Biomass gasification using carbon dioxide: Effect of temperature, CO_2/C ratio and the study of reactions influencing the process

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Table S1: Calculations for minimum fluidization velocity:

Ergun's correlation for pressure drop per unit length across packed of solid particles is shown in equation [A.1].

$$\frac{\Delta P}{L} = \frac{150\,(1-\varepsilon)^2}{\phi^2\varepsilon^2}\frac{\mu u}{dp^2} + \frac{1.75(1-\varepsilon)u^2\rho_g}{\varepsilon^3\phi dp} \qquad [A.1]$$

where, ε is the void fraction (porosity), ϕ is the sphericity of the bed solids, μ is the dynamic viscosity, and ρ_g the gas density. However, when the particle of bed fluidizes, the drag forces equal the buoyancy of the particle, thus the drag force is given by [A.2]

$$F_D = \Delta PA = AL\,(1-\varepsilon)(\rho_p - \rho_g)g \qquad [A.2]$$

These equations are solved simultaneously to obtain the minimum fluidization velocity, Umf, as defined in equation [A.3]:

$$Re_{mf} = [C_1^2 - C_2Ar]^{0.5} - C_1 \qquad [A.3]$$

$$Ar = \frac{\rho_g(\rho_p - \rho_g)g dp^3}{\mu^2} \qquad [A.4]$$

The values of C_1 and C_2 have been approximated in literature[38] over a wide range of fluid properties and particle sizes and the equation is written as:

$$Re_{mf} = [33.7^2 + 0.0408Ar]^{0.5} - 33.7 \qquad [A.5]$$

For sand (ρ_p =2776 kg/m³ & mean particle size dp= 263 μm), the minimum fluidization velocity was found out to be 0.0636 m/s.

Table S2: Intra particle mass transfer limitation calculations:

Thiele modulus (ϕ) is the measurement of reaction rate with respect to the rate of diffusion. Lower values of ϕ (less than 0.3) imply that the rate of diffusion is high and the process is kinetically controlled

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whereas higher values imply that the system shows mass transfer resistance. Simplifying, the value of ϕ can be calculated using equation [B.1].

$$\phi = \frac{d_p}{6}\sqrt{\frac{R_{obs}}{De_{CO_2}}} \qquad \text{[B.1]}$$

where dp = particle diameter, R_{obs} = observed reaction rate, and De = effective diffusivity which is calculated using equation [B.2].

$$De = \frac{D_{CO_2}\phi_p\,\sigma_c}{\tau} \qquad \text{[B.2]}$$

Where ϕ_p = particle porosity calculated to be 0.32, σ_c = Constriction factor and τ = tortuosity. The value of R_{obs} is calculated using the specific reaction rate obtained from a study by Van Dan Aarsen, et al. as mentioned in Appendix A. The calculated values of De and R_{obs} are plugged in equation [B.1] to yield the value of ϕ = 0.106. This implies that the process is kinetically controlled and the influence of mass transfer can be neglected.

Table S3: Heat transfer limitations between bulk phase and particle

A heat balance between the particle and surrounding medium at the particle surface can be written as:

$$h * A_p * (T - T_S) = \Delta H * R_r \qquad \text{[C.1]}$$

Where h is the heat transfer coefficient (W/m^2K), A_p is the surface area of the particle (m^2), T and T_S are the temperatures (K) of the surrounding medium and the particle respectively, ΔH is the heat of reaction (kJ/mol) taking place inside the particle and R_r is the rate of reaction (mol/s). The value of h is determined using the correlation [C.2]:

$$Nu = 0.3\ Re^{1.3} \qquad \text{[C.2]}$$

Parameters in this study:

dp (biomass) = $315*10^{-6}$ m; u = 0.11 m/s; Viscosity = $1.76*10^{-5}$ Pa s; ρ_g = 1.251 kg/m^3; K = 0.024 W/mK

The value of h obtained from this correlation = 76.4 W/m^2K

Due to presence of multiple reactions in the current process, ΔH and R_r cannot be specified. Considering Boudouard reaction, ΔH = 172 kJ/mol. Van Dan Aarsen, et al.[26] studied the char – CO_2 gasification in a fluidized bed and reported the following values at 815°C:

R" (specific reaction rate) = $75.9*10^{-6}$(mol/m^2s); S_o (specific surface area) = $1.05*10^8$ (m^2/m^3). Equation [C.1] becomes:

$$h * A_p * (T - T_S) = \Delta H * R'' * S_o * V_p \qquad \text{[C.3]}$$

From the above correlation, the value of (T-Ts) obtained = 1.1. Therefore, the bulk temperature of the particle has to be corrected by 1.1°C