TGF\_b model

#Abbreviation

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v: rate reaction

t: time

y: state variable

x: constant parameter

dydt: time derivative of y

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#Description of variable names

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- inact: inactive form

- act: active form

- S: SMAD

- p: phosphorylation

- m: mRNA

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# Rate reactions

v[1] = x[C.kf\_1\_TGFbeta]\*y[V.THBS1]\*y[V.TGFb\_inact]/(x[C.Kmf\_1\_TGFbeta] + y[V.TGFb\_inact])

v[2] = x[C.k\_on\_FMOD]\*y[V.FMOD]\*y[V.TGFb\_act]

v[3] = x[C.Rec\_act]\*y[V.TGFBR\_inact]\*y[V.TGFb\_act]

v[4] = x[C.pRec\_debind]\*y[V.TGFBR\_act]

v[5] = x[C.kf\_2\_TGFbeta]\*y[V.S2]\*y[V.TGFBR\_act]/(x[C.Kmf\_2\_TGFbeta]\*(1+y[V.S7]/x[C.k\_inhibit\_TGF])+y[V.S2])

v[6] = x[C.S\_dephosphos]\*y[V.ppS2]

v[7] = x[C.S\_dephos]\*y[V.pS2]

v[8] = x[C.kf\_3\_TGFbeta]\*y[V.S3]\*y[V.TGFBR\_act]/(x[C.Kmf\_3\_TGFbeta]\*(1+y[V.S7]/x[C.k\_inhibit\_TGF])+y[V.S3])

v[9] = x[C.S\_dephosphos]\*y[V.ppS3]

v[10] = x[C.S\_dephos]\*y[V.pS3]

v[11] = x[C.k\_on\_ppS2\_ppS3]\*y[V.ppS3]\*y[V.ppS2]

v[12] = x[C.S\_dephosphos]\*y[V.ppS2\_ppS3]

v[13] = x[C.k\_on\_ppS2\_ppS3\_S4]\*y[V.ppS2\_ppS3]\*y[V.S4]

v[14] = x[C.prod\_mS7]\*y[V.ppS2\_ppS3\_S4]\*\*x[C.n1\_TGF]/(x[C.Km\_1\_TGF]\*\*x[C.n1\_TGF]+y[V.ppS2\_ppS3\_S4]\*\*x[C.n1\_TGF])

v[15] = x[C.mS7\_turn]\*y[V.mS7]

v[16] = x[C.prod\_S7]\*y[V.mS7]

v[17] = x[C.prod\_mcFOS]\*y[V.TGFBR\_act]\*\*x[C.n2\_TGF]/(x[C.Km\_2\_TGF]\*\*x[C.n2\_TGF]+y[V.TGFBR\_act]\*\*x[C.n2\_TGF])

v[18] = x[C.mcFOS\_turn]\*y[V.mcFOS]

v[19] = x[C.prod\_cFOS]\*y[V.mcFOS]

v[20] = x[C.k\_off\_FMOD]\*y[V.FMOD\_complex]

v[21] = x[C.k\_off\_ppS2\_ppS3\_S4]\*y[V.ppS2\_ppS3\_S4]

v[22] = x[C.k\_off\_ppS2\_ppS3\_S4\_cFOS]\*y[V.ppS2\_ppS3\_S4\_cFOS]

v[23] = x[C.k\_on\_ppS2\_ppS3\_S4\_cFOS]\*y[V.ppS2\_ppS3\_S4]\*y[V.cFOS]

v[24] = x[C.prod\_mTHBS1]\*y[V.ppS2\_ppS3\_S4\_cFOS]\*\*x[C.n4\_TGF]/(x[C.Km\_4\_TGF]\*\*x[C.n4\_TGF]+y[V.ppS2\_ppS3\_S4\_cFOS]\*\*x[C.n4\_TGF])

v[25] = x[C.THBS1\_turn]\*y[V.mTHBS1]

v[26] = x[C.prod\_THBS1]\*y[V.mTHBS1]

v[27] = x[C.degrad\_cFOS]\*y[V.cFOS]

# Equations of the model

dydt[V.TGFb\_inact] = - v[1]

dydt[V.TGFb\_act] = + v[1] - v[2] - v[3] + v[20]

dydt[V.FMOD] = - v[2] + v[20]

dydt[V.FMOD\_complex] = + v[2] - v[20]

dydt[V.TGFBR\_inact] = - v[3] + v[4]

dydt[V.TGFBR\_act] = + v[3] - v[4]

dydt[V.S2] = - v[5] + v[7]

dydt[V.S3] = - v[8] + v[10]

dydt[V.S4] = - v[13] + v[21]

dydt[V.pS2] = + v[6] - v[7] + v[12]

dydt[V.pS3] = + v[9] - v[10] + v[12]

dydt[V.ppS2] = + v[5] - v[6] - v[11]

dydt[V.ppS3] = + v[8] - v[9] - v[11]

dydt[V.ppS2\_ppS3] = + v[11] - v[12] - v[13] + v[21]

dydt[V.ppS2\_ppS3\_S4] = + v[13] - v[23] - v[21] + v[22]

dydt[V.mS7] = + v[14] - v[15]

dydt[V.S7] = + v[16]

dydt[V.mcFOS] = + v[17] - v[18]

dydt[V.cFOS] = + v[19] - v[27] - v[23] + v[22]

dydt[V.ppS2\_ppS3\_S4\_cFOS] = + v[23] - v[22]

dydt[V.mTHBS1] = + v[24] - v[25]

dydt[V.THBS1] = + v[26]

# Best fit parameter

x[C.kf\_1\_TGFbeta] = 4.923e-01

x[C.Kmf\_1\_TGFbeta] = 2.529e+00

x[C.k\_on\_FMOD] = 1.000e+00

x[C.k\_off\_FMOD] = 1.000e+00

x[C.Rec\_act] = 5.970e-01

x[C.pRec\_debind] = 8.082e-03

x[C.S2tot] = 6.000e-02

x[C.S3tot] = 3.800e-01

x[C.S4tot] = 4.400e-03

x[C.kf\_2\_TGFbeta] = 4.664e-01

x[C.Kmf\_2\_TGFbeta] = 4.889e+00

x[C.k\_inhibit\_TGF] = 1.569e+00

x[C.S\_dephosphos] = 1.001e-01

x[C.S\_dephos] = 1.947e+00

x[C.kf\_3\_TGFbeta] = 9.264e-01

x[C.Kmf\_3\_TGFbeta] = 1.004e-01

x[C.k\_on\_ppS2\_ppS3] = 8.995e-01

x[C.k\_on\_ppS2\_ppS3\_S4] = 9.071e-01

x[C.k\_off\_ppS2\_ppS3\_S4] = 3.579e-01

x[C.prod\_mS7] = 2.069e-01

x[C.n1\_TGF] = 1.000e+00

x[C.Km\_1\_TGF] = 2.299e-01

x[C.mS7\_turn] = 8.564e+00

x[C.prod\_S7] = 2.258e-01

x[C.prod\_mcFOS] = 1.848e+01

x[C.n2\_TGF] = 1.000e+00

x[C.Km\_2\_TGF] = 2.049e-02

x[C.mcFOS\_turn] = 2.056e-02

x[C.prod\_cFOS] = 1.134e-01

x[C.k\_on\_ppS2\_ppS3\_S4\_cFOS] = 6.391e-01

x[C.k\_off\_ppS2\_ppS3\_S4\_cFOS] = 2.785e-01

x[C.prod\_mTHBS1] = 2.157e+02

x[C.n4\_TGF] = 1.000e+00

x[C.Km\_4\_TGF] = 1.102e-01

x[C.THBS1\_turn] = 5.464e-03

x[C.prod\_THBS1] = 3.524e+00

x[C.w\_THBS1] = 1.234e-01

x[C.w\_TGFBR1] = 2.282e-01

x[C.w\_TGFBR2] = 3.128e-01

x[C.w\_SMAD7] = 1.021e-01

x[C.w\_cFOS] = 1.047e-01

x[C.degrad\_cFOS] = 1.000e-01

# None zero initial values for 'Control' condition

# y0[V.TGFb\_act] =0 for 'Control'

y0[V.TGFb\_inact] = 0.013

y0[V.TGFBR\_inact] = 4.475e+01

y0[V.S2] = 6.000e-02

y0[V.S3] = 3.800e-01

y0[V.S4] = 4.400e-03

y0[V.mS7] = 2.105e+00

y0[V.mcFOS] = 1.225e-01

y0[V.mTHBS1] = 5.581e+02

# None zero initial values for 'TGFβ1' condition

# y0[V.TGFb\_act] = 0.0902 for 'TGFβ1'

y0[V.TGFb\_inact] = 0.013

y0[V.TGFb\_act] =0.0902

y0[V.TGFBR\_inact] = 4.475e+01

y0[V.S2] = 6.000e-02

y0[V.S3] = 3.800e-01

y0[V.S4] = 4.400e-03

y0[V.mS7] = 2.105e+00

y0[V.mcFOS] = 1.225e-01

y0[V.mTHBS1] = 5.581e+02