Ammonia Synthesis Reactor

This script demonstrates a degree of freedom analysis and solution of material balances for a simple model of an ammonia synthesis reactor. The problem is quoted from Example 2.8, page 108, of Murphy (2005).

Contents

Required Functions

- `CVX`
- `displaytable.m`

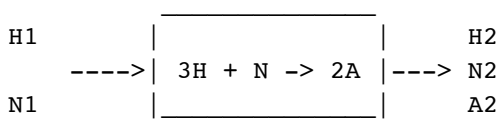
Problem Statement (Murphy, Example 2.8, page 108)

"A gas mixture of hydrogen and nitrogen is fed to a reactor, where they react to form ammonia, NH_3. The N_2 flowrate into the reactor is 150 gmol/h and the hydrogen is fed at a ratio of 4 gmol H_2 per gmol N_2. The balanced chemical reaction is

$$N_2 + 3H_2 \longrightarrow 2NH_3$$

Of the nitrogen fed to the reactor, 30% leaves in the reactor outlet stream; the rest is consumed by reaction. The reactor operates at steady state. Determine the DOF."

Flow Diagram



CVX Model

The CVX modell demonstrate identifies 6 variables, and 6 equations. Therefore there are 0 degrees of freedom.

```
cvx_begin quiet

    % Stream Variables (5)
    variables H1 N1             % Stream 1
    variables H2 N2 A2          % Stream 2

    % System Variables (1)
    variables X                 % Extent of reaction

    % Stream Specifications (3)
    N1 == 150;                  % Inlet flow of N2, gmol/h
    H1 == 4*N1;                 % 4:1 molar ratio of H2 to N2
    N2 == (1-0.7)*N1;           % 70% conversion of N2
```

```
    % Material Balances (3)
    0 == H1 - H2 - 3*X;         % Hydrogen
    0 == N1 - N2 - X;           % Nitrogen
    0 ==    - A2 + 2*X;         % Ammonia

cvx_end
```

Display Stream Table

This part requires `displaytable.m` to be present in the Matlab path. If necessary, download here https://raw.githubusercontent.com/jckantor/CBE20255/master/matlab/displaytable.m and place in your Matlab directory.

```
species = {'H2','N2','NH3'};
S = [H1 H2; N1 N2; 0  A2];

displaytable(S,species,'STRM');
```

```
     STRM(1)  STRM(2)
H2       600      285
N2       150       45
NH3        0      210
```

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