Simple mass transfer simulation using a single-particle heterogeneous reaction approach in rice husk combustion and rice husk ash extraction

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Abstract. Rice husk conversion to silica is usually carried out through combustion to produce ash and then continued with ash extraction to obtain silica. There is a model to simulate the single-particle combustion, which abandoned the simplification. However, the model is complex and seems complicated for early beginners. This study, hence, aims to discuss the simple mass transfer simulation using a single-particle heterogeneous reaction approach. The shrinking core model was targeted for rice husk combustion time prediction, whereas mass transfer effectiveness analysis was used in rice husk ash extraction simulation. According to this study, a shorter combustion time is reached under smaller particle diameter, more spherical particle, and higher oxygen concentration. The result showed that a combustion time of 133 minutes is obtained for oxygen diffusion to rice husk with diameter 5.8 mm, sphericity 0.5, and oxygen concentration 21%-vol. Besides, in order to improve the rice husk ash extraction overall mass transfer effectiveness from 0.01 to 0.1, extraction should be done under particle diameter of 0.2 mm, sphericity of 0.8, and agitator tip velocity of 5 cm/s. All of the parameters lessen the mass transfer limitation due to diffusion, and in consequence, intrinsic kinetic becomes a major factor.

1. Introduction

Rice husk is one of the special Indonesian biomass (besides bamboo leaves) because of its superior silica content in ash rather than other biomass, which can exceed 90% [1,2]. Rice husk as biomass is not only directed to alternative energy sources but also for industrial green chemicals [3–5]. For silica production purposes, rice husk is combusted, and the ash produced is then extracted with alkaline [6–9].

The rice husk combustion modelling study by Anshar et al. (2014) was intended to predict the maximum combustion temperature as well as the flue gas exhaust composition [10]. Meanwhile, a study on rice husk utilization for energy purposes by Chang et al. (2017) was aimed at predicting the maximal combustion temperature and specific rice husk consumption [11]. Also, the calculation of rice husk potential as an energy source in Pakistan relied on the energy amount produced [12]. Other than that, the rice husk ash extraction study mainly focused on direct experiments and mostly discussed the several
factors influencing its performance, i.e., acid leaching duration, acid concentration, alkaline amount, alkaline concentration, extraction duration, and extraction temperature [5,7,13–15]. Likewise, there is an orthogonal collocation model to simulate the single-particle pyrolysis and combustion, which abandoned the simplification and was able to simulate the current particle pyrolysis and combustion with high accuracy [16]. However, the simulation has high complexity and seems complicated for early beginners. As aforementioned, the simple mass transfer approach for rice husk combustion and rice husk ash extraction is still rarely reported. Therefore, this study aims to present it. Two case studies were provided, those are rice husk combustion time prediction with shrinking core model and rice husk ash extraction overall mass transfer effectiveness determination under various particle diameter, particle sphericity, and agitator tip velocity. It should be highlighted that the shrinking core model used in this simulation ignored the drying, devolatilization, and oxidation stages in the rice husk combustion, so the combustion phenomenon was considered to occur solely due to the interaction of a single rice husk particle with oxygen. The simulation followed the procedure from Levenspiel (1999) for shrinking core model [17]. The mass transfer approach was also assumed similar to the simple external diffusion on heterogeneous reactions, as stated in Fogler (1992) [18,19].

2. Case study I: Shrinking core model for predicting rice husk combustion time
The observation on coal or biomass combustion is still favored when described with the shrinking core model [17]. This model assumed single particle combustion with no particle size changes, as illustrated in Figure 1.

![Figure 1. Shrinking core model in rice husk combustion](image)

The mathematical model is derived from the steady-state shell mass balance of oxygen diffusion from the outer particle surface ($J_A$) and the mass balance of the particle due to reaction with oxygen (Figure 2). The calculation follows equation 1a [17,18]. Both sides in equation 1a are then divided by $4\pi r \Delta r$, taking $\Delta r \to 0$, and replacing $J_A$ with $-D \frac{dC_A}{dr}$ (First Fick’s Law, where $D$ is effective oxygen diffusivity in the rice husk particle). Yet, as a result of neglecting the presence of devolatilization and oxidation stages, oxygen is assumed not reacted with devolatilized products during diffusion toward rice husk particle surface. In addition, although rice husk has high porosity (63-69%) [20], the diffusion of oxygen through the porous matrix was also neglected and resulted in $r_A = 0$. Equation 1a will further rearrange to form equation 1b [17,21]. The boundary conditions are at $r = R_0$, $C_A = C_{A0}$ and at $r = R$, $C_A = 0$. By considering those boundary conditions, solving equation 1b will lead to equation 1c.
The particle has a sphericity factor of \((\phi)\), and for oxygen diffusion to particle limitation, particle core shrinkage flux should equal to oxygen diffusion rate at the position of \(R\). The maximum conversion of rice husk combustion is achieved when \(R = 0\). The equation of combustion time \((t_c)\) is written as equation 2 [17,22].

\[
t_c = \frac{\rho R_0^2}{6 \phi D C_{A0}}
\] (2)

For oxygen diffusion to the gas film limitation at steady-state conditions, the particle core shrinkage flux should equal to oxygen diffusion rate to gas film. The maximum conversion of rice husk combustion is also achieved when \(R = 0\) and the equation of combustion time \((t_c)\) is given in equation 3 [17,22]. The \(C_{A0}\) is the initial oxygen concentration in the bulk fluid and due to the gas film limitation, \(C_{A,s}\) is the oxygen concentration at the particle surface is 0.

\[
t_c = \frac{\rho R_0^2}{3 \phi k C_{A0}}
\] (3)

The oxygen to the gas film diffusion constant \((k)\) is examined with dimensionless analysis, which requires Reynold \((Re)\), Schmidt \((Sc)\), and Sherwood \((Sh)\) Numbers. Again to be noted, this simulation ignores the water and devolatilized products that flow out away from the rice husk particle or commonly known as Stefan flow [16,23]. Thus, the Frössling correlation can be utilized as specified in equation 4 [18].

\[
Sh = 2 + 0,6(Re)^{\frac{1}{2}}(Sc)^{\frac{1}{3}} \rightarrow \frac{k d_p}{D \varphi} = 2 + 0,6 \left(\frac{\rho u d_p}{\mu \varphi}\right)^{\frac{1}{2}} \left(\frac{\mu}{\rho D}\right)^{\frac{1}{3}}
\] (4)

Rice husk particle combustion time calculation is conducted at a pressure of 1 bar and a temperature of 700°C. Particle is considered to have a sphericity factor which varies at 0.3; 0.5; and 0.8, particle diameter \((d_p)\) was varied from 0.2 to 5.8 mm. The oxygen concentration was varied by 12%-vol and 21%-vol, and oxygen linear velocity is 0 m/s due to the absence of airflow in fixed bed combustion. Other physical data properties involved are presented in table 1.
Table 1. Physical data for rice husk combustion time calculation [21,24].

| Parameter                  | Value  | Units     |
|----------------------------|--------|-----------|
| Rice Husk Particle Density | 600    | kg/m³     |
| Gas-Particle Diffusivity   | 2.5 x 10⁻⁶ | m²/s   |
| Gas-Air Diffusivity        | 1.9 x 10⁻⁵ | m²/s   |
| Gas Viscosity              | 4.0 x 10⁻⁵ | Pa.s    |
| Gas Density                | 0.3    | kg/m³     |

The combustion reaction occurs spontaneously [15], so this calculation and only considers diffusion limitation. Figures 3 and 4 show the rice husk combustion time results for the diffusion determining step are increased along with larger particle diameter. Both figures also declare that at 12%-vol of oxygen concentration, combustion time is about two times longer than normal condition, 21%-vol of oxygen concentration. In contrast, combustion time is found longer under low particle sphericity. The particle with a sphericity of 0.3 gives three times greater combustion time than the sphericity of 0.8. Herein signifies that the sphericity factor becomes an influencing factor in rice husk combustion when diffusion is a determining step.

![Oxygen diffusion to particle limitation](image1)

**Figure 3.** Rice husk combustion time for oxygen diffusion to particle limitation.

![Oxygen diffusion to gas film limitation](image2)

**Figure 4.** Rice husk combustion time for oxygen diffusion to gas film limitation.

Rice husk fixed bed combustion usually occurred for about 2 hours [25]. The combustion simulation result reveals that rice husk with an average diameter of 5.8 mm and an average sphericity factor of 0.5 gives a combustion time of 133 minutes under 21%-vol of oxygen concentration. Although so many
aspects are ignored in this simple mass transfer simulation, the shrinking core model is still able to predict the rice husk combustion time, which is relatively consistent with the common experiments. This is implied that the appropriate rate-determining step is oxygen diffusion to particle, while the oxygen diffusion to gas film and reaction stages undergo in an immediate moment.

3. Case study II: Overall mass transfer effectiveness in rice husk ash extraction

Rice husk ash extraction was carried out using an alkaline solvent $MOH$. The extraction follows the reaction: $(SiO_2)_{ash} + 2MOH \rightarrow (M_2SiO_3)_{aq} + H_2O$ [4,5,7,26]. Subsequently, the extracted solution is filtered, and the filtrate is then titrated with acid $HX$ until it forms a precipitate with a gel-like texture $[5,9]$. The precipitation follows the reaction: $(M_2SiO_3)_{aq} + 2HX \rightarrow 2MX + SiO_2 \downarrow + H_2O$ [4,5,7,26]. Finally, the precipitate is dried $[5,9]$. Similar to rice husk combustion, there are three types of rate-determining steps in rice husk ash extraction: external diffusion (alkaline diffusion to ash particle), internal diffusion (alkaline diffusion into the ash pore structure), and reaction between alkaline and silica in ash particle. Since the reaction occurs spontaneously without a catalyst, a suitable determining step is external and internal diffusions. The extraction kinetic rate is not intrinsic but ought to involve the overall mass transfer effectiveness ($\Omega$) $[19]$.

The overall mass transfer effectiveness is derived from the shell mass balance of alkaline solvent in the rice husk ash particle, equation 5. The particle is assumed spherical and has an internal surface area of $S_a$ as well as density of $\rho_p$. The boundary conditions for equation 5 are when $r = R$, $C_A = C_{A,S}$ (alkaline concentration at the ash surface); and when $r = 0$, $\frac{dC_A}{dr} = 0$.

$$\frac{d^2C_A}{dr^2} + 2 \frac{dC_A}{dr} - \frac{kCA_s\rho_p}{D} = 0$$

This section introduces the parameter $\phi$ as the Thiele Modulus, defined as the ratio between the intrinsic reaction rate and the diffusion rate $[19]$. The mathematical form of the modulus is given in equation 6a. Substitution of equation 6a to equation 5b and solving the differential equation will lead to equation 6b.

$$\phi = R \sqrt{\frac{kCA_s\rho_p}{D}^{-1}}$$

$$C_A = C_{A,S} \frac{R \sinh(\phi \frac{r}{R})}{r \sinh(\phi)}$$

Afterward, the internal mass transfer effectiveness ($\eta$), which is the ratio of actual reaction rate by the intrinsic reaction rate is expressed in equation 7. To evaluate the alkaline concentration in the bulk fluid ($C_{A,0}$), the relationship between the bulk and surface concentration should be determined. The area involved in the bulk fluid is particle area ($A_p$), whereas the area at the surface is pore area ($A_S$) which is far greater than particle area. Following the aforementioned explanation, the reaction rate is substantially the same as the mass transfer rate steady-state condition. Finally, the overall mass transfer effectiveness is expressed in equation 8 $[19]$.

$$\eta = \frac{3}{\phi^2} [\phi \coth(\phi) - 1]$$

$$\Omega = \eta \left(1 + \frac{\eta kA_S}{k_cA_p}\right)^{-1}$$

The mass transfer coefficient in the particle side ($k_c$) is evaluated by Thones-Kramers correlation involving Sherwood ($Sh'$), Reynold ($Re'$), and Schmidt ($Sc'$) Numbers. The correlation is shown in
equation 9 and accurate for porosity ($\varepsilon$) between 0.25-0.5, $Re'$ which is in the range of 40-4000, and $Sc'$ between 1-4000 [18].

$$Sh' = (Re')^{\frac{1}{2}}(Sc')^{\frac{1}{3}} \rightarrow \frac{k_c d_p \varepsilon}{D(1 - \varepsilon) \varphi} = \left(\frac{\mu_d d_p}{\mu (1 - \varepsilon) \varphi}\right)^{\frac{1}{2}} \left(\frac{\mu}{\rho D}\right)^{\frac{1}{3}} \tag{9}$$

Figure 5a is the alkaline concentration plot inside the particle at various Thiele Modulus values of 0.2, 1, 5, and 25. It can be seen that at a small modulus, there is a slight alkaline concentration gradient between the outer and inner particles, which indicates that chemical reaction is a rate-determining step [19]. At the center of the particle, the alkaline concentration remains significant. On the other hand, a greater modulus value enlarges the alkaline concentration gradient, even before the alkaline far penetrates the center of the particle. When alkaline reaches the center of the particle, the alkaline concentration is very low, which signifies diffusion is a rate-determining step. In order to reduce the modulus value, rice husk ash extraction should be performed with a small particle diameter and high mass transfer coefficient, which could be realized by vigorous stirring [27].

Simulation is performed at varying ash particle diameter ($d$) from 0.2 to 5.8 mm; sphericity factor 0.3 and 0.8; agitator tip velocity 4-5 cm/s; solution density 1300 kg/m$^3$; solution viscosity 0.2838 cP; bed porosity 0.3; diffusivity of particle in the solution 10$^{-9}$ m$^2$/s; internal pore area 530 m$^2$/g; external particle systems area 3.57$\times$10$^{-4}$ m$^2$/g; and the reaction rate constant 4.42$\times$10$^{-10}$ m$^3$/m$^2$/s. Under this case, Schmidt Number lies at 21.83, and Reynold Number varied between 49.08 and 3926.31, which implies these conditions still meet the accuracy criteria of the Thoenes-Kramers correlation. The simulation results are given in Figure 5b.

The calculation shows that overall mass transfer effectiveness is augmented from 0.01 to 0.1 along with reducing ash particle diameter from 5.8 mm to 0.2 mm, higher ash particle sphericity from 0.3 to 0.8, and larger agitator tip velocity from 4 to 5 cm/s. To gain high overall mass transfer effectiveness, the rice husk ash extraction should be achieved by intensifying agitator tip velocity, enhancing ash particle sphericity, and reducing ash particle diameter at once [5].

The agitator tip velocity is associated with external diffusion, while particle diameter and sphericity are related to internal diffusion [17]. High agitator tip velocity generates great turbulence and significantly reduces external mass transfer resistance [22,27]. The more spherical particle, as well as smaller particle diameter, are realized through applying acid leaching prior to rice husk ash extraction.
Higher effectiveness value implies less mass transfer limitation due to intrinsic extraction kinetic plays a dominant role.

4. Concluding remarks
The simple mass transfer simulation for predicting rice husk combustion time and rice husk ash extraction performance has been successfully investigated. From this study, the shrinking core model is somewhat suitable for rice husk combustion time prediction with the oxygen diffusion to the particle becoming a rate-determining step. The average particle diameter of 5.8 mm and particle sphericity factor of 0.5 give a combustion time of 133 minutes under 21%-vol of oxygen concentration. Meanwhile, the external and internal diffusions become a rate-determining step for rice husk ash extraction. Reducing the ash particle diameter from 5.8 mm to 0.2 mm, increasing ash particle sphericity from 0.3 to 0.8, and intensifying agitator tip velocity from 4 to 5 cm/s enhance the overall mass transfer effectiveness from 0.01 to 0.1. Consequently, extraction should be provided under smaller ash particle diameter, higher sphericity, and intense agitator tip velocity. The smaller ash particle diameter, as well as higher sphericity, can be realized by applying acid leaching to rice husk ash prior to extraction.

5. References
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