

Tabelle 1: Reaktionen und Parameter für ein Modell, das einige zentrale Vorgänge in Leukozyten beschreibt, die hauptsächlich durch die Peroxidase bestimmt werden (per3+, coI, coII und coIII sind Formen der Peroxidase, MLTH ist Melatonin)

Reaktion	Reaktionsgeschwindigkeit (R_i)	Konstante
<i>Reaktionen im Phagosom:</i>		
1. $H_2O_2 + per^{3+} \xrightleftharpoons[k_{-1}]{k_1} coI$	$k_1[H_2O_2]_p[Per^{3+}]_p - k_{-1}[coI]_p$	$k_1 = 5.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$ $k_{-1} = 58 \text{ s}^{-1}$
2. $coI + MLTH \xrightarrow{k_2} coII + MLT^\cdot$	$k_2[coI]_p[MLTH]_p$	$k_2 = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$
3. $coII + MLTH \xrightarrow{k_3} per^{3+} + MLT^\cdot$	$k_3[coII]_p[MLTH]_p$	$k_3 = 4.0 \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$
4. $per^{3+} + O_2^- \xrightarrow{k_4} coIII$	$k_4[per^{3+}]_p[O_2^-]_p$	$k_4 = 1.1 \times 10^6 \text{ M}^{-1} \text{ s}^{-1}$
5. $2H^+ + 2O_2^- \xrightarrow{k_5} H_2O_2 + O_2$	$k_5[O_2^-]_p^2$	$k_5 = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$
6. $coIII + O_2^- \xrightarrow{k_6} coI + O_2$	$k_6[coIII]_p[O_2^-]_p$	$k_6 = 1.0 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$
<i>Reaktionen im Cytoplasma:</i>		
7. $NADPH + O_2 \xrightarrow{k_7} NADP^+ + H_2O_2$	$k_7[NADPH]_c[O_2]_c$	$k_7 = 1 \text{ M}^{-1} \text{ s}^{-1}$
8. $NADP^\cdot + O_2 \xrightarrow{k_8} NADP^+ + O_2^-$	$k_8[NADP^\cdot]_c[O_2]_c$	$k_8 = 5.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$
9. $2H^+ + 2O_2^- \xrightarrow{k_9} H_2O_2 + O_2$	$k_9[O_2^-]_c^2$	$k_9 = 5.0 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$
10. $MLT^\cdot + NADPH \xrightarrow{k_{10}} MLTH + NADP^\cdot$	$k_{10}[MLT^\cdot]_c[NADPH]_c$	$k_{10} = 1.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$
11. $2NADP^\cdot \xrightarrow{k_{11}} (NADP)_2$	$k_{11}[NADP^\cdot]_c^2$	$k_{11} = 6.0 \times 10^7 \text{ M}^{-1} \text{ s}^{-1}$
12. $\xrightarrow{k_{12}} NADPH$	k_{12}	$k_{12} = 25 \text{ } \mu\text{M s}^{-1}$
13. $\xrightleftharpoons[k_{-13}]{k_{13}} O_2(\text{cytoplasma})$	$k_{13} - k_{-13}[O_2]_c$	$k_{13} = 12.5 \text{ } \mu\text{M s}^{-1}$ $k_{-13} = 4.5 \times 10^{-2} \text{ s}^{-1}$
<i>Diffusionsterme:</i>		
14. $O_2(\text{phagosom}) \xrightleftharpoons[k_{14}]{k_{14}} O_2(\text{cytoplasma})$	$k_{14}([O_2]_p - [O_2]_c)$	$k_{14} = 30 \text{ s}^{-1}$
15. $H_2O_2(\text{phagosom}) \xrightleftharpoons[k_{15}]{k_{15}} H_2O_2(\text{cytoplasma})$	$k_{15}([H_2O_2]_p - [H_2O_2]_c)$	$k_{15} = 30 \text{ s}^{-1}$
16. $MLTH(\text{phagosom}) \xrightleftharpoons[k_{16}]{k_{16}} MLTH(\text{cytoplasma})$	$k_{16}([MLTH]_p - [MLTH]_c)$	$k_{16} = 10 \text{ s}^{-1}$
17. $MLT^\cdot(\text{phagosom}) \xrightleftharpoons[k_{17}]{k_{17}} MLT^\cdot(\text{cytoplasma})$	$k_{17}([MLT^\cdot]_p - [MLT^\cdot]_c)$	$k_{17} = 10 \text{ s}^{-1}$
18. $O_2^-(\text{phagosom}) \xrightleftharpoons[k_{18}]{k_{18}} O_2^-(\text{cytoplasma})$	$k_{18}([O_2^-]_p - [O_2^-]_c)$	$k_{18} = < 0.01 \text{ s}^{-1}$
<i>NADPH oxidase:</i>		
19. $NADPH(\text{cytoplasma}) + 2O_2(\text{phagosom}) \rightarrow NADP^+(\text{cytoplasma}) + 2O_2^-(\text{phagosom})$	$\frac{V\alpha(1+\alpha)}{(L+(1+\alpha)^2)} \frac{[O_2]_p}{K_O + [O_2]_p}; \alpha = \frac{[NADPH]_c}{K_{NADPH}}$	$V = 288 \text{ } \mu\text{M s}^{-1}$ $L = 550$ $K_O = 1.5 \text{ } \mu\text{M}$ $K_{NADPH} = 60 \text{ } \mu\text{M}$

Tabelle 2: Differentialgleichungen

Phagosom:

$$\frac{d[per^{3+}]_p}{dt} = -R_1 + R_3 - R_4$$

$$\frac{d[coI]_p}{dt} = R_1 - R_2 + R_6$$

$$\frac{d[coII]_p}{dt} = R_2 - R_3$$

$$\frac{d[coIII]_p}{dt} = R_4 - R_6$$

$$\frac{d[H_2O_2]_p}{dt} = -R_1 + R_5 - R_{15}$$

$$\frac{d[O_2^-]_p}{dt} = -R_4 - 2R_5 - R_6 - R_{18} + 2R_{19}$$

$$\frac{d[O_2]_p}{dt} = R_5 + R_6 - R_{14} - 2R_{19}$$

$$\frac{d[MLTH]_p}{dt} = -R_2 - R_3 - R_{16}$$

$$\frac{d[MLT^-]_p}{dt} = R_2 + R_3 - R_{17}$$

Cytoplasma:

$$\frac{d[NADPH]_c}{dt} = -R_7 - R_{10} + R_{12} - R_{19}$$

$$\frac{d[NADP^-]_c}{dt} = -R_8 + R_{10} - 2R_{11}$$

$$\frac{d[H_2O_2]_c}{dt} = R_7 + R_9 + f R_{15}$$

$$\frac{d[O_2^-]_c}{dt} = R_8 - 2R_9 + f R_{18}$$

$$\frac{d[O_2]_c}{dt} = -R_7 - R_8 + R_9 + R_{13} + f R_{14}$$

$$\frac{d[MLTH]_c}{dt} = R_{10} + f R_{16}$$

$$\frac{d[MLT^-]_c}{dt} = -R_{10} + f R_{17}$$
