

## SI Appendix

### General information and Assumption

Total oil consumption in the United States is 20.656 million barrels per day(1) =  $7.54 \times 10^9$  barrels per year. Share of US Oil Consumption for Transportation is 67% and same share for Light Duty Vehicles (LDV) is 40%. Therefore, total US oil consumption for transportation

$$= 5.05 \times 10^9 \text{ barrel} / \text{yr} = 5.05 \times 10^9 \text{ barrel} \times 158 \frac{\text{liter}}{1 \text{ barrel}} \times 0.87 \frac{\text{kg}}{\text{l}} = \frac{6.94 \times 10^{11} \text{ kg diesel}}{\text{yr}}$$

**All these numbers are taken from NRC report (2) unless specified otherwise.**

Carbon content in coal 75 wt% for all coal cases

Carbon content in biomass 42.5 wt% for all biomass cases

LHV of Coal = 27.098 MJ/kg

LHV of Biomass = 17.549 MJ/kg

HHV of coal = 27.91 MJ/kg (12000 BTU/lb)

HHV of biomass = 18.607 MJ/kg (8000 BTU/lb)

LHV of CO = 283.502 kJ/mol

LHV of H<sub>2</sub> = 242 kJ/mol = 120.1 MJ/kg = 33.3 kWh/kg

HHV of H<sub>2</sub> = 286 kJ/mol = 141.9 MJ/kg = 39.4 kWh/kg

LHV of CH<sub>4</sub> = 801.363 kJ/mol

HHV of CH<sub>4</sub> = 891 kJ/mol

LHV of diesel assuming C<sub>15</sub>H<sub>32</sub> = 43.987 MJ/kg. This value is obtained by complete combustion of C<sub>15</sub>H<sub>32</sub> assuming T = 150°C and gaseous H<sub>2</sub>O.

#### Heat of reaction



O<sub>2</sub> requirement for coal gasifier is 1 kg O<sub>2</sub>/kg coal feed.

O<sub>2</sub> requirement for biomass gasifier is 0.8 kg O<sub>2</sub>/kg dry biomass feed.

WGS shift as well as FT reactor operates at 35 atm and 250 °C

Assuming as available 1000 W/m<sup>2</sup> incident solar energy, 10% efficiency of conversion to H<sub>2</sub> based on HHV (8.5% based on LHV) and that solar energy is available 20% of the

$$\text{time} = 1000 \frac{\text{W}}{\text{m}^2} \times 0.1 \times 0.2 = 20 \frac{\text{W}}{\text{m}^2}$$

Converting this number into desirable units of kWh/m<sup>2</sup>/yr,

$$\frac{20 \text{ J}}{\text{m}^2 \text{ s}} \times \frac{1 \text{ kWh}}{3.6 \times 10^6 \text{ J}} \times \frac{3600 \text{ sec}}{1 \text{ hr}} \times \frac{24 \text{ hr}}{1 \text{ day}} \times \frac{365 \text{ day}}{1 \text{ year}} = \frac{175.2 \text{ kWh}}{\text{m}^2 \text{ yr}}$$

**Table 1: Conventional-I Biomass Case: Conventional process with gasifier at 50% efficiency. Data from Table E-23, MS Bio-C of the NRC report (2)**

$$\frac{10 \text{ ton biomass}}{\text{hectare} \times \text{yr}} = \frac{10 \times 10^3 \text{ kg biomass}}{10^4 \text{ m}^2 \text{ yr}} = \frac{1 \text{ kg biomass}}{\text{m}^2 \text{ yr}} = \frac{0.425 \text{ kg C}}{\text{m}^2 \text{ yr}}$$

1. From the NRC report, 18396 kg/h of dry biomass provides 1531.24 kmol/h of syngas containing 307.46 kmol/h CO, 307.47 kmol/h H<sub>2</sub>, 344.06 kmol/h CO<sub>2</sub> and 572.26 kmol/h H<sub>2</sub>O. Gasifier operating temperature and pressure were taken to be 1250 K and 35 atm.

2. Amount of biomass needed

$$18396 + 15\% \text{ of original biomass for drying} = 18396 + 3246 = 21642 \text{ kg/h}$$

3. CO<sub>2</sub> emission  $\frac{451.02 \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{19849 \text{ kg}}{\text{hr}}$

$$19849 \text{ kg/h} + 15\% \text{ from dryer} = 19849 + 3246 \times 0.425 \times \frac{44.01}{12.01} = 19849 + 5055 = 24904 \text{ kg/h}$$

4. Total energy used (energy in biomass + energy required for production of oxygen)

$$\begin{aligned} & 21642 \frac{\text{kg}}{\text{h}} \times 17.549 \frac{\text{MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} + \\ & \frac{18396 \text{ kg biomass}}{\text{h}} \times \frac{0.8 \text{ kg O}_2}{\text{kg biomass}} \times \frac{0.39 \text{ kWh}}{\text{kg}} \times \frac{3.6 \text{ MJ}}{1 \text{ kWh}} \times \frac{100}{40} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & = 105.5 + 14.349 = 119.85 \text{ MW} \end{aligned}$$

In these calculations, we do not account for energy to grow and transport the biomass to the gasifier.

5. Amount of diesel produced from ASPEN model using NRC syngas data for 18396 kg/hr of dry biomass = 13.37 kmol/hr

6. Energy content in diesel

$$\frac{13.37 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.99 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 34.69 \text{ MW}$$

7. Overall efficiency of the process  $\frac{34.69}{119.85} \times 100 = 28.95\%$

8. Amount of biomass required

$$\frac{6.94 \times 10^{11} \text{ kg diesel}}{\text{yr}} \times \frac{21642 \text{ kg biomass}}{13.37 \text{ kmol diesel} \times 212.42 \text{ kg/kmol}} = 5.29 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}$$

$$\text{Land area required} = \frac{5.29 \times 10^{12} \frac{\text{kgC}}{\text{yr}}}{\frac{1 \text{ kg biomass}}{\text{m}^2 \text{ yr}}} = 5.29 \times 10^{12} \text{ m}^2$$

$$\text{Total US land area} = 9.2 \times 10^6 \text{ km}^2 = 9.2 \times 10^{12} \text{ m}^2 \text{ (3)}$$

$$\text{Per cent of total US land area} = \frac{5.29 \times 10^{12} \times 100}{9.2 \times 10^{12}} = 57.8$$

9. Fraction of carbon in original biomass that shows up as diesel product

$$\frac{13.37 \times 15 \times 12.01}{21642 \times 0.425} = 0.262$$

**Table 1: H<sub>2</sub>CAR-I Biomass Case: Proposed process with gasifier at 50% efficiency. Data from Table E-23, MS Bio-C of the NRC report (2)**

From ASPEN simulation, for the H<sub>2</sub>CAR process, 13.37 kmol/hr of diesel is produced from 480 kmol/hr of syngas. In ASPEN simulation, conversion per pass from the hydrocarbon conversion reactor on the basis of CO fed to the reactor was taken to be 90%. The unreacted CO, H<sub>2</sub> and all CO<sub>2</sub> from the reactor exhaust was recycled to a simulated gasifier operating at 1250 K and 35 atm. 487 kmol/h of H<sub>2</sub> was added to the simulated gasifier to obtain H<sub>2</sub>/CO ratio of 2 in the exit stream. Furthermore, some O<sub>2</sub> was added in the inlet stream to supply energy for reverse Water Gas Shift (WGS) reaction as well as other heat requirements. The effluent stream from the simulated gasifier was taken to be at thermodynamic equilibrium(4, 5). From the NRC data in Table E-23, 18396 kg of dry biomass produces 1531.24 kmol/hr of syngas.

1. Amount of biomass needed

$$= \frac{480 \text{ kmol}}{\text{hr}} \times \frac{18396 \text{ kg biomass}}{1531.24 \text{ kmol}} = \frac{5766.6 \text{ kg biomass}}{\text{hr}}$$

2. Fraction of biomass in proposed process compared to biomass requirement in current process (Conventional-I) to produce same quantity of liquid fuel

$$\frac{5766.6}{21642} = 0.267$$

3. CO<sub>2</sub> in purge stream that will have to be recovered and recycled to keep carbon capture efficiency high

$$\frac{(0.22232 + 1.086904 + 0.091335) \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{61.64 \text{ kg CO}_2}{\text{hr}}$$

The emission of CO and CH<sub>4</sub> in purge stream is also accounted in CO<sub>2</sub> emission.

4. Extra H<sub>2</sub> required to dry the biomass

$$\frac{1017.7 \text{ kg biomass}}{\text{hr}} \times \frac{17.549 \text{ MJ (LHV)}}{\text{kg biomass}} \times \frac{\text{kg H}_2}{120.1 \text{ MJ}} = \frac{148.71 \text{ kg H}_2}{\text{hr}} = \frac{73.76 \text{ kmol H}_2}{\text{hr}}$$

5. Total energy when using energy from solar panels to produce H<sub>2</sub>. For ASPEN modeling, amount of H<sub>2</sub> from carbon-free energy source fed to gasifier to produce 13.37 kmol/hr of diesel equals 487 kmol/hr

$$\begin{aligned} & \frac{5766.6 \text{ kg biomass}}{\text{h}} \times \frac{17.549 \text{ MJ (LHV)}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & + \frac{(487 + 73.763) \text{ kmol H}_2}{\text{h}} \times \frac{242 \text{ MJ}}{\text{kmol}} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & = 28.111 + 37.696 = 65.81 \text{ MW} \end{aligned}$$

6. Energy content in diesel

$$\frac{13.36711 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.987 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 34.69 \text{ MW}$$

7. Overall efficiency of the process  $\frac{34.69}{65.81} \times 100 = 52.7\%$

8. Total quantity of biomass required

$$\frac{6.94 \times 10^{11} \text{ kg diesel}}{\text{yr}} \times \frac{5766.6 \text{ kg biomass}}{13.37 \text{ kmol diesel} \times 212.42 \text{ kg/kmol}} = 1.41 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}$$

$$\text{Land area required} = \frac{1.41 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}}{\frac{1 \text{ kg biomass}}{m^2 \text{ yr}}} = 1.41 \times 10^{12} m^2$$

$$\text{Per cent of total US land area} = \frac{1.41 \times 10^{12} \times 100}{9.2 \times 10^{12}} = 15.4$$

#### 9. Solar panel land area requirement

$$\text{Total } H_2 \text{ required to support 67\% of US oil consumption equals}$$

$$= \frac{6.94 \times 10^{11} \text{ kg diesel} \times (487 + 73.76) \text{ kmol} \times 2.02 \text{ kg } H_2}{\text{yr} \times 13.37 \text{ kmol} \times 212.42 \text{ kg diesel/kmol}} = \frac{2.77 \times 10^{11} \text{ kg } H_2}{\text{yr}}$$

Energy required to produce based on HHV of  $H_2$

$$= \frac{2.77 \times 10^{11} \text{ kg}}{\text{yr}} \times 39.4 \frac{\text{kWh}}{\text{kg}} = 1.09 \times 10^{13} \frac{\text{kWh}}{\text{year}}$$

$$\text{Solar panel area required} = \frac{1.09 \times 10^{13}}{175.2} = 6.22 \times 10^{10} m^2$$

$$\text{Per cent of total land area} = \frac{6.22 \times 10^{10}}{9.2 \times 10^{12}} \times 100 = 0.68$$

Combined land area for biomass and solar panels = 16.1 %

**Calculations for Table 1 Conventional – II Biomass case: Conventional process with gasifier at 70% efficiency and future optimism. Data from Table E-24, MS Bio-F of the NRC report (2)**

$$\frac{15 \text{ ton biomass}}{\text{hectare} \times \text{yr}} = \frac{15 \times 10^3 \text{ kg biomass}}{10^4 \text{ m}^2 \text{ yr}} = \frac{1.5 \text{ kg biomass}}{\text{m}^2 \text{ yr}} = \frac{0.6375 \text{ kg C}}{\text{m}^2 \text{ yr}}$$

1. Amount of biomass needed

$$11908 + 15\% \text{ of original biomass for drying} = 11908 + 2101 = 14009 \text{ kg/h}$$

2. CO<sub>2</sub> emission  $\frac{249.52 \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{10981 \text{ kg}}{\text{hr}}$

$$10981 \text{ kg/h} + 15\% \text{ from dryer} = 10981 + 2101 \times 0.425 \times \frac{44.01}{12.01} = 10981 + 3271.9 = 14253 \text{ kg/h}$$

3. Total energy used (energy in biomass + energy required for production of oxygen)

$$\begin{aligned} & 14009 \frac{\text{kg}}{\text{h}} \times 17.55 \frac{\text{MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} + \\ & \frac{11908 \text{ kg biomass}}{\text{h}} \times \frac{0.8 \text{ kg O}_2}{\text{kg biomass}} \times \frac{0.39 \text{ kWh}}{\text{kg}} \times \frac{3.6 \text{ MJ}}{1 \text{ kWh}} \times \frac{100}{40} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & = 68.29 + 9.2882 = 77.58 \text{ MW} \end{aligned}$$

5. From ASPEN modeling, 12.14 kmol/hr of diesel is produced from 11908 kg/hr of dry biomass. Energy content in diesel

$$\frac{12.14 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.99 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 31.52 \text{ MW}$$

6. Overall efficiency of the process  $\frac{31.52}{77.58} \times 100 = 40.63\%$

7. Quantity of biomass required

$$\frac{6.94 \times 10^{11} \text{ kg diesel}}{\text{yr}} \times \frac{14009 \text{ kg biomass}}{12.14 \text{ kmol diesel} \times 212.42 \text{ kg/kmol}} = 3.77 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}$$

$$3.77 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}$$

$$\text{Land area required} = \frac{3.77 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}}{1.5 \frac{\text{kg biomass}}{\text{m}^2 \text{ yr}}} = 2.51 \times 10^{12} \text{ m}^2$$

$$\text{Per cent of total US land area} = \frac{2.51 \times 10^{12} \times 100}{9.2 \times 10^{12}} = 27.5$$

8. Fraction of carbon in original biomass that shows up as diesel product

$$\frac{12.14 \times 15 \times 12.01}{14009 \times 0.425} = 0.37$$

**Calculations for Table 1: H<sub>2</sub>CAR - II Biomass Case: Proposed process with gasifier at 70% efficiency and future optimism. Data from Table E-24, MS Bio-F of the NRC report (2)**

Process was simulated using ASPEN in a manner analogous to the one described for Proposed-I Biomass case.

1. From ASPEN simulation, for the proposed process, 12.15 kmol/hr of diesel is produced from 433 kmol/hr of syngas. From the NRC data in Table E-24, 11908 kg of dry biomass produces 1011.3 kmol/hr of syngas. Amount of biomass needed

$$\frac{433 \text{ kmol}}{\text{hr}} \times \frac{11908 \text{ kg biomass}}{1011.13 \text{ kmol}} = \frac{5098.6 \text{ kg biomass}}{\text{hr}}$$

2. Fraction of biomass in proposed process compared to biomass requirement in current process (conventional-II) to produce same quantity of liquid fuel

$$\frac{5098.6}{14009} = 0.36$$

3. CO<sub>2</sub> in purge stream that will have to be recovered and recycled to keep carbon capture efficiency high

$$\frac{(0.2 + 0.59 + 0.028) \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{36.307 \text{ kg CO}_2}{\text{hr}}$$

4. Extra H<sub>2</sub> required to dry the biomass

$$\frac{899.69 \text{ kg biomass}}{\text{hr}} \times \frac{17.55 \text{ MJ (LHV)}}{\text{kg biomass}} \times \frac{\text{kg H}_2}{120.1 \text{ MJ}} = \frac{131.46 \text{ kg H}_2}{\text{hr}} = \frac{65.21 \text{ kmol H}_2}{\text{hr}}$$

5. From ASPEN modeling, amount of H<sub>2</sub> from carbon-free energy source fed to gasifier to produce 12.15 kmol/hr of diesel equals 374.5 kmol/hr. Therefore, total energy when using energy from solar panels to produce H<sub>2</sub>

$$\begin{aligned} & \frac{5098.6 \text{ kg biomass}}{\text{h}} \times \frac{17.5 \text{ MJ (LHV)}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & + \frac{(374.5 + 65.21) \text{ kmol H}_2}{\text{h}} \times \frac{242 \text{ MJ}}{\text{kmol}} \times \frac{1 \text{ h}}{3600 \text{ s}} \\ & = 24.85 + 29.56 = 54.4 \text{ MW} \end{aligned}$$

6. Energy content in diesel  $\frac{12.15 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.99 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 31.5 \text{ MW}$

7. Overall efficiency of the process  $\frac{31.5}{54.4} \times 100 = 58\%$

8. Total quantity of biomass required

$$\frac{6.94 \times 10^{11} \text{ kg diesel}}{\text{yr}} \times \frac{5098.6 \text{ kg biomass}}{12.15 \text{ kmol diesel} \times 212.42 \text{ kg/kmol}} = 1.37 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}}$$

$$\text{Land area required} = \frac{1.37 \times 10^{12} \frac{\text{kgC}}{\text{yr}}}{\frac{1.5 \text{ kg biomass}}{\text{m}^2 \text{ yr}}} = 9.15 \times 10^{11} \text{ m}^2$$

$$\text{Per cent of total US land area} = \frac{9.15 \times 10^{11} \times 100}{9.2 \times 10^{12}} = 9.98$$

9. Solar panel land area requirement

$$\begin{aligned} \text{Total } H_2 \text{ required to support 67\% of US oil consumption equals} \\ = \frac{6.94 \times 10^{11} \text{ kg diesel} \times (374.5 + 65.21) \text{ kmol} \times 2.02 \text{ kg } H_2}{\text{yr} \times 12.15 \text{ kmol} \times 212.42 \text{ kg diesel/kmol}} = \frac{2.39 \times 10^{11} \text{ kg } H_2}{\text{yr}} \end{aligned}$$

Energy required to produce based on HHV of  $H_2$

$$= \frac{2.39 \times 10^{11} \text{ kg}}{\text{yr}} \times 39.4 \frac{\text{kWh}}{\text{kg}} = 9.4 \times 10^{12} \frac{\text{kWh}}{\text{year}}$$

$$\text{Solar panel area required} = \frac{9.4 \times 10^{12}}{175.2} = 5.37 \times 10^{10} \text{ m}^2$$

$$\text{Total US land area} = 9.2 \times 10^6 \text{ km}^2 = 9.2 \times 10^{12} \text{ m}^2$$

$$\text{Per cent of total land area} = \frac{5.37 \times 10^{10}}{9.2 \times 10^{12}} \times 100 = 0.59$$

Combined land area of biomass and solar panels = 10.6%

10. Total  $H_2$  requirement

$$= \frac{6.94 \times 10^{11} \text{ kg diesel} \times (374.5 + 65.21) \text{ kmol} \times 2.02 \text{ kg } H_2}{\text{yr} \times 12.15 \text{ kmol} \times 212.42 \text{ kg diesel/kmol}} = \frac{2.39 \times 10^{11} \text{ kg } H_2}{\text{yr}}$$

11. Energy content of biomass

$$1.37 \times 10^{12} \frac{\text{kg biomass}}{\text{yr}} \times \frac{17.549 \text{ MJ (LHV)}}{\text{kg}} \times \frac{1 \text{ yr}}{3.1536 \times 10^7 \text{ sec}} \times \frac{1 \text{ TW}}{10^6 \text{ MW}} = 0.76 \text{ TW}$$

12. Energy content of  $H_2$

$$238.51 \times 10^9 \frac{\text{kg } H_2}{\text{yr}} \times 120.1 \frac{\text{MJ (LHV)}}{\text{kg}} \times \frac{1 \text{ yr}}{3.1536 \times 10^7 \text{ sec}} \times \frac{1 \text{ TW}}{10^6 \text{ MW}} = 0.91 \text{ TW}$$



**Calculations for Table 2 conventional coal case: Current process for coal gasification with gasifier efficiency = 75%. Data from Table E-8, CS coal-C of the NRC report (2)**

From the NRC report, 326994 kg/h of coal provides 41438.5 kmol/h of syngas containing 14502 kmol/h CO, 10501 kmol/h H<sub>2</sub>, 5935.5 kmol/h CO<sub>2</sub> and 10500 kmol/h H<sub>2</sub>O.

1. Amount of coal used  $\frac{326994 \text{ kg}}{\text{hr}}$
2. CO<sub>2</sub> emission  $\frac{12285.2 \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{5.41 \times 10^5 \text{ kg}}{\text{hr}}$
3. Total energy used  

$$\frac{326994 \text{ kg coal}}{\text{h}} \times \frac{27.098 \text{ MJ (LHV)}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} + \frac{326994 \text{ kg O}_2}{\text{h}} \times \frac{0.39 \text{ kWh}}{\text{kg}} \times \frac{3.6 \text{ MJ}}{1 \text{ kWh}} \times \frac{100}{40} \times \frac{1 \text{ h}}{3600 \text{ s}}$$

$$= 2461.4 + 318.82 = 2780.2 \text{ MW}$$
4. Amount of diesel produced from ASPEN runs = 543.49 kmol
5. Energy content in diesel  

$$\frac{543.49 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.987 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 1410.6 \text{ MW}$$
6. Overall efficiency of the process  $\frac{1410.6}{2780.2} \times 100 = 50.7\%$
7. Years coal will last  
 Total reserves of recoverable coal in US are 275 billion tons. Present coal consumption in US is 1.128 billion tons. Therefore, to produce  

$$= \frac{6.94 \times 10^{11} \text{ kg diesel} \times 326994 \text{ kg coal}}{\text{yr} \times 543.49 \text{ kmol} \times 212.42 \text{ kg/kmol diesel}} = 1.97 \times 10^{12} \frac{\text{kg coal required}}{\text{yr}}$$
  
 Coal will last for =  $\frac{275}{(1.128 + 1.97)} = 88.9 \text{ yrs}$  versus 243.8 yrs that coal will last if utilized at current consumption rate.
8. Fraction of carbon in coal that shows up as diesel product  

$$\frac{543.49 \times 15 \times 12.01}{326994 \times 0.75} = 0.4$$
9. CO<sub>2</sub> to be sequestered =  $\frac{5.4 \times 10^5}{326994} \times 1.97 \times 10^{12} = \frac{3.25 \times 10^{12} \text{ kg}}{\text{yr}}$   

$$= \frac{3.25 \times 10^{12}}{\text{yr}} \times \frac{12}{44} = 0.9 \text{ GtC/yr}$$

CO<sub>2</sub> to be sequestered is reported in Table 2.

**Table 2: H<sub>2</sub>CAR Coal Case: Coal gasification with gasifier efficiency = 75%. Data from Table E-8, CS coal-C of the NRC report (2)**

From ASPEN simulation we find that for the proposed process we need 16712 kmol/hr of syngas to make 543.49 kmol/hr of diesel. From NRC report, 326994 kg/hr of coal produces 41438.5 kmol/hr of syngas.

1. Amount of coal used  $\frac{326994 \text{ kg/hr} \times 16712}{41438.5} = 131880 \text{ kg/hr}$

2. Fraction of coal in proposed process compared to coal in current process to produce same quantity of liquid fuel  $\frac{131880}{326994} = 0.4$

3. CO<sub>2</sub> in purge stream that will have to be separated and recycled to keep carbon capture efficiency high.

$$\frac{(17.88 + 9.03 + 2.06) \text{ kmol}}{\text{hr}} \times \frac{44.01 \text{ kg}}{1 \text{ kmol}} = \frac{1275.2 \text{ kg}}{\text{hr}}$$

4. From ASPEN model, amount of H<sub>2</sub> fed to the gasifier = 17440 kmol/hr. Assuming H<sub>2</sub> produced from solar energy, total energy used

$$\frac{131880 \text{ kg coal}}{\text{h}} \times \frac{27.1 \text{ MJ(LHV)}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} + \frac{17440 \text{ kmol}}{\text{h}} \times \frac{242 \text{ MJ}}{\text{kmol}} \times \frac{1 \text{ h}}{3600 \text{ s}}$$

$$= 992.69 + 1172.4 = 2165.1 \text{ MW}$$

5. Energy content in diesel

$$\frac{543.5 \text{ kmol}}{\text{h}} \times \frac{212.42 \text{ kg}}{1 \text{ kmol}} \times \frac{43.99 \text{ MJ}}{\text{kg}} \times \frac{1 \text{ h}}{3600 \text{ s}} = 1410.6 \text{ MW}$$

6. Overall efficiency of the process when H<sub>2</sub> is from solar energy

$$\frac{1410.6}{2165.1} \times 100 = 65.2\%$$

7. Years coal will last:

Total reserves of recoverable coal in US are 275 billion tons. Present coal consumption in US is 1.128 billion tons. Therefore, to produce

$$= \frac{6.94 \times 10^{11} \text{ kg diesel} \times 131880 \text{ kg coal}}{\text{yr} \times 543.5 \text{ kmol} \times 212.42 \text{ kg/kmol diesel}} = 7.93 \times 10^{11} \frac{\text{kg coal required}}{\text{yr}}$$

Coal will last for  $= \frac{275}{(1.128 + 0.79)} = 143.14 \text{ yrs}$  versus 243.79 yrs that coal will last if utilized at current consumption rate.

From ASPEN model, amount of H<sub>2</sub> fed to gasifier = 17440 kmol/hr. Therefore, total H<sub>2</sub> requirement

$$= \frac{17440 \text{ kmol/hr} \times 2.02 \text{ kg/kmol} \times 6.94 \times 10^{11} \text{ kg diesel/yr}}{543.5 \text{ kmol/hr} \times 212.42 \text{ kg/kmol}} = 2.12 \times 10^{11} \frac{\text{kg H}_2}{\text{yr}}$$

8. Solar panel land area requirement

Total H<sub>2</sub> required to support 67% of US oil consumption equals  $= \frac{2.12 \times 10^{11} \text{ kg H}_2}{\text{yr}}$

Energy required to produce based on HHV of H<sub>2</sub>

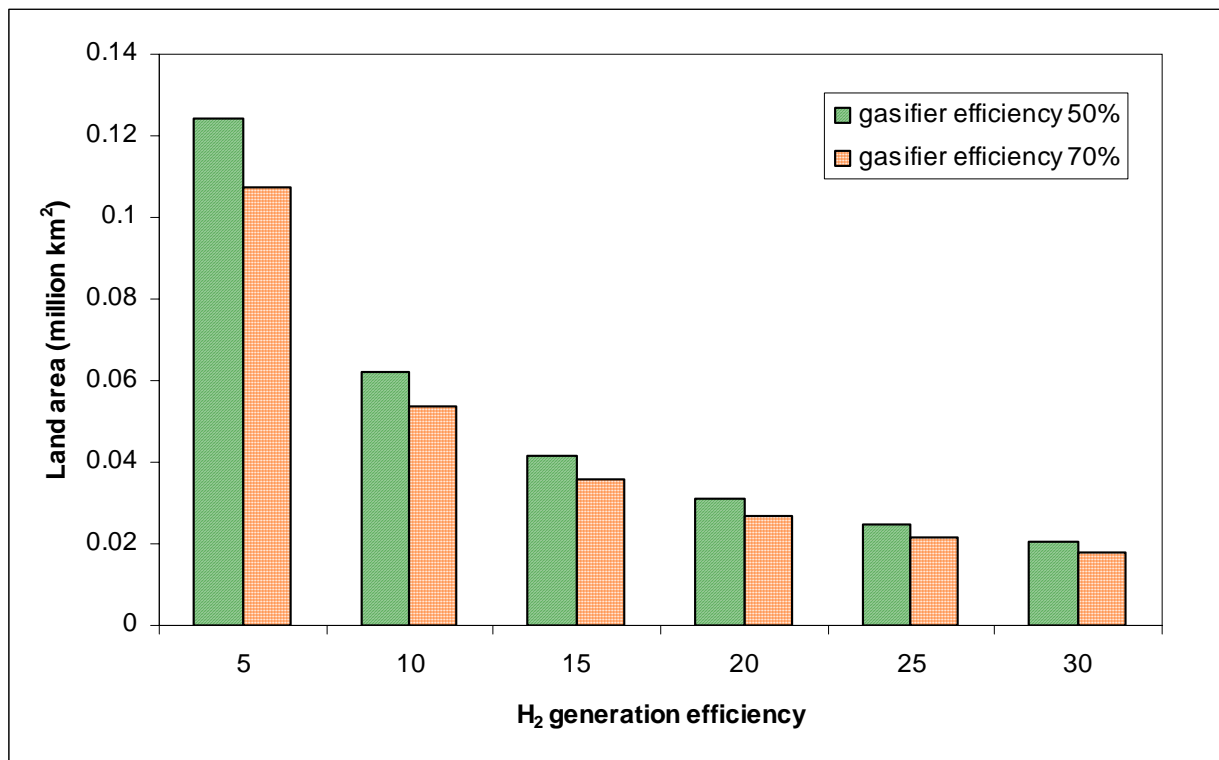
$$= \frac{2.12 \times 10^{11} \text{ kg}}{\text{yr}} \times 39.4 \frac{\text{kWh}}{\text{kg}} = 8.33 \times 10^{12} \frac{\text{kWh}}{\text{year}}$$

$$\text{Solar panel area required} = \frac{8.33 \times 10^{12}}{175.2} = 4.76 \times 10^{10} \text{ m}^2$$

$$\text{Total US land area} = 9.2 \times 10^6 \text{ km}^2 = 9.2 \times 10^{12} \text{ m}^2$$

$$\text{Per cent of total land area} = \frac{4.76 \times 10^{10}}{9.2 \times 10^{12}} \times 100 = 0.52$$

Figure 1 shows the land area requirement for only H<sub>2</sub> production with respect to the H<sub>2</sub> generation efficiency. The H<sub>2</sub> generation efficiency refers to the percentage of solar incident energy that is harnessed as H<sub>2</sub> in the form of its high heating value (HHV). For land area calculation, average availability of solar energy per day is taken to be 20%. In contrast to negligible effect of gasifier efficiency on the biomass land area, improvement in gasifier efficiency helps in reducing the H<sub>2</sub> requirement. For the H<sub>2</sub>CAR process, one may envision that the net energy in the gasifier is supplied through oxidation of H<sub>2</sub>, so increase in the efficiency of the gasifier helps in decreasing the H<sub>2</sub> requirement for the process.



**Figure 1: Land area requirement for H<sub>2</sub> production for varying H<sub>2</sub> generation efficiencies from solar energy**

### AEE\* Calculation for Biomass

Energy content of Biomass =  $17.5 \times 10^3 \text{ kJ/kg}$

Biomass growth rate =  $m \text{ kg/m}^2/\text{yr}$

Energy harnessed per  $\text{m}^2$  per year =  $17.5 \times m \times 10^3 \text{ kJ}$

Solar insolation =  $1 \text{ kW/m}^2$  for 20% of 24 hr. day

$$\text{AEE} = \left( \frac{17.5 \times m \times 10^3}{1 \times 365 \times 24 \times 3600 \times 0.2} \right) \times 100$$

Thus, for  $2.5 \text{ kg/m}^2/\text{yr}$ , AEE = 0.69%

### AEE Calculation for H<sub>2</sub> production

Photovoltaic Efficiency = P

Electrolyzer Efficiency = 60% (based on HHV)

Hydrogen Conversion Efficiency =  $0.6 \times 0.845 \times P$  (LHV)

AEE =  $0.6 \times 0.845 \times P$

Thus, for 15% Photovoltaic efficiency, AEE = 7.61%

Using above formulations, AEE can be calculated for varying photovoltaic efficiency and biomass growth rate and the results are presented in the table below.

### Tabular Representation of data

H <sub>2</sub> Production		Biomass Growth		Ratio of <b>Current</b> AEE for H <sub>2</sub> production/ <b>AEE for</b> <b>biomass growth rate</b>
PV efficiency (%)	AEE (%)	Biomass Growth Rate (kg/m <sup>2</sup> /yr)	AEE (%)	
10	5.07	1	0.28	27.2
15 (current)	7.61	1.5	0.42	18.1
20	10.15	2.5	0.69	11.0
25	12.68	4	1.10	6.9
35	17.76	5	1.38	5.5
50	25.37	6.25	1.73	4.4

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\* AEE: Annualized Energy Efficiency

*Technical Feasibility of a Billion-Ton Annual Supply*

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