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An improved index to predict the slagging propensity of woody biomass on high-temperature regions in utility boilers

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ABSTRACT

Ash deposition-related issues adversely affect the thermal transfer and cause corrosion to biomass fired utility boilers. Various models have been proposed to estimate the slagging propensities for firing biomass fuels of different origins. However, there is no reliable general applicable method that is available for assessing biomass fuel slagging propensities without carrying out extensive experimental testing. In addition, empirical correlations developed for coal produce large inaccuracies when applied to biomass. In this paper, a predictive slagging index, I_n, has been built by analysing the slagging formations of a range of woody biomass fuels, using the thermodynamic equilibrium modelling tool FactSage, together with the partial least squares regression (PLSR) coupled with cross-validation. The new index has been validated and supported by experimental observations from various literatures. The results obtained with the new index showed a substantially greater success rate in predicting the woody biomass ash slagging propensity when compared with the experimental observations from the literature than the other five conventional slagging indices. The predictive index, I_n, also successfully predicts the slagging propensities with high accuracy when extended to the application of herbaceous biomass and blended fuel between woody biomass and peat.

1. Introduction

Biomass as a fuel is gaining popularity as the demand for alternative energy sources grows since it is neutral of carbon, and its use decreases the reliance on fossil fuels. Biomass combustion, on the other hand, illustrates a number of technical challenges. Ash deposits accumulate inside the furnace and on the heat exchangers, such as the superheater tubes which not only hinders the transfer of heat in the super-heat exchangers, lowering the boiler's overall thermal efficiency, but it can also cause serious corrosion [1–4]. Slagging is usually associated with the deposit of fly ash in the 'flame exposure region' subject to radiant heat transfer. The deposited fly ash becomes adhesive when the local temperature is close to, or beyond, the ash melting point. Molten or semi-fused ash and sintered deposit comprise most of the slagging. In the initial stage of the formation of slag, a thin layer of powdery deposits will form on the cool tube surfaces. When the molten and sintered deposits combine with one another, a thin porous layer is formed, and this acts as an insulator to the heat transfer surfaces. Then, a layer of molten ash eventually may form on the top of the surface exposed to the gas.

To ensure that biomass combustion is safe in power generation boilers due to the slagging formation, the slagging tendency of biomass combustion must be predicted [5,6] so that measures can be taken to reduce the slagging if necessary [7–9]. There has been gaining a lot of interest among the researchers to investigate the slagging formation issues in the boiler. Recently, the evaluation indices or criterion numbers have been prioritised as a means of solving slagging issues in the biomass boiler. The widely used method at the moment is to carry out the predictive analysis on the biomass ash compositions on the

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slagging formation. This is because these methods are low cost, and it is very convenient for the researchers to obtain the chemical compositions of the biomass fuel. The significance of predicting slagging characteristics is broadly known but the major present methods still depend on basic empirical indices obtained from the past [10]. These indices are assumed to offer accurate predictions when implemented to ash samples obtained from the intended blend of boiler firing. Moreover, usually, the predictions are completed in the laboratory prior to firing a new fuel blend in order to anticipate any possible issues because full-scale firing is high risk and could damage the boiler [11].

Previous studies [12–17] produced many empirical indices containing the ash-forming materials thought to be most significant for slagging, allowing for a comparison of fuel assortments and their behaviour on ash melting or slag formation in biomass combustion. For example, the base-to-acid ratio, $R_{b/a}$ index was first created for coal, but it is also used to predict ash melting for biomass. Garcia-Maraver [18] mentioned that there are contradictions in the B/A ratio slagging tendency indicator and diverged from the results of previous findings, where a reduction in the B/A ratio led to a rise in hemispherical temperature (HT) and fluid temperature (FT) and a decrease in slag propensity. The studies by Garcia-Maraver [18] stated that the majority of the biomass is extremely highly prone to slagging with some of the biomass cases, such as grass that showed low B/A values. Hence, the idea to apply the B/A ratio to the biomass situation is not ideal due to many disagreements in the previous research to study biomass slagging propensity. Previous researchers decided that one of the predominant components in slag specimens from biomass fuels is silica, which corroborates the melting composition of "sticky" silicates that produce slagging. The proportion of fuel ash that forms slag in burners is strongly correlated with the silica concentration of the fuel ash [18], hence the silica content of biomass can be utilised as a slagging indicator. According to the data analysis produced by Öhman [19], the essential Si content (SiO_2) is in the range of 20–25 wt% of the fuel ash. This deduction was supported by the studies [20–22]. However, sand or soil contaminants can increase silica levels in biomass fuels. The SiO_2 index demonstrated high possibility to create ash deposits for straws, biomass mixtures, and grasses [18]. These values of SiO_2 are in agreement with previous research [23,24] that examined the SiO_2 levels in these kinds of biomasses and the impact on the plant's rigidness or sturdiness. In contrast, several woody biomass types were prone to create ash residues. This occurs because high Si, as found in biomass fuels, from an external contamination [10,25–27]. Woody biomass should have very low levels of Si without contamination, thereby preventing the creation of sticky silicates and other slagging difficulties at common firing temperatures (1000 °C - 1100 °C) [19]. Hence, the silica content is not suitable to apply in predicting biomass slagging behaviour because it is limited to the condition and situation of the biomass itself. Yu [28] proposed an index for wood-based biomass, $A = (CaO + MgO)/(SiO_2 + Al_2O_3 + K_2O + Fe_2O_3)$. However, the index used to judge the property of ash slagging is not accurate because of the differences in each biomass fuel contents [28]. Öhman indicated that differences in total ash and ash forming constituents of the fuel had a significant impact on the burners' performance [29]. To the authors' knowledge, the studies on ash composition based empirical slagging indices have been developed to predict the slagging tendency but the outcomes do not fully satisfy the objectives. This is because the researches are mostly based on the fuel and ash composition but do not consider the thermal chemical condition of the ash itself and thus are lack of understanding of the biomass ash chemistry.

In this paper, a new semi-empirical index based on chemical equilibrium calculation, ash composition and ash content is developed to predict the slagging behaviours of biomass combustion in fixed-bed combustor technology. The current research is focused on predicting the woody biomass slagging propensities. Wood pellets are currently mainly used for large-scale electricity generation; more of these wood pellets are proposed to be used for heating and combined heat and power in the future. The thermodynamic equilibrium calculation (TEC) has been employed to determine the melt fraction of biomass fuels. Then the partial least squares regression (PLSR) coupled with cross-validation has been used to develop a new formula to predict the slagging index based on the experimental ash composition and the melt fraction from TEC. The results obtained with the designed index show a substantially greater success rate in predicting the biomass ash slagging propensity when compared with the experimental observations from the literature. The predictive tool developed is able to assist the users in determining biomass characteristics and behaviours during firing in the fixed-bed boiler.

2. Material and methods

In this section, the explanation will focus on the data used to develop the prediction method to estimate the slagging propensities of biomass. A total of 28 biomass ash composition datasets were collected from the literature, as shown in Table 1, which consists of ash compositions, ash content (%) and experimental slagging observations. 8 major ash compositions (MgO, Al_2O_3, SiO_2, K_2O, CaO, Fe_2O_3, Na_2O, P_2O_5) were included in the simulations; however, TiO_2 and SO_3 were excluded due to its low amount in the ash. The first 13 datasets (number 1–13) are experimental ash composition data and have been considered as training datasets and the last 15 (number 14–28) will be used as testing datasets. The training and testing datasets will be computed using thermodynamic equilibrium modelling in Section 2.1 to predict the value of melting fraction formed based on the ash compositions. The melting fraction formed will then be multiplied by the ash content of the fuel to create a FactSage slagging index, I_f. The results obtained will be used in Section 2.2, where the PLS regression analysis will be employed to create a new formula, I_n, to predict the slagging propensity. Finally, I_n will be validated with the experimental slagging observations.

The training datasets 1–13 consist of experimental ashes from 13 types of pure wood-based biomass that were chosen due to the availability in the literature [14,29–34] of the experimental observation data for the biomass slagging behaviour to determine the slagging propensities of biomass fuels in the combustion. The remaining 15 testing datasets (number 14–28) consisting of pure woody biomass were selected based on the fuel and ash analysis carried out by the previous researchers [14,29–34]. This data will be used to validate the model equation developed using PLS regression and to show the capability of the expression formed to predict the slagging observation without needed to conduct combustion tests.

2.1. Thermodynamic equilibrium model

Generally, to predict the ash and slagging formation during the firing of the biomasses, a thermodynamic equilibrium calculation is often employed as it appears to be able to show a reasonable forecast of the ash conversion process without carrying out complex experiments for every single biomass, although the process in a real furnace may not be fully in equilibrium [35–38]. The FactSage thermochemical software has been widely applied in solid fuel firing analysis for computing multiphase multicomponent at equilibrium conditions, with adequate fuel composition, atmosphere and temperature settings. It builds upon the Gibbs power reduction and includes large databases for oxide or silicate and salt composition structures [35–38]. Both unmixed compounds and solution stages are included in the databases. The unmixed compound (pure compound) are composed of stoichiometric element composition, whereas, there are optimized frameworks for the solution stages in the solution databases. The techniques applied to initiate the thermodynamic database have been thoroughly analysed in the past [35–38]. The FactSage 8.1 thermodynamic software was used in this paper to predict the biomass melting fraction for the fuels (1–13) listed in Table 1. The model was set up as follows.

Table 1
Chemical ash composition for various types of wood-based biomass [13,16,29–34].

Num.	Biomass	MgO	Al_2O_3	SiO_2	K_2O	CaO	Fe_2O_3	Na_2O	P_2O_5	Ash content (%)	Experimental Observation
1	Pine chips	10.90	4.02	5.49	11.31	45.42	0.95	0.05	7.14	0.25	Low
2	Stemwood II	12.83	1.86	8.67	19.98	47.96	1.05	0.05	7.60	0.31	Low
3	Oak chips	8.13	2.83	1.32	31.94	24.83	0.38	3.64	10.33	0.55	Low
4	Softwood sawdust	5.40	5.10	28.59	14.89	33.17	5.05	1.78	6.02	0.50	Low
5	Sawdust	10.00	10.14	12.91	7.27	28.14	9.58	8.13	13.83	0.2	Low
6	Bark-spruce	4.71	3.23	15.18	10.56	60.73	0.66	0.45	4.49	3.6	Moderate
7	Bark-pine	4.96	11.76	21.88	12.32	46.23	1.80	1.06	5.13	1.9	Moderate
8	Bark	5.08	9.15	31.33	10.67	33.36	3.90	1.84	4.68	4.4	Moderate
9	Scots pine II	5.93	0	50.04	15.25	23.10	0	0	5.68	0.5	Moderate
10	Scots pine III	4.96	0	50.72	17.45	20.27	0	0	6.59	1.1	Moderate
11	Logging residues II	5.84	3.26	31.99	11.95	34.65	1.62	2.33	8.36	2.7	Moderate
12	Wood II	5.50	1.25	48.51	15.18	22.32	1.16	0.72	5.37	0.76	High
13	Bark II	4.69	4.54	28.70	11.39	41.37	2.19	1.64	5.49	3.6	High
14	Stemwood	7.33	0	7.88	19.53	61.87	0	0	3.38	0.2	Low
15	Wood	9.60	2.40	10.12	22.07	48.94	1.55	1.04	4.28	0.30	Low
16	Scots pine	8.88	6.09	25.08	8.33	37.85	2.44	6.60	4.72	0.45	Low
17	Oak sawdust	7.46	2.39	15.80	9.32	39.23	2.48	2.88	2.03	0.82	Low
18	Energy wood	6.87	2.32	11.82	16.64	52.18	1.97	1.86	6.33	1.0	Low
19	Eucalyptus chips	14.11	1.58	4.86	18.83	25.85	0.49	4.04	16.30	0.33	Low
20	Pine sawdust	13.55	4.51	9.72	11.53	39.14	4.87	0.47	3.54	0.53	Low
21	Pulpwood	12.34	0	4.34	29.35	53.97	0	0	5.84	0.7	Low
22	Wood pellets	10.21	8.58	21.09	25.04	28.77	2.69	3.62	4.30	0.57	Low
23	Softwood sawdust II	4.71	6.06	37.58	12.07	27.15	4.93	2.88	4.62	0.7	Moderate
24	Logging residues III	5.16	3.29	32.71	11.51	36.25	1.45	1.19	8.45	2.5	Moderate
25	Pinecone chips	11.03	4.55	9.12	40.03	13.62	0.24	4.09	6.44	1.21	Moderate
26	Scots pine IV	5.17	0	53.85	15.55	25.43	0	0	6.88	1.3	Moderate
27	Logging residues	1.41	11.31	70.47	4.05	6.34	3.80	2.63	1.36	6.4	High
28	Bark III	2.41	9.73	52.19	5.77	20.27	5.09	2.47	2.07	8.6	High

i The model is set up assuming equilibrium conditions with the databases FACTPS, FTsalt and FToxid.
ii. Table 1 consists of 8 major ash compositions (MgO, Al_2O_3, SiO_2, K_2O, CaO, Fe_2O_3, Na_2O, P_2O_5) from experimental ash composition and oxygen was applied as the input to the model.
iii. The temperature for the equilibrium simulations was set to be in the range of 1150–1250 °C. This temperature has been benchmarked based on the common biomass fixed-bed boiler operating temperature [32].
iv. The "SLAGA" model, with two-phase immiscibility, was used in the calculations as the solution species [39].
v. Record the average reading of slagging weight formed for each fuel resulting from the equilibrium simulation.
vi. The slagging weight formed from the equilibrium simulation will be divided with 1g of the ash to obtain melt fraction. The melt fraction will be multiplied with the ash content for each fuel to obtain Factsage slagging index I_f.

2.2. Partial least square regression coupled with cross validation

The mathematical approach PLSR associated features and generalises the multivariate regression and analysis of the principal component analysis [9]. It is able to analyse larger data, multivariate systems with a high degree of correlation and is better than the multiple regression method [40]. This method is frequently used to identify both the stopping criterion and the total amount of latent variables while performing cross-validation with only a single observation at a time [40–42]. PLSR is particularly suitable for problems where fewer observation data are available such as those in the biomass slagging propensity analysis. For more information on the PLSR and the cross-validation technique, please refer to Refs. [9,40,41,43–45]. PLSR coupled with cross-validation techniques were employed to process the training datasets, see Table 1 & Table 2. This has resulted in an equation formed as a function of the biomass ash compositions. The equation obtained was modified by multiplying the expression with the ash content to obtain new formula to predict the slagging indices, I_n.

Table 2
Melting fraction data of the biomass obtained from the FactSage 8.1 model.

Num.	Biomass	Melt fraction	I_f	Experiment observation	Ash content (%)
1	Pine chips	0.48	0.12	Low	0.25
2	Stemwood II	0.51	0.16	Low	0.31
3	Oak chips	0.46	0.25	Low	0.55
4	Softwood sawdust	0.76	0.38	Low	0.50
5	Sawdust	0.82	0.16	Low	0.20
6	Bark-spruce	0.56	2.09	Moderate	3.60
7	Bark pine	0.60	1.14	Moderate	1.90
8	Bark	0.61	2.68	Moderate	4.40
9	Scots pine II	0.90	0.45	Moderate	0.50
10	Scots pine III	0.86	0.95	Moderate	1.10
11	Logging residues II	0.81	2.20	Moderate	2.70
12	Wood II	1.00	0.76	High	0.76
13	Bark II	0.80	2.88	High	3.60

3. Results & discussion

3.1. Melting fraction predicted by using thermodynamic equilibrium calculations

The melt fraction is defined by the weight ratio of the slag liquid formed based on 1 g of the fuel ash by thermodynamic equilibrium calculations. Theoretically, the maximum value of melt fraction must be 1.0 where total of 1g of ash is fully melt into slag-liquid. The melt fraction idea was introduced by Isaak et al. [46] and stated that more liquid will be present in the deposit as the temperatures increase. It was experimentally reported that the stickiness of deposits will increase with the increase in deposit temperature [46]. Therefore, the temperature indirectly impacts on the deposit stickiness by affecting the amount of liquid phase in the deposit. Zhou et al. [47] presented a sample melting curve that illustrates the particle melt fraction with respect to the particle temperature, which clearly shows that the melt fraction of the ash increases with an increase in temperature. The melting fraction concept became popular in forecasting the biomass ash deposition [1,47,48]. Beckmann et al. [49] illustrated the melting curve of Middleburg coal ash by using FactSage 6.1. Fig. 1 shows the melt fraction (SLAG-liq, red line) graph of Oak chips (3) and it is clearly illustrates that the degree of melt increases with an increase in the temperature. Based on Fig. 1, the Oak chips start to melt at 750 °C where the melt fraction is 0.05 and increase linearly to the degree of melt (0.46) at 1150 °C. It must be noted that the different biomass fuel will have different degree of melting behavior due to the difference in its ash compositions. For example, Oak chips give melt fraction of 0.46 while Bark spruce (please refer to Table 2) indicate its melt fraction of 0.56 at 1150–1250 °C. Thus, the degree of melt presented in our Factsage simulation is in agreement with the typical melting curve presented by Zhou et al. [49] and melting curve of Middleburg coal by Beckmann et al. [51]. In this paper, the study is focused on the determination of the melt fraction in the high-temperature regions (1150–1250 °C) only.

The melting fraction has been obtained from the FactSage thermodynamic equilibrium model for the 13 woody biomass fuels (training datasets). Then, the melting fraction was multiplied with ash content to introduce the Factsage slagging index, I_f. The I_f value will be represented as proportional of the actual slag in the fuel with respect to the ash content. This is because, the I_f value will be considered as a quantitative measurement of the slag for the biomass fuel ash and will be compared with the experimental observation which is the qualitative measurement (low, moderate, high). Please refer to the [17,29,33] for a detailed explanation of the experimental observation's classifications. Table 2 shows the melt fraction based on 1g of fuel ash input and I_f value with respect to the ash content and experimental observation for each fuel in the training datasets. Fig. 2 shows the positive trend on the relationship between the FactSage slagging index, I_f and experimental observation. This indicates that the value of slagging index from FactSage will increase corresponding to experimental observations moving from low to moderate and high of biomass fuel slagging propensities. The ash content of the fuel is very important in determining the values of the Factsage slagging index, I_f as shown in Table 2. For example, the melt fraction of biomass fuel Oak chips (3) and bark-spruce (6) in Table 2 are both 0.56. However, the experiment observation [30,32] stated that the slagging severity for the two fuels are low and moderate, respectively. This is due to the difference in the ash content for the two fuels. Oak chips (3) has low ash content which is 0.55% compared to the 3.60% in Bark-spruce (6). The experimental observation is consistent with the predicted I_f, which are 0.25 for Oak chips (3) and 2.09 for bark-spruce (6). Hence, the ash content will influence the slagging severity level. It is noted that, according to the method of ternary diagram proposed by

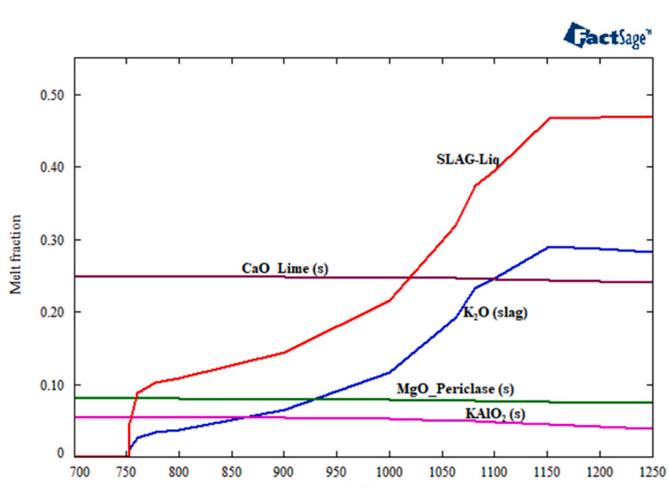

Fig. 1. Solid-liquid phase for Oak chips (3) obtained by FactSage equilibrium simulation.

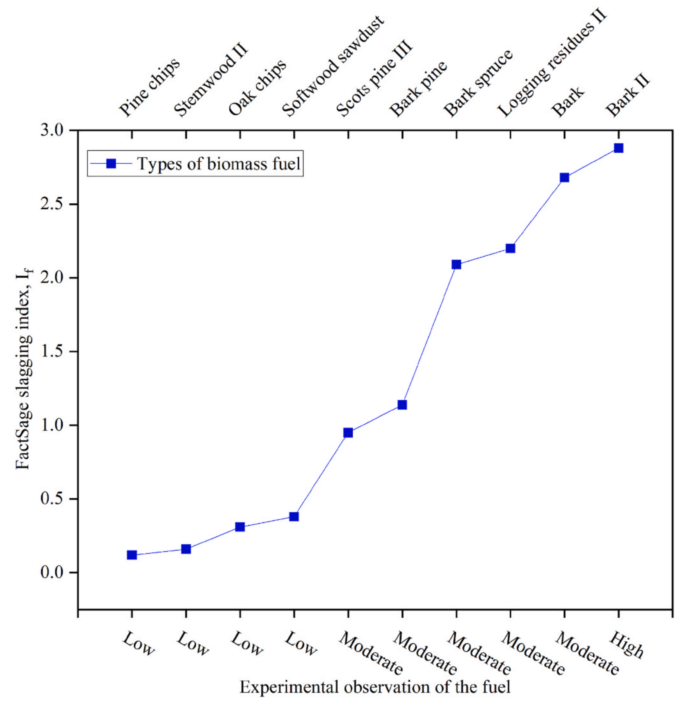

Fig. 2. Relationship between FactSage slagging index, I_f and experimental observations of slagging of biomass fuels.

Näzelius et al. [17], both Oak chips (3) and Bark-spruce (6) are in the low slagging area. This indicates that the method by Näzelius et al. [17] fails to correctly evaluate the slagging potential for Bark-spruce (6). This is because the method did not take into consideration ash content. Therefore, it should be cautious to use the method to predict the slagging potential of fuels with significant differences in ash content. Please refer to the appendix section (b), Figure 9 for the comparison of slagging index between with and without ash content.

3.2. New predictive indices, I_n

The method to predict the slagging propensities of biomass can help the power plant operator predict the quality of the fuel before firing the biomass. The aim of this section is to develop a new predictive index formula that can be used to forecast the slagging propensity of woody biomass based on the fuel ash composition only, without performing a thermodynamic equilibrium calculation process, since FactSage software is not widely used among power plant operators. The new predictive index formula, I_n, is developed based on I_f as shown in Table 2, by using the PLS regression analysis coupled with cross-validation together with chemical ash compositions (training datasets 1–13) from Table 1. After performing PLSR coupled with the cross-validation method, the root means square error (RMSE), R^2, and slope for the training data were 0.006, 0.998 and 0.996, respectively. These indicate a good model fit [50]. The expression of I_n is obtained as follows:

$$\begin{aligned} I_n = \Big| \big[& 0.43 - 2.476 \times 10^{-1}\,(MgO + CaO) + 7.147 \times 10^{-1}\,SiO_2 \\ & + 3.674 \times 10^{-1}\,(K_2O + Na_2O) + 18.875 \times 10^{-1}\,Fe_2O_3 \\ & + 11.306 \times 10^{-1} P_2O_5 \big] \Big| \times \text{Ash content } (\%) \end{aligned} \quad (3.1)$$

*Condition applying eq (3.1).

a. The **mass fractions** of the ash compositions must be applied for the oxide parameters in Equation (3.1).
b. The **I_n index** will always a **positive value** due to the lowest value of melt fraction is 0.18.

It is noted from Equation (3.1) that the MgO + CaO has a negative coefficient, which implies that the predicted slagging index, I_n will decrease with an increase in the values of MgO + CaO. On the other hand, the parameters (SiO_2, $K_2O + Na_2O$, Fe_2O_3 and P_2O_5) related to the slagging formation of biomass fuel are found to have a positive coefficient which means that the predicted slagging index, I_n will be high with an increased value of these four parameters. These elements with positive coefficients are highly prone to slagging formation and silica is the most common component of the biomass slag [20,22,51]. The regression coefficient of potassium combined with sodium is the smallest value among the positive coefficients, which is +0.3674. This indicates that the potassium element can be considered a low impact on the biomass slagging behaviour when the content of silica oxide is low, especially for wood-based biomass. For example, Oak chips (3) was observed to have a high amount of K_2O (31.94 wt%) among the training datasets (1–13), a low SiO_2 (1.32 wt%) and a significant amount of CaO (24.83 wt%) and this has resulted in 0.25 in the FactSage slagging index, I_f based on Table 2. Experiments carried out by Ref. [30] showed that the Oak chips (3) has low slagging propensities. Hence, the presence of a high amount of potassium ~32 wt% does not give a big impact on the slag formation of Oak chips (3). This is because the Oak chips (3) has low Silica oxide and high content of Calcium oxide as well as a low ash content, which is 0.55%. It was suspected that the potassium is not able to accelerate the slagging formation with a small amount of silica oxide present in the fuel (3). Fig. 1 shows the solid-liquid phase equilibrium composition from the FactSage simulation for Oak chips (3) fuel. The graph shows a low value of potassium (K_2O-liq) formed in all the slag phase (slag-liq) which is about 0.29 g based on 1 g input of fuel ash. Small amount of potassium appears in the solid phase, such as $KAlO_2$. Another example can be observed is logging residues (27) from Table 1, the potassium content is the lowest among the datasets which is 4.05 wt%, a very high SiO_2 (70.47 wt%) and low value of CaO (6.34 wt%). The experiment carried out by Ref. [32] indicated that the logging residues is observed as severe slag. This showed that the amount of potassium is not significant in the formation of slagging without the presence of high silica and low calcium contents.

3.3. *Analysis and application of the new predictive indices, I_n*

This section mainly focuses on the validation of the new predictive indices, I_n, against the testing datasets (14–28) in Table 1 by using the fuel ash analysis from the literature [14,17,29–34]. Table 3 shows the comparison of the biomass slagging tendency between the experimental observations and predicted indices of the testing fuels. Logging residues (27) and Bark III (28) were observed to have severe slagging in the experimental observation [29,32]. This can be related to the high value of silica oxide and the low amount of calcium oxide content compared to other types of pure woody biomass fuels based on their chemical ash compositions. In addition, the total ash content for the logging residues (27) and Bark III (28) are 6.40% and 8.60% respectively. The predicted index value for the logging residues (27) is 6.50, while for the Bark III (28) is 7.7 which both fuels (27 & 28) are considered as high value of the index. On the other hand, the clean wood fuel (Stemwood, Scots pine, Energy wood, Eucalyptus chips, Pulpwood, Wood pellets) and wood sawdust (Oak sawdust & Pine sawdust) are low in slagging behaviour based on the experimental observation. This is because the clean wood fuel and wood sawdust have a low amount of silica oxide and a high amount of calcium oxide content as shown in Table 1. Their predictive indices, using I_n equation (3.1), are ranging from 0.08 to 0.52, respectively, and all the I_n values found are low index values. The Softwood sawdust II, Logging residues III, Pinecone chips and Scots pine IV were observed as moderate slagging, with the predictive index values being 0.57, 1.83, 0.80 and 1.10, respectively. Overall, it can be concluded that the pure woody biomass with silica-rich fuel tends to have a high slagging tendency while the biomass fuels with a high amount of calcium have a low slagging potential. In the absence of soil contamination, the clean wood chips and sawdust pellets have a low intrinsic silica concentration and this results in them being low slag fuel sources [30]. Fig. 3 shows the correlation between the FactSage slagging index, I_f (blue line) and predictive slagging index, I_n (red line). As we know that the predictive slagging index, I_n was developed based on the FactSage slagging index by using the PLSR method coupled with the cross-validation method. The testing data were simulated using the FactSage equilibrium calculation to obtain the melting fraction and multiply it with the ash contents to create I_f. We can clearly see that both indices which are I_f and I_n are in mutual agreement and have the same trend as the calculated slagging index.

Table 3
Comparison of the biomass slagging tendency between the experimental observation and prediction indices of the testing data (woody biomass).

Num.	Type of biomass	Prediction Indices, I_n	Experimental observation
14	Stemwood	0.08	Low
15	Wood	0.16	Low
16	Scots pine	0.29	Low
17	Oak sawdust	0.44	Low
18	Energy wood	0.52	Low
19	Eucalyptus chips	0.20	Low
20	Pine sawdust	0.30	Low
21	Pulpwood	0.30	Low
22	Wood pellets	0.40	Low
23	Softwood sawdust II	0.57	Moderate
24	Logging residues III	1.83	Moderate
25	Pinecone chips	0.80	Moderate
26	Scots pine IV	1.10	Moderate
27	Logging residues	6.50	High
28	Bark III	7.70	High

3.4. *Comparison of the new biomass slagging predictive indices, I_n, with the 5 different types of existing expressions*

The performance of the new predictive equation for I_n is compared with the 5 different types of existing indices equations. These 5 different types of expression are developed to predict the coal ash behaviour but were also used to compare the biomass ash slagging, for example by Garcia-Maraver [18]. Fig. 4 illustrates the number of predicted samples out of the 15 testing fuels that match the experimental observations for each index. The new index proposed in this paper shows that I_n successfully predicted (*please refer to the appendix section (a) on the new*

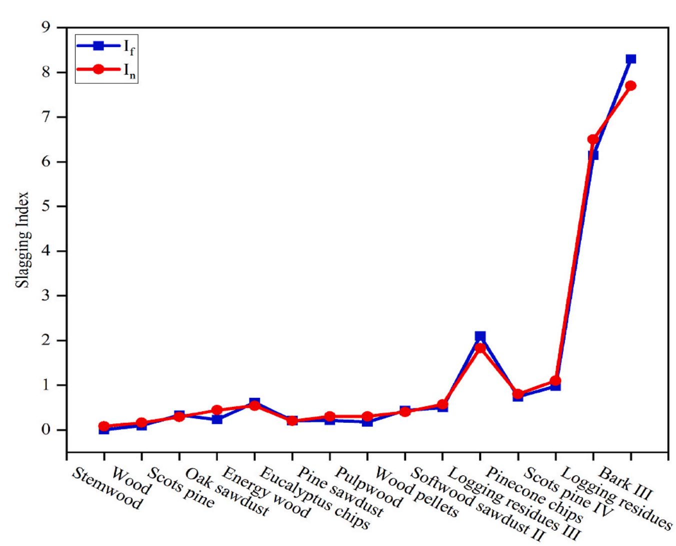

Fig. 3. Comparison between FactSage slagging index, I_f (blue line) and predictive slagging index, I_n (red line). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

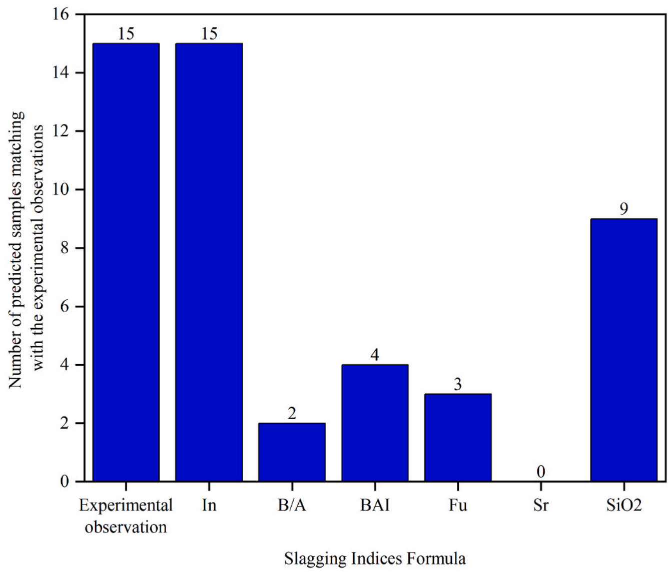

Fig. 4. Comparison of the number of predicted samples matching with the experimental observations [28,30] between I_n and 5 existing indices.

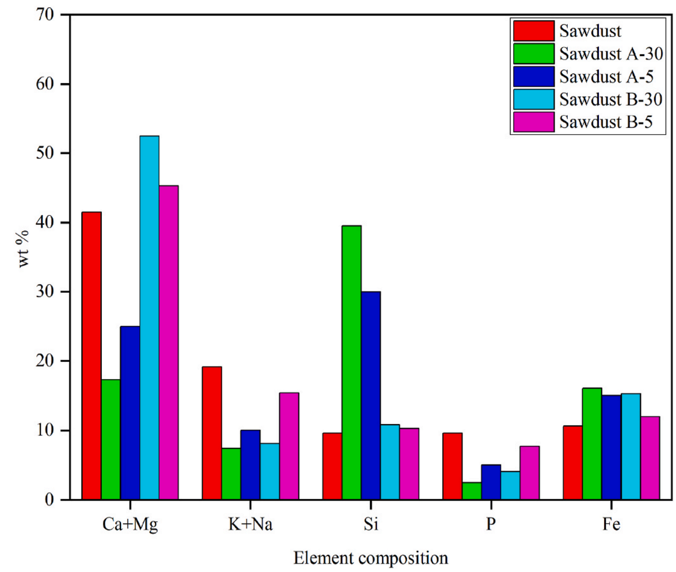

Fig. 5. Elemental fuel ash compositions of the Sawdust and blends of Sawdust with Peat A/B [33].

slagging boundary indicator development to determine the severity of slagging propensities) all the samples matching with the experimental observations. On the other hand, the 4 existing indices (B/A, BAI, Fu, Sr) were only able to predict the maximum 4 samples correctly while the use of SiO_2 content was able to accurately predict 9 samples (out of 15) showing that SiO_2 is indeed one of the dominating species of slagging formation for these fuels.

4. Performance of the indices, I_n for woody biomass with peat addition

4.1. Woody biomass with peat addition

The experimental data presented by Näzelius [33], which consists of 12 blends of Sawdust and Energy crops with various amounts of Peat: Sawdust 100%; Sawdust + Peat A & B (with ratios 0–30 wt %); Energy wood 100%; Energy wood + Peat A & B (0–30 wt %), is used in this study. There is an increasing demand for Peat as new materials in the solid recovered fuel industry [33]. However, Peat is known to have high ash content, which is potentially problematic in the combustion compared to stem wood. The biomass datasets of Näzelius [33] are divided into two groups, which are Case 1 (Sawdust + Peat A/B) and Case 2 (Energy wood + Peat A/B). In the experiments by Näzelius [33], two types of Peat (Peat A and Peat B) were pelletized into stem wood sawdust and energy wood at three different ratios (5–30 wt%), respectively. Peat A is the traditional Scandinavian fuel peat that has higher levels of ash and silica (carex), and Peat B has lower levels of ash and a higher Ca/Si ratio [33]. Please refer to Table 8 in the appendix section (c) for the ash element compositions of the raw materials used by Nazelius et al. [33]. The experiment was carried out in a P-labelled and underfed commercial pellet burner (15 kW) [33].

4.1.1. Case 1 (Sawdust + Peat A/B)

Fig. 5 shows the average elemental ash compositions of the sawdust and blends of sawdust with Peat A/B. Silica compositions were the lowest in the pure sawdust (red column) while were the highest with the addition of Peat A into the sawdust. It can be clearly seen that the influence of Peat addition on the sawdust resulted in a gradually increasing amount of silica in the blending compositions between Peat A/B and sawdust at ratios of 5–30 wt%. Another major effects of Peat A addition on the sawdust that can be observed in Fig. 5 are the amount of calcium and magnesium formed. The pure sawdust without the addition of Peat A has a high amount of Ca + Mg which is 41.49 wt%, however, after the addition of Peat A with ratios of 5 and 30 wt%, the amount of Ca + Mg significantly decreases from 25 wt% to 17.28 wt% respectively. The mixture between sawdust and Peat B with ratios of 5 and 30 wt% generally increase the amount of Ca + Mg from 45.30 wt% to 52.47 wt% and no significant changes in Si level for both ratios. This was expected due high Ca/Si ratio in Peat B.

Table 4 presents a comparison of slagging between the predictions using I_n and the experimental observations from Näzelius [33]. The predicted indices, I_n for Sawdust A-30 is 2.49 and was observed as severe slagging in the experimental result [33]. The I_n of Sawdust B-5 was 0.32, which can be ranked as low slagging, which was consistent with the experimental observation. The pure sawdust value of I_n forecasted was relatively small which is 0.16 while Näzelius et al. mentioned that there was no slagging observed during the experiment [33]. This is due to the high calcium + magnesium and low silica in the ash although the content of potassium + sodium is relatively high. The I_n estimated for Sawdust A-5 and Sawdust B-30 were 0.60 and 0.43, respectively, and these were shown as moderate slagging (experimental observation). Overall, only Sawdust B-30 failed to satisfy the experimental observation as the predicted I_n was categorized as low slagging propensity while it was observed as moderate slagging in the experiment.

4.1.2. Case 2 (Energy wood + Peat A/B)

Fig. 6 presents the bar graph of ash compositions of pure Energy wood with the addition of Peat A & B. Pure Energy wood has a low silica

Table 4
Comparison of the biomass slagging tendency between the experimental observation and prediction indices of Case 1.

Type of biomass	Prediction Indices, I_n	Prediction observation indicator for slagging	Experimental observation [33]
Sawdust	0.16	Low	None
Sawdust A-30	2.49	High	High
Sawdust A-5	0.60	Moderate	Moderate
Sawdust B-30	0.43	Low	Moderate
Sawdust B-5	0.32	Low	Low

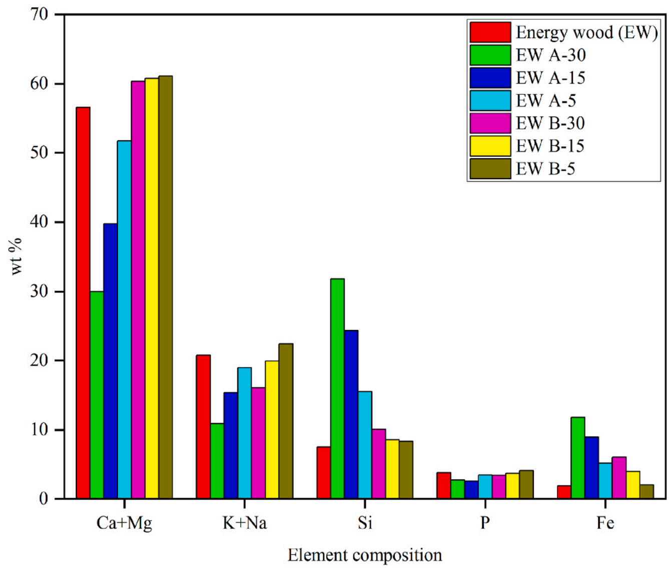

Fig. 6. Elemental fuel ash compositions of the Energy wood and blends of Energy wood with Peat A/B [33].

content and high content of Ca + Mg. In addition, we can clearly see that the major effect of Peat A addition to the Energy wood is the drastic decrease in the calcium and magnesium value. The silica will continue to increase with the addition of Peats. Table 5 shows the comparison of slagging between the predictions and the experimental observations for blends of Energy wood with Peat A/B. Pure Energy wood has high value of Ca + Mg elements and the predicted slagging index, I_n value was 0.52 which is ranked as low slagging. Näzelius et al. mentioned that there was no slagging observed during the firing of the pure energy wood [33]. The EW A-30 and EW A-15 predicted by I_n were 3.01 and 2.17, respectively, while the experimental observation considered them as being severe slagging due to the burner need to shut down during firing [33]. This is suspected to be due to the high amount of Si and the low amount of Ca + Mg in their fuel compositions. The predictive indices, I_n for EW A-5 was forecasted to be 0.88, while it was observed as moderate slagging in the experimental observation [33]. In addition, the slagging observation based on an experiment conducted by Näzelius et al. indicated that all the blended ratios for Peat B 5–30 wt% with energy wood have low slagging formation while the I_n indices prediction were 0.53, 0.54 and 0.55, respectively. Overall, the predictive index, I_n developed is able to predict up to 80% accuracy for the mixture of biomass between Sawdust, Energy wood and Peat A/B.

4.2. Herbaceous biomass

The experimental data illustrated by Weber et al. [52,53] which consists of 6 types of herbaceous biomass which are Mixed wood, Poplar,

Table 5
Comparison of the biomass slagging tendency between the experimental observation and prediction indices of Case 2.

Type of biomass	Prediction Indices, I_n	Prediction observation indicator for slagging	Experimental observation [33]
Energy wood (EW)	0.52	Low	None
EW A-30	3.01	High	High
EW A-15	2.17	High	High
EW A-5	0.88	Moderate	Moderate
EW B-30	0.55	Low	Low
EW B-15	0.54	Low	Low
EW B-5	0.53	Low	Low

Palm kernel expeller (PKE), Switchgrass II, Grain residue and Fermentation residue. The biomasses were fired to investigate the issues of deposits formed at high-temperature regions (950–1200 °C). Fig. 7 presented the fuel ash composition of 6 types of herbaceous biomass determined by X-ray fluorescence. Mixed wood has an extremely high amount of Ca + Mg and the.

lowest amount of Silica among others. Fuel ash composition in Fermentation residue is contradicted from Mixed wood which is the lowest amount of calcium + magnesium and the highest value of Si. Poplar has the highest amount of phosphorus which is approximately 41 wt%. The I_n was employed to determine the slagging indices of every single biomass from Fig. 7. The results later will be compared between the prediction indices, I_n and the rank of the biomass (Mixed wood, Poplar, Palm kernel expeller (PKE), Switchgrass II, Grain residue and Fermentation residue) slagging propensity from low to high. The slagging propensity rank was determined by analysing the deposited mass versus ash input after 2 h of deposits collected at high-temperature surfaces (>1000 °C) [53]. The rank of the 6 various types of biomasses can be illustrated in Table 6. Based on, the prediction indices, I_n was successfully predict the slagging propensity for all biomass with respect to the biomass slagging propensity ranking provided by the literature [53]. However, it must be noted that the main objective of this paper is to develop the slagging propensity for woody biomasses only. The author strongly suggested always taking a precaution when applying the herbaceous biomass to the I_n formula. This is because the ash composition for herbaceous biomass is more exotic compared to woody biomass. This can be clearly seen in the distribution of ash composition for herbaceous biomass in Fig. 7.

5. Conclusion

This paper has demonstrated that it is practical to employ thermodynamical equilibrium modelling together with PLSR with cross-validation to accurately predict the slagging propensity of firing biomass in utility boilers. The new slagging index, I_n was developed by analysing the melting fraction predicted by the FactSage software taking into consideration the ash content of the fuels and using the numerical PLS regression coupled with a cross-validation technique. The proposed method has been validated against the experimental observations from the literature on wood-based biomass in fixed bed and grate type of combustors. The findings show that the slagging propensity index may be classifiable into 3 main groups: low slagging when $I_n \leq 0.55$; 0.55 <

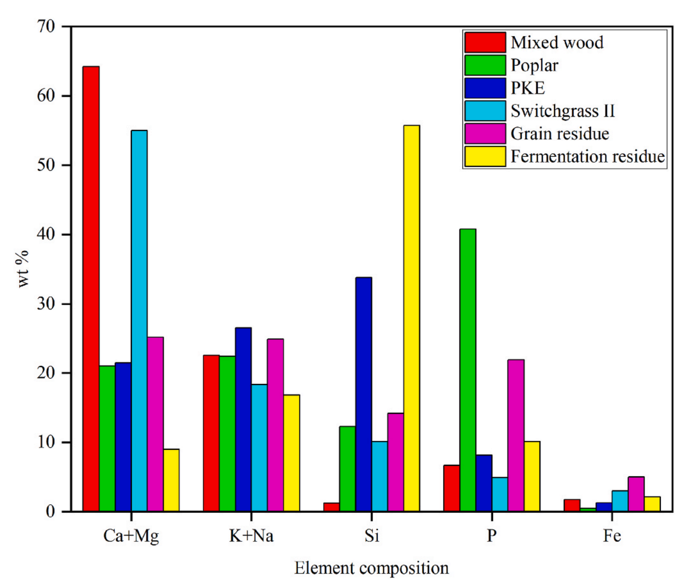

Fig. 7. Fuel ash compositions of the 6 types of herbaceous biomass [52,53].

Table 6
Comparison of the biomass slagging tendency between the deposited mass versus ash [53]and prediction indices, I_n.

Num.	Type of biomass	Prediction Indices, I_n	Ranking of the biomass slagging propensity from low to high
1	Mixed wood	0.93	1
2	Poplar	1.70	2
3	PKE	3.70	3
4	Switchgrass II	4.88	4
5	Grain residue	6.33	5
6	Fermentation residue	6.59	6

moderate slagging <2.10; and high slagging when $I_n \geq 2.10$.

For the tested woody biomass fuels, the new index, I_n shows a substantially greater success rate than 5 existing indices in assessing the boiler slagging potential. Furthermore, the predictive index, I_n has been extended to herbaceous biomass and blended applications between woody biomass and Peat. The result shows that the I_n expression is able to predict the slagging potential with high accuracy. It can be confirmed that the main element that contributes to the slagging formation in the biomass firing fixed-bed is silica oxides. Woody biomass with higher values of calcium elements will have a low tendency to slag while those with a higher value of silica oxides will have a high probability of slagging.

It should be noted that the new predictive slagging index, I_n has taken into consideration the level of the ash contents of the biomass fuels. The index must be applied in high-temperature regions of the fixed bed and grate-type boilers operation. In addition, the new predictive index, I_n is based on wood-based biomass with high SiO_2 and CaO contents. Therefore, care should be taken when extending the predicted indices I_n developed in this paper to other types of biomass fuels, in particular very high potassium fuels. The authors strongly recommend that future experimental studies at industrial/full scales should be performed to obtain a large dataset of experimental observations in real application. This will improve and increase the accuracy of the predictive indices to accurately predict the biomass slagging propensities.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

a). Slagging boundary indicator

The slagging boundary indicator represent the severity in the slagging of the biomass. The indicator is significant in guiding the users, especially power plant operators of energy power generation in determining the wood-based biomass fuel slagging behaviours. Figure 8 illustrates the graph showing the relations between experimental observation and predictive slagging index, I_n. It can be clearly observed that the predictive slagging index is positively correlated with the experimental observations for most fuels. According to Fig. 8, the boundary value between low and moderate slagging regions may be 0.55 (please refer to the green dotted line in Figure 8). This value has been decided based on the median interval between the lowest value of I_n for the moderate experimental observation and the highest value for the low slagging observation. The boundary number between moderate and high slagging may be 2.10 (please see the red dotted line in Figure 8). This is because the moderate observation fuel shows a consistently linear increase of the index value, I_n which is from 0.57 to 1.99 while the predictive index value, I_n for the high-slagging fuel starts from 2.17 to 7.70. This value has been determined by applying the median interval method between moderate and high slag propensity. The availability of experimental observations for high-slagging fuel is really needed in order to improve and determine the boundary of slagging behaviour between moderate and high in the future. Large datasets may require in the future to fine-tune and improve more on the boundary values. Currently, the author has been classifying the indicator of the slagging predictive index into 3 main groups: low slagging ≤0.55; 0.55 < moderate slagging <2.10; high slagging ≥2.10 as shown in Table 7.

Table 7
Slagging predictive index, I_n indicator

Slagging index boundary	Slagging predictive index, I_n
Low	≤0.55
Moderate	0.56–2.09
High	≥2.10

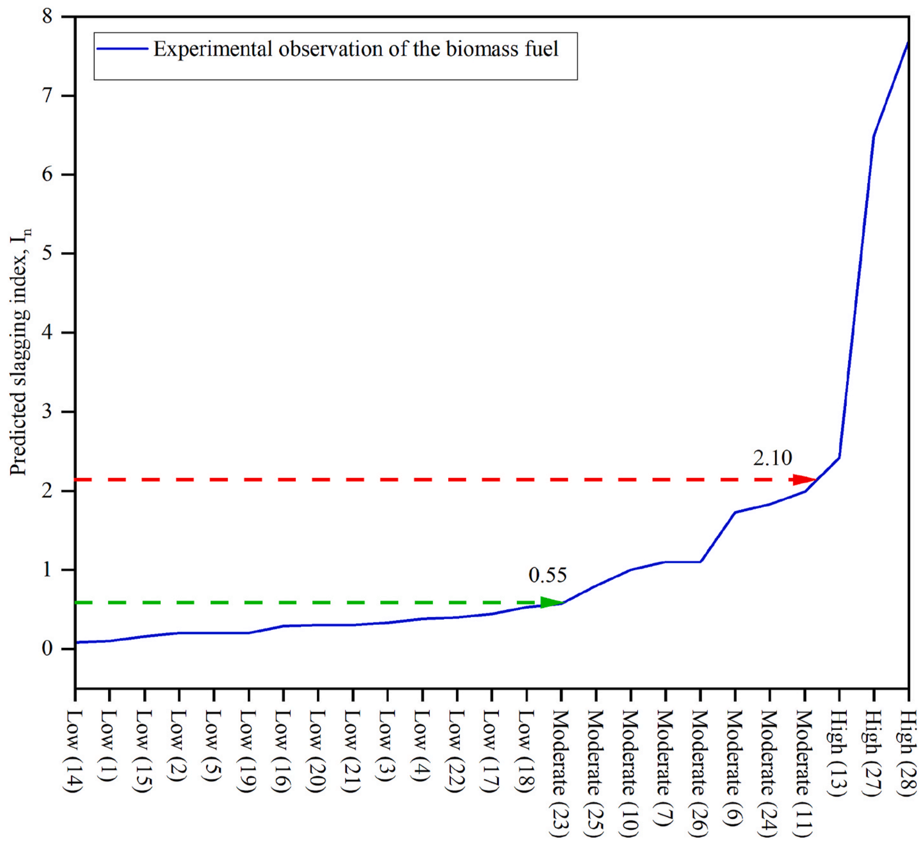

Fig. 8. Correlation between predictive slagging index, I_n and the experimental observations of the biomass fuel. (The x-axis is representing the fuel number based on list in Table 1).

b). Comparison of the performance of the slagging index with and without ash content

Figure 9 shows the comparison of the performance of the slagging indicator with and without ash content. It is observed that the trend (without ash content) in the red colour line cannot agree with the slagging observation increasing from low to moderate while the trend in the green colour line agrees with the observation. This may indicate that the ash content cannot be ignored in determining the severity of the slagging for the biomass fuels.

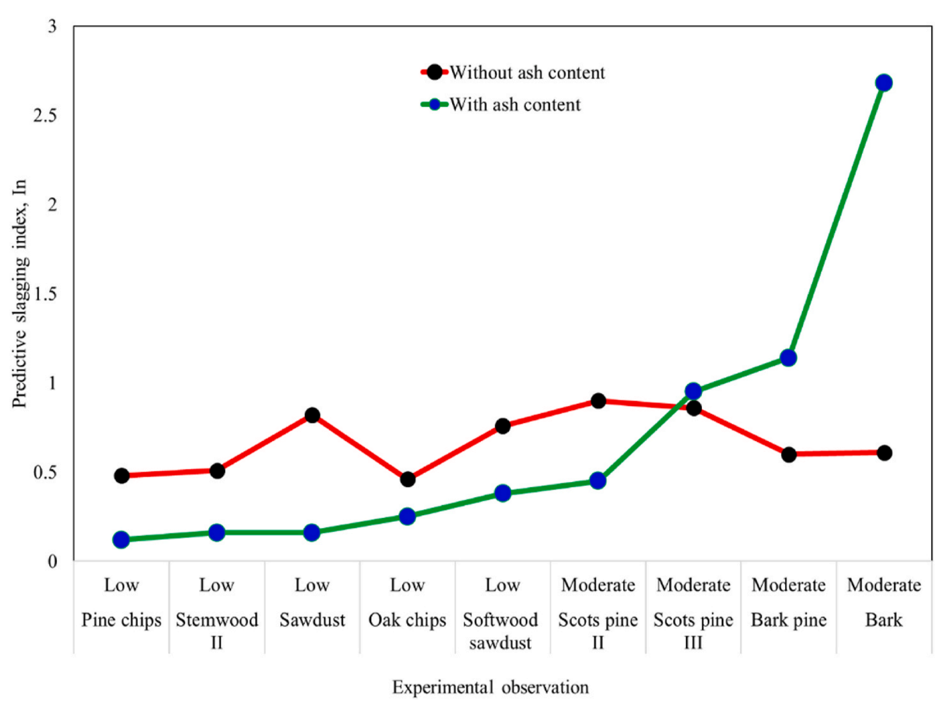

Fig. 9. Comparison of the performance of the slagging index with and without ash content.

c). Chemical ash Compositions for sub-chapter 4 (supplementary data)

Table 8
Chemical ash compositions for 4 different types of biomass [33].

Element	Sawdust (wt%)	Energy wood (wt%)	Peat A (wt%)	Peat B (wt%)
Mg	<0.01	0.03	0.08	0.08
Al	<0.01	0.01	0.44	0.05
Si	<0.01	0.04	1.06	0.06
P	<0.01	0.02	0.05	0.01
K	<0.01	0.10	0.07	0.01
Ca	0.03	0.27	0.29	0.22
Fe	0.01	0.01	0.42	0.09
Na	<0.01	0.01	0.07	0.01
Ash (%)	0.20	1.00	5.30	1.10

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