



Production of Hydrogen Through a Sulfur-Iodine Cycle Based on the Electrochemical Bunsen Reaction

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Background & Description:

The production of hydrogen through the sodium iodine cycle based on the electrochemical Bunsen reaction involves a series of chemical reactions that use water as the feedstock to produce hydrogen. This process is a promising and sustainable method for large-scale hydrogen production as it relies on renewable sources of energy and has minimal environmental impact. By using this process, hydrogen can be produced efficiently, which can be used in various applications such as fuel cells and as a feedstock to produce chemicals.

The production of hydrogen through sodium iodine cycle based on electrochemical Bunsen reaction involves three main reactions: Bunsen reaction, hydrogen iodide decomposition, and hydrogen sulfide decomposition.

1. Electrochemical Bunsen Reaction:

$$2H_2O + SO_2 + I_2 \, \rightarrow \, 2HI + H_2SO_4$$
 , Conversion Rate: 100%

- 2. H₂SO₄ Decomposition section:
 - a. H₂SO₄ Decomposer:

$$H_2SO_4 \rightarrow H_2O + SO_3$$
, Conversion Rate: 100%

b. SO3 Decomposer

$$SO_3 \rightarrow SO_2 + 0.5O_2$$
, Conversion Rate: 78%

3. HI Decomposition section:

$$2HI \rightarrow H_2 + I_2$$
, Conversion Rate: 40%

In this flowsheet, S-01 is the main feed of water, S-18 and S-31 are recycled HI and H₂SO₄ feeds respectively whereas S-26 and S-16 are the H₂ and O₂ product stream respectively.





Software & Flowsheet specifications:

1. DWSIM Version: 5.8.3

2. Thermodynamics: NRTL

3. Temperature: Kelvin

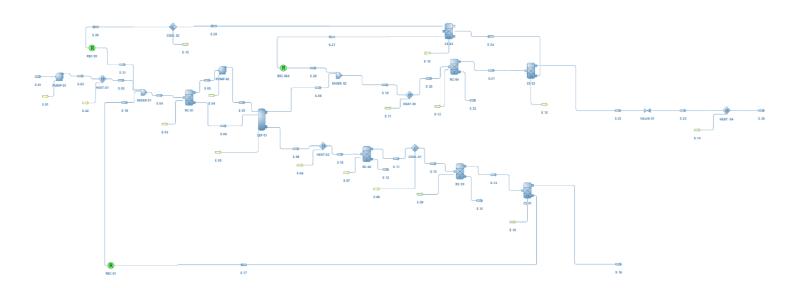
4. Pressure: MPa

5. Molar flow rate: mol/s

6. Mass flow rate: g/s

7. Volumetric flow rate: m³/s

Flowsheet:







Results:

| BUNSEN REACTOR | | | | | | | | | | | | |
|---|---------|---------|---------|----------|------------|----------|----------|----------|-------|--|--|--|
| Object | S-01 | S-02 | S-03 | S-04 | S-05 | S-06 | S-18 | S-31 | | | | |
| Temperature | 298.15 | 298.19 | 313 | 313.274 | 313 | 313 | 313 | 313 | К | | | |
| Pressure | 0.1 | 0.5 | 0.5 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | MPa | | | |
| Mass Flow | 18.0153 | 18.0153 | 18.0153 | 1919.25 | 206.491 | 1712.76 | 0 | 1901.24 | g/s | | | |
| Molar Flow | 1 | 1 | 1 | 36.53 | 1.68951 | 34.8405 | 0 | 35.53 | mol/s | | | |
| Molar Flow (Mixture) / Water | 1 | 1 | 1 | 24.989 | 0.0874991 | 24.9015 | 0 | 23.989 | mol/s | | | |
| Molar Flow (Mixture) / Hydrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s | | | |
| Molar Flow (Mixture) / Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s | | | |
| Molar Flow (Mixture) / Hydrogen iodide | 0 | 0 | 0 | 4.431 | 1.60044 | 2.83056 | 0 | 4.431 | mol/s | | | |
| Molar Flow (Mixture) / Iodine | 0 | 0 | 0 | 7.11 | 0.00156544 | 7.10843 | 0 | 7.11 | mol/s | | | |
| Molar Flow (Mixture) / Sulfur dioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s | | | |
| Molar Flow (Mixture) / Hydrogen Sulfide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s | | | |
| Molar Flow (Mixture) / Sulfur trioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s | | | |

| H2SO4 DECOMPOSITION | | | | | | | | | | | | |
|---|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-------|
| Object | S-06 | S-09 | S-10 | S-11 | S-12 | S-13 | S-14 | S-15 | S-16 | S-17 | S-18 | |
| Temperature | 313 | 329.304 | 1123 | 1123 | 1123 | 1123 | 313 | 313 | 313 | 313 | 313 | К |
| Pressure | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | MPa |
| Mass Flow | 1712.76 | 1564.46 | 1564.46 | 1564.46 | 0 | 1564.46 | 0 | 1564.46 | 15.9994 | 0 | 0 | g/s |
| Molar Flow | 34.8405 | 33.4337 | 33.4337 | 33.4337 | 0 | 33.4337 | 0 | 33.4337 | 0.5 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Water | 24.9015 | 24.6136 | 24.6136 | 24.6136 | 0 | 24.6136 | 0 | 24.6136 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Hydrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.5 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Hydrogen iodide | 2.83056 | 1.7172 | 1.7172 | 1.7172 | 0 | 1.7172 | 0 | 1.7172 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Iodine | 7.10843 | 7.10287 | 7.10287 | 7.10287 | 0 | 7.10287 | 0 | 7.10287 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Sulfur dioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Hydrogen Sulfide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Sulfur trioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | mol/s |

| HI DECOMPOSITION | | | | | | | | | | | | | | | |
|---|-------------|------------|-------------|-------------|-----------|----------|----------|-----------|---------|---------|----------|----------|----------|----------|-------|
| Object | 5-07 | 5-08 | 5-19 | S-20 | 5-21 | 5-22 | 5-23 | S-24 | S-25 | S-26 | S-27 | 5-28 | S-29 | 5-30 | |
| Temperature | 1435.69 | 329.304 | 713.123 | 723 | 723 | 723 | 723 | 723 | 723 | 313 | 723 | 723 | 723 | 313 | К |
| Pressure | 1.17 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | 0.1 | 0.1 | 0.101325 | 0.101325 | 0.101325 | 0.101325 | MPa |
| Mass Flow | 206.491 | 354.796 | 4728.36 | 4728.36 | 4728.36 | 0 | 2.01588 | 4727.27 | 2.01588 | 2.01588 | 4373.56 | 4373.56 | 1901.24 | 1901.24 | g/s |
| Molar Flow | 1.68951 | 3.0963 | 69.2857 | 69.2857 | 69.8285 | 0 | 1 | 69.2857 | 1 | 1 | 66.1894 | 66.1894 | 35.53 | 35.53 | mol/s |
| Molar Flow (Mixture) / Water | 0.0874991 | 0.375368 | 0.375368 | 0.375368 | 0.375368 | 0 | 0 | 0.375368 | 0 | 0 | 0 | 0 | 23.989 | 23.989 | mol/s |
| Molar Flow (Mixture) / Hydrogen | 0 | 0 | 0 | 0 | 0.542761 | 0 | 1 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Oxygen | 0 | 0 | 1.82 135 | 1.82135 | 1.82 135 | 0 | 0 | 1.82135 | 0 | 0 | 1.82135 | 1.82 135 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Hydrogen iodide | 1.60044 | 2.7138 | 2.7138 | 2.7138 | 1.62828 | 0 | 0 | 1.62828 | 0 | 0 | 0 | 0 | 4.431 | 4.431 | mol/s |
| Molar Fraction (Mixture) / Iodine | 0.000926564 | 0.00230267 | 0.000102904 | 0.000102904 | 0.0156477 | 0 | 0 | 0.0157702 | 0 | 0 | 0 | 0 | 0.200113 | 0.200113 | |
| Molar Flow (Mixture) / Sulfur dioxide | 0 | 0 | 57.4833 | 57.4833 | 57.4833 | 0 | 0 | 57.4833 | 0 | 0 | 57.4833 | 57.4833 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Hydrogen Sulfide | 0 | 0 | 4.52426 | 4.52426 | 4.52426 | 0 | 0 | 4.52426 | 0 | 0 | 4.52426 | 4.52426 | 0 | 0 | mol/s |
| Molar Flow (Mixture) / Sulfur trioxide | 0 | 0 | 2.3605 | 2.3605 | 2.3605 | 0 | 0 | 2.3605 | 0 | 0 | 2.3605 | 2.3605 | 0 | 0 | mol/s |

Conclusion:

Thus, the flowsheet for the production of hydrogen through the sodium-iodine cycle based on the electrochemical Bunsen reaction resulted in the formation of 1 mol/s of H_2 and 0.5 mol/s of H_2 from an initial input of 1 mol/s of H_2 O. This was achieved through the use of a sodium-iodine cycle, which involved various unit operations such as chemical conversion, and separation.

Reference: