EQUAÇÃO ESTEQUIOMÉTRICA DA REACÇÃO DE CRESCIMENTO

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \beta CH_xO_yN_z + \gamma CO_2 + \delta H_2O$$

EQUAÇÃO ESTEQUIOMÉTRICA DA REACÇÃO DE CRESCIMENTO COM BAIXA PRODUÇÂO DE PRODUTOS EXTRACELULARES β=0

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \gamma CO_2 + \delta H_2O$$

QUOCIENTE RESPIRATÓRIO

$$\gamma / b = RQ$$

$\gamma / b = RQ$ é o quociente respiratório

exemplo:

se $RQ = 0.85 \Leftrightarrow b = \gamma / 0.85 \Leftrightarrow b = 118$

EQUAÇÃO ESTEQUIOMÉTRICA DA REACÇÃO DE CRESCIMENTO

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \beta CH_xO_yN_z + \gamma CO_2 + \delta H_2O$$

Coeficientes estequiométricos:

1 - fonte de carbono
a - amónia
b - oxigénio

α – **biomassa**
β – **produto extracelular**
γ – **anidrido carbónico**
δ – **água**

base de cálculo: 1 mole de fonte de carbono (ex.: glucose)

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \beta CH_xO_yN_z + \gamma CO_2 + \delta H_2O$$

se $\beta \approx 0$

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \gamma CO_2 + \delta H_2O$$

	1	a	b	α	β	γ	δ
C	6	0	0	1.0α	0	1.0γ	0
H	12	$3a$	0	1.8α	0	0	2δ
N	0	a	0	0.2α	0	0	0
O	6	0	$2b$	0.5α	0	2.0γ	1δ

	1	a	b	α	β	γ	δ
C	6	0	0	1.0α	0	1.0γ	0
H	12	3a	0	1.8α	0	0	2δ
N	0	a	0	0.2α	0	0	0
O	6	0	2b	0.5α	0	2.0γ	1δ

C (balanço ao carbono) $6=\alpha+\gamma$
H (balanço ao hidrogénio) $12+3a=1.8\alpha+2.0\delta$
N (balanço ao azoto) $a=0.2\alpha$
O (balanço ao oxigénio) $6+2b=0.5\alpha+2.0\gamma+\delta$
íncógnitas: a,b, α,β,γ e δ
equações: 4 e o quociente respiratório (RQ)
RQ=γ/β=0.85

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \beta CH_xO_yN_z + \gamma CO_2 + \delta H_2O$$

	1	a	b	α	β	γ	δ
C	6	0	0	1.0α	0	1.0γ	0
H	12	3a	0	1.8α	0	0	2δ
N	0	a	0	0.2α	0	0	0
O	6	0	2b	0.5	0	2.0	1δ
RQ			1b			0.85γ	

	1	a	b	α	β	γ	δ
C	6	0	0	1.0α	0	1.0γ	0
H	12	3a	0	1.8α	0	0	2δ
N	0	a	0	0.2α	0	0	0
O	6	0	2b	0.5	0	2.0	1δ
RQ			118b			1.0γ	

	1	a	b	α	β	γ	δ
C	6	0	0	1.0α	0	1.0γ	0
H	12	3a	0	1.8α	0	0	2δ
N	0	a	0	0.2α	0	0	0
O	6	0	2b	0.5	0	2.0	1δ
RQ			118b			1.0γ	

$$\begin{bmatrix} 6 + 0a + 0b = 1\alpha + 0\beta + 1.0\gamma + 0\delta \\ 12 + 3a + 0b = 1.8\alpha + 0\beta + 0\gamma + 2\delta \\ 0 + a + 0b = 0.2\alpha + 0\beta + 0\gamma + 0\delta \\ 6 + 0a + 2b = 0.5\alpha + 0\beta + 2.0\gamma + 1\delta \\ 0 + 0a + 118b = 0\alpha + 0\beta + 1.0\gamma + 0\delta \end{bmatrix}$$

$$\begin{bmatrix} 6 + 0a + 0b = 1\alpha + 0\beta + 1.0\gamma + 0\delta \\ 12 + 3a + 0b = 1.8\alpha + 0\beta + 0\gamma + 2\delta \\ 0 + a + 0b = 0.2\alpha + 0\beta + 0\gamma + 0\delta \\ 6 + 0a + 2b = 0.5\alpha + 0\beta + 2.0\gamma + 1\delta \\ 0 + 0a + 1.18b = 0\alpha + 0\beta + 1.0\gamma + 0\delta \end{bmatrix}$$

$$\begin{bmatrix} 1.00\alpha + 0.00\beta + 1.00\gamma + 0.00\delta - 0.00a - 0.00b = 6 \\ 1.80\alpha + 0.00\beta + 0.00\gamma + 2.00\delta - 3.00a - 0.00b = 12 \\ 0.20\alpha + 0.00\beta + 0.00\gamma + 0.00\delta - 1.00a - 0.00b = 0 \\ 0.50\alpha + 0.00\beta + 2.00\gamma + 1.00\delta - 0.00a - 2.00b = 6 \\ 0.00\alpha + 0.00\beta + 1.00\gamma + 0.00\delta - 0.00a - 1.18b = 0 \end{bmatrix}$$

SISTEMA DE EQUAÇÕES:

$$\begin{bmatrix} 1.00\alpha + 0.00\beta + 1.00\gamma + 0.00\delta - 0.00a - 0.00b = 6 \\ 1.80\alpha + 0.00\beta + 0.00\gamma + 2.00\delta - 3.00a - 0.00b = 12 \\ 0.20\alpha + 0.00\beta + 0.00\gamma + 0.00\delta - 1.00a - 0.00b = 0 \\ 0.50\alpha + 0.00\beta + 2.00\gamma + 1.00\delta - 0.00a - 2.00b = 6 \\ 0.00\alpha + 0.00\beta + 1.00\gamma + 0.00\delta - 0.00a - 1.18b = 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{MATRIZ DE} \\ \text{COEFICIENTES} \end{bmatrix} * \begin{bmatrix} \text{MATRIZ DE} \\ \text{INCÓGNITAS} \end{bmatrix} = \begin{bmatrix} \text{MATRIZ DE} \\ \text{RESULTADOS} \end{bmatrix}$$

$$\begin{matrix} \alpha & \gamma & \delta & a & b \end{matrix}$$
$$\begin{bmatrix} 1.00 & 1.00 & 0.00 & -0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -1.18 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix} * \begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix}\text{MATRIZ DE}\\ \text{COEFICIENTES}\end{bmatrix} * \begin{bmatrix}\text{MATRIZ DE}\\ \text{INCÓGNITAS}\end{bmatrix} = \begin{bmatrix}\text{MATRIZ DE}\\ \text{RESULTADOS}\end{bmatrix}$$

$$\begin{bmatrix}\text{MATRIZ DE}\\ \text{INCÓGNITAS}\end{bmatrix} = \begin{bmatrix}\text{MATRIZ DE}\\ \text{COEFICIENTES}\end{bmatrix}^{-1} * \begin{bmatrix}\text{MATRIZ DE}\\ \text{RESULTADOS}\end{bmatrix}$$

$$\begin{bmatrix}\text{MATRIZ DE}\\ \text{COEFICIENTES}\end{bmatrix}^{-1} = \text{é a matriz inversa dos coeficientes}$$

$$\begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -118 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix} * \begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix}\text{MATRIZ DE}\\ \text{INCÓGNITAS}\end{bmatrix} = \begin{bmatrix}\text{MATRIZ DE}\\ \text{COEFICIENTES}\end{bmatrix}^{-1} * \begin{bmatrix}\text{MATRIZ DE}\\ \text{RESULTADOS}\end{bmatrix}$$

$$\begin{bmatrix}\text{MATRIZ DE}\\ \text{COEFICIENTES}\end{bmatrix}^{-1} = \text{é a matriz inversa dos coeficientes}$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -118 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix}^{-1} * \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -1.18 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix}^{-1} * \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} \text{MATRIZ INVERSA} \\ \\ \text{DOS COEFICIENTES} \end{bmatrix} = \begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -1.18 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix}^{-1}$$

$$\begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -1.18 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix}^{-1} = \begin{bmatrix} 0.75 & 1.23 & -3.70 & 4.18 & -2.47 \\ 0.25 & -1.23 & 3.70 & -4.18 & 2.47 \\ -0.45 & -0.24 & 0.72 & -2.51 & 1.48 \\ 0.15 & 0.25 & -1.74 & 0.84 & -0.49 \\ 0.21 & -1.05 & 3.14 & -4.39 & -2.09 \end{bmatrix}$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 1.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 1.80 & 0.00 & 2.00 & -3.00 & 0.00 \\ 0.20 & 0.00 & 0.00 & -1.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & -1.18 \\ 0.50 & 2.00 & 1.00 & 0.00 & -2.00 \end{bmatrix}^{-1} * \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 0.75 & 1.23 & -3.70 & 4.18 & -2.47 \\ 0.25 & -1.23 & 3.70 & -4.18 & 2.47 \\ -0.45 & -0.24 & 0.72 & -2.51 & 1.48 \\ 0.15 & 0.25 & -1.74 & 0.84 & -0.49 \\ 0.21 & -1.05 & 3.14 & -4.39 & -2.09 \end{bmatrix} * \begin{bmatrix} 6 \\ 12 \\ 0 \\ 0 \\ 6 \end{bmatrix}$$

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \gamma CO_2 + \delta H_2O$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 4.52 \\ 1.48 \\ 3.29 \\ 0.90 \\ 1.26 \end{bmatrix}$$

$$C_6H_{12}O_6 + aNH_3 + bO_2 \Rightarrow \alpha CH_{1.8}O_{0.5}N_{0.2} + \gamma CO_2 + \delta H_2O$$

$$\begin{bmatrix} \alpha \\ \gamma \\ \delta \\ a \\ b \end{bmatrix} = \begin{bmatrix} 4.52 \\ 1.48 \\ 3.29 \\ 0.90 \\ 1.26 \end{bmatrix}$$

$$C_6H_{12}O_6 + 0.90NH_3 + 1.26O_2 \Rightarrow 4.52CH_{1.8}O_{0.5}N_{0.2} + 1.48CO_2 + 3.29H_2O$$

AUXILIAR DE CÁLCULOS COM MATRIZES

a) Produto de matrizes

$$\begin{bmatrix} a_{11} & a_{12} & \dots & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ a_{k1} & a_{k2} & \dots & \dots & a_{kn} \end{bmatrix} * \begin{bmatrix} b_{11} & b_{12} & \dots & \dots & b_{1p} \\ b_{21} & a_{22} & \dots & \dots & b_{2p} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & \dots & a_{np} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & \dots & \dots & c_{1p} \\ c_{21} & c_{22} & \dots & \dots & c_{2p} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ c_{k1} & a_{k2} & \dots & \dots & c_{kp} \end{bmatrix}$$

$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + \dots a_{1n}b_{n1}$$

$$c_{12} = a_{11}b_{12} + a_{12}b_{22} + \dots a_{1n}b_{n2}$$

$\Rightarrow A * B \neq B * A$

$\Rightarrow A * B = A * C$ **não implica B=C**

$\Rightarrow A * B = 0$ mesmo com $A \neq 0$ e $B \neq 0$

$$c_{kp} = a_{k1}b_{1p} + a_{k2}b_{2p} + \dots + a_{kn}b_{np}$$

O produto de matrizes não é propriedade comutativa

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

$$x1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}} \qquad x_2 = \frac{\begin{vmatrix} a_{11} & b_1 & a_{13} \\ a_{21} & b_2 & a_{23} \\ a_{31} & b_3 & a_{33} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}} \qquad x_3 = \frac{\begin{vmatrix} a_{11} & a_{12} & b_1 \\ a_{21} & a_{22} & b_2 \\ a_{31} & a_{32} & b_3 \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}}$$