d3_2} \cdot \left[\text{IkBeIKKNFkB}\right]\right)$$
 (83)

Table 115: Properties of each parameter.

| Id | Name | SBO Value | Unit | Constant |
|------------|------------|-----------|---|----------|
| a9 d3_2 | a9 d3_2 | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | |

7.41 Reaction int_2ein

This is a reversible reaction of two reactants forming one product.

Name int_2ein

Reaction equation

$$IkBeIKK + NFkB_cytoplasm \Longrightarrow IkBeIKKNFkB$$
 (84)

Reactants

Table 116: Properties of each reactant.

| Id | Name | SBO |
|---------|---------|-----|
| IkBeIKK | IkBeIKK | |

| Id | Name | SBO |
|----------------|------|-----|
| NFkB_cytoplasm | NFkB | |

Product

Table 117: Properties of each product.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBeIKKNFkB | IkBeIKKNFkB | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

 $v_{41} = \text{vol}(\text{cytoplasm}) \cdot (\text{a6_3} \cdot [\text{IkBeIKK}] \cdot [\text{NFkB_cytoplasm}] - \text{d6_3} \cdot [\text{IkBeIKKNFkB}])$ (85)

Table 118: Properties of each parameter.

| Id | Name | SBO V | Value | Unit | Constant |
|--------------|--------------|-------|-------|---|----------|
| a6_3 d6_3 | a6_3 d6_3 | | | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ $(60 \text{ s})^{-1}$ | A |

7.42 Reaction deg_e

This is an irreversible reaction of one reactant forming no product.

Name deg_e

Reaction equation

$$IkBe_cytoplasm \longrightarrow \emptyset$$
 (86)

Reactant

Table 119: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBe_cytoplasm | IkBe | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{42} = \text{vol}(\text{cytoplasm}) \cdot \text{deg}_{2}\text{c} \cdot [\text{IkBe_cytoplasm}]$$
 (87)

Table 120: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|--------|--------|-----------------------------|----------|
| deg3_c | deg3_c | $0.18 (60 \text{ s})^{-1}$ | |

7.43 Reaction deg_e_n

This is an irreversible reaction of one reactant forming no product.

Name deg_e_n

Reaction equation

IkBe_nucleus
$$\longrightarrow \emptyset$$
 (88)

Reactant

Table 121: Properties of each reactant.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBe_nucleus | IkBen | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{43} = \text{vol}(\text{nucleus}) \cdot \text{deg}_{3}\text{n} \cdot [\text{IkBe_nucleus}]$$
 (89)

Table 122: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|-------|-----------------------|----------------|
| deg3_n | deg3_n | | 0.18 | $(60 \text{ s})^{-1}$ | \blacksquare |

7.44 Reaction deg_en_n

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

Name deg_en_n

Reaction equation

$$IkBeNFkB_nucleus \longrightarrow NFkB_nucleus$$
 (90)

Reactant

Table 123: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBeNFkB_nucleus | IkBeNFkBn | |

Product

Table 124: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| NFkB_nucleus | NFkBn | |

Kinetic Law

 $\textbf{Derived unit} \ \left(60 \ s\right)^{-1} \cdot \mu mol$

$$v_{44} = \text{vol}(\text{nucleus}) \cdot \text{deg6_n} \cdot [\text{IkBeNFkB_nucleus}]$$
 (91)

Table 125: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|------------------|-----------------------|----------------|
| deg6_n | deg6_n | | $6\cdot 10^{-5}$ | $(60 \text{ s})^{-1}$ | $ \checkmark $ |

7.45 Reaction deg_en

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

Name deg_en

Reaction equation

$$IkBeNFkB_cytoplasm \longrightarrow NFkB_cytoplasm$$

Reactant

Table 126: Properties of each reactant.

| Id | Name | SBO |
|-----------------------------|----------|-----|
| ${\tt IkBeNFkB_cytoplasm}$ | IkBeNFkB | |

Product

Table 127: Properties of each product.

| Id | Name | SBO |
|----------------|------|-----|
| NFkB_cytoplasm | NFkB | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{45} = \text{vol}(\text{cytoplasm}) \cdot \text{deg6_c} \cdot [\text{IkBeNFkB_cytoplasm}]$$
 (93)

Table 128: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|-------------------|-----------------------|---------------|
| deg6_c | deg6_c | | $6 \cdot 10^{-5}$ | $(60 \text{ s})^{-1}$ | $ \mathbf{Z}$ |

7.46 Reaction deg_ei

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

Name deg_ei

Reaction equation

IkBeIKK
$$\longrightarrow$$
 IKK (94)

Reactant

(92)

Table 129: Properties of each reactant.

| Id | Name | SBO |
|---------|---------|-----|
| IkBeIKK | IkBeIKK | |

Product

Table 130: Properties of each product.

| Id | Name | SBO |
|-----|------|-----|
| IKK | IKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{46} = \text{vol}\left(\text{cytoplasm}\right) \cdot \text{r3} \cdot \left[\text{IkBeIKK}\right]$$
 (95)

Table 131: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|----|------|------------------------------|----------|
| r3 | r3 | $0.036 (60 \text{ s})^{-1}$ | Ø |

7.47 Reaction deg_ein

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

Name deg_ein

Reaction equation

$$IkBeIKKNFkB \longrightarrow NFkB_cytoplasm + IKK$$
 (96)

Reactant

Table 132: Properties of each reactant.

| Id | Name | SBO |
|-------------|-------------|-----|
| IkBeIKKNFkB | IkBeIKKNFkB | |

Products

Table 133: Properties of each product.

| 1 | | <u> </u> |
|-----------------------|-------------|----------|
| Id | Name | SBO |
| NFkB_cytoplasm IKK | NFkB IKK | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \mu \text{mol}$

$$v_{47} = \text{vol}(\text{cytoplasm}) \cdot \text{r6} \cdot [\text{IkBeIKKNFkB}]$$
 (97)

Table 134: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|----|------|-----------------------------|----------|
| r6 | r6 | $0.18 (60 \text{ s})^{-1}$ | |

7.48 Reaction loc_e

This is a reversible reaction of one reactant forming one product.

Name loc_e

Reaction equation

$$IkBe_cytoplasm \Longrightarrow IkBe_nucleus$$
 (98)

Reactant

Table 135: Properties of each reactant.

| Id | Name | SBO |
|----------------|------|-----|
| IkBe_cytoplasm | IkBe | |

Product

Table 136: Properties of each product.

| Id | Name | SBO |
|--------------|-------|-----|
| IkBe_nucleus | IkBen | |

Kinetic Law

Derived unit $\left(60\,s\right)^{-1} \cdot \mu mol$

 $v_{48} = \text{vol}(\text{cytoplasm}) \cdot \text{tp1e} \cdot [\text{IkBe_cytoplasm}] - \text{vol}(\text{nucleus}) \cdot \text{tp2e} \cdot [\text{IkBe_nucleus}]$ (99)

Table 137: Properties of each parameter.

| 0.018 $(60 \text{ s})^{-1}$ | ✓ |
|-----------------------------|--|
| | $0.018 (60 \text{ s})^{-1} \\ 0.012 (60 \text{ s})^{-1}$ |

7.49 Reaction loc_en

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

Name loc_en

Reaction equation

 $IkBeNFkB_nucleus \longrightarrow IkBeNFkB_cytoplasm \tag{100}$

Reactant

Table 138: Properties of each reactant.

| Id | Name | SBO |
|------------------|-----------|-----|
| IkBeNFkB_nucleus | IkBeNFkBn | |

Product

Table 139: Properties of each product.

| Id | Name | SBO |
|-----------------------------|----------|-----|
| ${\tt IkBeNFkB_cytoplasm}$ | IkBeNFkB | |

Kinetic Law

Derived unit $\left(60\,\mathrm{s}\right)^{-1}\cdot\mu\mathrm{mol}$

$$v_{49} = \text{vol}(\text{nucleus}) \cdot \text{k2_e} \cdot [\text{IkBeNFkB_nucleus}]$$
 (101)

Table 140: Properties of each parameter.

| Id | Name | SBO Value Unit | Constant |
|------|------|------------------------------|----------|
| k2_e | k2_e | $0.414 (60 \text{ s})^{-1}$ | |

7.50 Reaction IKK_deg

This is an irreversible reaction of one reactant forming no product.

Name IKK_deg

Reaction equation

$$IKK \longrightarrow \emptyset \tag{102}$$

Reactant

Table 141: Properties of each reactant.

| Id | Name | SBO |
|-----|------|-----|
| IKK | IKK | |

Kinetic Law

 $\textbf{Derived unit} \ \left(60 \ s\right)^{-1} \cdot \mu mol$

$$v_{50} = \text{vol}\left(\text{cytoplasm}\right) \cdot \text{k_IKK_deg} \cdot [\text{IKK}]$$
 (103)

Table 142: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|-----------|---------|-----|-------|-----------------------|----------------|
| k_IKK_deg | IKK_deg | | 0.0 | $(60 \text{ s})^{-1}$ | \overline{Z} |

7.51 Reaction itxn_a

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Name itxn_a

Reaction equation

$$\emptyset \xrightarrow{NFkB_nucleus} IkBa_mRNA$$
 (104)

Modifier

Table 143: Properties of each modifier.

| Id | Name | SBO |
|--------------|-------|-----|
| NFkB_nucleus | NFkBn | |

Product

Table 144: Properties of each product.

| Id | Name | SBO |
|-----------|-------|-----|
| IkBa_mRNA | IkBat | |

Kinetic Law

Derived unit $10^{-6} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_{51} = \text{vol}(\text{nucleus}) \cdot \text{tr}2\text{a.i} \cdot [\text{NFkB_nucleus}]^2$$
 (105)

Table 145: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|--------|--------|-----|-------|---|-----------|
| tr2a_i | tr2a_i | | 1.98 | $\mu \text{mol}^{-1} \cdot (60 \text{ s})^{-1} \cdot 1$ | \square |

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.

8.1 Species IkBa_mRNA

Name IkBat

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

This species takes part in five reactions (as a reactant in mdeg_a, tsl_a and as a product in txn_a, tsl_a, itxn_a).

$$\frac{d}{dt}IkBa_{m}RNA = v_1 + v_3 + v_{51} - v_2 - v_3$$
 (106)

8.2 Species IkBa_cytoplasm

Name IkBa

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

This species takes part in five reactions (as a reactant in int_ai, int_an, deg_a, loc_a and as a product in tsl_a).

$$\frac{d}{dt} IkBa_cytoplasm = v_3 - v_4 - v_5 - v_9 - v_{15}$$
 (107)

8.3 Species IkBa_nucleus

Name IkBan

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

This species takes part in three reactions (as a reactant in int_an_n, deg_a_n and as a product in loc_a).

$$\frac{d}{dt}$$
IkBa_nucleus = $v_{15} - v_6 - v_{10}$ (108)

8.4 Species IkBaIKK

Name IkBaIKK

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

This species takes part in three reactions (as a reactant in int_2ain, deg_ai and as a product in int_ai).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IkBaIKK} = v_4 - v_8 - v_{13} \tag{109}$$

8.5 Species IkBaNFkB_cytoplasm

Name IkBaNFkB

Initial concentration $0.06~\mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in int_2ani, deg_an and as a product in int_an, loc_an).

$$\frac{d}{dt} IkBaNFkB_{cytoplasm} = v_5 + v_{16} - v_7 - v_{12}$$
 (110)

8.6 Species IkBaNFkB_nucleus

Name IkBaNFkBn

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

This species takes part in three reactions (as a reactant in deg_an_n, loc_an and as a product in int_an_n).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{IkBaNFkB_nucleus} = v_6 - v_{11} - v_{16} \tag{111}$$

8.7 Species IkBaIKKNFkB

Name IkBaIKKNFkB

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

This species takes part in three reactions (as a reactant in deg_ain and as a product in int_2ani, int_2ain).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{IkBaIKKNFkB} = v_7 + v_8 - v_{14} \tag{112}$$

8.8 Species NFkB_cytoplasm

Name NFkB

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

This species takes part in 13 reactions (as a reactant in int_an, int_2ain, int_2bin, int_bn, loc_n, int_en, int_2ein and as a product in deg_an, deg_ain, deg_bin, deg_bn, deg_en, deg_ein).

$$\frac{d}{dt} NFkB_cytoplasm = v_{12} + v_{14} + v_{19} + v_{21} + v_{45} + v_{47} - v_5 - v_8 - v_{25} - v_{28} - v_{33} - v_{38} - v_{41}$$
(113)

8.9 Species IKK

Name IKK

Initial concentration $0.0010 \ \mu mol \cdot l^{-1}$

This species takes part in 13 reactions (as a reactant in int_ai, int_2ani, int_2bni, int_bi, int_ei, int_2eni, IKK_deg and as a product in deg_ai, deg_ain, deg_bin, deg_bi, deg_ei, deg_ein).

$$\frac{\mathrm{d}}{\mathrm{d}t}IKK = v_{13} + v_{14} + v_{19} + v_{20} + v_{46} + v_{47} - v_4 - v_7 - v_{26} - v_{29} - v_{37} - v_{40} - v_{50}$$
 (114)

8.10 Species NFkB_nucleus

Name NFkBn

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

This species takes part in eight reactions (as a reactant in int_an_n, int_bn_n, int_en_n and as a product in deg_an_n, deg_bn_n, loc_n, deg_en_n and as a modifier in itxn_a).

$$\frac{d}{dt} NFkB_nucleus = v_{11} + v_{22} + v_{33} + v_{44} - v_6 - v_{27} - v_{39}$$
 (115)

8.11 Species IkBbIKK

Name IkBbIKK

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

This species takes part in three reactions (as a reactant in deg_bi, int_2bin and as a product in int_bi).

$$\frac{d}{dt}IkBbIKK = v_{29} - v_{20} - v_{25}$$
 (116)

8.12 Species IkBbIKKNFkB

Name IkBbIKKNFkB

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

This species takes part in three reactions (as a reactant in deg_bin and as a product in int_2bin, int_2bni).

$$\frac{d}{dt}IkBbIKKNFkB = v_{25} + v_{26} - v_{19}$$
 (117)

8.13 Species IkBbNFkB_nucleus

Name IkBbNFkBn

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

This species takes part in three reactions (as a reactant in loc_bn, deg_bn_n and as a product in int_bn_n).

$$\frac{d}{dt} IkBbNFkB_nucleus = v_{27} - v_{17} - v_{22}$$
 (118)

8.14 Species IkBbNFkB_cytoplasm

Name IkBbNFkB

Initial concentration $0.03 \ \mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in deg_bn, int_2bni and as a product in loc_bn, int_bn).

$$\frac{d}{dt} IkBbNFkB_cytoplasm = v_{17} + v_{28} - v_{21} - v_{26}$$
 (119)

8.15 Species IkBb_nucleus

Name IkBbn

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

This species takes part in three reactions (as a reactant in deg_b_n, int_bn_n and as a product in loc_b).

$$\frac{d}{dt} \text{IkBb_nucleus} = v_{18} - v_{23} - v_{27}$$
 (120)

8.16 Species IkBb_cytoplasm

Name IkBb

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

This species takes part in five reactions (as a reactant in loc_b, deg_b, int_bn, int_bi and as a product in tsl_b).

$$\frac{d}{dt} \text{IkBb_cytoplasm} = v_{30} - v_{18} - v_{24} - v_{28} - v_{29}$$
 (121)

8.17 Species IkBb_mRNA

Name IkBbt

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

This species takes part in four reactions (as a reactant in tsl_b, mdeg_b and as a product in tsl_b, txn_b).

$$\frac{d}{dt}IkBb_mRNA = v_{30} + v_{32} - v_{30} - v_{31}$$
 (122)

8.18 Species IkBe_mRNA

Name IkBet

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

This species takes part in four reactions (as a reactant in mdeg_e, tsl_e and as a product in txn_e, tsl_e).

$$\frac{d}{dt}IkBe_mRNA = v_{34} + v_{36} - v_{35} - v_{36}$$
 (123)

8.19 Species IkBe_cytoplasm

Name IkBe

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

This species takes part in five reactions (as a reactant in int_ei, int_en, deg_e, loc_e and as a product in tsl_e).

$$\frac{d}{dt} \text{IkBe_cytoplasm} = v_{36} - v_{37} - v_{38} - v_{42} - v_{48}$$
 (124)

8.20 Species IkBe_nucleus

Name IkBen

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

This species takes part in three reactions (as a reactant in int_en_n, deg_e_n and as a product in loc_e).

$$\frac{d}{dt} \text{IkBe_nucleus} = v_{48} - v_{39} - v_{43}$$
 (125)

8.21 Species IkBeNFkB_cytoplasm

Name IkBeNFkB

Initial concentration 0.01 µmol·1⁻¹

This species takes part in four reactions (as a reactant in int_2eni, deg_en and as a product in int_en, loc_en).

$$\frac{d}{dt} IkBeNFkB_cytoplasm = v_{38} + v_{49} - v_{40} - v_{45}$$
 (126)

8.22 Species IkBeNFkB_nucleus

Name IkBeNFkBn

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

This species takes part in three reactions (as a reactant in deg_en_n, loc_en and as a product in int_en_n).

$$\frac{d}{dt} IkBeNFkB_nucleus = v_{39} - v_{44} - v_{49}$$
 (127)

8.23 Species IkBeIKKNFkB

Name IkBeIKKNFkB

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

This species takes part in three reactions (as a reactant in deg_ein and as a product in int_2eni, int_2ein).

$$\frac{d}{dt} \text{IkBeIKKNFkB} = v_{40} + v_{41} - v_{47}$$
 (128)

8.24 Species IkBeIKK

Name IkBeIKK

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

This species takes part in three reactions (as a reactant in int_2ein, deg_ei and as a product in int_ei).

$$\frac{d}{dt}IkBeIKK = v_{37} - v_{41} - v_{46}$$
 (129)

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