Formula for chemical systems

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2.9 Chemical Reaction System

- collection of chemical species, each composed of a number of elements

ex. For chemical system w/ species CH_4, S_2, CS_2, H_2S,

For elements C, H, S, formula vectors are:

$CH_4: \begin{bmatrix}1\\4\\0\end{bmatrix}$, $S_2: \begin{bmatrix}0\\0\\2\end{bmatrix}$, $CS_2: \begin{bmatrix}1\\0\\2\end{bmatrix}$, $H_2S: \begin{bmatrix}0\\2\\1\end{bmatrix}$ (C, H, S)

Formula matrix: $A = \begin{array}{c} \\ C \\ H \\ S \end{array}\begin{array}{c} \begin{array}{cccc} CH_4 & S_2 & CS_2 & H_2S \end{array} \\ \begin{bmatrix} 1 & 0 & 1 & 0 \\ 4 & 0 & 0 & 2 \\ 0 & 2 & 2 & 1 \end{bmatrix} \end{array}$

For n_1 moles of CH_4, n_2 moles of S_2, n_3 moles of CS_2, n_4 moles of H_2S

$\vec{b} = n_1\begin{bmatrix}1\\4\\0\end{bmatrix} + n_2\begin{bmatrix}0\\0\\2\end{bmatrix} + n_3\begin{bmatrix}1\\0\\2\end{bmatrix} + n_4\begin{bmatrix}0\\2\\1\end{bmatrix} \longrightarrow b_1, b_2, b_3$ = molar amounts of species

↳ $\vec{b} = A\vec{n} \longrightarrow \vec{n} = [n_1, n_2, n_3, n_4]$ (species abundance vector)

ex. Chemical Reaction: $CH_4 + 2S_2 = CS_2 + 2H_2S$

$\begin{bmatrix}1\\4\\0\end{bmatrix} + 2\begin{bmatrix}0\\0\\2\end{bmatrix} = \begin{bmatrix}1\\0\\2\end{bmatrix} + 2\begin{bmatrix}0\\2\\1\end{bmatrix}$

- every possible chemical reaction in the system corresponds to a vector in $N(A)$

$A = \begin{bmatrix}1&0&1&0\\4&0&0&2\\0&2&2&1\end{bmatrix}$, $\text{ref}(A) = \begin{bmatrix}1&0&0&1/2\\0&1&0&1\\0&0&1&-1/2\end{bmatrix}$

$\therefore N(A) = \text{span}\left\{\begin{bmatrix}-1/2\\-1\\1/2\\1\end{bmatrix}\right\}$

Finding corresponding chemical reaction

① Use basis vectors → integer multiples of $N(A)$

$N(A) = \text{span}\left\{\begin{bmatrix}-1/2\\-1\\1/2\\1\end{bmatrix}\right\} = \text{span}\left\{\begin{bmatrix}-1\\-2\\1\\2\end{bmatrix}\right\}$

② $A\begin{bmatrix}-1\\-2\\1\\2\end{bmatrix} = A\left(\begin{bmatrix}0\\0\\1\\2\end{bmatrix} - \begin{bmatrix}1\\2\\0\\0\end{bmatrix}\right) = 0 \longrightarrow A\begin{bmatrix}0\\0\\1\\2\end{bmatrix} = A\begin{bmatrix}1\\2\\0\\0\end{bmatrix}$ → Reaction structure

(reaction coeff.)

③ $1CS_2 + 2H_2S = 1CH_4 + 2S_2$

↳ 1 × col#3 + 2 × col#4 = 1 × col#1 + 2 × col#2

ex. Chemical System w/ CH_4, S_2, CS_2, H_2S, H_2

$B = \begin{array}{c} \\ C \\ H \\ S \end{array}\begin{array}{c} \begin{array}{ccccc} CH_4 & S_2 & CS_2 & H_2S & H_2 \end{array} \\ \begin{bmatrix} 1&0&1&0&0 \\ 4&0&0&2&2 \\ 0&2&2&1&0 \end{bmatrix} \end{array} \longrightarrow \text{ref}(B) = \begin{bmatrix}1&0&0&1/2&1/2\\0&1&0&1&1/2\\0&0&1&-1/2&-1/2\end{bmatrix}$

$N(B) = \text{span}\left\{\begin{bmatrix}-1\\-2\\1\\2\\0\end{bmatrix}, \begin{bmatrix}-1\\-1\\1\\0\\2\end{bmatrix}\right\}$

↳ $x_4 = s$, $x_5 = t$

$2x_1 + s + t = 0 \longrightarrow x_1 = -1/2\,s - 1/2\,t$

$2x_2 + 2s + t = 0 \longrightarrow x_2 = -s - 1/2\,t$

$2x_3 - s - t = 0 \longrightarrow x_3 = 1/2\,s + 1/2\,t$

$\longrightarrow s\begin{bmatrix}-1\\-2\\2\\1\\0\end{bmatrix} + t\begin{bmatrix}-1\\-1\\1\\0\\2\end{bmatrix}$

- ∴ 2 possible chemical reactions: [0] [1]

$\left\{ \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \end{bmatrix} \right\}$ $\quad 2x_3 - s - t = 0 \rightarrow x_3 = \frac{1}{2}s + \frac{1}{2}t$ $\quad \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \end{bmatrix}$

- $\therefore$ 2 possible chemical reactions:

① $CS_2 + 2H_2S = CH_4 + 2S_2 \longrightarrow A\begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \\ 0 \end{bmatrix} = A\begin{bmatrix} 1 \\ 1 \\ 8 \\ 8 \end{bmatrix}$

② $CS_2 + 2H_2 = CH_4 + S_2$

- All other chem reactions are lin. combs of ① & ②

ex. $5① + 2②$: $7CS_2 + 10H_2S + 4H_2 = 7CH_4 + 12S_2$