

Supporting Information:

S.1 Heat exchange modeling

The below empirical specific heat equations are used for gaseous heat exchange per (Çengel et al., 2012):

$$c_{pH_2}(T) = a_{H_2}T + b_{H_2}T^2 + c_{H_2}T^3 + d_{H_2}T^4$$

$$c_{pCH_4}(T) = a_{CH_4}T + b_{CH_4}T^2 + c_{CH_4}T^3 + d_{CH_4}T^4$$

Table S1. Coefficients for empirical specific heat equations.

	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>
H_2	29.11	-0.1916×10^{-2}	0.4003×10^{-5}	-0.8704×10^{-9}
CH_4	19.89	5.024×10^{-2}	1.269×10^{-5}	-11.01×10^{-9}

S.2 Plug flow reactor model

In order to validate the mathematical model for the reactor kinetics, we employ Aspen HYSYS process simulation software. The Aspen HYSYS model was a kinetically controlled plug flow reactor with a single pyrolysis reaction. The kinetic parameters derived experimentally by Upham et al. (2017) were employed. Various reactor dimensions, volumes, and gas holdup values were explored. The mole fraction produced was found to only be a function of the residence time. The residence time can be converted to a reactive volume by multiplying by the volumetric flow rate, allowing for various reactor configurations to be compared on an identical baseline. Several simulations were conducted and the mole fraction of H_2 in product gas stream is compared in Figure S1 to that predicted by the model derived in Upham et al., 2017, and the model used in this work.

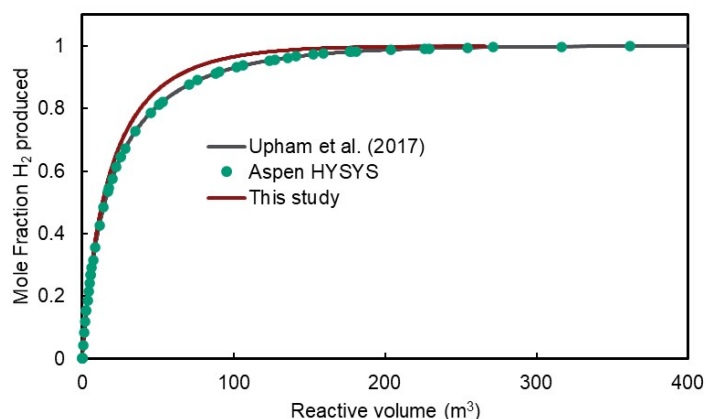


Figure S1. Results of our mathematical model as compared to the model derived in Upham et al. (2017) and the outputs of a similarly tuned Aspen HYSYS reactor model.

While the mathematical formulation used by Upham et al. (2017) and ASPEN HYSYS accounts for the changing concentration of reactants across the plug-flow reactor, it does not appear that these models account for any consequent changes as mole creation results in a larger volume and reactant surface area.

S.3 Capital Cost correlations:

The Chemical Engineering literature contains a well-established body of work on the topic of capital cost estimation for novel process equipment. Table S2, below, includes all capital cost estimation equations employed and their source. Some equations include adjustment factors for materials, f_m , and all values were updated to 2017 \$ using CEPCI.

Table S2. Capital cost estimation equations employed for a variety of equipment and materials.

Equipment (e)	Purchased cost (PC_e)	Source
Heat exchanger	$f_m(28000 + 54A_{HXR}^{1.2})$	$f_m = 1.7$ (Towler & Sinnott, 2012)
Pressure vessel	$(11600 + 34m_{shell}^{0.85})$	(Towler & Sinnott, 2012)
Cyclone	$f_m exp^{0.12 \ln V_{g2}}$	$f_m = 9$ (Ulrich & Vasudevan, 2004)
Bag filter	$exp^{9.9 + 0.5575 \ln V_{g2}}$	(Ulrich & Vasudevan, 2004)
Transformer	$\frac{(\dot{Q}_{loss} + \dot{Q}_{reactor}) \$ 42850}{\frac{10^6 W}{MW}}$	(CAISO, 2018)
Materials	Purchased cost (PC_e)	Source
Insulation	$C_{C-ins} \rho_{C-ins} V_{C-ins}$	$C_{C-ins} = \frac{\$0.1}{kg}$ (Parkinson, 2018)
Ceramic (Mg-O)	$C_{Mg-o} \rho_{Mg-o} V_{Mg-o}$	$C_{Mg-o} = \frac{\$0.36}{kg}$ (Parkinson, 2018)
Molten metal (Ni-Bi)	$(C_{Ni} x_{Ni} + C_{Bi} x_{Bi}) \rho_m (1 - \varepsilon) V_R$	$x_{Ni} = 0.1$ $x_{Bi} = 0.9$ $C_{Ni} = \frac{\$6}{lb}$ (InvestmentMine.com) $C_{Bi} = \frac{\$5}{lb}$ (Rotometals.com)
Resistive elements (Si-C)	$C_{Si-c} \rho_{Si-c} V_{Si-c}$	$C_{Si-c} = \frac{\$36}{kg}$ (Stack, 2016)

S.4 Operational cost estimates

Power consumption of the cyclone, $\dot{W}_{cyclone}$ [W] is estimated from equations in Ulrich et al. (2004).

$$\dot{W}_{cyclone} = 2000 \dot{V}_{g2a} \quad (1)$$

S.5 Radial conduction modeling

A multi-layered radial conduction model was employed to estimate the shell losses from the pyrolysis reactor:

$$\dot{Q}_{ceramic} = \frac{2\pi R^2 k_{MgO}(T_{r1} - T_{r2})}{L_{MgO}} + \frac{2\pi H k_{MgO}(T_{r1} - T_{r2})}{\log \frac{R + 2L_{MgO}}{R + L_{MgO}}}$$

$$\dot{Q}_{insulation} = \frac{2\pi R^2 k_{ins}(T_{r2} - T_{r3})}{L_{ins}} + \frac{2\pi H k_{ins}(T_{r2} - T_{r3})}{\log \frac{R + 2L_{MgO} + L_{ins}}{R + 2L_{MgO}}}$$

$$\dot{Q}_{steel} = \frac{2\pi R^2 k_{steel}(T_{r3} - T_{r4})}{L_{steel}} + \frac{2\pi H k_{steel}(T_{r3} - T_{r4})}{\log \frac{R + 2L_{MgO} + L_{ins} + L_{steel}}{R + 2L_{MgO} + L_{ins}}}$$

$$\dot{Q}_{loss, rad} = 2\pi H \sigma_{rad} (T_{r4}^4 - T_{amb}^4) (R + 2L_{MgO} + L_{ins} + L_{steel}) + 2\pi R^2 \sigma_{rad} (T_{r4}^4 - T_{amb}^4) \quad (5)$$

$$\dot{Q}_{loss, conv} = 2\pi H h_{conv} (T_{r4} - T_{amb}) (R + 2L_{MgO} + L_{ins} + L_{steel}) + 2\pi R^2 h_{conv} (T_{r4} - T_{amb}) \quad (6)$$

$$\dot{Q}_{loss} = \dot{Q}_{loss, rad} + \dot{Q}_{loss, conv} \quad (7)$$

$$\dot{Q}_{loss} = \dot{Q}_{steel} = \dot{Q}_{insulation} = \dot{Q}_{ceramic} \quad (8)$$