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BIOMASS PROTOCOL:
A Process Simulation Approach

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Parâmetros

Tolerância (sugerida): $Tol = 0.05$

Massa atômica (Hysys 8.8):

- $M_C^0 = 12.0108003616333$
- $M_H^0 = 1.00800001621246$
- $M_O^0 = 16.0000000000000$
- $M_N^0 = 14.0065002441406$
- $\underline{M}^0 = \begin{bmatrix} M_C^0 \\ M_H^0 \\ M_O^0 \\ M_N^0 \end{bmatrix}$

Exemplo de componentes modelos (1ª tentativa):

- $HHV_{sacarose}^{molar}\ (kJ/kmol) = 5611650$
- $HHV_{antraceno}^{molar}(kJ/kmol) = 1430510$
- $HHV_{anidmaleic}^{molar}(kJ/kmol) = 2364320$
- $HHV_{piridazina}^{molar}\ (kJ/kmol) = 7052350$

Pré-Processamento Tipo I

Entra composição aprox. e elementar em base de fração mássica ($\underline{m}$):

- *af (ash-free):* $\underline{m}^{af} = [\ m_{H2O}^{af}\ , m_{FC}^{ar}\ ,\ m_{VM}^{ar}]$ | $\sum_j m_j^{af} = 1$
- *ar (as received)*: $\underline{m}^{ar} = [\ m_{ash}^{ar}\ ,\ m_{FC}^{ar}\ ,\ m_{VM}^{ar}\ ,\ m_{H2O}^{ar}\ ]$ | $\sum_j m_j^{ar} = 1$
- *db (dry basis)*: $\underline{m}^{db} = [\ m_{ash}^{db}\ ,\ m_C^{db}\ ,\ m_H^{db}\ ,\ m_O^{db}\ ,\ m_N^{db}\ ]$ | $\sum_j m_j^{db} = 1$
- *daf (dry-ash-free basis)*: $\underline{m}^{daf} = [m_C^{daf}, m_H^{daf}, m_O^{daf}, m_N^{daf}]$ | $\sum_j m_j^{daf} = 1$

0, $$HHV_{ref}^{daf} = \left(\frac{1}{1 - m_{H2O}^{ar} - m_{ash}^{ar}}\right) HHV_{ref}^{ar} = \left(\frac{1}{1 - m_{ash}^{db}}\right) HHV_{ref}^{db} = \left(\frac{1}{1 - m_{H2O}^{af}}\right) HHV_{ref}^{af}$$

1, $$w_i^0 = \ m_i^{daf} = \left(\frac{1}{1 - m_{ash}^{db}}\right) m_i^{db}\ , \qquad \forall\ i\ \epsilon\ \{\ C, H, O, N\ \}$$

2, $$y_i^0 = \frac{w_i^0}{M_i^0}\ , \qquad \forall\ i\ \epsilon\ \{\ C, H, O, N\ \}$$

3, $$MM^0 = \frac{1}{\sum_i y_i^0}$$

4, $$z_i^0 = MM^0 * y_i^0\ , \qquad \forall\ i\ \epsilon\ \{\ C, H, O, N\ \}$$

Pré-Processamento Tipo II

Entra fórmula mínima: relação molar $[H/C], [O/C], [N/C]$

Entra composição aprox. em base de fração mássica ($\underline{m}$):

- *af (ash-free):* $\underline{m}^{af} = [\ m^{af}_{H2O}\ , m^{ar}_{FC}\ ,\ m^{ar}_{VM}\ ] \quad | \quad \sum_j m^{af}_j = 1$
- *ar (as received)*: $\underline{m}^{ar} = [\ m^{ar}_{ash}\ ,\ m^{ar}_{FC}\ ,\ m^{ar}_{VM}\ ,\ m^{ar}_{H2O}\ ] \quad | \quad \sum_j m^{ar}_j = 1$
- *db (dry basis)*: $\underline{m}^{db} = [\ m^{db}_{ash}\ ,\ m^{ar}_{FC}\ ,\ m^{ar}_{VM}\ ] \quad | \quad \sum_j m^{db}_j = 1$

0, $$HHV^{daf}_{ref} = \left(\frac{1}{1 - m^{ar}_{H2O} - m^{ar}_{ash}}\right) HHV^{ar}_{ref} = \left(\frac{1}{1 - m^{db}_{ash}}\right) HHV^{db}_{ref} = \left(\frac{1}{1 - m^{af}_{H2O}}\right) HHV^{af}_{ref}$$

1, $$z^0_C = \frac{1}{1 + [H/C] + [O/C] + [N/C]}$$

2, $$z^0_H = z^0_C * [H/C]$$

3, $$z^0_O = z^0_C * [O/C]$$

4, $$z^0_N = z^0_C * [N/C]$$

Main Routine

5, Entra componentes modelos: $\begin{cases} comp1\text{: } C_{[a_{11}]}H_{[a_{12}]}O_{[a_{13}]}N_{[a_{14}]},\ HHV_1^{molar}\ conhecido \\ comp2\text{: } C_{[a_{21}]}H_{[a_{22}]}O_{[a_{23}]}N_{[a_{24}]},\ HHV_2^{molar}\ conhecido \\ comp3\text{: } C_{[a_{31}]}H_{[a_{32}]}O_{[a_{33}]}N_{[a_{34}]},\ HHV_3^{molar}\ conhecido \\ comp4\text{: } C_{[a_{41}]}H_{[a_{42}]}O_{[a_{43}]}N_{[a_{44}]},\ HHV_4^{molar}\ conhecido \end{cases}$

6, Montar matriz de nº de átomos e vetor HHV: $\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$, $\underline{HHV}^{molar} = \begin{bmatrix} HHV_1^{molar} \\ HHV_2^{molar} \\ HHV_3^{molar} \\ HHV_4^{molar} \end{bmatrix}$

7, $\underline{\boldsymbol{M}} = \underline{\underline{\boldsymbol{A}}}.\underline{\boldsymbol{M^0}}$, $\underline{M}^0 = \left[M_C^0, M_H^0, M_O^0, M_N^0 \right]^T$

8, $\underline{\boldsymbol{x}}^* = \underline{\boldsymbol{z^0}}.\underline{\underline{\boldsymbol{A}}}^{-1}$, $\underline{z}^0 = [\ z_C^0\ ,\ z_H^0\ ,\ z_O^0\ ,\ z_N^0\ ]$

9, $\underline{\boldsymbol{x}} = \dfrac{\underline{\boldsymbol{x}}^*}{\sum_i x_i^*}$, $\underline{x} = [\ x_1\ ,\ x_2\ ,\ x_3\ ,\ x_4\ ]$

10, Se $0 \le x_i \le 1,\ \forall i \epsilon \{1, \dots, 4\}$, prosseguir.

$Senão,$ escolher nova combinação de componentes modelos e retornar para passo 5.

Validação via HHV

11. $MM = \underline{\boldsymbol{x}} . \underline{\boldsymbol{M}}$

12. $H\widehat{H}V^{daf} = MM^{-1} . \underline{\boldsymbol{x}} . \boldsymbol{H}\underline{\boldsymbol{H}}\boldsymbol{V}^{\boldsymbol{molar}}$

13, $Erro = \varepsilon = \dfrac{H\widehat{H}V^{daf} - HHV_{ref}^{daf}}{HHV_{ref}^{daf}}$

14, $Se \quad |\varepsilon| \leq Tol$, prosseguir (modelo validado).

$Senão$, escolher uma nova combinação de componentes modelos e retornar para passo 5.

Processamento Final

$$15, \qquad h_i = M_i . x_i \quad , \qquad \forall\, i \in \{1, \dots, 4\}$$

$$16, \qquad w_i = h_i / MM \quad , \qquad \forall\, i \in \{1, \dots, 4\}$$

Simulação sem cinzas:

$$17a, \qquad m_i^{*,af} = w_i \left(1 - \frac{m_{H2O}^{ar}}{1 - m_{ash}^{ar}} \right),$$

$$= w_i \left(1 - m_{H2O}^{af} \right),$$

$$\forall\, i \in \{1, \dots, 4\}$$

$$18b, \qquad \underline{m}^{*,ar} = [m_1^{*,af}, m_2^{*,af}, m_3^{*,af}, m_4^{*,af}, m_{H2O}^{af}]$$

Simulação com cinzas:

$$17b, \qquad m_i^{*,ar} = w_i \left(1 - m_{H2O}^{af} - m_{H2O}^{af} \right),$$

$$\forall\, i \in \{1, \dots, 4\}$$

$$18b, \qquad \underline{m}^{*,ar} = [m_1^{*,ar}, m_2^{*,ar}, m_3^{*,ar}, m_4^{*,ar}, m_{H2O}^{ar}, m_{ash}^{ar}]$$