

Initial Conditions:

	CD3 ζ	LCK	Phosphatase
molecules/ μm^2	1	1000	10-100000

Parameter Values:

	k_{cat} (min $^{-1}$)	$K_{M,A1}$ (μm^{-2})	$K_{M,A2}$ (μm^{-2})	$K_{M,B1}$ (μm^{-2})	$K_{M,B2}$ (μm^{-2})	$K_{M,C1}$ (μm^{-2})	$K_{M,C2}$ (μm^{-2})	X_I
LCK parameters	360	97	332	270	154	485	405	0.115
Phosphatase parameters	360	11	36	32	18	67	57	0.1

Equations:

$$\frac{dpY_{A1}}{dt} = \frac{\left(K_{\text{cat}} / K_{M,A1} \right) (Y_{A1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} - \frac{\left(P_{\text{cat}} / P_{M,A1} \right) (pY_{A1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

$$\frac{dY_{A1}}{dt} = - \frac{\left(K_{\text{cat}} / K_{M,A1} \right) (Y_{A1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} + \frac{\left(P_{\text{cat}} / P_{M,A1} \right) (pY_{A1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

$$\frac{dpY_{A2}}{dt} = \frac{\left(K_{\text{cat}} / K_{M,A2} \right) (Y_{A2})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} - \frac{\left(P_{\text{cat}} / P_{M,A2} \right) (pY_{A2})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

$$\begin{aligned} & \frac{dpY_{C1}}{dt} \\ = & \frac{\left(K_{cat}/K_{M,C1} \right) (Y_{C1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} \\ - & \frac{\left(P_{cat}/P_{M,C1} \right) (pY_{C1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}} \end{aligned}$$

$$\begin{aligned} & \frac{dY_{C1}}{dt} \\ &= - \frac{\left(K_{cat}/K_{M,C1} \right) (Y_{C1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} \\ &+ \frac{\left(P_{cat}/P_{M,C1} \right) (pY_{C1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}} \end{aligned}$$

$$\begin{aligned} & \frac{dpY_{C2}}{dt} \\ &= \frac{\left(\frac{K_{cat}}{K_{M,C2}} \right) (Y_{C2})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} \\ &\quad - \frac{\left(\frac{P_{cat}}{P_{M,C2}} \right) (pY_{C2})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}} \end{aligned}$$

$$\begin{aligned} & \frac{dY_{C2}}{dt} \\ &= - \frac{\left(K_{cat} / K_{M,C2} \right) (Y_{C2})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} \\ &+ \frac{\left(P_{cat} / P_{M,C2} \right) (pY_{C2})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}} \end{aligned}$$