



Ordinary Differential Equations System

Full Model

Parameter	Value	Value Units
$volume_{cell}$	1e-018	meter ³
k_{rate}	0	molecule/second

2 Rate Laws

2.1 Reaction 1

	Reactants	Products
Species	Gene_RIBOKEY YcgE_protein	Gene_RIBOKEY mRNA_key YcgE_protein

Reaction Rate

$$v_1 = k_{trans_RIBOKEY} \cdot \frac{Km^2}{(Km^2 + YcgE_{protein}^2)} \cdot Gene_{RIBOKEY} \quad (1)$$

	Parameter	Value	Value Units
Parameters	$k_{trans_RIBOKEY}$	0.00848	1/second
	Km	8000	molecule

2.2 Reaction 2

	Reactants	Products
Species	mRNA_key	degraded_key

Reaction Rate

$$v_2 = essencia_{coli.mRNA_key} \cdot dmRNA_{Gene_test} \quad (2)$$

	Parameter	Value	Value Units
Parameters	$dmRNA_{Gene_test}$	0.0023105	1/second

2.3 Reaction 3

	Reactants	Products
Species	Gene_antiRIBOKEY VirG_P	mRNA_antikey Gene_antiRIBOKEY VirG_P

Reaction Rate

$$v_3 = k_{trans_antikey} \cdot \frac{VirG_P}{(Km + VirG_P)} \cdot Gene_{antiRIBOKEY} \quad (3)$$

	Parameter	Value	Value Units
Parameters	$k_{trans_antikey}$	0.00848	1/second
	Km	3000	molecule

2.4 Reaction 4

	Reactants	Products
Species	mRNA_antikey	degraded_antikey

Reaction Rate

$$v_4 = dmRNA_{key_complementary} \cdot essencia_{coli.mRNA_antikey} \quad (4)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{key_complementary}$	0.0023105	1/second

2.5 Reaction 5

Species	Reactants	Products
	mRNA_key mRNA_antikey	Annealed_mRNA

Reaction Rate

$$v_5 = K_{annealing} \cdot essencia_{coli.mRNA.key} \cdot essencia_{coli.mRNA.antikey} \quad (5)$$

Parameters	Parameter	Value	Value Units
	$K_{annealing}$	100	1/(second*molecule)

2.6 Reaction 6

Species	Reactants	Products
	Annealed_mRNA	degraded_an_mRNA

Reaction Rate

$$v_6 = dannealed_{mRNA} \cdot essencia_{coli.Annealed.mRNA} \quad (6)$$

Parameters	Parameter	Value	Value Units
	$dannealed_{mRNA}$	0.004621	1/second

2.7 Reaction 7

Species	Reactants	Products
	closed_mRNA_Sam8	mRNA_Sam8_degraded

Reaction Rate

$$v_7 = dmRNA_{Sam8} \cdot Vanillin_{production.closed.mRNA.Sam8} \quad (7)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{Sam8}$	0.0023105	1/second

2.8 Reaction 8

Species	Reactants	Products
	mRNA_Sam5	mRNA_Sam5_degraded

Reaction Rate

$$v_8 = dmRNA_{Sam5} \cdot Vanillin_{production.mRNA.Sam5} \quad (8)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{Sam5}$	0.0023105	1/second

2.9 Reaction 9

Species	Reactants	Products
	closed_mRNA_COMT	mRNA_COMT_degraded

Reaction Rate

$$v_9 = dmRNA_{COMT} \cdot Vanillin_{production.closed.mRNA.COMT} \quad (9)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{COMT}$	0.0023105	1/second

2.10 Reaction 10

Species	Reactants	Products
	YcgF_protein_inactive blue_light	YcgF_protein_active

Reaction Rate

$$v_{10} = k_{dimer} \cdot Sensor_{Bluelight.YcgF_protein_inactive}^2 \cdot Sensor_{Bluelight.blue_light} - k_{diss} \cdot Sensor_{Bluelight.YcgF_protein_active} \quad (10)$$

Parameters	Parameter	Value	Value Units
	k_{dimer}	8e-011	1/(second*molecule ²)
	k_{diss}	0.0058	1/second

2.11 Reaction 11

Species	Reactants	Products
	YcgF_protein_active YcgE_protein	YcgF_YcgE_complex

Reaction Rate

$$v_{11} = k_{bind} \cdot Sensor_{Bluelight.YcgF_protein_active} \cdot Sensor_{Bluelight.YcgE_protein} - k_{unbind} \cdot Sensor_{Bluelight.YcgF_YcgE_complex} \quad (11)$$

Parameters	Parameter	Value	Value Units
	k_{bind}	10	1/(second*molecule)
	k_{unbind}	1	1/second

2.12 Reaction 12

Species	Reactants	Products
	mRNA_YcgF	degraded_mRNA_YcgF

Reaction Rate

$$v_{12} = dmRNA_{YcgF} \cdot Sensor_{Bluelight.mRNA_YcgF} \quad (12)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{YcgF}$	0.0023105	1/second

2.13 Reaction 13

Species	Reactants	Products
	Gene_YcgF	Gene_YcgF mRNA_YcgF

Reaction Rate

$$v_{13} = k_{Transcription.YcgF} \cdot Sensor_{Bluelight.Gene.YcgF} \quad (13)$$

Parameters	Parameter	Value	Value Units
	$k_{Transcription.YcgF}$	0.0154	1/second

2.14 Reaction 14

	Reactants	Products
Species	mRNA_YcgF	YcgF_protein_inactive mRNA_YcgF

Reaction Rate

$$v_{14} = k_{Translation_YcgF} \cdot Sensor_{Bluelight.mRNA.YcgF} \quad (14)$$

Parameters

Parameter	Value	Value Units
$k_{Translation_YcgF}$	0.167	1/second

2.15 Reaction 15

	Reactants	Products
Species	Gene_YcgE	Gene_YcgE mRNA_YcgE

Reaction Rate

$$v_{15} = k_{Transcription_YcgE} \cdot Sensor_{Bluelight.Gene.YcgE} \quad (15)$$

Parameters

Parameter	Value	Value Units
$k_{Transcription_YcgE}$	0.00848	1/second

2.16 Reaction 16

	Reactants	Products
Species	mRNA_YcgE	mRNA_YcgE YcgE_protein

Reaction Rate

$$v_{16} = k_{Translation_YcgE} \cdot Sensor_{Bluelight.mRNA.YcgE} \quad (16)$$

Parameters

Parameter	Value	Value Units
$k_{Translation_YcgE}$	0.167	1/second

2.17 Reaction 17

	Reactants	Products
Species	mRNA_YcgE	degraded_mRNA_YcgE

Reaction Rate

$$v_{17} = dmRNA_{YcgE} \cdot Sensor_{Bluelight.mRNA.YcgE} \quad (17)$$

Parameters

Parameter	Value	Value Units
$dmRNA_{YcgE}$	0.0023105	1/second

2.18 Reaction 18

	Reactants	Products
Species	mRNA_Fcs	mRNA_Fcs_degraded

Reaction Rate

$$v_{18} = Vanillin_{production.mRNA.Fcs} \cdot dmRNA_{Fcs} \quad (18)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{Fcs}$	0.0023105	1/second

2.19 Reaction 19

Species	Reactants	Products
	mRNA_Ech	mRNA_Ech_degraded

Reaction Rate

$$v_{19} = Vanillin_{production.mRNA.Ech} \cdot dmRNA_{Ech} \quad (19)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{Ech}$	0.0023105	1/second

2.20 Reaction 20

Species	Reactants	Products
	open_mRNA_Sam8	Sam8
	open_mRNA_Sam8_complex	open_mRNA_Sam8 open_mRNA_Sam8_complex

Reaction Rate

$$v_{20} = k_{Transl_Sam8} \cdot (Vanillin_{production.open.mRNA.Sam8} + Vanillin_{production.open.mRNA.Sam8.complex}) \quad (20)$$

Parameters	Parameter	Value	Value Units
	k_{Transl_Sam8}	0.16667	1/second

2.21 Reaction 21

Species	Reactants	Products
	mRNA_Sam5	Sam5 mRNA_Sam5

Reaction Rate

$$v_{21} = k_{Transl_Sam5} \cdot Vanillin_{production.mRNA.Sam5} \quad (21)$$

Parameters	Parameter	Value	Value Units
	k_{Transl_Sam5}	0.167	1/second

2.22 Reaction 22

Species	Reactants	Products
	open_mRNA_COMT	open_mRNA_COMT
	open_mRNA_COMT_complex	COMT open_mRNA_COMT_complex

Reaction Rate

$$v_{22} = k_{Transl_COMT} \cdot (Vanillin_{production.open.mRNA.COMT} + Vanillin_{production.open.mRNA.COMT.complex}) \quad (22)$$

Parameters	Parameter	Value	Value Units
	k_{Transl_COMT}	0.16667	1/second

2.23 Reaction 23

	Reactants	Products
Species	mRNA_Fcs	mRNA_Fcs Fcs

Reaction Rate

$$v_{23} = k_{Transl_Fcs} \cdot Vanillin_{production.mRNA_Fcs} \quad (23)$$

Parameters

Parameter	Value	Value Units
k_{Transl_Fcs}	0.167	1/second

2.24 Reaction 24

	Reactants	Products
Species	mRNA_Ech	mRNA_Ech Ech

Reaction Rate

$$v_{24} = k_{Transl_Ech} \cdot Vanillin_{production.mRNA_Ech} \quad (24)$$

Parameters

Parameter	Value	Value Units
k_{Transl_Ech}	0.167	1/second

2.25 Reaction 25

	Reactants	Products
Species	Tyrosine Sam8	p-coummaric_acid Sam8

Reaction Rate

$$v_{25} = k_{react_Sam8} \cdot Sam8 \cdot \frac{Tyrosine}{(Km \cdot 602 + Tyrosine)} \quad (25)$$

Parameters

Parameter	Value	Value Units
k_{react_Sam8}	0.015	1/second
Km	15.5	micromolarity

2.26 Reaction 26

	Reactants	Products
Species	p-coummaric_acid Sam5	Caffeic_acid Sam5

Reaction Rate

$$v_{26} = k_{react_Sam5} \cdot Sam5 \cdot [p - \frac{coummaric_{acid}}{([p - coummaric_{acid}] + Km \cdot 602)}] \quad (26)$$

Parameters

Parameter	Value	Value Units
k_{react_Sam5}	4.2385	1/second
Km	432	micromolarity

2.27 Reaction 27

	Reactants	Products
Species	Caffeic_acid COMT	Ferulic_acid COMT

Reaction Rate

$$v_{27} = k_{react.COMT} \cdot COMT \cdot \frac{Caffeic_{acid}}{(Km \cdot 602 + Caffeic_{acid})} \quad (27)$$

	Parameter	Value	Value Units
Parameters	$k_{react.COMT}$	0.03319	1/second
	Km	43	micromolarity

2.28 Reaction 28

	Reactants	Products
Species	Ferulic_acid Fcs	Feruloyl CoA Fcs

Reaction Rate

$$v_{28} = k_{act} \cdot Fcs \cdot \frac{Ferulic_{acid}}{(Km + Ferulic_{acid})} \quad (28)$$

	Parameter	Value	Value Units
Parameters	k_{act}	0.074068	1/second
	Km	43	micromolarity

2.29 Reaction 29

	Reactants	Products
Species	Feruloyl CoA Ech	Vanillin_intracellular Ech

Reaction Rate

$$v_{29} = k_{react.Ech} \cdot Ech \cdot \frac{[FeruloylCoA]}{([FeruloylCoA] + Km \cdot 602)} \quad (29)$$

	Parameter	Value	Value Units
Parameters	$k_{react.Ech}$	0.9578	1/second
	Km	2.4	micromolarity

2.30 Reaction 30

	Reactants	Products
Species	Sam8	degraded_Sam8

Reaction Rate

$$v_{30} = dSam8 \cdot Vanillin_{production.Sam8} \quad (30)$$

	Parameter	Value	Value Units
Parameters	$dSam8$	0.00028881	1/second

2.31 Reaction 31

	Reactants	Products
Species	Sam5	degraded_Sam5

Reaction Rate

$$v_{31} = dSam5 \cdot Vanillin_{production.Sam5} \quad (31)$$

Parameters	Parameter	Value	Value Units
	$dSam5$	0.00028881	1/second

2.32 Reaction 32

Species	Reactants	Products
	COMT	degraded.COMT

Reaction Rate

$$v_{32} = dCOMT \cdot Vanillin_{production.COMT} \quad (32)$$

Parameters	Parameter	Value	Value Units
	$dCOMT$	0.00028881	1/second

2.33 Reaction 33

Species	Reactants	Products
	Fcs	degraded.Fcs

Reaction Rate

$$v_{33} = dFcs \cdot Vanillin_{production.Fcs} \quad (33)$$

Parameters	Parameter	Value	Value Units
	$dFcs$	1.9254e-005	1/second

2.34 Reaction 34

Species	Reactants	Products
	Ech	degraded.Ech

Reaction Rate

$$v_{34} = dEch \cdot Vanillin_{production.Ech} \quad (34)$$

Parameters	Parameter	Value	Value Units
	$dEch$	1.9254e-005	1/second

2.35 Reaction 35

Species	Reactants	Products
	mRNA_VirG	mRNA_VirG VirG

Reaction Rate

$$v_{35} = k_{Transl_VirG} \cdot Sensor_{Vanillin.mRNA.VirG} \quad (35)$$

Parameters	Parameter	Value	Value Units
	k_{Transl_VirG}	0.16667	1/second

2.36 Reaction 36

Species	Reactants	Products
	Gene_VirG	Gene_VirG mRNA_VirG

Reaction Rate

$$v_{36} = k_{Transcr_VirG} \cdot Gene_{VirG} \quad (36)$$

Parameters	Parameter	Value	Value Units
	$k_{Transcr_VirG}$	0.000848	1/second

2.37 Reaction 37

Species	Reactants	Products
	mRNA_VirG	degraded_mRNA_VirG

Reaction Rate

$$v_{37} = dmRNA_{VirG} \cdot Sensor_{Vanillin.mRNA_VirG} \quad (37)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{VirG}$	0.0023105	1/second

2.38 Reaction 38

Species	Reactants	Products
	VirG VirA_P	VirG_P VirA

Reaction Rate

$$v_{38} = k_1 \cdot Sensor_{Vanillin.VirG} \cdot Sensor_{Vanillin.VirA_P} \quad (38)$$

Parameters	Parameter	Value	Value Units
	k_1	1e-006	1/(second*molecule)

2.39 Reaction 39

Species	Reactants	Products
	Gene_VirA	mRNA_VirA Gene_VirA

Reaction Rate

$$v_{39} = k_{Transcr_VirA} \cdot Gene_{VirA} \quad (39)$$

Parameters	Parameter	Value	Value Units
	$k_{Transcr_VirA}$	0.000848	1/second

2.40 Reaction 40

Species	Reactants	Products
	mRNA_VirA	degraded_mRNA_VirA

Reaction Rate

$$v_{40} = dmRNA_{VirA} \cdot Sensor_{Vanillin.mRNA_VirA} \quad (40)$$

Parameters	Parameter	Value	Value Units
	$dmRNA_{VirA}$	0.0023105	1/second

2.41 Reaction 41

	Reactants	Products
Species	mRNA_VirA	VirA mRNA_VirA

Reaction Rate

$$v_{41} = k_{Transl_VirA} \cdot mRNA_{VirA} \quad (41)$$

	Parameter	Value	Value Units
Parameters	k_{Transl_VirA}	0.167	1/second

2.42 Reaction 42

	Reactants	Products
Species	Vanillin_input VirA	VirA_P Vanillin_input

Reaction Rate

$$v_{42} = k_1 \cdot Sensor_{Vanillin.Vanillin_input} \cdot Sensor_{Vanillin.VirA} - k_2 \cdot Sensor_{Vanillin.VirA_P} \quad (42)$$

	Parameter	Value	Value Units
Parameters	k_1	1e-008	1/(second*molecule)
	k_2	0.1	1/second

2.43 Reaction 43

	Reactants	Products
Species	closed_mRNA_Sam8 mRNA_key	open_mRNA_Sam8_complex

Reaction Rate

$$v_{43} = k_{complex} \cdot essencia_{coli.mRNA_key} \cdot Vanillin_{production.closed_mRNA_Sam8} - k_{dis} \cdot Vanillin_{production.open_mRNA_Sa} \quad (43)$$

	Parameter	Value	Value Units
Parameters	$k_{complex}$	0.00237	1/(second*molecule)
	k_{dis}	0.00416	1/second

2.44 Reaction 44

	Reactants	Products
Species	closed_mRNA_Sam8	open_mRNA_Sam8

Reaction Rate

$$v_{44} = k_{open} \cdot Vanillin_{production.closed_mRNA_Sam8} - k_{closed} \cdot Vanillin_{production.open_mRNA_Sam8} \quad (44)$$

	Parameter	Value	Value Units
Parameters	k_{open}	7.5	1/second
	k_{closed}	500	1/second

2.45 Reaction 45

	Reactants	Products
Species	open_mRNA_Sam8_complex	o_mRNA_Sam8_complex_degraded

Reaction Rate

$$v_{45} = \text{dopen}_{mRNA_Sam8_complex} \cdot Vanillin_{production.open_mRNA_Sam8_complex} \quad (45)$$

Parameters

Parameter	Value	Value Units
$\text{dopen}_{mRNA_Sam8_complex}$	0.0023105	1/second

2.46 Reaction 46**Species**

Reactants	Products
open_mRNA_Sam8	o_mRNA_Sam8_degraded

Reaction Rate

$$v_{46} = \text{dopen}_{mRNA_Sam8} \cdot Vanillin_{production.open_mRNA_Sam8} \quad (46)$$

Parameters

Parameter	Value	Value Units
dopen_{mRNA_Sam8}	0.0023105	1/second

2.47 Reaction 47**Species**

Reactants	Products
mRNA_key closed_mRNA_COMT	open_mRNA_COMT_complex

Reaction Rate

$$v_{47} = k_{complex} \cdot \text{essencia}_{coli.mRNA_key} \cdot Vanillin_{production.closed_mRNA_COMT} - k_{dis} \cdot Vanillin_{production.open_mRNA_COMT} \quad (47)$$

Parameters

Parameter	Value	Value Units
$k_{complex}$	0.00237	1/(second*molecule)
k_{dis}	0.00416	1/second

2.48 Reaction 48**Species**

Reactants	Products
closed_mRNA_COMT	open_mRNA_COMT

Reaction Rate

$$v_{48} = k_{open} \cdot Vanillin_{production.closed_mRNA_COMT} - k_{closed} \cdot Vanillin_{production.open_mRNA_COMT} \quad (48)$$

Parameters

Parameter	Value	Value Units
k_{open}	7.5	1/second
k_{closed}	500	1/second

2.49 Reaction 49**Species**

Reactants	Products
open_mRNA_COMT_complex	o_mRNA_COMT_complex_degraded

Reaction Rate

$$v_{49} = \text{dopen}_{mRNA_COMT_complex} \cdot Vanillin_{production.open_mRNA_COMT_complex} \quad (49)$$

Parameters	Parameter	Value	Value Units
	$dopen_{mRNA_COMT_complex}$	0.0023105	1/second

2.50 Reaction 50

Species	Reactants	Products
	open_mRNA_COMT	o_mRNA_COMT_degraded

Reaction Rate

$$v_{50} = dopen_{mRNA_COMT} \cdot Vanillin_{production.open_mRNA_COMT} \quad (50)$$

Parameters	Parameter	Value	Value Units
	$dopen_{mRNA_COMT}$	0.0023105	1/second

2.51 Reaction 51

Species	Reactants	Products
	VirA	VirA_degraded

Reaction Rate

$$v_{51} = dVirA \cdot Sensor_{Vanillin.VirA} \quad (51)$$

Parameters	Parameter	Value	Value Units
	$dVirA$	1.9254e-005	1/second

2.52 Reaction 52

Species	Reactants	Products
	VirG	VirG_degraded

Reaction Rate

$$v_{52} = dVirG \cdot Sensor_{Vanillin.VirG} \quad (52)$$

Parameters	Parameter	Value	Value Units
	$dVirG$	1.9254e-005	1/second

2.53 Reaction 53

Species	Reactants	Products
	VirA_P	VirA_P_degraded

Reaction Rate

$$v_{53} = dVirA_P \cdot Sensor_{Vanillin.VirA_P} \quad (53)$$

Parameters	Parameter	Value	Value Units
	$dVirA_P$	1.9254e-005	1/second

2.54 Reaction 54

Species	Reactants	Products
	VirG_P	VirG_P_degraded

Reaction Rate

$$v_{54} = dVirG_P \cdot Sensor_{Vanillin.VirG_P} \quad (54)$$

Parameters	Parameter	Value	Value Units
	$dVir_{GP}$	1.9254e-005	1/second

2.55 Reaction 55

Species	Reactants	Products
	Vanillin_intracellular	Vanillin_extracellular

Reaction Rate

$$v_{55} = k_{diffusion} \cdot S_{cell} \cdot \left(\frac{Vanillin_{production} \cdot Vanillin_{intracellular}}{volume_{cell} - \frac{essencia_{coli} \cdot Vanillin_{extracellular}}{number_{cells}}} \right) \quad (55)$$

Parameters	Parameter	Value	Value Units
	$k_{diffusion}$	0.0001127	meter/second
	$volume_{liquid}$	5e-005	meter ³
	$number_{cells}$	150000000000	molecule/molecule
	S_{cell}	2.0106e-012	meter ²

2.56 Reaction 56

Species	Reactants	Products
	Vanillin_extracellular	Vanillin_air

Reaction Rate

$$v_{56} = S_{air} \cdot k_{ol} \cdot \left(\frac{essencia_{coli} \cdot Vanillin_{extracellular}}{volume_{liquid} - \frac{essencia_{coli} \cdot Vanillin_{air}}{H \cdot \frac{volume_{air}}{3600}}} \right) \quad (56)$$

Parameters	Parameter	Value	Value Units
	$volume_{liquid}$	5e-005	meter ³
	S_{air}	0.005	meter ²
	H	1.36e-005	molecule/molecule
	$volume_{air}$	Inf	meter ³
	k_{ol}	0.00028	meter/hour

2.57 Reaction 57

Species	Reactants	Products
	YcgF_protein_inactive	degraded_YcgF

Reaction Rate

$$v_{57} = k_{deg} \cdot YcgF_{protein.inactive} \quad (57)$$

Parameters	Parameter	Value	Value Units
	k_{deg}	1.9254e-005	1/second

2.58 Reaction 58

Species	Reactants	Products
	YcgF_protein.active	degraded_YcgF_dimer

Reaction Rate

$$v_{58} = k1 \cdot YcgF_{protein.active} \quad (58)$$

Parameters	Parameter	Value	Value Units
	k_1	1.9254e-005	1/second

2.59 Reaction 59

Species	Reactants	Products
	YcgE_protein	degraded_YcgE

Reaction Rate

$$v_{59} = k_1 \cdot Y_{cgE_{protein}} \quad (59)$$

Parameters	Parameter	Value	Value Units
	k_1	1.9254e-005	1/second

2.60 Reaction 60

Species	Reactants	Products
	YcgF_YcgE_complex	degraded_YcgF_YcgE

Reaction Rate

$$v_{60} = k_1 \cdot Y_{cgF_{YcgE_{complex}}} \quad (60)$$

Parameters	Parameter	Value	Value Units
	k_1	1.9254e-005	1/second

2.61 Reaction 61

Species	Reactants	Products
	operon_Sams_COMT_ECH_FCS	operon_Sams_COMT_ECH_FCS mRNA_Fcs mRNA_Ech closed_mRNA_Sam8 mRNA_Sam5 closed_mRNA_COMT

Reaction Rate

$$v_{61} = k_{trans} \cdot V_{anillin_{production.operon_Sams_COMT_ECH_FCS}} \quad (61)$$

Parameters	Parameter	Value	Value Units
	k_{trans}	0.00848	1/second

2.62 Reaction 62

Species	Reactants	Products
	Vanillin_extracellular	DUMMY

Reaction Rate

$$v_{62} = k_{rate} \quad (62)$$

Parameters	Parameter	Value	Value Units
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3 Equations

3.1 Species: Gene_RIBOKEY

$$\frac{d[Gene_{RIBOKEY}]}{dt} = +v_1 - v_1 \quad (63)$$

3.2 Species: mRNA_key

$$\frac{d[mRNA_{key}]}{dt} = +v_1 - v_2 - v_5 - v_{43} - v_{47} \quad (64)$$

3.3 Species: degraded_key

$$\frac{d[degraded_{key}]}{dt} = +v_2 \quad (65)$$

3.4 Species: Gene_antiRIBOKEY

$$\frac{d[Gene_{antiRIBOKEY}]}{dt} = +v_3 - v_3 \quad (66)$$

3.5 Species: mRNA_antikey

$$\frac{d[mRNA_{antikey}]}{dt} = +v_3 - v_4 - v_5 \quad (67)$$

3.6 Species: degraded_antikey

$$\frac{d[degraded_{antikey}]}{dt} = +v_4 \quad (68)$$

3.7 Species: Annealed_mRNA

$$\frac{d[Annealed_{mRNA}]}{dt} = +v_5 - v_6 \quad (69)$$

3.8 Species: degraded_an_mRNA

$$\frac{d[degraded_{an.mRNA}]}{dt} = +v_6 \quad (70)$$

3.9 Species: Vanillin_extracellular

$$\frac{d[Vanillin_{extracellular}]}{dt} = +v_{55} - v_{56} - v_{62} \quad (71)$$

3.10 Species: Vanillin_air

$$\frac{d[Vanillin_{air}]}{dt} = +v_{56} \quad (72)$$

3.11 Species: DUMMY

$$\frac{d[DUMMY]}{dt} = +v_{62} \quad (73)$$

3.12 Species: YcgF_protein_inactive

$$\frac{d[YcgF_{protein.inactive}]}{dt} = -v_{10} + v_{14} - v_{57} \quad (74)$$

3.13 Species: YcgF_protein_active

$$\frac{d[YcgF_{protein_active}]}{dt} = +v_{10} - v_{11} - v_{58} \quad (75)$$

3.14 Species: blue_light

$$\frac{d[blue_light]}{dt} = -v_{10} \quad (76)$$

3.15 Species: YcgE_protein

$$\frac{d[YcgE_{protein}]}{dt} = +v_1 - v_1 - v_{11} + v_{16} - v_{59} \quad (77)$$

3.16 Species: YcgF_YcgE_complex

$$\frac{d[YcgF_{YcgE_complex}]}{dt} = +v_{11} - v_{60} \quad (78)$$

3.17 Species: Gene_YcgF

$$\frac{d[Gene_{YcgF}]}{dt} = +v_{13} - v_{13} \quad (79)$$

3.18 Species: Gene_YcgE

$$\frac{d[Gene_{YcgE}]}{dt} = +v_{15} - v_{15} \quad (80)$$

3.19 Species: mRNA_YcgF

$$\frac{d[mRNA_{YcgF}]}{dt} = -v_{12} + v_{13} + v_{14} - v_{14} \quad (81)$$

3.20 Species: degraded_mRNA_YcgF

$$\frac{d[degraded_{mRNA_{YcgF}}]}{dt} = +v_{12} \quad (82)$$

3.21 Species: degraded_mRNA_YcgE

$$\frac{d[degraded_{mRNA_{YcgE}}]}{dt} = +v_{17} \quad (83)$$

3.22 Species: mRNA_YcgE

$$\frac{d[mRNA_{YcgE}]}{dt} = +v_{15} + v_{16} - v_{16} - v_{17} \quad (84)$$

3.23 Species: degraded_YcgF

$$\frac{d[degraded_{YcgF}]}{dt} = +v_{57} \quad (85)$$

3.24 Species: degraded_YcgE

$$\frac{d[degraded_{YcgE}]}{dt} = +v_{59} \quad (86)$$

3.25 Species: degraded_YcgF_dimer

$$\frac{d[\text{degraded}_{YcgF_dimer}]}{dt} = +v_{58} \quad (87)$$

3.26 Species: degraded_YcgF_YcgE

$$\frac{d[\text{degraded}_{YcgF_YcgE}]}{dt} = +v_{60} \quad (88)$$

3.27 Species: VirG_P

$$\frac{d[VirG_P]}{dt} = +v_3 - v_3 + v_{38} - v_{54} \quad (89)$$

3.28 Species: Gene_VirA

$$\frac{d[Gene_{VirA}]}{dt} = +v_{39} - v_{39} \quad (90)$$

3.29 Species: Gene_VirG

$$\frac{d[Gene_{VirG}]}{dt} = +v_{36} - v_{36} \quad (91)$$

3.30 Species: degraded_mRNA_VirG

$$\frac{d[\text{degraded}_{mRNA_VirG}]}{dt} = +v_{37} \quad (92)$$

3.31 Species: mRNA_VirG

$$\frac{d[mRNA_{VirG}]}{dt} = +v_{35} - v_{35} + v_{36} - v_{37} \quad (93)$$

3.32 Species: VirG

$$\frac{d[VirG]}{dt} = +v_{35} - v_{38} - v_{52} \quad (94)$$

3.33 Species: mRNA_VirA

$$\frac{d[mRNA_{VirA}]}{dt} = +v_{39} - v_{40} + v_{41} - v_{41} \quad (95)$$

3.34 Species: degraded_mRNA_VirA

$$\frac{d[\text{degraded}_{mRNA_VirA}]}{dt} = +v_{40} \quad (96)$$

3.35 Species: VirA

$$\frac{d[VirA]}{dt} = +v_{38} + v_{41} - v_{42} - v_{51} \quad (97)$$

3.36 Species: VirA_P

$$\frac{d[VirA_P]}{dt} = -v_{38} + v_{42} - v_{53} \quad (98)$$

3.37 Species: Vanillin_input

$$\frac{d[Vanillin_{input}]}{dt} = +v_{42} - v_{42} \quad (99)$$

3.38 Species: VirA_degraded

$$\frac{d[VirA_{degraded}]}{dt} = +v_{51} \quad (100)$$

3.39 Species: VirG_degraded

$$\frac{d[VirG_{degraded}]}{dt} = +v_{52} \quad (101)$$

3.40 Species: VirA_P_degraded

$$\frac{d[VirA_{P_degraded}]}{dt} = +v_{53} \quad (102)$$

3.41 Species: VirG_P_degraded

$$\frac{d[VirG_{P_degraded}]}{dt} = +v_{54} \quad (103)$$

3.42 Species: closed_mRNA_Sam8

$$\frac{d[closed_{mRNA_Sam8}]}{dt} = -v_7 - v_{43} - v_{44} + v_{61} \quad (104)$$

3.43 Species: mRNA_Sam5

$$\frac{d[mRNA_{Sam5}]}{dt} = -v_8 + v_{21} - v_{21} + v_{61} \quad (105)$$

3.44 Species: closed_mRNA_COMT

$$\frac{d[closed_{mRNA_COMT}]}{dt} = -v_9 - v_{47} - v_{48} + v_{61} \quad (106)$$

3.45 Species: mRNA_Sam8_degraded

$$\frac{d[mRNA_{Sam8_degraded}]}{dt} = +v_7 \quad (107)$$

3.46 Species: mRNA_Sam5_degraded

$$\frac{d[mRNA_{Sam5_degraded}]}{dt} = +v_8 \quad (108)$$

3.47 Species: mRNA_COMT_degraded

$$\frac{d[mRNA_{COMT_degraded}]}{dt} = +v_9 \quad (109)$$

3.48 Species: mRNA_Fcs

$$\frac{d[mRNA_{Fcs}]}{dt} = -v_{18} + v_{23} - v_{23} + v_{61} \quad (110)$$

3.49 Species: mRNA_Ech

$$\frac{d[mRNA_{Ech}]}{dt} = -v_{19} + v_{24} - v_{24} + v_{61} \quad (111)$$

3.50 Species: mRNA_Fcs_degraded

$$\frac{d[mRNA_{Fcs_degraded}]}{dt} = +v_{18} \quad (112)$$

3.51 Species: mRNA_Ech_degraded

$$\frac{d[mRNA_{Ech_degraded}]}{dt} = +v_{19} \quad (113)$$

3.52 Species: Tyrosine

$$\frac{d[Tyrosine]}{dt} = -v_{25} \quad (114)$$

3.53 Species: Sam8

$$\frac{d[Sam8]}{dt} = +v_{20} + v_{25} - v_{25} - v_{30} \quad (115)$$

3.54 Species: Sam5

$$\frac{d[Sam5]}{dt} = +v_{21} + v_{26} - v_{26} - v_{31} \quad (116)$$

3.55 Species: COMT

$$\frac{d[COMT]}{dt} = +v_{22} + v_{27} - v_{27} - v_{32} \quad (117)$$

3.56 Species: Fcs

$$\frac{d[Fcs]}{dt} = +v_{23} + v_{28} - v_{28} - v_{33} \quad (118)$$

3.57 Species: Ech

$$\frac{d[Ech]}{dt} = +v_{24} + v_{29} - v_{29} - v_{34} \quad (119)$$

3.58 Species: p-coummaric_acid

$$\frac{d[p-coummaric_acid]}{dt} = +v_{25} - v_{26} \quad (120)$$

3.59 Species: Caffeic_acid

$$\frac{d[Caffeic_acid]}{dt} = +v_{26} - v_{27} \quad (121)$$

3.60 Species: Ferulic_acid

$$\frac{d[Ferulic_acid]}{dt} = +v_{27} - v_{28} \quad (122)$$

3.61 Species: Feruloyl CoA

$$\frac{d[FeruloylCoA]}{dt} = +v_{28} - v_{29} \quad (123)$$

3.62 Species: Vanillin_intracellular

$$\frac{d[Vanillin_{intracellular}]}{dt} = +v_{29} - v_{55} \quad (124)$$

3.63 Species: degraded_Sam8

$$\frac{d[degraded_{Sam8}]}{dt} = +v_{30} \quad (125)$$

3.64 Species: degraded_Sam5

$$\frac{d[degraded_{Sam5}]}{dt} = +v_{31} \quad (126)$$

3.65 Species: degraded_COMT

$$\frac{d[degraded_{COMT}]}{dt} = +v_{32} \quad (127)$$

3.66 Species: degraded_Fcs

$$\frac{d[degraded_{Fcs}]}{dt} = +v_{33} \quad (128)$$

3.67 Species: degraded_Ech

$$\frac{d[degraded_{Ech}]}{dt} = +v_{34} \quad (129)$$

3.68 Species: open_mRNA_Sam8

$$\frac{d[open_{mRNA_Sam8}]}{dt} = +v_{20} - v_{20} + v_{44} - v_{46} \quad (130)$$

3.69 Species: open_mRNA_Sam8_complex

$$\frac{d[open_{mRNA_Sam8_complex}]}{dt} = +v_{20} - v_{20} + v_{43} - v_{45} \quad (131)$$

3.70 Species: o_mRNA_Sam8_complex_degraded

$$\frac{d[o_{mRNA_Sam8_complex_degraded}]}{dt} = +v_{45} \quad (132)$$

3.71 Species: o_mRNA_Sam8_degraded

$$\frac{d[o_{mRNA_Sam8_degraded}]}{dt} = +v_{46} \quad (133)$$

3.72 Species: open_mRNA_COMT

$$\frac{d[open_{mRNA_COMT}]}{dt} = +v_{22} - v_{22} + v_{48} - v_{50} \quad (134)$$

3.73 Species: open_mRNA_COMT_complex

$$\frac{d[\text{open_mRNA_COMT_complex}]}{dt} = +v_{22} - v_{22} + v_{47} - v_{49} \quad (135)$$

3.74 Species: o_mRNA_COMT_complex_degraded

$$\frac{d[o_mRNA_COMT_complex_degraded]}{dt} = +v_{49} \quad (136)$$

3.75 Species: o_mRNA_COMT_degraded

$$\frac{d[o_mRNA_COMT_degraded]}{dt} = +v_{50} \quad (137)$$

3.76 Species: operon_Sams_COMT_ECH_FCS

$$\frac{d[\text{operon_Sams_COMT_ECH_FCS}]}{dt} = +v_{61} - v_{61} \quad (138)$$

4 Compartments**4.1 *essencia_coli***

Species	Initial Amount	Initial Amount Units
Gene_RIBOKEY	1.5	molecule
mRNA_key	0	molecule
degraded_key	0	molecule
Gene_antiRIBOKEY	20	molecule
mRNA_antikey	0	molecule
degraded_antikey	0	molecule
Annealed_mRNA	0	molecule
degraded_an_mRNA	0	molecule
Vanillin_extracellular	0	molecule
Vanillin_air	0	molecule
DUMMY	0	molecule

4.2 *Sensor_Bluelight*

Species	Initial Amount	Initial Amount Units
YcgF_protein_inactive	0	molecule
YcgF_protein_active	0	molecule
blue_light	33	molecule
YcgE_protein	0	molecule
YcgF_YcgE_complex	0	molecule
Gene_YcgF	1	molecule
Gene_YcgE	1	molecule
mRNA_YcgF	0	molecule
degraded_mRNA_YcgF	0	
degraded_mRNA_YcgE	0	
mRNA_YcgE	0	molecule
degraded_YcgF	0	
degraded_YcgE	0	
degraded_YcgF_dimer	0	
degraded_YcgF_YcgE	0	

4.3 Sensor_{vanillin}

Species	Initial Amount	Initial Amount Units
VirG_P	0	molecule
Gene_VirA	1	molecule
Gene_VirG	1	molecule
degraded_mRNA_VirG	0	
mRNA_VirG	0	molecule
VirG	0	molecule
mRNA_VirA	0	molecule
degraded_mRNA_VirA	0	
VirA	0	molecule
VirA_P	0	molecule
Vanillin_input	0	molecule
VirA_degraded	0	molecule
VirG_degraded	0	
VirA_P_degraded	0	
VirG_P_degraded	0	

4.4 Vanillin_production

Species	Initial Amount	Initial Amount Units
closed_mRNA_Sam8	0	molecule
mRNA_Sam5	0	molecule
closed_mRNA_COMT	0	molecule
mRNA_Sam8_degraded	0	
mRNA_Sam5_degraded	0	
mRNA_COMT_degraded	0	
mRNA_Fcs	0	molecule
mRNA_Ech	0	molecule
mRNA_Fcs_degraded	0	
mRNA_Ech_degraded	0	
Tyrosine	300000	molecule
Sam8	0	molecule
Sam5	0	molecule
COMT	0	molecule
Fcs	0	molecule
Ech	0	molecule
p-coummaric_acid	0	molecule
Caffeic_acid	0	molecule
Ferulic_acid	0	molecule
Feruloyl CoA	0	molecule
Vanillin_intracellular	0	molecule
degraded_Sam8	0	molecule
degraded_Sam5	0	molecule
degraded_COMT	0	molecule
degraded_Fcs	0	molecule
degraded_Ech	0	molecule
open_mRNA_Sam8	0	molecule
open_mRNA_Sam8_complex	0	molecule
o_mRNA_Sam8_complex_degraded	0	
o_mRNA_Sam8_degraded	0	
open_mRNA_COMT	0	molecule
open_mRNA_COMT_complex	0	molecule
o_mRNA_COMT_complex_degraded	0	
o_mRNA_COMT_degraded	0	
operon_Sams_COMT_ECH_FCS	1	molecule