Chemical dynamics CHEM674

Laplace and linear algebra methods

University of Delaware

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Outline

- Laplace methods
- Linear algebra methods

Laplace transform

The transform F(p) of a function f(t) subjected to the Laplace transformation is defined by the integral:

$$F(p) = \mathcal{L}[f(t)] = \int_0^\infty e^{-pt} f(t)\,dt$$

Laplace transform

The transform F(p) of a function f(t) subjected to the Laplace transformation is defined by the integral:

$$F(p) = \mathcal{L}[f(t)] = \int_0^\infty e^{-pt} f(t)\,dt$$

The Laplace transform of a given function maybe determined by direct integration :

$$F(p) = \mathcal{L}[e^{-at}] = \int_0^\infty e^{-at}\, e^{-pt} dt = \int_0^\infty e^{-(a+p)t} dt$$

$$= -\frac{1}{a+p}\left[e^{-(a+p)t}\right]_0^\infty$$

$$= \frac{1}{p+a} \qquad (p > -a)$$

Properties of the Laplace transform

Laplace transform of a linear combination of functions.

$$f(t) = f_1(t) + f_2(t) + \cdots + f_n(t)$$

$$\mathcal{L}[f(t)] = \int_0^\infty [f_1(t) + f_2(t) + \cdots + f_n(t)]e^{-pt}\,dt$$

$$= \int_0^\infty f_1(t)e^{-pt}\,dt + \int_0^\infty f_2(t)e^{-pt}\,dt + \cdots + \int_0^\infty f_n(t)e^{-pt}\,dt$$

$$\mathcal{L}[f(t)] = F_1(p) + F_2(p) + \cdots + F_n(p)$$

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Properties of the Laplace transform

The Laplace transform of the derivative of f(t), i.e., f’(t), can be readily obtained.

$$\mathcal{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

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$$\mathcal{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

$$\int u\frac{\mathrm{d}v}{\mathrm{d}x}\,\mathrm{d}x = u\,v - \int v\frac{\mathrm{d}u}{\mathrm{d}x}\mathrm{d}x$$

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u=exp(-pt)
dv=f'(t)dt

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$$\mathcal{L}[f'(t)] = f(t)e^{-pt}\Big]_0^\infty + p\int_0^\infty f(t)e^{-pt}\,dt$$

u=exp(-pt)
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Properties of the Laplace transform

The Laplace transform of the derivative of f(t), i.e., f'(t), can be readily obtained.

$$\mathscr{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

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u=exp(-pt)
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$$\mathscr{L}[f'(t)] = p\mathscr{L}[f(t)] - f(0)$$

Properties of the Laplace transform

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$$\mathcal{L}[f'(t)] = p\mathcal{L}[f(t)] - f(0) \qquad \mathcal{L}[f''(t)] = p\mathcal{L}[f'(t)] - f'(0)$$

Properties of the Laplace transform

$$\mathcal{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

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$$\mathcal{L}[f'(t)] = p\mathcal{L}[f(t)] - f(0)$$

$$\mathcal{L}[f''(t)] = p\mathcal{L}[f'(t)] - f'(0)$$

$$\mathcal{L}[f''(t)] = p(p\mathcal{L}[f(t)] - f(0)) - f'(0)$$

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Properties of the Laplace transform

$$\mathcal{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

$$\mathcal{L}[f'(t)] = f(t)e^{-pt}\Big]_0^\infty + p\int_0^\infty f(t)e^{-pt}\,dt$$

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$$\mathcal{L}[f''(t)] = p\mathcal{L}[f'(t)] - f'(0)$$

$$\mathcal{L}[f''(t)] = p(p\mathcal{L}[f(t)] - f(0)) - f'(0)$$

$$\mathcal{L}[f''(t)] = p^2\mathcal{L}[f(t)] - pf(0) - f'(0)$$

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Properties of the Laplace transform

$$\mathcal{L}[f'(t)] = \int_0^\infty f'(t)e^{-pt}\,dt$$

$$\mathcal{L}[f^{(n)}(t)] = p^n\mathcal{L}[f(t)] - \sum_{i=1}^{n} f^{(i-1)}(0)p^{n-1}$$

$$\mathcal{L}[f'(t)] = f(t)e^{-pt}\Big]_0^\infty + p\int_0^\infty f(t)e^{-pt}\,dt$$

$$\mathcal{L}[f'(t)] = p\mathcal{L}[f(t)] - f(0)$$

$$\mathcal{L}[f''(t)] = p\mathcal{L}[f'(t)] - f'(0)$$

$$\mathcal{L}[f''(t)] = p(p\mathcal{L}[f(t)] - f(0)) - f'(0)$$

$$\mathcal{L}[f''(t)] = p^2\mathcal{L}[f(t)] - pf(0) - f'(0)$$

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Properties of the Laplace transform

The transform of an integral of a function f(t) may be expressed as

$$\mathcal{L}\left[\int_0^t f(t)\,dt\right] = \frac{\mathcal{L}[f(t)]}{p}$$

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Thus, for rate equations that are linear with respect to the reactants, Laplace methods is great

Reversible reactions

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftarrows}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

At time t=0 both A_1 and A_2 are present, that is $[A_1] = [A_1]_0$ and $[A_2] = [A_2]_0$

$$[A_1]_0 + [A_2]_0 = [A_1] + [A_2]$$

Reversible reactions

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2] \qquad \mathscr{L}[f'(t)] = p\mathscr{L}[f(t)] - f(0)$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

Reversible reactions

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The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2] \qquad \mathscr{L}[f'(t)] = p\mathscr{L}[f(t)] - f(0)$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$(p + k_1)(\mathscr{L}[A_1]) - k_2\mathscr{L}[A_2] = [A_1]_0$$

$$-k_1(\mathscr{L}[A_1]) + (p + k_2)\mathscr{L}[A_2] = [A_2]_0$$

Reversible reactions

The determinant of a 2x2 matrix is denoted by $\begin{vmatrix} a & c \\ b & d \end{vmatrix}$

To evaluate a 2x2 determinant use $\begin{vmatrix} a & c \\ b & d \end{vmatrix} = ad - bc$

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftarrows}} A_2$$

Cramer's rule for a system of linear equations :

The solution to the system:

$$\begin{Bmatrix} a_1 x + b_1 y = c_1 \\ a_2 x + b_2 y = c_2 \end{Bmatrix}$$

Is given by:

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

Cramer's rule

$$\begin{cases} a_1 x + b_1 y = c_1 \\ a_2 x + b_2 y = c_2 \end{cases}$$

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

$$6x - 5y = -23$$
$$3x + 3y = 16$$

Cramer's rule

$$\begin{cases} a_1 x + b_1 y = c_1 \\ a_2 x + b_2 y = c_2 \end{cases}$$

$$6x - 5y = -23$$
$$3x + 3y = 16$$

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

$$x = \frac{\begin{vmatrix} -23 & -5 \\ 16 & 3 \end{vmatrix}}{\begin{vmatrix} 6 & -5 \\ 3 & 3 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} 6 & -23 \\ 3 & 16 \end{vmatrix}}{\begin{vmatrix} 6 & -5 \\ 3 & 3 \end{vmatrix}}$$

Cramer's rule

$$\begin{cases} a_1x + b_1y = c_1 \\ a_2x + b_2y = c_2 \end{cases}$$

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

$$6x - 5y = -23$$
$$3x + 3y = 16$$

$$x = \frac{\begin{vmatrix} -23 & -5 \\ 16 & 3 \end{vmatrix}}{\begin{vmatrix} 6 & -5 \\ 3 & 3 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} 6 & -23 \\ 3 & 16 \end{vmatrix}}{\begin{vmatrix} 6 & -5 \\ 3 & 3 \end{vmatrix}}$$

$$x = \frac{(-23)(3) - (16)(-5)}{(6)(3) - (3)(-5)} = \frac{-69 + 80}{18 + 15} = \frac{11}{33} = \frac{1}{3}$$

$$y = \frac{(6)(16) - (3)(-23)}{(6)(3) - (3)(-5)} = \frac{96 + 69}{18 + 15} = \frac{165}{33} = 5$$

Cramer's rule

$$\begin{cases} a_1x + b_1y + c_1z = d_1 \\ a_2x + b_2y + c_2z = d_2 \\ a_3x + b_3y + c_3z = d_3 \end{cases}$$

The determinant of a 3x3 matrix is denoted by $\begin{vmatrix} a & d & g \\ b & e & h \\ c & f & i \end{vmatrix}$

To evaluate a 3x3 determinant use $\begin{vmatrix} a & d & g \\ b & e & h \\ c & f & i \end{vmatrix} = a\begin{vmatrix} e & h \\ f & i \end{vmatrix} - b\begin{vmatrix} d & g \\ f & i \end{vmatrix} + c\begin{vmatrix} d & g \\ e & h \end{vmatrix}$

Cramer's rule for a system of linear equations :

The solution to the system:

Is given by: $x = \frac{D_x}{D}$ $y = \frac{D_y}{D}$ $z = \frac{D_z}{D}$

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} \quad D_x = \begin{vmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d_3 & b_3 & c_3 \end{vmatrix} \quad D_y = \begin{vmatrix} a_1 & d_1 & c_1 \\ a_2 & d_2 & c_2 \\ a_3 & d_3 & c_3 \end{vmatrix} \quad D_z = \begin{vmatrix} a_1 & b_1 & d_1 \\ a_2 & b_2 & d_2 \\ a_3 & b_3 & d_3 \end{vmatrix}$$

Cramer's rule

$$\begin{cases} a_1 x + b_1 y + c_1 z = d_1 \\ a_2 x + b_2 y + c_2 z = d_2 \\ a_3 x + b_3 y + c_3 z = d_3 \end{cases}$$

$$\begin{aligned} -x + 2y + 3z &= -7 \\ -4x - 5y + 6z &= -13 \\ 7x - 8y - 9z &= 39 \end{aligned}$$

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

Cramer's rule

$$\begin{cases} a_1x + b_1y + c_1z = d_1 \\ a_2x + b_2y + c_2z = d_2 \\ a_3x + b_3y + c_3z = d_3 \end{cases}$$

$$\begin{aligned} -x + 2y + 3z &= -7 \\ -4x - 5y + 6z &= -13 \\ 7x - 8y - 9z &= 39 \end{aligned}$$

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

$$D = \begin{vmatrix} -1 & 2 & 3 \\ -4 & -5 & 6 \\ 7 & -8 & -9 \end{vmatrix}$$

Cramer's rule

$$\begin{cases} a_1x + b_1y + c_1z = d_1 \\ a_2x + b_2y + c_2z = d_2 \\ a_3x + b_3y + c_3z = d_3 \end{cases}$$

$$\begin{aligned} -x + 2y + 3z &= -7 \\ -4x - 5y + 6z &= -13 \\ 7x - 8y - 9z &= 39 \end{aligned}$$

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix}$$

$$D = \begin{vmatrix} -1 & 2 & 3 \\ -4 & -5 & 6 \\ 7 & -8 & -9 \end{vmatrix} = -1\begin{vmatrix} -5 & 6 \\ -8 & -9 \end{vmatrix} - (-4)\begin{vmatrix} 2 & 3 \\ -8 & -9 \end{vmatrix} + 7\begin{vmatrix} 2 & 3 \\ -5 & 6 \end{vmatrix}$$

$$D = -1\left[(-5)(-9) - (6)(-8)\right] + 4\left[(2)(-9) - (3)(-8)\right] + 7\left[(2)(6) - (3)(-5)\right]$$

$$D = -1(45 + 48) + 4(-18 + 24) + 7(12 + 15) = \underline{120}$$

Cramer’s rule

$$\begin{cases} a_1x + b_1y + c_1z = d_1 \\ a_2x + b_2y + c_2z = d_2 \\ a_3x + b_3y + c_3z = d_3 \end{cases}$$

$$\begin{aligned} -x + 2y + 3z &= -7 \\ -4x - 5y + 6z &= -13 \\ 7x - 8y - 9z &= 39 \end{aligned}$$

$$x = \frac{D_x}{D} \qquad y = \frac{D_y}{D} \qquad z = \frac{D_z}{D}$$

$$D = -1(45+48) + 4(-18+24) + 7(12+15) = \underline{120}$$

$$D_x = \begin{vmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d_3 & b_3 & c_3 \end{vmatrix} \qquad D_x = \begin{vmatrix} -7 & 2 & 3 \\ -13 & -5 & 6 \\ 39 & -8 & -9 \end{vmatrix} = -7\begin{vmatrix} -5 & 6 \\ -8 & -9 \end{vmatrix} - (-13)\begin{vmatrix} 2 & 3 \\ -8 & -9 \end{vmatrix} + 39\begin{vmatrix} 2 & 3 \\ -5 & 6 \end{vmatrix} = -7(45+48) + 13(-18+24) + 39(12+15) = \underline{480}$$

$$D_y = \begin{vmatrix} a_1 & d_1 & c_1 \\ a_2 & d_2 & c_2 \\ a_3 & d_3 & c_3 \end{vmatrix} \qquad D_y = \begin{vmatrix} -1 & -7 & 3 \\ -4 & -13 & 6 \\ 7 & 39 & -9 \end{vmatrix} = -1\begin{vmatrix} -13 & 6 \\ 39 & -9 \end{vmatrix} - (-4)\begin{vmatrix} -7 & 3 \\ 39 & -9 \end{vmatrix} + 7\begin{vmatrix} -7 & 3 \\ -13 & 6 \end{vmatrix} = -1(117-234) + 4(63-117) + 7(-42+39) = \underline{-120}$$

$$D_z = \begin{vmatrix} a_1 & b_1 & d_1 \\ a_2 & b_2 & d_2 \\ a_3 & b_3 & d_3 \end{vmatrix} \qquad D_z = \begin{vmatrix} -1 & 2 & -7 \\ -4 & -5 & -13 \\ 7 & -8 & 39 \end{vmatrix} = -1\begin{vmatrix} -5 & -13 \\ -8 & 39 \end{vmatrix} - (-4)\begin{vmatrix} 2 & -7 \\ -8 & 39 \end{vmatrix} + 7\begin{vmatrix} 2 & -7 \\ -5 & -13 \end{vmatrix} = -1(-195-104) + 4(78-56) + 7(-26-35) = \underline{-40}$$

Cramer's rule

$$\begin{cases} a_1x + b_1y + c_1z = d_1 \\ a_2x + b_2y + c_2z = d_2 \\ a_3x + b_3y + c_3z = d_3 \end{cases}$$

$$\begin{aligned} -x + 2y + 3z &= -7 \\ -4x - 5y + 6z &= -13 \\ 7x - 8y - 9z &= 39 \end{aligned}$$

$$x = \frac{D_x}{D} \qquad y = \frac{D_y}{D} \qquad z = \frac{D_z}{D}$$

$$D = -1(45 + 48) + 4(-18 + 24) + 7(12 + 15) = \underline{120}$$

$$x = \frac{480}{120} = 4 \qquad y = \frac{-120}{120} = -1 \qquad z = \frac{-40}{120} = -\frac{1}{3}$$

Reversible reactions

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

$$\mathcal{L}[f'(t)] = p\mathcal{L}[f(t)] - f(0)$$

The differential equation for this mechanism is:

$$(p + k_1)(\mathcal{L}[A_1]) - k_2\mathcal{L}[A_2] = [A_1]_0$$
$$-k_1(\mathcal{L}[A_1]) + (p + k_2)\mathcal{L}[A_2] = [A_2]_0$$

$$\begin{cases} a_1x + b_1y = c_1 \\ a_2x + b_2y = c_2 \end{cases}$$

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

Reversible reactions

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$$-k_1(\mathcal{L}[A_1]) + (p + k_2)\mathcal{L}[A_2] = [A_2]_0$$

$$\begin{cases} a_1 x + b_1 y = c_1 \\ a_2 x + b_2 y = c_2 \end{cases}$$

$$\mathcal{L}[A_1] = \frac{\begin{vmatrix} [A_1]_0 & -k_2 \\ [A_2]_0 & (p + k_2) \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}} \qquad \mathcal{L}[A_2] = \frac{\begin{vmatrix} p + k_1 & [A_1]_0 \\ -k_1 & [A_2]_0 \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}}$$

$$x = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

Reversible reactions

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftarrows}} A_2$$

$$\mathscr{L}[f'(t)] = p\mathscr{L}[f(t)] - f(0)$$

The differential equation for this mechanism is:

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$$\mathscr{L}[A_1] = \frac{\begin{vmatrix} [A_1]_0 & -k_2 \\ [A_2]_0 & (p + k_2) \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}} \quad \mathscr{L}[A_2] = \frac{\begin{vmatrix} p + k_1 & [A_1]_0 \\ -k_1 & [A_2]_0 \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}}$$

$$\Rightarrow$$

$$\mathscr{L}[A_1] = \frac{(p + k_2)[A_1]_0}{p(p + (k_1 + k_2))} + \frac{k_2[A_2]_0}{p(p + (k_1 + k_2))}$$

$$\mathscr{L}[A_2] = \frac{(p + k_1)[A_2]_0}{p(p + (k_1 + k_2))} + \frac{k_1[A_1]_0}{p(p + (k_1 + k_2))}$$

Reversible reactions

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

$$\mathscr{L}[f'(t)] = p\mathscr{L}[f(t)] - f(0)$$

The differential equation for this mechanism is:

$$(p + k_1)(\mathscr{L}[A_1]) - k_2\mathscr{L}[A_2] = [A_1]_0$$
$$-k_1(\mathscr{L}[A_1]) + (p + k_2)\mathscr{L}[A_2] = [A_2]_0$$

Inverse Laplace transform :

$$\mathscr{L}^{-1}[F(p)] = f(t)$$

$$\mathscr{L}[A_1] = \frac{\begin{vmatrix} [A_1]_0 & -k_2 \\ [A_2]_0 & (p + k_2) \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}} \quad \mathscr{L}[A_2] = \frac{\begin{vmatrix} p + k_1 & [A_1]_0 \\ -k_1 & [A_2]_0 \end{vmatrix}}{\begin{vmatrix} p + k_1 & -k_2 \\ -k_1 & p + k_2 \end{vmatrix}}$$

$$\Rightarrow$$

$$\mathscr{L}[A_1] = \frac{(p + k_2)[A_1]_0}{p(p + (k_1 + k_2))} + \frac{k_2[A_2]_0}{p(p + (k_1 + k_2))}$$

$$\mathscr{L}[A_2] = \frac{(p + k_1)[A_2]_0}{p(p + (k_1 + k_2))} + \frac{k_1[A_1]_0}{p(p + (k_1 + k_2))}$$

Reversible reactions

Inverse Laplace transform :

$$\mathcal{L}^{-1}[F(p)] = f(t)$$

$$\mathcal{L}[A_1] = \frac{(p + k_2)[A_1]_0}{p(p + (k_1 + k_2))} + \frac{k_2[A_2]_0}{p(p + (k_1 + k_2))}$$

TABLE 2-1.2 Some Useful Laplace Transform Pairs

No.	$F(p)$	$f(t)$
1	$\frac{1}{p^2}$	t
2	$\frac{1}{p+a}$	e^{-at} Valid for complex a.
3	$\frac{1}{p(p+a)}$	$\frac{1}{a}(1 - e^{-at})$
4	$\frac{1}{(p+a)(p+b)}$	$\frac{1}{(b-a)}(e^{-at} - e^{-bt})$
5	$\frac{1}{p(p+a)(p+b)}$	$\frac{1}{ab}\left[1 + \frac{1}{(a-b)}(be^{-at} - ae^{-bt})\right]$
6	$\frac{1}{(p+a)(p+b)(p+c)}$	$\frac{1}{(b-a)(c-a)}e^{-at} + \frac{1}{(a-b)(c-b)}e^{-bt} + \frac{1}{(a-c)(b-c)}e^{-ct}$
7	$\frac{1}{(p+a)^2}$	te^{-at}
8	$\frac{1}{p(p+a)^2}$	$\frac{1}{a^2}[1 - e^{-at} - ate^{-at}]$.
9	$\frac{p}{(p+a)(p+b)}$	$\frac{1}{(a-b)}[ae^{-at} - be^{-bt}]$
10	$\frac{p}{(p-a)(p-b)}$	$\frac{1}{(a-b)}[ae^{at} - be^{bt}]$
11	$\frac{p}{(p+a)(p+b)(p+c)}$	$\frac{-a}{(b-a)(c-a)}e^{-at} - \frac{b}{(a-b)(c-b)}e^{-bt} - \frac{c}{(a-c)(b-c)}e^{-ct}$
12	$\frac{p}{(p+a)^2}$	$(1 - at)e^{-at}$
13	$\frac{p+a}{(p+b)(p+c)}$	$\frac{1}{(c-b)}[(a-b)e^{-bt} - (a-c)e^{-ct}]$
14	$\frac{p^2}{(p+a)(p+b)(p+c)}$	$\frac{a^2}{(b-a)(c-a)}e^{-at} + \frac{b^2}{(a-b)(c-b)}e^{-bt} + \frac{c^2}{(a-c)(b-c)}e^{-ct}$

Reversible reactions

Inverse Laplace transform :

$$\mathcal{L}^{-1}[F(p)] = f(t)$$

$$\mathcal{L}[A_1] = \frac{(p + k_2)[A_1]_0}{p(p + (k_1 + k_2))} + \frac{k_2[A_2]_0}{p(p + (k_1 + k_2))}$$

$$[A_1] = \frac{[A_1]_0}{(k_1 + k_2)}(k_2 + k_1 e^{-(k_1+k_2)t}) + \frac{[A_2]_0 k_2}{(k_1 + k_2)}(1 - e^{-(k_1+k_2)t})$$

TABLE 2-1.2 Some Useful Laplace Transform Pairs

No.	$F(p)$	$f(t)$
1	$\frac{1}{p^2}$	t
2	$\frac{1}{p+a}$	e^{-at} Valid for complex a.
3	$\frac{1}{p(p+a)}$	$\frac{1}{a}(1 - e^{-at})$
4	$\frac{1}{(p+a)(p+b)}$	$\frac{1}{(b-a)}(e^{-at} - e^{-bt})$
5	$\frac{1}{p(p+a)(p+b)}$	$\frac{1}{ab}\left[1 + \frac{1}{(a-b)}(be^{-at} - ae^{-bt})\right]$
6	$\frac{1}{(p+a)(p+b)(p+c)}$	$\frac{1}{(b-a)(c-a)}e^{-at} + \frac{1}{(a-b)(c-b)}e^{-bt} + \frac{1}{(a-c)(b-c)}e^{-ct}$
7	$\frac{1}{(p+a)^2}$	te^{-at}
8	$\frac{1}{p(p+a)^2}$	$\frac{1}{a^2}[1 - e^{-at} - ate^{-at}]$.
9	$\frac{p}{(p+a)(p+b)}$	$\frac{1}{(a-b)}[ae^{-at} - be^{-bt}]$
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13	$\frac{p+a}{(p+b)(p+c)}$	$\frac{1}{(c-b)}[(a-b)e^{-bt} - (a-c)e^{-ct}]$
14	$\frac{p^2}{(p+a)(p+b)(p+c)}$	$\frac{a^2}{(b-a)(c-a)}e^{-at} + \frac{b^2}{(a-b)(c-b)}e^{-bt} + \frac{c^2}{(a-c)(b-c)}e^{-ct}$

Reversible reactions

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$$[A_1] = \frac{[A_1]_0}{(k_1 + k_2)}(k_2 + k_1 e^{-(k_1+k_2)t}) + \frac{[A_2]_0 k_2}{(k_1 + k_2)}(1 - e^{-(k_1+k_2)t})$$

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Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

At time t=0 both A_1 and A_2 are present, that is $[A_1] = [A_1]_0$ and $[A_2] = [A_2]_0$

$$[A_1]_0 + [A_2]_0 = [A_1] + [A_2]$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

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$$\mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

$$\mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[\mathrm{A}_1]}{dt} = k_1[\mathrm{A}_1] - k_2[\mathrm{A}_2]$$

$$-\frac{d[\mathrm{A}_2]}{dt} = k_2[\mathrm{A}_2] - k_1[\mathrm{A}_1]$$

$$\begin{pmatrix} \frac{d[\mathrm{A}_1]}{dt} \\ \frac{d[\mathrm{A}_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [\mathrm{A}_1] \\ [\mathrm{A}_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

We define an orthogonal matrix **P** which is invertible such that :

$$\mathbf{A} = \mathbf{PB}$$

In addition :

$$\mathbf{P}^{-1}\mathbf{KP} = \Lambda$$

where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

Linear algebra methods

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

The differential equation for this mechanism is:

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where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

d**B**/dt = $\mathbf{P}^{-1}$d**A**/dt = $\mathbf{P}^{-1}\mathbf{KA}$ = $\mathbf{P}^{-1}\mathbf{KPB}$

$$\frac{d\mathbf{B}}{dt} = \mathbf{P}^{-1}\mathbf{KPB} = \Lambda\mathbf{B}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[\mathrm{A}_1]}{dt} = k_1[\mathrm{A}_1] - k_2[\mathrm{A}_2]$$

$$-\frac{d[\mathrm{A}_2]}{dt} = k_2[\mathrm{A}_2] - k_1[\mathrm{A}_1]$$

$$\begin{pmatrix} \frac{d[\mathrm{A}_1]}{dt} \\ \frac{d[\mathrm{A}_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [\mathrm{A}_1] \\ [\mathrm{A}_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

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In addition :

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where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

$$\frac{d\mathbf{B}}{dt} = \mathbf{P}^{-1}\mathbf{KPB} = \Lambda\mathbf{B}$$

↓ Solution

$$\mathbf{B} = e^{\Lambda t}\mathbf{B}_i$$

$\mathbf{B}_i$ is the vector of initial values of **B**

And at t = 0: $\mathbf{A}_i = \mathbf{PB}_i$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

We define an orthogonal matrix **P** which is invertible such that :

$$\mathbf{A} = \mathbf{PB} \Longrightarrow \mathbf{P}^{-1}\mathbf{A} = \mathbf{B}$$

In addition :

$$\mathbf{P}^{-1}\mathbf{KP} = \Lambda$$

where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

$$\frac{d\mathbf{B}}{dt} = \mathbf{P}^{-1}\mathbf{KPB} = \Lambda\mathbf{B}$$

$$\Downarrow$$

$$\mathbf{B} = e^{\Lambda t}\mathbf{B}_i$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

The differential equation for this mechanism is:

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

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$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

We define an orthogonal matrix **P** which is invertible such that :

$$\mathbf{A} = \mathbf{PB} \longrightarrow \mathbf{P}^{-1}\mathbf{A} = \mathbf{B}$$

In addition :

$$\mathbf{P}^{-1}\mathbf{KP} = \Lambda$$

where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

$$\frac{d\mathbf{B}}{dt} = \mathbf{P}^{-1}\mathbf{KPB} = \Lambda\mathbf{B}$$

$$\downarrow$$

$$\mathbf{B} = e^{\Lambda t}\mathbf{B}_i$$

$$\downarrow$$

$$\boxed{\mathbf{P}^{-1}\mathbf{A} = e^{\Lambda t}\mathbf{B}_i = e^{\Lambda t}\mathbf{P}^{-1}\mathbf{A}_i}$$

Linear algebra methods

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

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$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

We define an orthogonal matrix **P** which is invertible such that :

$$\mathbf{A} = \mathbf{PB} \Longrightarrow \mathbf{P}^{-1}\mathbf{A} = \mathbf{B}$$

In addition :

$$\mathbf{P}^{-1}\mathbf{KP} = \Lambda$$

where Λ is the matrix of negative eigenvalues with $-\lambda_1, -\lambda_2, \ldots -\lambda_n$

$$\mathbf{P}^{-1}\mathbf{A} = e^{\Lambda t}\mathbf{B}_i = e^{\Lambda t}\mathbf{P}^{-1}\mathbf{A}_i$$

Multiplying through by **P** from the left :

$$\mathbf{A} = \mathbf{P}e^{\Lambda t}\mathbf{P}^{-1}\mathbf{A}_i$$

Linear algebra methods

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

$$\mathbf{A} = \mathbf{P}\, e^{\Lambda t}\, \mathbf{P}^{-1}\, \mathbf{A}_i$$

We must find the matrix **P** that diagonalizes **K**t :

$$\det(\mathbf{K} - \Lambda \mathbf{1}) = 0$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

$$-\frac{d[A_2]}{dt} = k_2[A_2] - k_1[A_1]$$

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$$\det(\mathbf{K} - \Lambda \mathbf{I}) = 0$$

$$(-k_1 - \lambda)(-k_2 - \lambda) - k_1 k_2 = 0$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[\mathrm{A}_1]}{dt} = k_1[\mathrm{A}_1] - k_2[\mathrm{A}_2]$$

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$$\begin{pmatrix} \dfrac{d[\mathrm{A}_1]}{dt} \\ \dfrac{d[\mathrm{A}_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [\mathrm{A}_1] \\ [\mathrm{A}_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

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$$(-k_1 - \lambda)(-k_2 - \lambda) - k_1 k_2 = 0$$

$$\lambda_1 = 0 \quad \text{and} \quad \lambda_2 = -(k_1 + k_2)$$

$$\mathbf{P}_1 = \begin{pmatrix} k_2 \\ k_1 \end{pmatrix} \quad \text{and} \quad \mathbf{P}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

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The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

$$\mathbf{A} = \mathbf{P}\, e^{\Lambda t}\, \mathbf{P}^{-1}\, \mathbf{A}_i$$

We must find the matrix **P** that diagonalizes **K**t :

$$\det(\mathbf{K} - \Lambda\mathbf{1}) = 0$$

$$(-k_1 - \lambda)(-k_2 - \lambda) - k_1 k_2 = 0$$

$$\lambda_1 = 0 \quad \text{and} \quad \lambda_2 = -(k_1 + k_2)$$

$$\mathbf{P}_1 = \begin{pmatrix} k_2 \\ k_1 \end{pmatrix} \quad \text{and} \quad \mathbf{P}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\mathbf{P} = \begin{pmatrix} k_2 & 1 \\ k_1 & -1 \end{pmatrix}$$, which diagonalizes **K**t

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[A_1]}{dt} = k_1[A_1] - k_2[A_2]$$

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$$\begin{pmatrix} \frac{d[A_1]}{dt} \\ \frac{d[A_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix}$$

The differential equation for this mechanism is:

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

$$\mathbf{A} = \mathbf{P}\, e^{\Lambda t}\, \mathbf{P}^{-1}\, \mathbf{A}_i$$

$$\lambda_1 = 0 \quad \text{and} \quad \lambda_2 = -(k_1 + k_2)$$

$$\mathbf{P} = \begin{pmatrix} k_2 & 1 \\ k_1 & -1 \end{pmatrix} \qquad \mathbf{P}^{-1} = \begin{pmatrix} \frac{1}{(k_1 + k_2)} & \frac{1}{(k_1 + k_2)} \\ \frac{k_1}{(k_1 + k_2)} & \frac{-k_2}{(k_1 + k_2)} \end{pmatrix}$$

$$\mathbf{A} = \begin{pmatrix} [A_1] \\ [A_2] \end{pmatrix} = \frac{A_0}{(k_1 + k_2)} \begin{pmatrix} k_2 + k_1 e^{-(k_1 + k_2)t} \\ k_1 + k_1 e^{-(k_1 + k_2)t} \end{pmatrix}$$

Linear algebra methods

$$A_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} A_2 \qquad \mathbf{K} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}$$

$$-\frac{d[\mathrm{A}_1]}{dt} = k_1[\mathrm{A}_1] - k_2[\mathrm{A}_2]$$

$$-\frac{d[\mathrm{A}_2]}{dt} = k_2[\mathrm{A}_2] - k_1[\mathrm{A}_1]$$

The differential equation for this mechanism is:

$$\begin{pmatrix} \frac{d[\mathrm{A}_1]}{dt} \\ \frac{d[\mathrm{A}_2]}{dt} \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix} \begin{pmatrix} [\mathrm{A}_1] \\ [\mathrm{A}_2] \end{pmatrix}$$

$$\frac{d\mathbf{A}}{dt} = \mathbf{KA}$$

$$\mathbf{A} = \mathbf{P}\, e^{\Lambda t}\, \mathbf{P}^{-1}\, \mathbf{A}_i$$

$$\lambda_1 = 0 \quad \text{and} \quad \lambda_2 = -(k_1 + k_2)$$

$$\mathbf{P} = \begin{pmatrix} k_2 & 1 \\ k_1 & -1 \end{pmatrix} \qquad \mathbf{P}^{-1} = \begin{pmatrix} \frac{1}{(k_1 + k_2)} & \frac{1}{(k_1 + k_2)} \\ \frac{k_1}{(k_1 + k_2)} & \frac{-k_2}{(k_1 + k_2)} \end{pmatrix}$$

$$\mathbf{A} = \begin{pmatrix} [\mathrm{A}_1] \\ [\mathrm{A}_2] \end{pmatrix} = \frac{A_0}{(k_1 + k_2)} \begin{pmatrix} k_2 + k_1 e^{-(k_1 + k_2)t} \\ k_1 + k_1 e^{-(k_1 + k_2)t} \end{pmatrix}$$

This approach is fine for any set of first-order or pseudo first-order equations.