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Prediction of Agglomeration at High Temperatures during the Combustion of Selected Biomass Fuels in a Laboratory Scale Fixed Bed – Factsage Inputs

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ABSTRACT: *In this research work, Factsage software had been utilized to predict the eutectic points on both the binary and the ternary phase diagrams. Eutectic point on phase diagram is largely influenced by the percentage of the inorganics (K_2O, KOH, Na_2O or SiO_2) in the mixture. Factsage software predicts the eutectic points (eutectic temperatures) on both the binary and the ternary phase diagrams at elevated temperatures. With the addition of additive (kaolin) to the bed materials, agglomeration was predicted to occur in the combustion bed at 1200 ^{0}C on the binary phase diagrams if the biomass fuel is dominated by potassium, K. Consequently, if the biomass fuel is dominated by sodium, Na, agglomeration was predicted to occur at 1700 ^{0}C in the combustion bed. However, on the ternary phase diagrams, with the addition of kaolin to the bed materials, initial agglomeration was predicted to occur at 1550 ^{0}C if the biomass fuel is dominated by potassium, K but rose to 1700 ^{0}C if the biomass fuel is dominated by sodium, Na. This justifies the affirmation that, Sodium, Na has a higher melting temperature than potassium, K. Fusion of particles occur in the combustion bed at the eutectic temperatures. Pressure was discovered to have noticeable effects on agglomeration during the combustion of the selected biomass fuels. At a pressure of 5 bar, in a Potassium K dominated biomass fuels, the eutectic temperature was predicted to occur in the bed at 1600 ^{O}C as against 1200 ^{O}C when the pressure in the combustion chamber was 1bar. In a Sodium Na dominated biomass fuels, the eutectic temperature at which agglomeration would occur in the bed was predicted to be 2000 ^{O}C. The higher the pressure, the lower is the risk of agglomeration in the combustion beds.*

Keywords: *Eutectic, FactSage, Fusion, Kaolin, Phase diagrams, Agglomeration, Gooch crucible*

I. INTRODUCTION

Both the binary and the ternary phase diagrams are very significant in the determination of eutectic points as related to agglomeration formation during the combustion of the selected biomass fuels in the combustion chamber. Factsage package contains FACT-Win / FACT and CHEMSAGE, SOLGASMIX thermochemical. It comprises of several databases, information, calculation and manipulation modules, which permits access to the control of pure substances and solution database. The Gibbs energy minimization workhorse of Factsage is the equilibrium module and some other common programs [1].

Factsage software contains thermochemical software and databases. It runs on PC operating under MS windows. It has been used extensively to predict eutectic point on phase diagrams at which melting and fusion of solid particles in a fixed bed combustor during the combustion process of blends of biomass fuels with coal [2].

1.1 Background of the Study

The eutectic points refer to the points on phase diagrams (binary and ternary) where melting and fusion of biomass fuel particles occur during the combustion of single/blends of biomass fuels with coal. Factsage software specifically determines the behaviour and characteristics of substances on phase diagram using their thermodynamic properties. Phase diagram is a broad module that allows the determination of different combinations of pressure,

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temperature, volume, compositions, chemical potential, and phase fraction. Phase diagram could be in the form of unary, binary, ternary or multi components phase diagrams [3]. The corresponding temperature to the eutectic point on the temperature axis is the eutectic temperature. It is also the equivalent agglomeration temperature in the combustor bed. The eutectic points on binary and the ternary phase diagrams varied considerably, even though, the operating conditions may be the same.

Combination of two software package F*A*C*T/FACT-Win and ChemSage otherwise referred to as FactSage was introduced in 2001. It is made up of several information, calculations, and modules that enable researchers to access pure substances and databases. Many thermochemical calculations can be performed with the series of modules available in the package. With this, thermochemical calculations can be processed to generate graphs, figures, and tables of high interest to the corrosion and chemical engineers, physical metallurgist, environmentalists, geochemists, electrochemists, ceramists, and other relevant fields of study [2]. This application permits acquisition of new databases, calculation, and manipulation of both phase diagrams and other complex phase. Version 6.1 was adopted in this research. The modules are grouped into different categories: Info, databases, calculate, and manipulate.

II. METHODOLOGY/MATERIALS

2.1 Locating Eutectic Points on the Binary Phase Diagram

Determination of the eutectic points on binary phase diagrams can be accomplished by utilizing a graph of temperature against the compositions of the two substances under study at a constant pressure, P. The system is at a gas phase (γ) or vapour state when the temperature of the system is very high while at a lower temperature, the system is at a liquid phase (α). At the intermediary between the gas and the liquid phase, is the solid phase (β) [3]. Between the two states (vapour and liquid), the system is at an equilibrium with each other therefore, fusion of the substances take place at this point. The particular spot, at which this occurs, is the eutectic point EP [4]. The eutectic point is very significant in this research work because, the temperature at eutectic point indicates the temperature at which agglomeration will occur in the laboratory-scale fixed bed whereby the Gooch ceramic crucible is the combustor. In binary phase diagram, temperature T is plotted against the mole fractions of the two substances under consideration, Figure 2.1

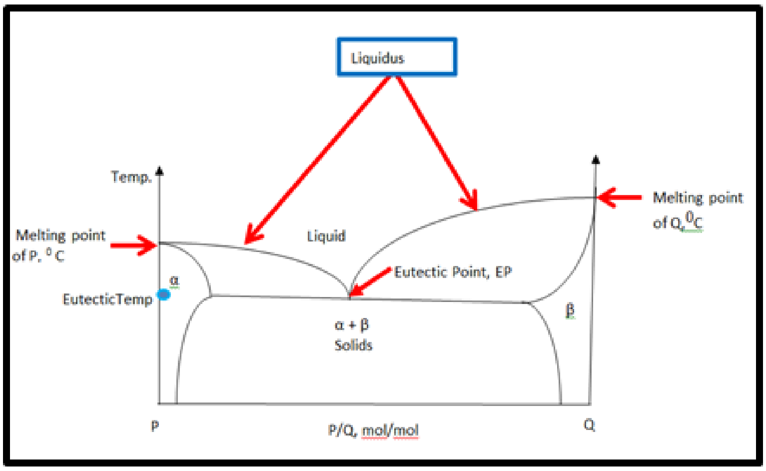

Figure 2-1 Schematic of a eutectic point on a typical binary phase diagram [5]

2.2 Locating Eutectic Points on the Ternary Phase Diagram

Ternary phase diagram is a phase diagram comprising of three concurrent components with four dimensions. That is the 3-components and the Temperature axis. It can be likened to a quadrilateral triangle. The composition of the component at the vortex is 100%. Moreover, the composition of each component at the two edges is 100% each [6]. Eutectic point is formed within the interior of the triangle and this depends on the compositions of each component in the entire system. The ternary eutectic point is the point at which, three boundary curves appear together at a triple junction in a ternary phase diagram [7]. The corresponding temperature at which eutectic point was formed is the eutectic temperature. It is the temperature at which the three components crystallizes out at isothermal as shown in triangle ABC, Figure 2.2

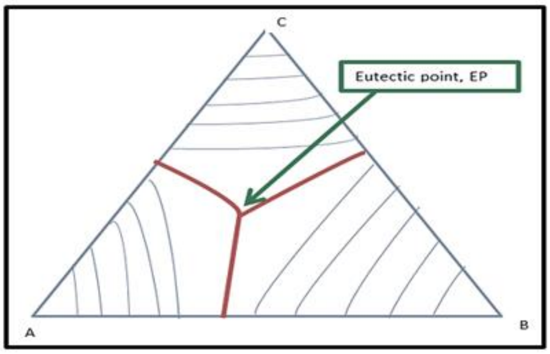

Figure 2-2: Schematic of Eutectic point on a typical ternary phase diagram [5]

III. ANALYSES OF RESULTS

Factsage software predicts the eutectic point which is the temperature at which agglomeration would occur in the combustion bed. Composition of individual component in moles in the mixture of kaolin/potassium oxide or in kaolin/sodium oxide during the combustion of biomass fuels, does not seems to have any significant effect or influence on the agglomeration formation in the bed. Eutectic point was formed at the same temperature 1200 0C when 10 moles and 12 moles of kaolin reacted with one mole of potassium oxide, Figures 3.1 and Figure 3.2 respectively.

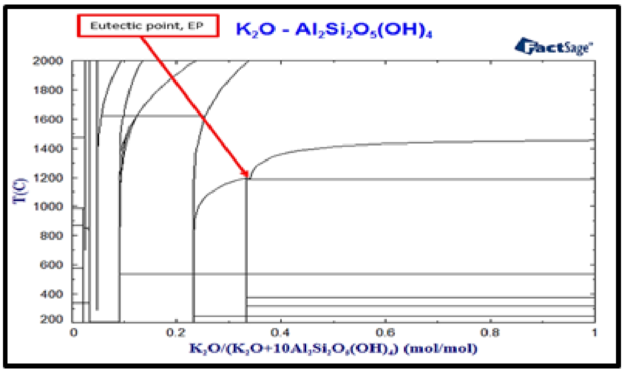

Figure 3-1: Profile of Eutectic points on binary phase diagrams at 1200 ^{0}C

Irrespective of variations in the composition, the eutectic point remained unaltered at 1200 0C in a potassium dominated biomass fuels, Figure 3.2

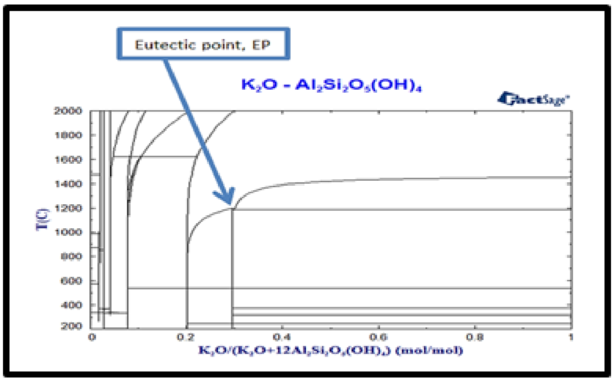

Figure 3-2: Profile of Eutectic points on binary phase diagrams at 1200 ^{0}C

In figure 3.2, two moles of potassium oxide reacted with one mole of kaolin in the combustion chamber, agglomeration occurred at a temperature of 1200 0C. This is equivalent to the eutectic temperature recorded when 2 moles of kaolin was added to 1 mole of potassium oxide under the same operating conditions, the same eutectic temperature of 1200 0C was also recorded, Figure 3.3

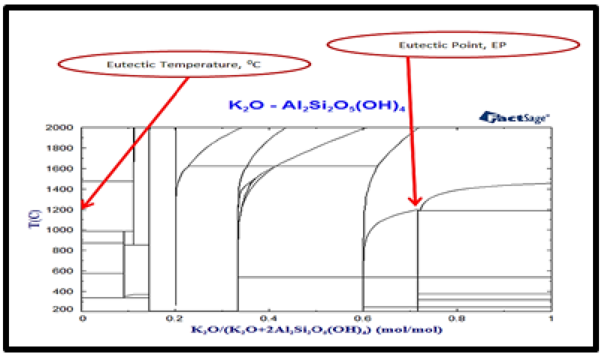

Figure 3-3: Profile of Eutectic points on binary phase diagrams at 1200 ^{0}C

Meanwhile, in a Sodium oxide, Na_2O dominated biomass fuels; simulation results indicated that agglomerates would be produce at a temperature of 1700^0 C irrespective of the volume of the additive or the biomass fuels in the composition.

3.1 Influence of Pressure on Agglomeration

Simulation results obtained from Factsage software clearly indicated that, operating the bed at a higher pressure would prolong the time for agglomeration formation in a fixed bed [8]. At a bed pressure of 1 bar in a Potassium K dominated biomass, the eutectic temperature at which agglomeration would occur in the bed is 1200 ^{O}C. Meanwhile, in a Sodium Na dominated biomass, the eutectic temperature at which agglomeration would occur in the bed is 1700 ^{O} C at 1bar. However, as the pressure increases, so also the agglomeration time and eutectic temperature increases. At a pressure of 5bar, in a Potassium K dominated biomass, the eutectic temperature at which agglomeration would occur in the bed is 1600 ^{O}C as against 1200 ^{O}C when the pressure in the combustion chamber was 1bar. At 5 bar, in a Sodium Na dominated biomass, the eutectic temperature at which agglomeration would occur in the bed is 2000 ^{O} C, Figures 3.4a and 3.4b.

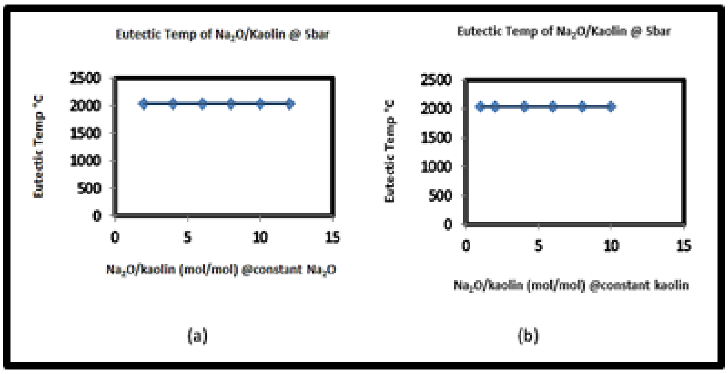

Figure 3 4: (a) Eutectic temperature between kaolin and Sodium oxide at constant Na_2O, on binary phase diagram at 2000 ^{0}C. (b) Eutectic temperature between kaolin and Sodium oxide at constant kaolin, on binary phase diagram at 2000 ^{0}C

In Comparison with fluidized bed combustor, bed pressure increases as air flow rate increases [9, 10]. Voidage at minimum fluidization Єmf, increases slightly with increasing bed pressure while minimum fluidization velocity decreases with rise in the operating pressure but it is negligible for beds having fine particles with diameter dp less than 100µm [11, 12, 13]. Particle voidage at minimum fluidization Єmf, increases with rise in the bed operating temperature for fine particles but may not have any effect on coarse particles. Minimum fluidization velocity U_{mf} of sand particles decreases with rise in bed operating temperature [14, 15, 16].

The higher the pressure in the bed, the higher the temperature at which agglomeration will occur in the bed. Considering the binary phase diagrams emanated from the combustion of the selected biomass fuels (willow, miscanthus, and white wood), only two components were compared simultaneously (kaolin and alkali compounds) while in the ternary phase diagrams, three components were compared together simultaneously (alkali compounds, kaolin, and silica).

IV. DISCUSSIONS

The eutectic temperature is the temperature at which fusion of alkali metals (K, Na) and silica (SiO_2) from the sand (bed materials) occurs in the combustion bed during the combustion process of the selected problematic biomass fuels. Variations in the composition of the components do not have any noticeable effects on the agglomeration and the eutectic points. Two components (additive and alkali oxides) were compared simultaneously on the binary phase diagrams. Alkali oxides considered are potassium oxide K_2O and sodium oxide Na_2O while the additive is kaolin, $Al_2Si_2O_5(OH)_4$. With the dominant alkali in the biomass fuels as potassium K, eutectic point was located on the phase diagram at a eutectic temperature of 1200 ^{0}C as indicated by the meeting point of the two liquidus on the tie lines.

In the same trend, four moles of kaolin was added to one mole of potassium oxide under the same operating conditions. A eutectic point was located at an equivalent temperature of 1200 ^{0}C despite an increase in the percentage composition of kaolin to four moles.

Increase or decrease in the proportion of the components, under the same operating conditions does not have any noticeable influence on the eutectic point or the eutectic temperatures. This assertion is further ascertained in this research. Utilizing Factsage software to predict the eutectic temperatures in a sodium dominated biomass fuels, a eutectic point was located on the binary phase diagrams at a temperature of 1600 ^{0}C irrespective of the volume of the individual component in the mixture. In a mixture of one mole of sodium oxide and one mole of kaolin, a eutectic point was located at an equivalent temperature on the binary phase diagram, Figure 4.1

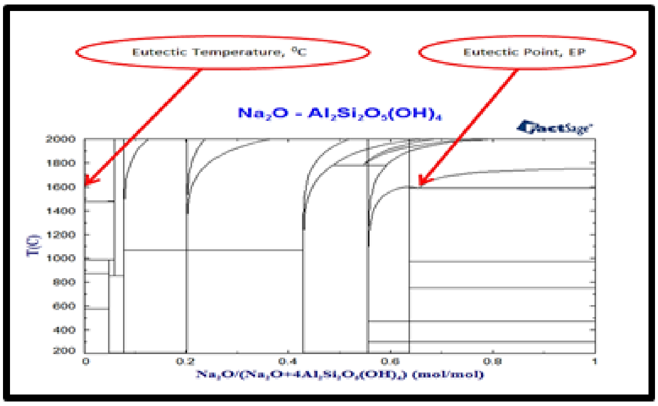

Figure 4.1: Profile of eutectic points on binary phase diagrams at 1600 ^{0}C

4.1 Influence of Additive on Agglomeration Tendencies

The impact of additive on the agglomeration tendencies during the combustion processes of the selected biomass fuels was considered. Simulation results indicated that, with the addition of kaolin to the bed contents, pressure has tremendous influence on the formation of agglomerates in the beds during the combustion of the problematic biomass fuels.

In the ternary phase diagram, no eutectic point was observed at temperatures of 1300 ^{0}C and 1400 ^{0}C. It is expected that, eutectic points would be formed at higher temperatures compared to the binary phase diagrams. This is because, three components interacted simultaneously K_2O - SiO_2 – $Al_2Si_2O_5(OH)_4$. This compound has a higher melting temperature than the K_2O - $Al_2Si_2O_5(OH)_4$ hence, higher eutectic points. Eutectic point was fully developed at 1600 ^{0}C, and 1650 ^{0}C Figures 4.2 and 4.3

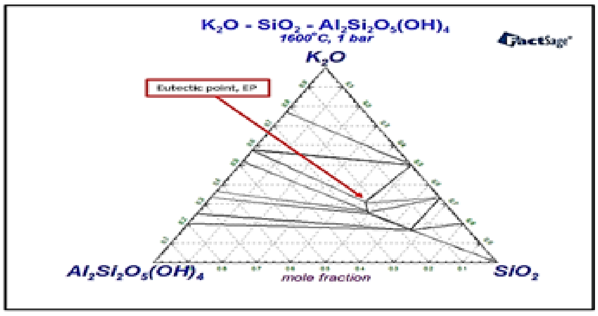

Figure 4-2 Profile of Eutectic point on a ternary phase diagram at 1600 ^{0}C, 1 bar

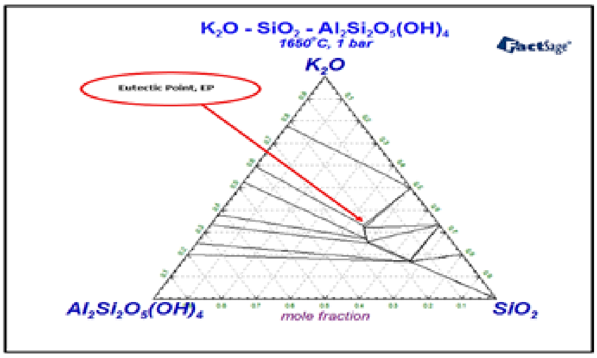

Figure 4-3: Eutectic point at 1650 ^{0}C, 1bar on ternary phase diagram

V. CONCLUSIONS

Temperature at which fusion of blends of biomass fuel particles with bed materials occurred when additive, kaolin was added was fully established. This led to the determination of the safe working temperature of the combustion equipment (SWT) which was recommended to be below the eutectic temperature, when additive (kaolin) was added. With the addition of additive (kaolin) to the bed contents, in Potassium, K dominated biomass fuels, agglomeration was predicted to occur in the bed at the elevated temperature of 1200 ^{0}C and pressure of 1 bar on binary phase diagrams. Two components (kaolin and potassium oxide) were considered simultaneously. Eutectic temperature in Sodium, Na dominated biomass fuel was at a higher temperature of 1700 ^{0}C at the same operating conditions. With the addition of additive (kaolin) to the bed materials, initial agglomeration was forecasted to occur in the bed at the temperature of 1550 ^{0}C and pressure of 1 bar on ternary phase diagrams where three components were considered simultaneously. Eutectic points became pronounced on the ternary phase diagram at 1600 ^{0}C, 1650 ^{0}C, and above. Variation in the value of the compositions of the components (kaolin and potassium oxide respectively) $Al_2Si_2O_5(OH)_4$ and K_2O was discovered not have any significant influence on the eutectic temperatures on both the binary and the ternary phase diagrams. Percentage of the components was in either mole or grams. Pressure has significant influence on the formation of agglomerates in a laboratory- scale fixed bed during the combustion of biomass fuels. This was confirmed with the results obtained from Factsage software applications to determine the eutectic temperatures on binary and ternary phase diagrams. The higher the pressure in the bed, the higher the eutectic temperature, the lower is the risk of agglomeration in the beds during the combustion processes of the biomass fuels. Outcome of this research also confirms FactSage software as a reliable tool in agglomeration experiments.

VI. ACKNOWLEDGEMENT

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