Figura 11 (pag. 188 della seconda edizione). Curve concentrazione-tempo per le reazioni elementari in serie

$t_{fin} := 3$

$t := 0, 0.01 .. t_{fin}$

Given

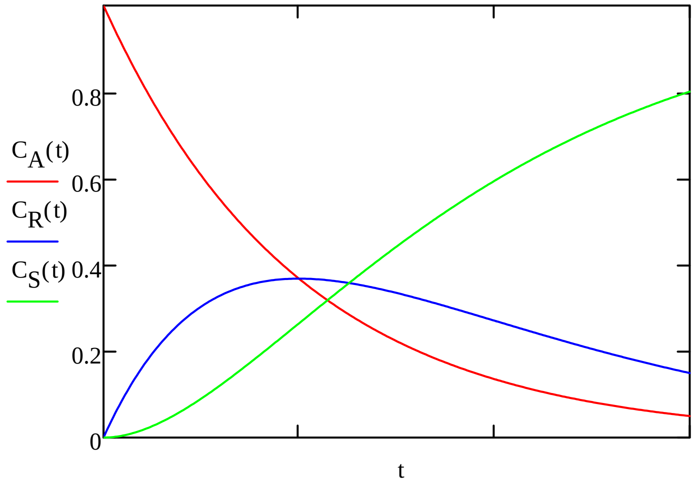
$$\frac{d}{dt}C_A(t) = -1 \cdot C_A(t) \qquad C_A(0) = 1$$

$$\frac{d}{dt}C_R(t) = 1 \cdot C_A(t) - 1 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) \qquad C_S(0) = 0$$

Figura 11A $\quad A \xrightarrow{1} R \xrightarrow{1} S$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Given

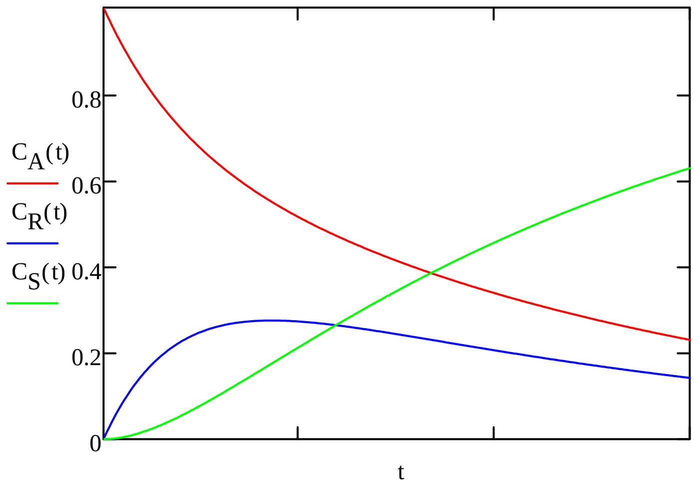
$$\frac{d}{dt}C_A(t) = -1 \cdot C_A(t) + 1 \cdot C_R(t) \qquad C_A(0) = 1$$

$$\frac{d}{dt}C_R(t) = 1 \cdot C_A(t) - 1 \cdot C_R(t) - 1 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) \qquad C_S(0) = 0$$

Figura 11B $\quad A \underset{1}{\overset{1}{\rightleftarrows}} R \xrightarrow{1} S$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$

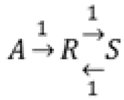


Given $\frac{d}{dt}C_A(t) = -1 \cdot C_A(t)$ $C_A(0) = 1$

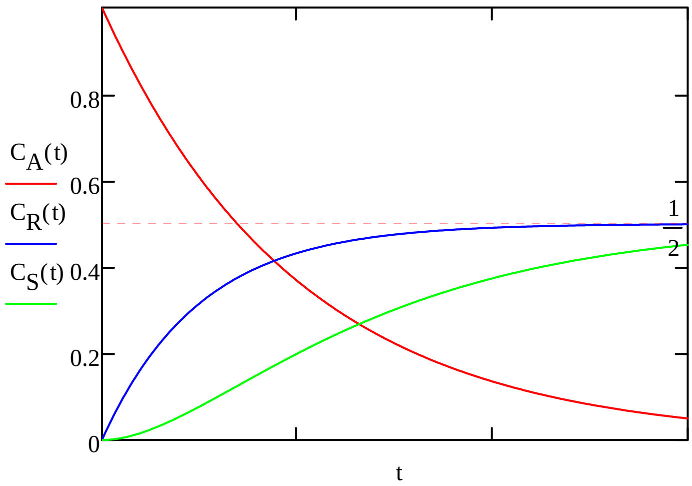
$\frac{d}{dt}C_R(t) = 1 \cdot C_A(t) - 1 \cdot C_R(t) + 1 \cdot C_S(t)$ $C_R(0) = 0$

$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) - 1 \cdot C_S(t)$ $C_S(0) = 0$

Figura 11C



$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$

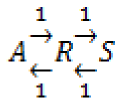


Given $\frac{d}{dt}C_A(t) = -1 \cdot C_A(t) + 1 \cdot C_R(t)$ $C_A(0) = 1$

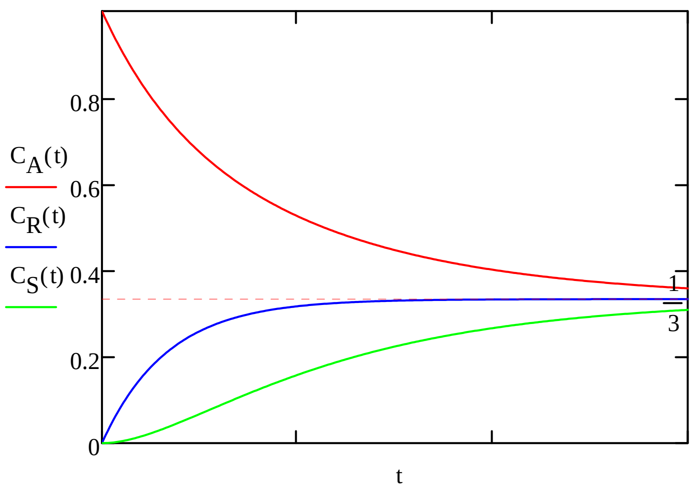
$\frac{d}{dt}C_R(t) = 1 \cdot C_A(t) - 1 \cdot C_R(t) + 1 \cdot C_S(t) - 1 \cdot C_R(t)$ $C_R(0) = 0$

$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) - 1 \cdot C_S(t)$ $C_S(0) = 0$

Figura 11D



$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Risolviamo l'equilibrio:

$K_1 = 1 = \frac{R_{eq}}{A_{eq}}$ $K_2 = 1 = \frac{S_{eq}}{R_{eq}}$

$A_{eq} + R_{eq} + S_{eq} = 1$

... risolvendo ...

$A_{eq} = R_{eq} = S_{eq} = \frac{1}{3}$

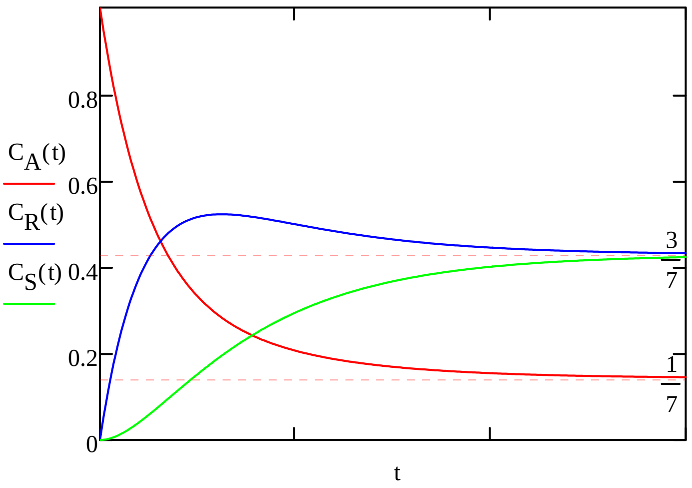
Given $\frac{d}{dt}C_A(t) = -3 \cdot C_A(t) + 1 \cdot C_R(t)$ $\quad C_A(0) = 1$

Figura 11E $\quad A \underset{1}{\overset{3}{\rightleftarrows}} R \underset{1}{\overset{1}{\rightleftarrows}} S$

$$\frac{d}{dt}C_R(t) = 3 \cdot C_A(t) - 1 \cdot C_R(t) + 1 \cdot C_S(t) - 1 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) - 1 \cdot C_S(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Risolviamo l'equilibrio:

$$K_1 = 3 = \frac{R_{eq}}{A_{eq}} \qquad K_2 = 1 = \frac{S_{eq}}{R_{eq}}$$

$$A_{eq} + R_{eq} + S_{eq} = 1$$

... risolvendo ...

$$A_{eq} = \frac{1}{7} \qquad R_{eq} = S_{eq} = \frac{3}{7}$$

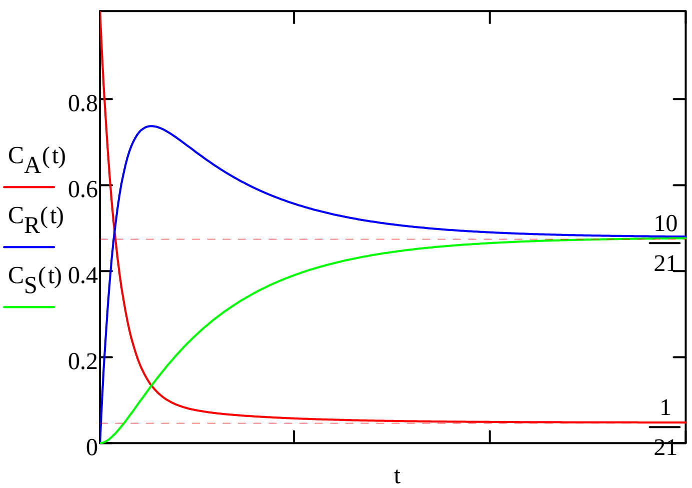
Given $\frac{d}{dt}C_A(t) = -10 \cdot C_A(t) + 1 \cdot C_R(t)$ $\quad C_A(0) = 1$

Figura 11F $\quad A \underset{1}{\overset{10}{\rightleftarrows}} R \underset{1}{\overset{1}{\rightleftarrows}} S$

$$\frac{d}{dt}C_R(t) = 10 \cdot C_A(t) - 1 \cdot C_R(t) + 1 \cdot C_S(t) - 1 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_R(t) - 1 \cdot C_S(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Risolviamo l'equilibrio:

$$K_1 = 10 = \frac{R_{eq}}{A_{eq}} \qquad K_2 = 1 = \frac{S_{eq}}{R_{eq}}$$

$$A_{eq} + R_{eq} + S_{eq} = 1$$

... risolvendo ...

$$A_{eq} = \frac{1}{21} \qquad R_{eq} = S_{eq} = \frac{10}{21}$$

Figura 12 (pag. 189 della seconda edizione). Curve concentrazione-tempo per le reazioni elementari in parallelo

Figura 12A

$$A \xrightarrow{1} R \qquad A \xrightarrow{1} S$$

Given

$$\frac{d}{dt}C_A(t) = -1\cdot C_A(t) - 1\cdot C_A(t) \qquad C_A(0) = 1$$

$$\frac{d}{dt}C_R(t) = 1\cdot C_A(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1\cdot C_A(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$

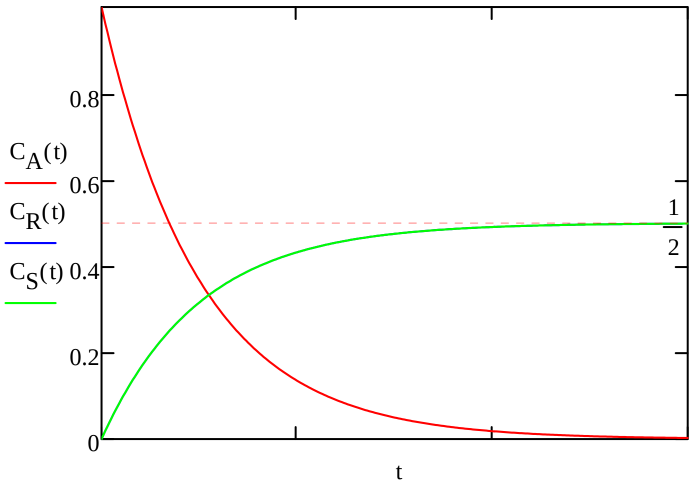


Figura 12B

$$A \underset{1}{\overset{1}{\rightleftarrows}} R \qquad A \xrightarrow{1} S$$

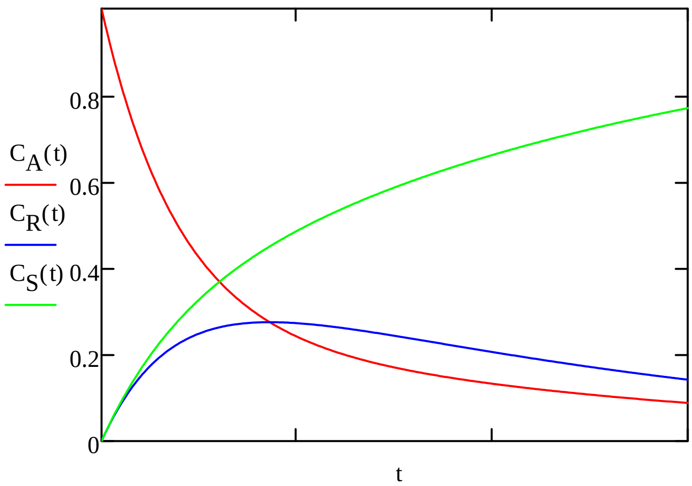
Given

$$\frac{d}{dt}C_A(t) = -1\cdot C_A(t) + 1\cdot C_R(t) - 1\cdot C_A(t) \qquad C_A(0) = 1$$

$$\frac{d}{dt}C_R(t) = 1\cdot C_A(t) - 1\cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1\cdot C_A(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Given $\frac{d}{dt}C_A(t) = -1 \cdot C_A(t) - 1 \cdot C_A(t) + 1 \cdot C_R(t) + 1 \cdot C_S(t)$ $C_A(0) = 1$ Figura 12C

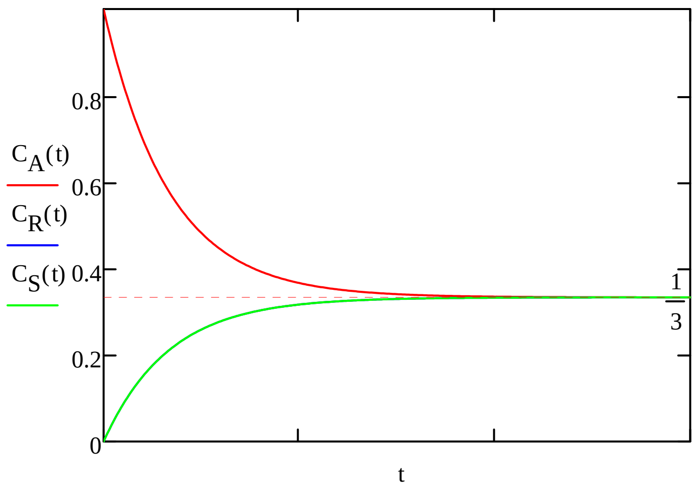
$$A \underset{1}{\overset{1}{\rightleftarrows}} R$$

$$A \underset{1}{\overset{1}{\rightleftarrows}} S$$

$$\frac{d}{dt}C_R(t) = 1 \cdot C_A(t) - 1 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_A(t) - 1 \cdot C_S(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



Given $\frac{d}{dt}C_A(t) = -3 \cdot C_A(t) + 3 \cdot C_R(t) - 1 \cdot C_A(t) + 1 \cdot C_S(t)$ $C_A(0) = 1$ Figura 12D

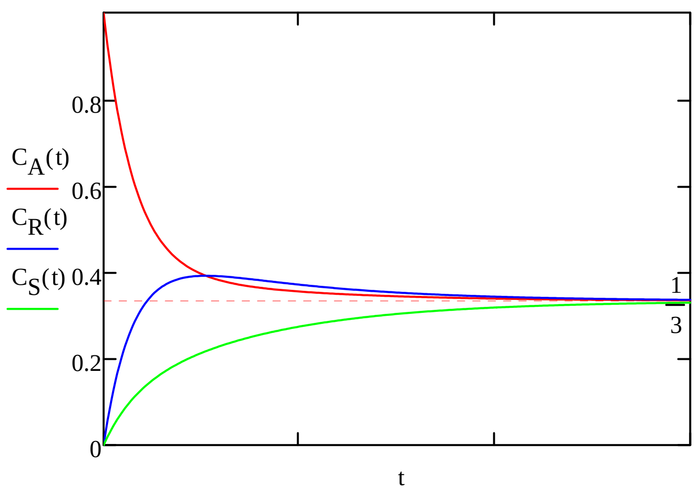
$$A \underset{3}{\overset{3}{\rightleftarrows}} R$$

$$A \underset{1}{\overset{1}{\rightleftarrows}} S$$

$$\frac{d}{dt}C_R(t) = 3 \cdot C_A(t) - 3 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_A(t) - 1 \cdot C_S(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$



$$A \underset{10}{\overset{10}{\rightleftarrows}} R \qquad A \underset{1}{\overset{1}{\rightleftarrows}} S$$

Figura 12D

Given $\frac{d}{dt}C_A(t) = -10 \cdot C_A(t) + 10 \cdot C_R(t) - 1 \cdot C_A(t) + 1 \cdot C_S(t)$ $\quad C_A(0) = 1$

$$\frac{d}{dt}C_R(t) = 10 \cdot C_A(t) - 10 \cdot C_R(t) \qquad C_R(0) = 0$$

$$\frac{d}{dt}C_S(t) = 1 \cdot C_A(t) - 1 \cdot C_S(t) \qquad C_S(0) = 0$$

$$\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} C_A \\ C_R \\ C_S \end{pmatrix}, t, t_{fin}, 1000\right]$$