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An improved numerical model for early detection of bed agglomeration in fluidized bed combustion

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Abstract

An improved predictive numerical index has been developed to predict the tendency of bed agglomeration in fluidized bed boilers. The index was developed based on the melt fraction resulting from the thermodynamic equilibrium model of fuel ash compositions together with SiO_2 as the bed material at temperatures ranging from 700 to 900 °C. The partial least square regression (PLSR) coupled with the cross-validation technique is utilized to establish the correlation for the bed agglomeration index, I_a. The improved index, I_a has been validated by experimental observations found in various literature sources. The results obtained using the improved index, I_a demonstrated a significantly higher success rate in predicting the bed

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agglomeration tendency of biomass fuel ash compared to the other four conventional bed agglomeration indices. In addition, K_2O is the main element that accelerates the formation of bed agglomeration in the biomass firing while CaO was found to reduce the tendency of bed agglomeration in the fluidized bed combustion system.

Keywords: Biomass; Bed agglomeration index; Thermodynamic equilibrium model; Silica sand; Fluidized bed

1 Introduction

Over the past few years, research has been focused on a comprehensive analysis of the agglomeration mechanisms occurring during biomass's fluidized bed combustion (FBC). This is included by looking at the aspects of potential early detection methods and operational countermeasures for agglomeration mechanisms in the FBC system [1]. First of all, it is important to understand the fundamental root cause of the agglomeration problems in the FBC systems. Agglomeration is fundamentally driven by the formation of eutectic alkali silicates due to the interaction between SiO_2 in the bed material or ash and alkali species such as K_2O and Na_2O [2-4]. The alkali silicate formation will determine the eutectic melting temperature as the primary instigator of bed agglomeration. The low melting temperature of eutectic compounds (<800 °C) [5] will cause bed agglomeration in the FBC due to the formation of melt at temperatures 800-900 °C [6]. In addition, it has been reported that the emergence of alkali phosphates also results in bed agglomeration [7, 8]. Bed agglomeration can cause an unfavourable flop of the fluidized bed, which is described as defluidization. As a result, several cases have been reported in the literature that the defluidization of the bed will lead to the shutdown of the fluidized bed combustors.

Visser et al. [9] identified two mechanisms responsible for the agglomeration of bed particles in the FBC system which are coating-induced and melt-induced agglomeration. Melting phenomena are crucial in both mechanisms. In the coating-induced mechanism, ash deposited on bed particles will form a liquid phase as a result of chemical reactions which causes multiple particles to stick to each other. Melt-induced agglomeration means the straight adherence of the bed elements through relatively liquified fuel-derived cinders. Melt-induced agglomeration relies on larger molten ash particles colliding with the bed particles, with the molten ash acting as a viscous glue [10-12]. However, coating-induced agglomeration has been identified as the predominant mechanism in the FBC system [2, 3]. Various researchers assessed bed particle composition and subsequently used thermodynamic calculations to identify potential melt phases. This suggests that all chemical reactions within the ash have achieved thermodynamic equilibrium corresponding to coating-induced agglomeration.

According to F. Scala et al. [1], the method of combination between thermodynamic equilibrium analysis and compression strength test was unable to predict the sintering tendency of biomass ash, this is due to the method not taking into consideration the interaction between ash and quartz as bed material. This also happened the same in the past when the researchers tested the ash fusion accuracy to predict the bed agglomeration temperatures. Therefore, it was concluded that the ex-situ method failed to predict the bed agglomeration behaviours [1]. Over the years, researchers have proposed various empirical indices for bed agglomeration in the FBC system. The alkali index is generally effective in predicting agglomeration, however, its accuracy diminishes when considering factors such as alternative bed materials or additives, as noted by various researchers [13-15]. Fernández Llorente et al. [16] determined that the ratio of alkaline earth oxides to alkaline oxides is a weak indicator of ash sintering likelihood and severity. Moreover, the bed agglomeration index (BAI) was introduced to measure the operational issues in FBC technology. Several publications report that silica-dominated in-bed agglomerations form in fluidized bed combustors at 760-900 ºC [14, 17]. The BAI index, however, does not take this element into account when making predictions about deposit generation. P. Billen et al. [18] proposed a method to predict the agglomeration in FBC by predicting melt formation and agglomeration using phase diagrams as a result of thermodynamic calculations. Recently, Nik Norizam et al. [19] successfully produced a numerical model to predict slagging propensity in the fixed bed reactor by using the melt formation theory. Melt formation is the formation of a liquid phase when the temperature exceeds the melting point of compounds in the ash. This can cause the ash and bed particles to stick together and agglomerate leading to melt-induced agglomeration. On the other hand, coating-induced agglomeration occurs when the ash reacts with the bed material and forms a coating on the bed particles. The melt phase in this case only forms after the ash interacts with the bed material. This coating facilitates the agglomeration of the ash and bed material.

To the best of the authors' knowledge, a number of research have been done in the past to develop bed agglomeration prediction indices in the FBC system, however, the applicability of the existing indices across different types of biomass to estimate the bed agglomeration tendency remains limited. This is because previous researchers have not focused sufficiently on the chemical reactions of fuel ash compositions in response to temperature changes within the system. Also, this can be supported by Morris et al. [2], who recommended determining bed agglomeration behaviour influenced by the fuel ash composition. In this paper, an improved semi-empirical index based on the thermodynamic equilibrium model (TEM) is developed for early detection of bed agglomeration combustion in FBC technology. The research aims to predict bed agglomeration in FBC biomass technology by analyzing chemical ash compositions, using TEM to assess the melting degree of biomass fuels with SiO_2 (quartz) as the bed material. Then the partial least square regression (PLSR) coupled with cross-validation has been employed to create a numerical model, I_a to estimate the bed agglomeration index based on the experimental ash composition and the degree of melt from TEM. The results obtained with the improved numerical model, I_a demonstrate a significantly greater success rate in forecasting the tendency of bed agglomeration as compared to experimental observations from the existing literature. This predictive tool would allow a better selection of fuels and a priori incorporation of countermeasures in the FBC system for the industrial operators.

2 Material and methods

In this section, the discussion focuses on the datasets employed to develop an improved index to predict the bed agglomeration tendency of biomass. A total of 35 datasets containing biomass ash compositions were gathered from relevant literature sources [7, 20-27], as illustrated in Table 1, which consists of ash compositions, ash content (%) and experimental observations of bed agglomeration tendency in the FBC boiler. 9 major ash compositions (Na_2O, MgO, Al_2O_3, SiO_2, P_2O_5, K_2O, CaO, SO_3, Fe_2O_3) and quartz (SiO_2) as a bed material were included in the model, however, TiO_2 was excluded due to its low content in the ash. The initial 20 datasets (1-20) represent experimental ash composition data and have been designated as training datasets, while the subsequent 15 datasets (21-35) will serve as testing datasets. The training and testing datasets will be analysed through thermodynamic equilibrium modelling in Section 2.1 to predict the melting fraction based on the ash compositions. The obtained results will be utilized in Section 2.2, where PLS regression analysis will be employed to formulate an expression, denoted as I_a, for predicting the bed agglomeration behaviour without the necessity for conducting combustion tests in the future. Subsequently, the effectiveness of I_a will be validated against experimental observations of bed agglomeration in the FBC system.

2.1 Thermodynamic equilibrium model

The application of thermodynamic equilibrium modelling (TEM) has become extensive in the industry as a tool to predict the ash transformation behaviour and the chemical and physical characteristics of ash in various ash-related processes, such as the issues of bed agglomeration in fluidized beds, heat transfer surfaces corrosion, and smelt bed behaviour patterns in boilers. The modelling was carried out using FactSage and the experimental data gathered during the measurements were utilised as model inputs to simulate the formation of the bed agglomeration in the FBC technology. It offers a reasonably accurate prediction of the ash conversion process without the need for intricate experiments for each biomass. However, it is important to note that the process in a real fluidized bed furnace may not entirely reach equilibrium although particles in a fluidized bed have much longer residence time than those in a pulverised combustor [28-31]. The FactSage thermochemical software is extensively employed for the analysis of solid fuel firing. It facilitates the computation of multiphase multicomponent equilibrium conditions, providing accurate results when configured with the appropriate fuel composition, atmosphere, and temperature settings [19]. It builds upon the Gibbs energy reduction and incorporates extensive databases for oxide, silicate, and salt composition structures [28-31]. The databases contained both unmixed compounds and solution stages. The pure compounds consist of stoichiometric element compositions, while the solution databases feature optimized frameworks for the solution stages. The methods employed to establish the thermodynamic database have been extensively examined in prior studies [28-31]. The FactSage 8.1 software was utilized in this study to predict the melting fraction, M_f of biomass fuels as listed in Table 1. The model extended the configuration set by Nik Norizam et al. [19] by integrating the bed material into the present model (iii) to simulate the bed agglomeration model in the FBC boiler, and the setting of the TEM is as follows:

i. The model is configured under the assumption of equilibrium conditions, utilizing the FACTPS, FTsalt, and FToxid databases.
ii. Table 1 includes 9 ash compositions (MgO, Al_2O_3, SiO_2, K_2O, CaO, Fe_2O_3, Na_2O, P_2O_5, SO_3) derived from experimental data. These compositions were normalised and labelled as input-stream 1 in the model.

Table 1 Chemical ash compositions for various types of biomass [7, 20-27].

Num.	Biomass	Na_2O	MgO	Al_2O_3	SiO_2	P_2O_5	K_2O	CaO	SO_3	Fe_2O_3	M_f	Ash content (%)	Agglomeration tendencies (experimental)
1	Logging residues	0.96	5.16	3.08	31.63	5.37	10.44	36.38	5.22	1.75	0.27	2.4	Low
2	Bark I	1.50	3.69	5.08	37.16	2.95	7.95	36.12	3.47	2.09	0.28	3.7	Low
3	Wheat straw	0.85	3.47	0.21	35.86	6.24	31.55	11.73	9.94	0.15	1.00	5.7	High
4	Sunflower husks	0.10	8.57	14.62	17.94	9.48	21.27	14.72	6.85	6.45	0.60	1.9	High
5	DDGS-logging residues	0.43	6.68	0.99	12.06	22.15	17.14	12.77	27.08	0.69	0.50	3.2	Low
6	DDGS-wheat straw	0.48	5.64	0.12	17.25	19.71	24.82	6.27	25.50	0.20	0.79	5.05	High
7	Logging residues-PA	0.95	4.99	3.03	31.12	7.82	10.27	35.09	5.01	1.72	0.28	2.4	Low
8	Pepper waste	1.05	4.55	8.40	15.40	11.20	35.36	10.04	10.62	3.38	0.95	7.4	High
9	Rice straw	0.70	9.24	3.34	33.66	0	10.33	36.62	0	6.11	0.19	n.m.	n/a
10	Corncob	3.27	10.34	5.21	46.27	0	21.94	5.24	0	7.71	0.70	n.m.	n/a
11	DDGS	0.20	6.99	0.03	3.27	28.65	19.35	2.31	38.98	0.22	0.70	4.4	High
12	DDGS-willow	0.37	6.67	0.38	5.06	25.35	19.69	10.73	31.39	0.36	0.55	3.3	High
13	Coconut shell	4.62	1.54	8.48	66.76	1.54	8.48	2.41	0.01	6.17	0.96	3.1	High
14	Rapeseed mean-bark	0.86	7.41	2.15	17.30	19.51	13.59	22.03	15.94	1.22	0.40	4.8	Low
15	Coffee (mbuni) husks	0.52	5.23	5.10	17.65	4.84	49.80	13.99	n.m.	2.88	1.3	4.1	High
16	Bark II	1.74	4.28	5.42	31.72	3.69	8.54	43.30	0	1.31	0.18	4.9	Low
17	Forest residues	1.23	6.18	2.48	18.04	6.44	16.08	42.28	5.26	2.01	0.16	n.m.	Low
18	Cotton stalk	4.52	11.08	4.06	7.80	9.03	40.23	21.34	0	1.93	0.67	1.75	High
19	Thistle	11.73	5.03	3.50	18.27	2.13	13.86	44.16	0	1.32	0.77	8.9	High
20	Almond shell	0.86	4.58	0.86	6.17	4.23	54.63	28.19	0	0.48	0.65	0.94	High

21	Rapeseed meal	0.20	9.95	0.24	2.16	32.29	17.83	11.31	25.48	0.55	0.40	7.4	Low
22	RM	0.19	9.91	0.23	2.38	32.16	17.74	11.47	25.33	0.60	0.43	6	Low
23	Logging residues-PA 2	0.89	4.71	2.86	29.36	13.01	9.69	33.11	4.73	1.50	0.39	2.4	Low
24	Rapeseed cake	7.32	8.41	0.20	1.29	35.69	18.32	13.35	15.07	0.35	0.70	7.5	High
25	Wheat straw 2	0.49	2.43	1.05	43.12	5.20	32.07	10.95	3.65	1.05	1.11	7.3	High
26	Brassica	1.25	3.82	2.25	14.05	6.59	27.75	43.37	0	0.92	0.34	7.7	Low
27	Cotton husks	1.32	7.59	1.32	10.93	4.05	50.20	20.95	1.72	1.92	0.90	3.2	High
28	Coffee husks	0.84	3.06	10.45	5.29	5.71	61.00	12.81	0.56	0.28	1.19	n.m.	High
29	Soy husks	6.27	8.40	8.76	2.01	5.80	36.09	25.33	4.38	2.96	0.70	5.1	High
30	Coffee (parchment) husks	0.64	4.76	5.78	21.34	4.37	47.43	12.60	0	3.08	1.1	0.9	High
31	Wood	0.84	1.26	5.74	17.93	2.94	0.70	63.31	0	7.28	0.1	0.5	Low
32	Peat	0.50	1.50	10.10	30.67	6.73	0.75	39.53	0	10.22	0.1	4.3	Low
33	RC-Bark10	7.24	8.26	0.22	2.52	35.13	18.31	14.85	13.09	0.37	0.68	7.2	High
34	RC-Bark20	6.89	8.01	0.46	3.84	32.91	17.47	16.04	13.79	0.59	0.67	7.0	High
35	RC-Bark30	6.75	7.80	0.76	5.52	31.98	17.36	17.83	11.36	0.65	0.66	6.7	High

a) All chemical compositions of ash were measured on dry basis in wt%.
b) M_f : Melt fraction obtained from equilibrium model.
c) n.m.: Not measured

iii. Quartz (SiO_2) was introduced into the system as input-stream 2 with a 1:1 ratio to the fuel. The temperature range of the equilibrium modelling was set between 700 and 900 °C in oxidizing conditions (excess of 10% O_2). This temperature range has been chosen based on the typical operating conditions of biomass FB boilers [2].

iv. The simulations utilized the "FToxid-SLAGA" and "FTsalt-SALTF" model, incorporating two-phase immiscibility as the solution database [32].

v. Record the weight range of the solid-liq phase formed for each fuel as a result of the equilibrium modelling.

vi. The solid-liq phase formed during the equilibrium calculation is fractioned by 1g of the ash to calculate the melt fraction, M_f.

2.2 Partial Least Square Regression Coupled with Cross Validation

The mathematical approach of Partial Least Squares Regression (PLSR) incorporates and generalizes the multivariate regression along with the analysis of the principal components [33]. It excels in analysing extensive datasets and multivariate systems with a high correlation, outperforming the multiple regression method [34]. This method is commonly employed to determine the stopping criterion and the total number of latent variables during cross-validation, considering only one observation at a time [34-36]. The PLSR is especially well-suited for problems with limited observational data, as encountered in the analysis of bed agglomeration behaviour of biomass. For additional details on PLSR and the cross-validation technique, please refer to the following references [33-35, 37-39]. The PLSR coupled with cross-validation techniques, was utilized for the analysis of the training datasets, as illustrated in Table 1. This process has led to the formulation of an equation, expressed as a function of the biomass ash compositions, to predict the improved bed agglomeration index (BAI), denoted as I_a.

3 Results & Discussion

3.1 Comparison melt fraction with and without presence of SiO_2 (quartz) predicted by TEM.

Isaak et al. [40] introduced the concept of melt fraction, suggesting that higher temperatures lead to an increased presence of liquid in deposits. Experimental findings by Isaak et al. [40] revealed a correlation between deposit stickiness and temperature, indicating that elevated temperatures result in stickier deposits due to an increased amount of liquid phase. Zhou et al. [41] indicated that the melting curve of ash melting fraction increases with an increase in temperatures. Moreover, the idea of melting fraction gained popularity in predicting the deposition of biomass ash [41-43]. Recently, Nik Norizam et al. [19] successfully developed a model to predict the slagging propensity in fixed bed boilers of woody biomass at high-temperature regions by employing the melting fraction concept obtained from the Factsage 8.1 equilibrium model. Based on Figure 1, the melt fraction was compared between the current FBC (with bed material) and the fixed bed model (without bed material). The motivation is to compare the melt fraction model with and without the presence of the bed material (quartz). The presence of bed material (rigid lines) has higher melt fractions compared to without the presence of quartz (dash lines). This proves that the presence of SiO_2 (quartz) as bed material actively reacts with the fuel ash compositions and produces a significant amount of agglomerates in FBC technology. Figure 1 demonstrates that Wheat straw (red line) exhibits a higher melting fraction than Bark I (blue line). Experimentally, it was observed that Wheat straw tends to have a high propensity for bed agglomeration, whereas Bark I exhibits a low tendency for bed agglomeration. This is because Wheat straw has a high ratio of K_2O/CaO compared to Bark I. The analysis of the chemical compositions of ash will be further explained in Section 3.2. In addition, Figure 1 clearly illustrates the melting degree increases with an increase in the temperature. Thus, the melting degree illustrated in TEM simulation is in

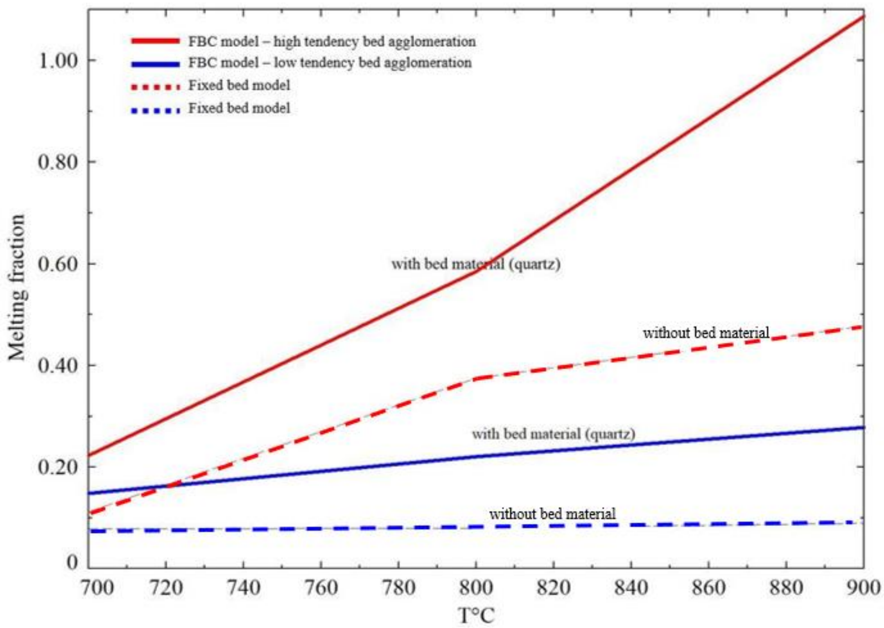

Figure 1 Comparison of the melt fraction between the FBC model with bed material and fixed-bed model without bed material.

agreement with the common melting curve demonstrated by Zhou et al. [41] and the melting fraction of woody biomass in fixed bed boiler by Nik Norizam et al. [19]. This paper concentrates on determining the melt fraction exclusively in the low-temperature range of 700-900 °C based on typically FBC operating conditions [2].

3.2 Analysis and application of an improved BAI, I_a

Predicting the bed agglomeration tendency in FBC can assist power plant operators in anticipating the fuel quality before biomass firing. The objective of this section is to create an improved numerical model for a bed agglomeration index, I_a. This numerical model is intended for predicting the bed agglomeration behaviour of biomass based on the fuel ash composition, eliminating the need for a thermodynamic equilibrium calculation process. This is particularly relevant as the FactSage software is not extensively utilized among power plant operators. The development of bed agglomeration index, I_a is based on the melting fraction, M_f and chemical ash compositions (training datasets 1-20) as shown in Table 1 by applying the method of PLS regression (PLSR) analysis, coupled with cross-validation. The root means square error

(RMSE), R^2, and slope for the training data were 0.031, 0.988 and 0.988, respectively which suggested a good fit of the model [44]. The expression of I_a is acquired as follows:

$$I_a = |[0.34 - 1.2055(MgO + CaO) + 1.6228(K_2O + Na_2O) + 7.113 \times 10^{-1}\, SiO_2 + 1.627 \times 10^{-1}(SO_3 + P_2O_5)]| \tag{3.1}$$

**Condition applying eq 3.1:*

*The **mass fractions** of the ash compositions must be applied for the oxide parameters in the Equation 3.1.*

The negative coefficient in Equation (3.1) for MgO+CaO indicates that an increase in the values of MgO+CaO will result in a decrease in the predicted value of BAI, I_a. Conversely, the parameters (SiO_2, K_2O+Na_2O, SO_3+P_2O_5) associated with the bed agglomeration tendencies of biomass fuel exhibit positive coefficients. This implies an increased value of these three parameters will result in a higher predicted number of BAI, I_a. Elements exhibiting positive coefficients are highly prone to the formation of bed agglomeration, with potassium being the most prevalent component in the agglomerates [2, 7, 20, 21, 24, 45]. Among the positive coefficients, the highest value is +1.6228, and it corresponds to the regression coefficient of potassium combined with sodium. This suggests that the presence of the potassium element significantly influences the bed agglomeration behaviour. Morris et al. [2] explained that agglomeration caused by melt-induced mechanism occurs when there is a sufficient content of silica and alkali metal in the fuel ash. Lin et al. [20] found that high potassium content in straw leads to the development of agglomerates and defluidization. According to Grimm et al. [7], the wheat straw (potassium rich fuel) showed high tendency of bed agglomeration upon firing in a 5 kW bubbling fluidized bed reactor. Figure 2 illustrates the solid-liquid phase for wheat straw obtained by the TEM simulation, it is clearly shown that most of the compounds containing potassium which consist of $K_2Ca_2Si_9O_{21}$, $K_2MgSi_5O_{12}$, K_2SO_4, and $KAlSi_3O_8$. This is in agreement with the study by Lin et al. [20] who suggested that compounds containing potassium have a tendency to persist in the bed and create potassium-rich ash with a low melting point during the combustion process. Moreover, experimental observation from Table 1 shows that about 95% of high bed agglomeration tendency was observed when the potassium value is higher than 10 wt%.

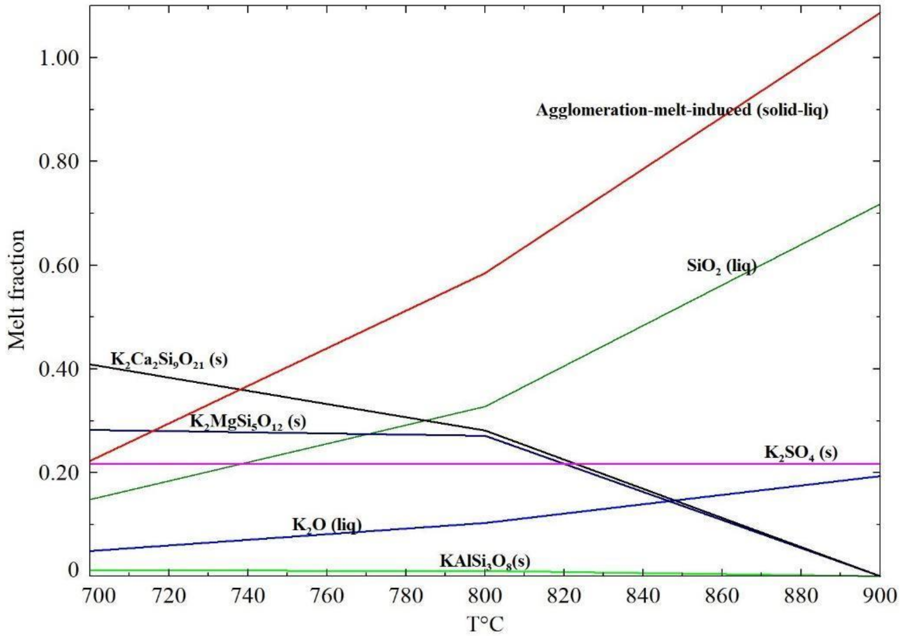

Figure 2 Solid-liquid phase for Wheat straw (3) obtained by the FactSage equilibrium modelling.

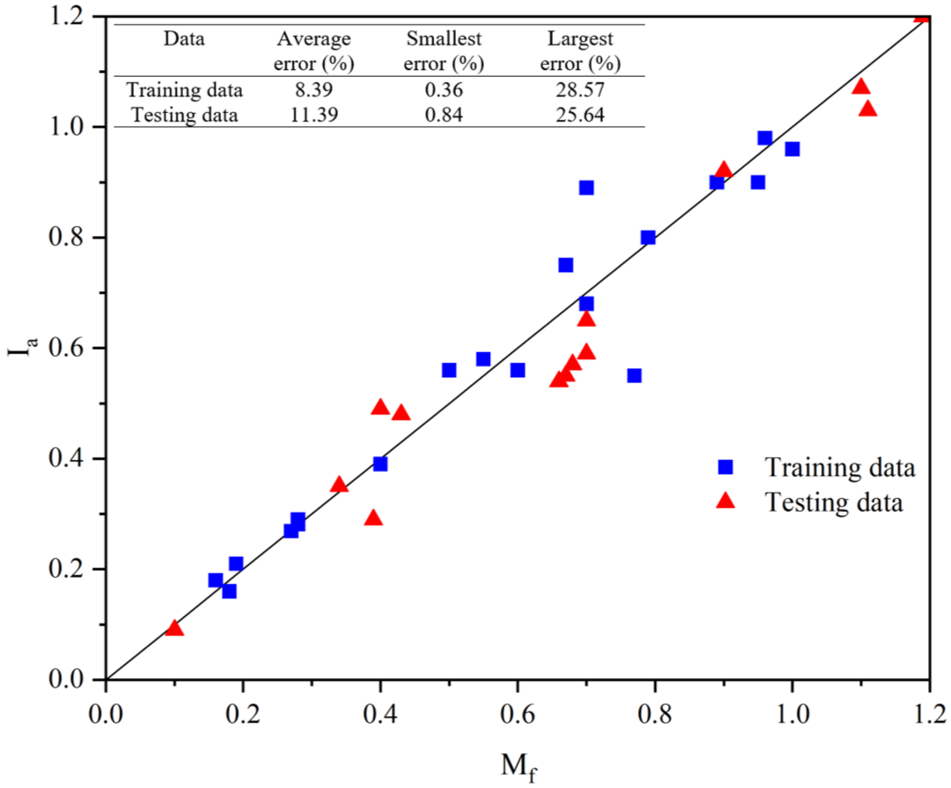

Figure 3 Comparison between melt fraction by TEM, M_f and predictive BAI index, I_a.

Figure 3 demonstrates a comparison between the melt fraction values, M_f and the predicted agglomeration index, I_a and the estimated error. The melt fraction for the 20 biomass fuels (training datasets) were determined using the TEM. The M_f value will serve as a quantitative measure of bed agglomeration behaviour and will be compared with the qualitative measurement (low and high) based on experimental observations. As explained in Section 3.1, the value of the melt fraction, M_f will increase corresponding to experimental observations of bed agglomeration from low to high tendency. For a comprehensive explanation of the classifications of the experimental observations, please refer to Table 2 [7, 20-24]. It can be observed that the predicted index, I_a closely matches the melt fraction, M_f for both the training and testing datasets. It was found that the average error for prediction bed agglomeration index, I_a is 11.39%, which indicates that both of the indices M_f and I_a are in agreement with each other and exhibit the same trend as the calculated agglomeration index.

Table 2 A comprehensive explanation of the classification for the bed agglomeration tendency by experimental observations.

Authors	Technique used to determine the bed agglomeration in FBC
Grimm et al. [7]	The study evaluates the bed agglomeration tendency based on the formation and characteristics of coating layers on bed particles, as well as the temperature at which agglomeration leads to defluidization.
Lin et al. [20]	The paper uses defluidization time as the primary metric to assess the agglomeration tendency in FBC, with temperature being a critical factor influencing this behavior. The shorter the time before defluidization occurs, the higher the agglomeration tendency.
Yu et al. [21]	The study is to determine the tendency of agglomeration in FBC of biomass by measuring the slip resistance between particles. An increase in slip resistance between particles will correspond to the defluidization and high tendency to bed agglomeration.
Llorente et al. [22]	The sintering degree of agglomerates of bed material was determined visually and the assessment of ash disintegration in the agglomerates and deposits.
Liu et al. [23]	The bed agglomeration tendency was measured by monitoring the chemical composition changes, observing the physical changes in the bed material particles, and correlating these with the operational stability of the CFB during the experiments.

Piotrowska et al. [24]	The bed agglomeration tendency was concluded by analysing the temperature and pressure to determine the initial and total defluidization temperature. The initial defluidization temperature indicated the growth of agglomerates. The bed agglomeration tendency will reduced with an increased in defluidization temperature.

Figure 4 shows the predicted value of the agglomeration index, I_a compared to the 15 experimental observations datasets (Table 1, numbers 21-35) from the literature [7, 20-27]. The results indicate that the value of I_a index below 0.5 corresponds to a low bed agglomeration tendency based on experimental observations. For example, Brassica (26) and Wood (31) were observed as low tendency of bed agglomeration in the experimental observation [22, 27]. This is due to the low ratio of K_2O/CaO. In contrast, biomass fuels with I_a value above 0.5 tend to show high bed agglomeration during combustion. Most of the biomass fuels that were observed to exhibit high bed agglomeration have a high K_2O/CaO ratio. For example, Cotton husks (27) and coffee husks (28) have high amounts of potassium which are 50.20 wt% and 61.00 wt%, respectively while the amount of calcium for both fuels are lower than the potassium content. The findings suggest that potassium-rich ash compositions typically led to higher bed agglomeration risks while biomass fuels with a high amount of calcium content shows lower bed agglomeration potential in fluidised quartz bed combustors.

However, the K_2O/CaO ratio alone is not sufficient to accurately predict bed agglomeration propensities. For example, Thistle (19) observed high agglomeration tendencies during the experiments despite having a low K_2O/CaO ratio. This discrepancy is because the K_2O/CaO ratio does not account for the elements that are prone to agglomeration such as sodium. Furthermore, Thistle (19) also showed a high melting fraction (0.77) in TEM analysis which indicated high tendency of bed agglomeration in fluidized bed reactor. On the other hand, Rapeseed meal (21) and RM (22) had high K_2O/CaO ratios, yet they showed low agglomeration propensities in the experiments. When their ash compositions were applied to

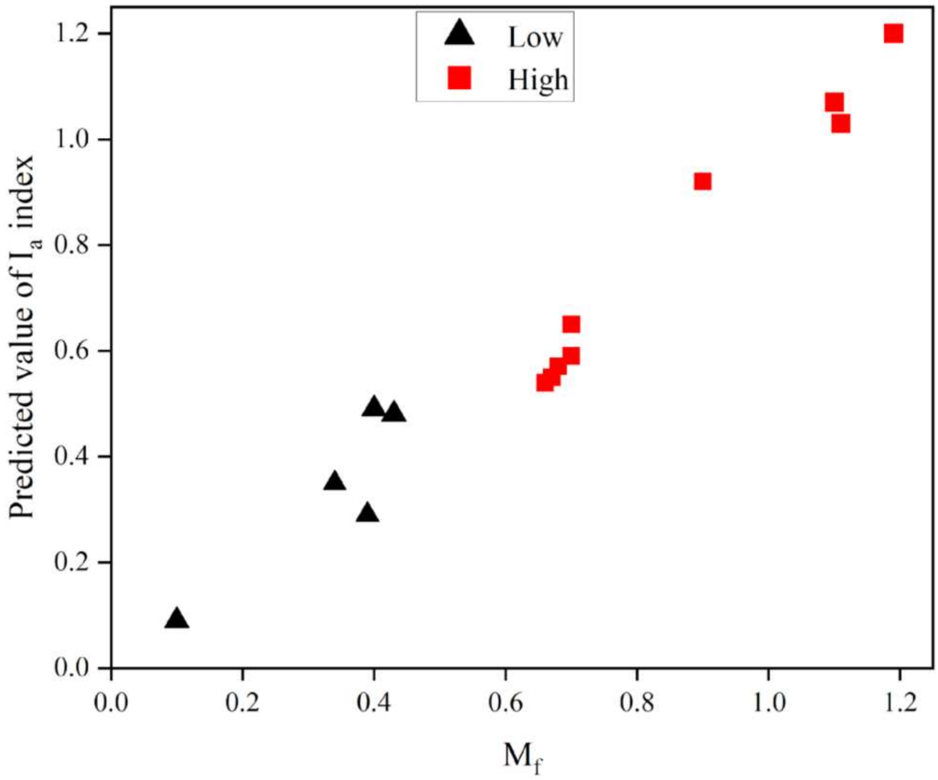

Figure 4 The predicted values in the proposed index, Ia versus experimental observations of bed agglomeration tendency.

the I_a index, the index accurately predicted their low agglomeration tendencies which aligned with experimental observations. This accuracy is because the I_a index considers multiple ash components beyond potassium and calcium, providing a more comprehensive prediction of agglomeration behaviour. In conclusion, the I_a index provides a more reliable assessment for predicting bed agglomeration in fluidized bed systems.

Figure 5 shows the performance of the improved model equation for I_a compared with four different existing index equations [10, 13-15, 46]. These four distinct expressions are created for predicting bed agglomeration behaviour in FBC technology [2]. Please refer to the appendix (Table 3) for a complete list of all the equations and their corresponding thresholds for each index. The Figure 5 illustrates the number of predicted samples, out of the 15 testing fuels (21-35), that correspond to the experimental observations for each index. It is observed that the ranking for the accuracy in the prediction performance, arranged from high to low, is as follows: I_a > I2 = (Na + K + Si) / (Ca + P + Mg) = BAI > I1 = (Na + K) / (2S + Cl) > Alkali

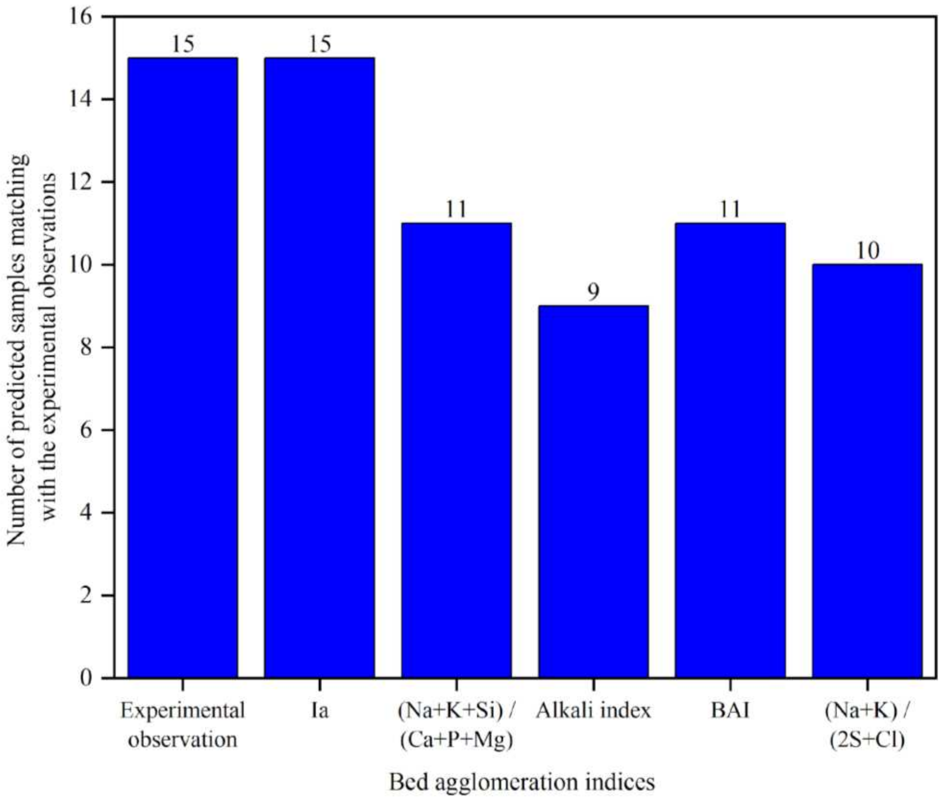

Figure 5 Comparison of the number of predicted samples matching with the experimental observations between I_a and 4 existing indices.

index. The new improved index, I_a, successfully predicted a total of 15 out of 15 samples in accordance with the experimental observations. On the other hand, the four existing indices (I2, Alkali index, BAI, I1) could only accurately predict a maximum of 73% of the total samples.

4 Conclusions

This study has successfully developed an improved semi-empirical index to predict the tendency of bed agglomeration in a FBC system. The index, I_a takes into account the chemical ash compositions when biomass is fired in fluidized bed combustors. The predictive tool created is capable of assisting industrial users in determining bed agglomeration behaviours when firing various types of biomass in FBC boilers. The newly improved bed agglomeration index, I_a was created by analysing the predicted melting fraction through TEM, considering the quartz as bed material used in the FBC system and chemical compositions of fuel ash, by employing the numerical PLS regression coupled with a cross-validation. The presented method has been verified using experimental observations from existing literature on biomass in the FBC technology. The results indicate that the BAI propensity index, I_a can be categorized into two primary groups: low bed agglomeration tendency when $I_a \leq 0.50$ and high bed agglomeration propensity when $I_a > 0.50$. In addition, the I_a demonstrates a significantly higher success rate compared to four existing indices in evaluating the tendency of bed agglomeration in fluidized bed type of boiler.

It can be confirmed that the primary element contributing to bed agglomeration formation is K_2O, while a high value of CaO will reduce the tendency of bed agglomeration in FBC. The index should be utilized during the low-temperature (700-900 °C) operation of fluidized bed boilers. In addition, the I_a index is developed based on fluidized quartz bed combustion, therefore, caution should be exercised when extending the predicted indices, I_a in this paper to other types of bed material used in FBC technology. The authors strongly recommend obtaining more extensive datasets of experimental observations by conducting tests at an industrial or full scale to improve the accuracy of the predictive indices in forecasting the tendency of bed agglomeration of FBC.

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Appendix

Table 3 list of all the equations and their corresponding thresholds for each index [10, 13-15, 46].

Index	Equation	Threshold for each index
I_a	$I_a = \lvert[0.34 - 1.2055(MgO + CaO) + 1.6228(K_2O + Na_2O) + 7.113 \times 10^{-1}\, SiO_2 + 1.627 \times 10^{-1}(SO_3 + P_2O_5)]\rvert$	Bed agglomeration tendency, I_a: low $\leq 0.50 <$ high
Alkali index	AI = (K_2O + Na_2O) kg/GJ	0.17 < AI < 0.34 agglomeration possible AI > 0.34 agglomeration near certain
Bed agglomeration index	$BAI = \frac{Fe_2O_3}{K_2O + Na_2O}$	Agglomeration when BAI < 0.15
Agglomeration index, I1	$I1 = \frac{Na + K}{2S + Cl}$	High agglomeration potential when I1 > 1
Agglomeration index, I2	$I2 = \frac{Na + K + Si}{Ca + P + Mg}$	High agglomeration potential when I2 > 1