Supplementary Information

Ceramic microreactors for on-site hydrogen production from high temperature steam reforming of propane

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Derivation of appropriate equations for kinetic analysis

Eqn (4) in the manuscript represents the PFR design equation. After substituting the power rate law expression for the rate term, the following equation is obtained:

$$\frac{\mathrm{d}X}{\mathrm{d}V} = \frac{k' C_{\mathrm{P}}^{\alpha} C_{\mathrm{W}}^{\beta}}{F_{\mathrm{P0}}} \tag{S1}$$

The concentrations must then be expressed in terms of the conversion of propane X. Table S1 lists the flow rates of relevant species at the inlet and after a certain value of X, where A is the inlet flow rate of propane, B is the inlet flow rate of steam, and D is the inlet flow rate of helium.

Table S1. Stoichiometric table for the steam reforming of propane.

Species	Inlet flow rate	Change in flow rate	Final flow rate
C_3H_8	A	$-AX$	$A(1-X)$
H_2O	B	$-3AX$	$B-3AX$
CO	0	$+3AX$	$3AX$
H_2	0	$+7AX$	$7AX$
He	D	0	D
Total	$A+B+D$	$+6AX$	$A(1+6X)+B+D$

Since the inlet flow rate of He was kept at 25 percent of the total inlet flow rate, then the following equation can be written:

$$4D = A + B + D \tag{S2}$$

The steam-to-carbon ratio (here, represented as α_{C}) can be used to express B in terms of A:

$$B = 3\alpha_{\mathrm{C}} A \tag{S3}$$

Using eqns (S2) and (S3), the final total flow rate in Table S1 can be expressed as the following:

$$A(1+6X) + B + D = A(6X + 4\alpha_{\mathrm{C}} + \frac{4}{3}) \tag{S4}$$

The concentration of any species *i* can be expressed in terms of the mol fraction of *i*, y_i, assuming ideal gas behavior, with the following equation:

$$C_i = \frac{P_i}{RT} = \frac{y_i P}{RT} \tag{S5}$$

The mol fraction can also be expressed as the ratio of the flow rate of species *i* to the total flow rate. Substituting this ratio for the quantity y_i yields the following expressions for the concentrations of propane and steam:

$$C_{\mathrm{P}} = \frac{P}{RT}\left(\frac{1-X}{6X+4\alpha_{\mathrm{C}}+4/3}\right) \tag{S6}$$

$$C_{\mathrm{W}} = \frac{P}{RT}\left(\frac{3(\alpha_{\mathrm{C}}-X)}{6X+4\alpha_{\mathrm{C}}+4/3}\right) \tag{S7}$$

Substituting eqns (S6) and (S7) into eqn (S1), the following equation is obtained:

$$\frac{\mathrm{d}X}{\mathrm{d}V} = \frac{k'}{F_{\mathrm{P0}}}\left(\frac{P}{RT}\right)^{\alpha+\beta}\left(\frac{1-X}{6X+4\alpha_{\mathrm{C}}+4/3}\right)^{\alpha}\left(\frac{3(\alpha_{\mathrm{C}}-X)}{6X+4\alpha_{\mathrm{C}}+4/3}\right)^{\beta} \tag{S8}$$

The Ergun equation describes the pressure drop gradient in a packed bed reactor and is represented by eqn (5):

$$\frac{\mathrm{d}P}{\mathrm{d}V} = -\frac{G}{101325 A_{\mathrm{C}} d_{\mathrm{P}} \rho}\cdot\frac{1-\varepsilon}{\varepsilon^3}\cdot\left[\frac{150(1-\varepsilon)\mu}{d_{\mathrm{P}}}+1.75G\right] \tag{5}$$

The superficial mass velocity, *G*, is calculated from the total volumetric flow rate and steam-to-carbon ratio. The density of the gas mixture, ρ, is equal to the molar density of the gas multiplied by its average molecular weight, represented by the following equation:

$$\rho = \frac{P}{RT}\sum_i y_i MW_i \tag{S9}$$

where MW_i is the molecular weight of species *i* (in kg mol^{-1}). Using the stoichiometric table, the mol fractions y_i are substituted into eqn (S9) along with the molecular weight of each species. This expression for ρ is then substituted into eqn (5), giving the following equation:

$$\frac{\mathrm{d}P}{\mathrm{d}V} = -\frac{GRT}{101325 A_{\mathrm{C}} d_{\mathrm{P}} P}\cdot\frac{1000(6X+4\alpha_{\mathrm{C}}+4/3)}{45.431-0.003X+58.051\alpha_{\mathrm{C}}}\cdot\frac{1-\varepsilon}{\varepsilon^3}\cdot\left[\frac{150(1-\varepsilon)\mu}{d_{\mathrm{P}}}+1.75G\right] \tag{S10}$$