Sunlight Ancient & Modern: The relative energy efficiency of hydrogen from coal and current biomass

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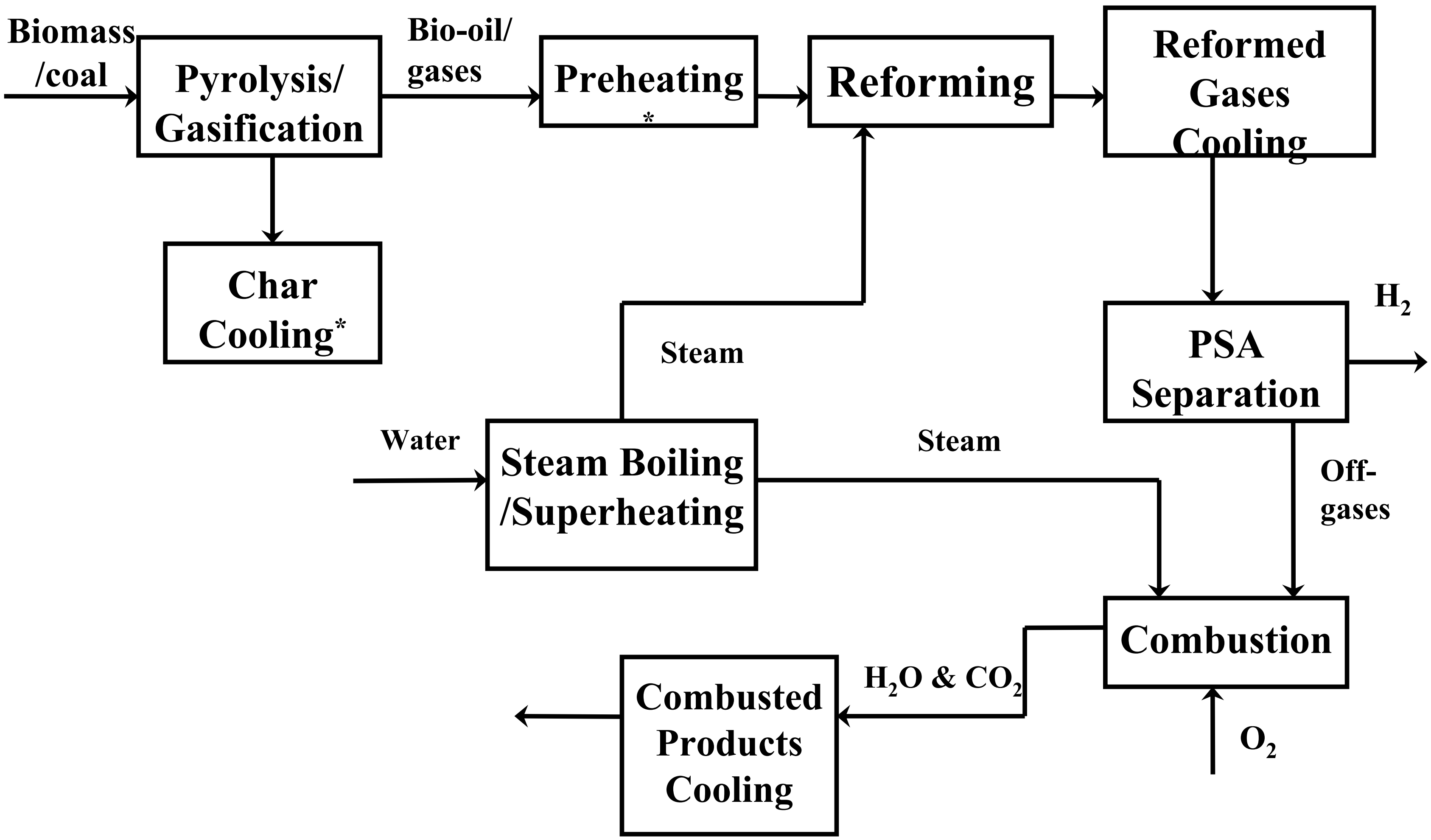
Objectives

- Establish transparent comparisons of baseline systems to produce hydrogen from various primary energy sources.

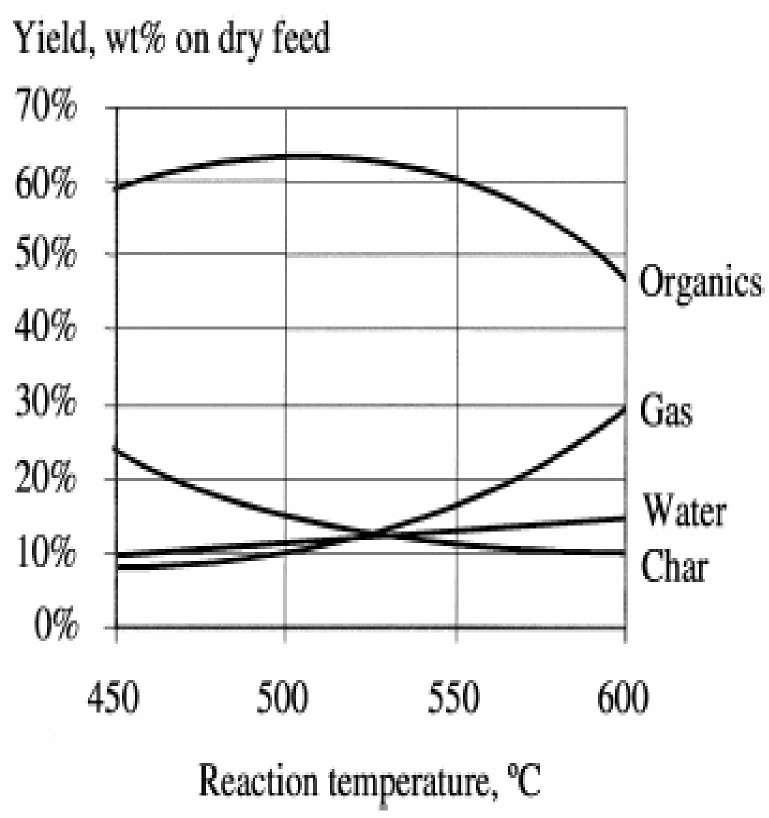
- Establish the critical parameters & assumptions to which system is sensitive.

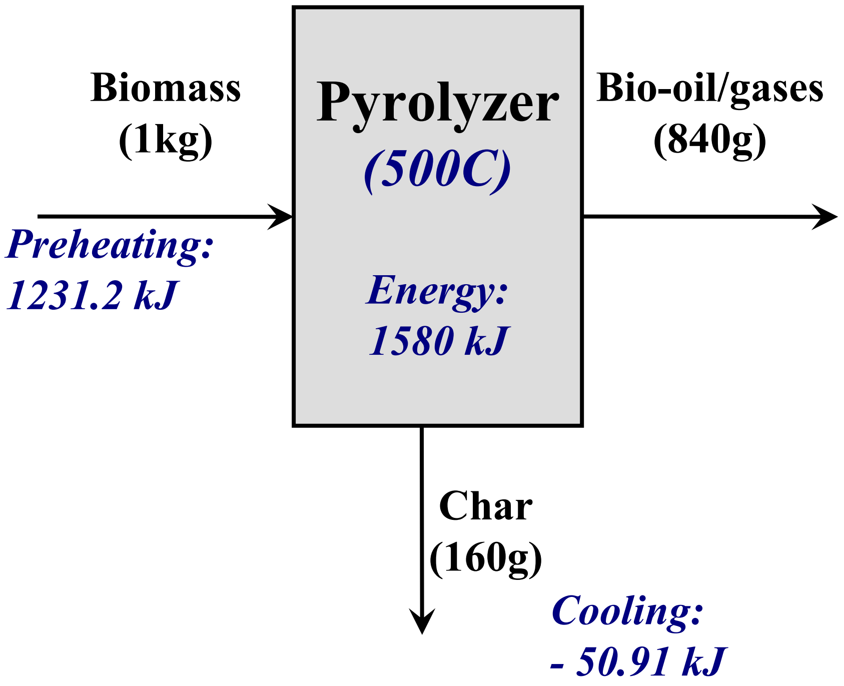
- Provide analyses for components of technological systems that combine hydrogen production with carbon sequestration.

Process Outline



Pyrolysis of Biomass





Bio-oil Composition Estimation

- Contains hundreds of components
- Concentrations vary significantly
- Depends on biomass, reaction conditions, etc.
- Limited experimental results

Estimation Method

$$\min \quad \sum \alpha_i (W_i - W_i^T)^2$$

$$s.t. \quad Lb_i \le W_i \le Ub_i$$

$$x_{ref} / Mw_{bio} = \sum x_i W_i / Mw_i$$

$$y_{ref} / Mw_{bio} = \sum y_i W_i / Mw_i$$

$$z_{ref} / Mw_{bio} = \sum z_i W_i / Mw_i$$

Bio-oil Composition Estimation (cont.)

Other compositions

$$\min \quad \sum (y/2 + x - z)_i W_i^L$$

$$s.t. \quad Lb_i \le W^L{}_i \le Ub_i$$

$$x_{ref} / Mw_{bio} = \sum x_i W_i^L / Mw_i$$

$$y_{ref} / Mw_{bio} = \sum y_i W_i^L / Mw_i$$

$$z_{ref} / Mw_{bio} = \sum z_i W_i^L / Mw_i$$

$$\sum (W_i^L - W_i^T)^2 \le \sum (W_i - W_i^T)^2$$

H2 production not sensitive to bio-oil composition

	W	WL	WU
Value of $\sum (y/2+x-z)_i W_i$	138.82	138.77	138.85

Steam Reforming (SR) reactions

$$C_xH_yO_z + (x-z)H_2O \leftrightarrow xCO + (x + y/2 + z)H_2$$

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

$$CH_4 + H_2O \leftrightarrow CO + 3H_2$$

Heat Integration for Biomass Conversion

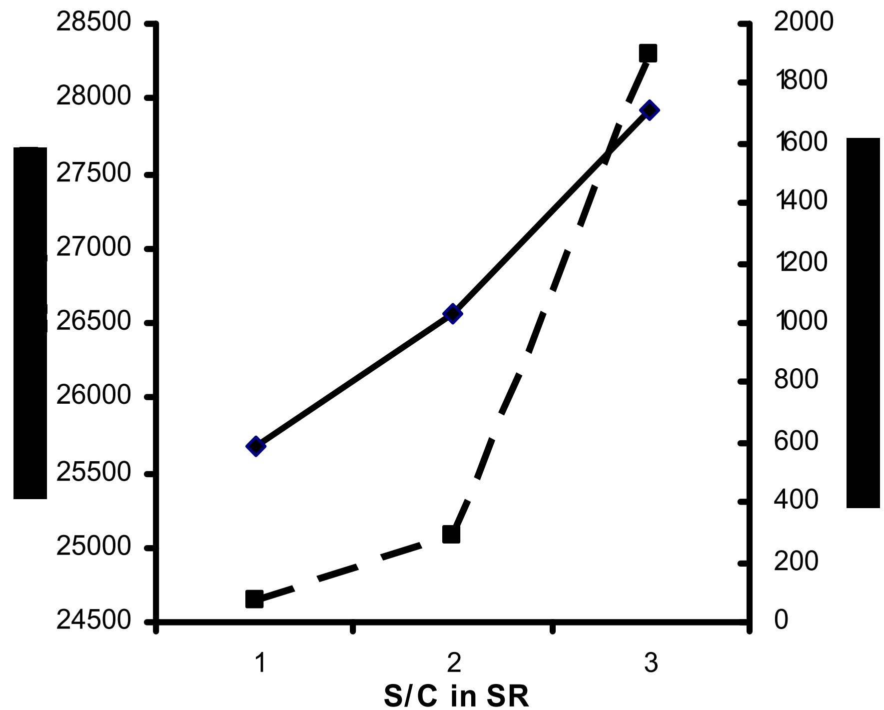
- **Heat sources**

 - Steam reforming products
 - Combusted products
 - Char

- **Heat sinks**

 - Pyrolysis
 - Steam reforming
 - Biomass preheating
 - Bio-oil/gases preheating
 - Steam making

Heat Integration by Pinch Analysis



Biomass Conversion Summary

Item	S/C = 1	S/C = 3	S/C = 3
H2 output/mol	40.95	51.17	55.7
H2O input/mol	555.71	604.22	643.98
H2O output/mol	545.99	584.28	619.48
Net Usage of water/mol	9.72	19.94	24.50
O2 input/mol	30.56	25.45	23.17
CO2 output/mol	43.29	43.29	43.29
Total Energy Input/kJ	25669	26563	27913
Total Energy Waste/kJ	72	286	1897
Mol H2 / MJ Energy Input	1.60	1.93	2.00

Gasification of Coal

Reactions

$$C + 1/2O_2 = CO$$

$$CO + 1/2O_2 = CO_2$$

$$H_2 + 1/2O_2 = H_2O$$

$$C + CO_2 \leftrightarrow 2CO$$

$$C + H_2O \leftrightarrow CO + H_2$$

$$C + 2H_2 \leftrightarrow CH_4$$

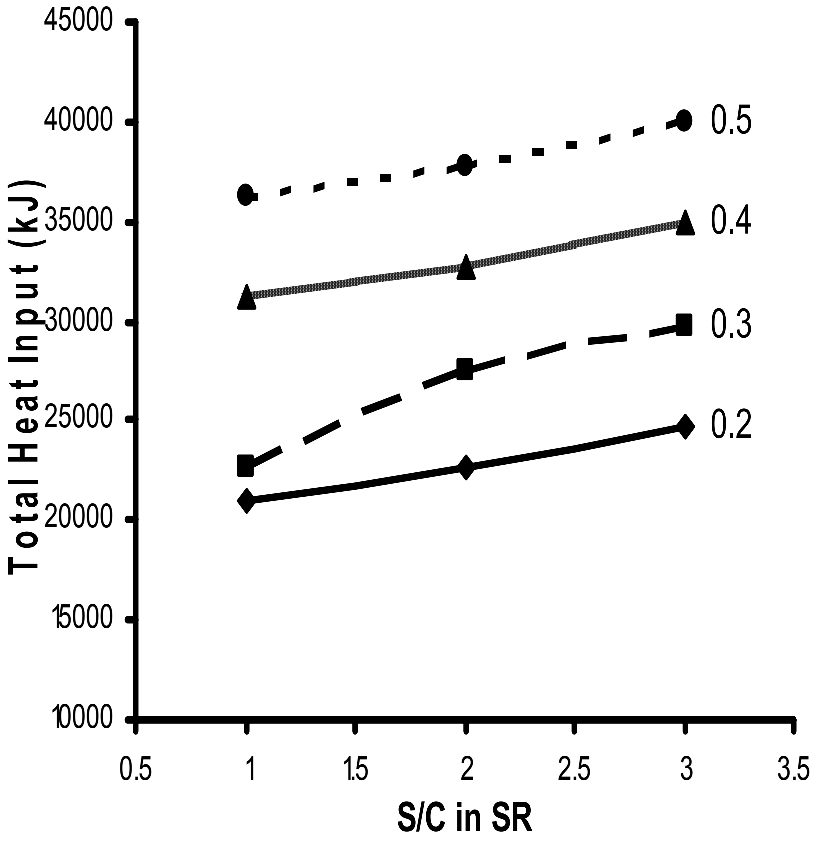
$$CO + H_2O \leftrightarrow CO_2 + H_2$$

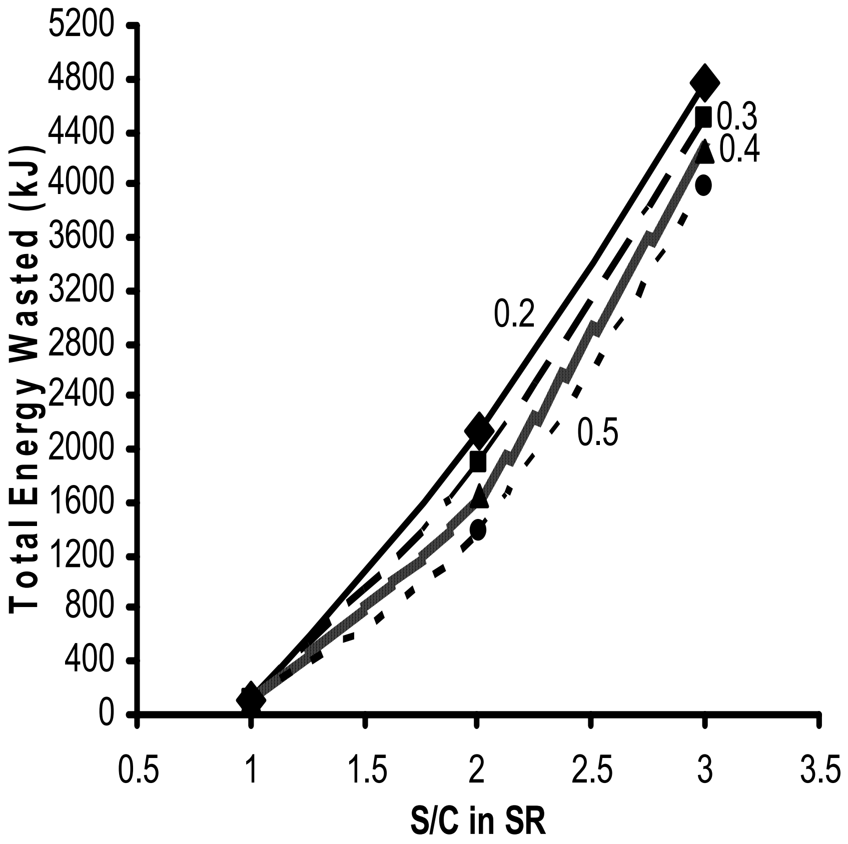
$$CH_4 + H_2O \leftrightarrow CO_2 + 3H_2$$

Simulation results

- Hydrogen production ability changed little with increasing temperature.
- Energy requirement increased significantly with temperature.
- Oxygen is not needed if S/C ratio is above 0.6.

Heat Integration for Coal Conversion





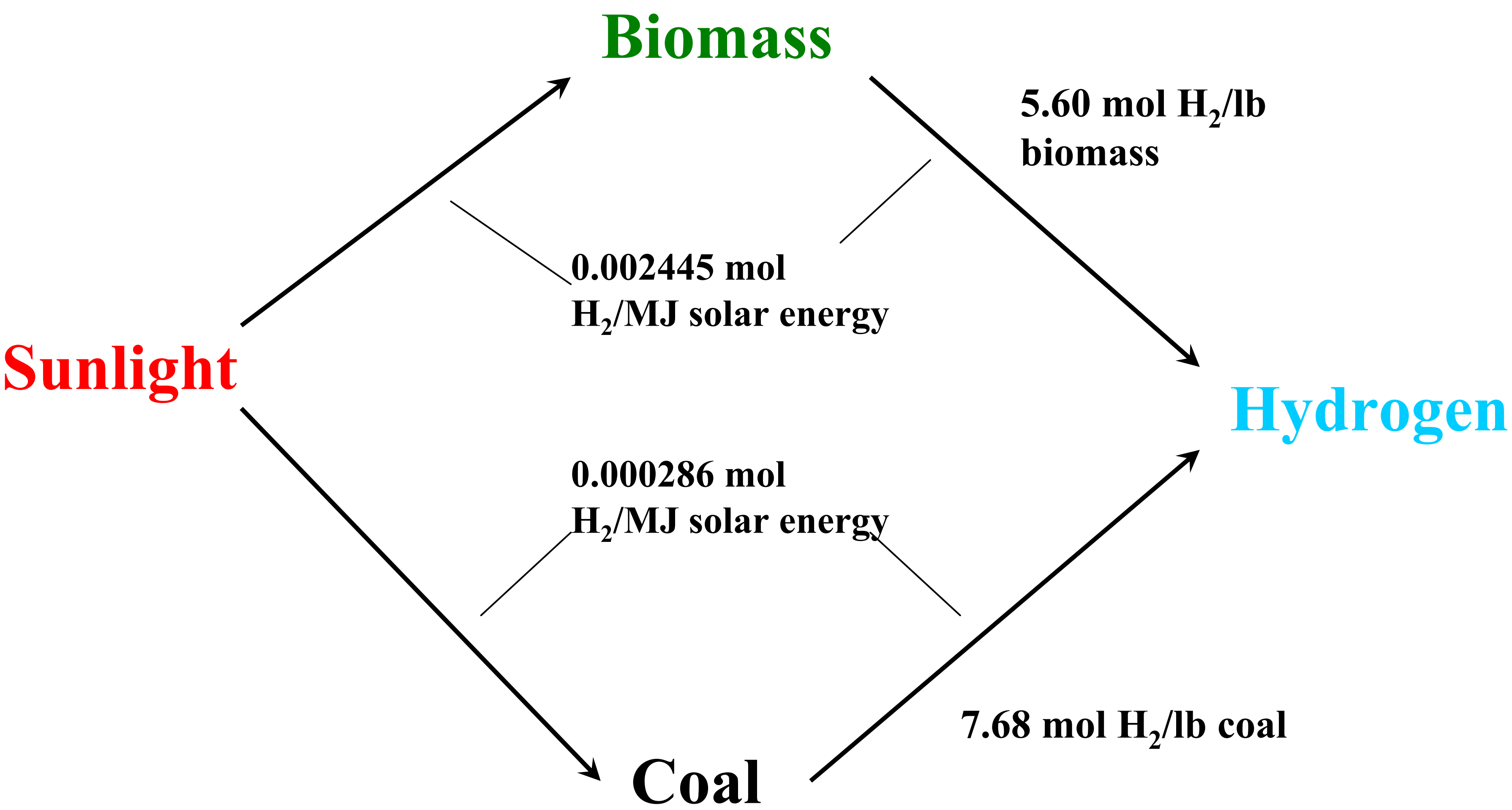
Coal Conversion Summary

Hydrogen production per unit energy input (Mol H2 / MJ Energy Input)

	S/C =1 in SR	S/C =2 in SR	S/C =3 in SR
S/C =0.2 in Gas.	2.46	2.60	2.70
S/C =0.3 in Gas.	2.07	2.43	2.44
S/C =0.4 in Gas.	2.00	2.23	2.26
S/C =0.5 in Gas.	1.87	2.10	2.13

Item	Value
Mol H2 / MJ Energy Input	2.70
H2 output/mol	66.48
H2O input/mol	826.08
H2O output/mol	788.00
Net Usage of water/mol	38.08
O2 input/mol	45.94
CO2 output/mol	68.05
Total Energy Input/kJ	24622
Total Energy Waste/kJ	4754

Comparison of the Two Systems



Conclusions

- **Higher energy density of coal leads to greater hydrogen production efficiency (no surprise.)**

- **Heat integration schemes are dependent of steam/carbon ratios and specific system conditions – must be holistically optimized.**

- **Bio-oil composition not a key factor.**

- **Overall efficiency of sunlight to hydrogen is significantly better for current sunlight due to putative inefficiencies of geological coal forming processes (but it’s in the past).**

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