Novel Model for the Release and Condensation of Inorganics for a Pressurized Fluidized-Bed Gasification Process: Effects of Gasification Temperature

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ABSTRACT: A model is established to investigate the release and condensation of inorganics for a wood steam/oxygen-blown fluidized-bed gasification process. In the established model, fates of major elements (C, H, O, N, S, and Cl) and minor elements (Al, Ca, Fe, K, Mg, Mn, Na, P, Si, Ti, and Zn) are modeled separately. The composition of gaseous species involving major elements is predicted using Aspen Plus based on a semiempirical model. The release of minor elements and the condensation of inorganics are predicted using software SimuSage. The combination of Aspen Plus with SimuSage is achieved by manually inputting the stream parameters calculated from Aspen Plus into SimuSage. On the basis of this developed model, effects of gasification temperature on the condensation of Na-, K-, and Cl-containing species during gas cooling are studied. Results show that the process model established by combining Aspen Plus and SimuSage is valid and can be used to investigate the release of inorganics during gasification and condensation of inorganics during gas cooling. Under the investigated gasification conditions, regardless of the bed material, there are two temperature ranges within which no salt melt is formed during gas cooling. As the gasification temperature increases, the high-temperature range without salt melt formation becomes successively wider.

1. INTRODUCTION

Gasification, as one of the thermochemical conversion pathways, efficiently converts different biomass feedstock into a product gas, comprising permanent gas components such as CO, CO₂, CH₄, and H₂. The product gas can be utilized to produce high-value-added chemicals, transportation fuels, and other energy carriers after upgrading. However, the product gas from a biomass-fueled gasifier commonly contains contaminants such as alkalis, particulates, HCl, H₂S, COS, NH₃, and HCN. The contaminant, alkalis, could poison catalysts in downstream process equipment. In addition, gaseous alkalis are condensable and can condense out of the gas phase when gas temperature decreases, generally resulting in problems such as ash deposition and equipment corrosion. It is therefore necessary to investigate the release and condensation of alkalis to eliminate these problems.

Both experimental measurements and chemical equilibrium calculation have been conducted for the release of alkali metals during biomass gasification. It is well known that factors including gasifier type, gasification conditions, feedstock impurities, tars, and bed materials can affect the release of alkali metals during biomass gasification. In terms of the condensation of inorganics during gas cooling, studies are generally performed based on thermodynamic equilibrium calculations. One typical equilibrium calculation study was conducted by Froment et al. using FactSage 5.4.1 to investigate the speciation of the condensed phase during gas cooling from 1300 to 25 °C. In FactSage, the product composition calculation is based on a global thermodynamic equilibrium model. This kind of model is characterized by underestimating the yields of CO₂, tars, light hydrocarbons, and char, as well as overestimating the yields of H₂ and CO. The inaccurate yields of major gas species may affect the release of alkali metals during gasification and may also affect the fate of inorganics during gas cooling. Furthermore, melts are not taken into account in the thermodynamic database used by Froment et al. This may lead to inaccurate prediction of the speciation of the condensed phase during both gasification and gas cooling. Therefore, a more accurate model and a proper thermodynamic database are required to improve the prediction of the release and condensation of inorganics.

Besides investigating the release of inorganics during gasification in a gasifier and the condensation of inorganics in equipment such as heat exchanger, there is a need to investigate...
the fate of inorganics at other positions of a gasification system. This is most practically performed by means of process modeling. At present, most developed process models do not consider inorganic elements, apart from nitrogen and sulfur.24−26 Moreover, ash is generally treated as an unconventional inert component, not participating in the chemical and phase equilibriums. Font Palma and Martin27 utilized process simulation software Aspen Plus to investigate the partition of inorganic constituents formed in a gasification process of 200 kW on-site power generation using poultry litter as the feedstock; only six inorganic elements and a limited number of species are considered in their work. Michael Stemmler et al.28 developed a process model using SimuSage with a pure substance database of FactSage 5.3. In their process model, the formation of only methane and ethylene is considered by reducing the amount of carbon and hydrogen. Other nonequilibrium factors such as the formation of char and tar are not considered. In short, there is a lack of accurate process modeling and use of thermodynamic databases involving both organic and inorganic elements.

In the present study, a process model is established by combining Aspen Plus with SimuSage. Because Aspen Plus has abundant model blocks and can also establish a user model by programming subroutines, it is used for predicting the composition of major gas components, light hydrocarbons, tars, unconverted carbon, and NH₃ based on a semiempirical model. SimuSage is a ChemApp-based set of Delphi components for flowsheeting, which can be used for process simulation using a customized thermodynamic database, despite that only limited types of blocks are available for the modeling. Because of the convenience of importing a customized thermodynamic database, SimuSage is used for determining the release of inorganics during gasification and condensation of inorganics during gas cooling. A comprehensive thermodynamic database extracted from FactSage 7.1 is used for SimuSage calculations, including data for gas, solid, and liquid phases (and solution phases). On the basis of the established model and the customized thermodynamic database, effects of gasification temperature on the condensation of Na+, K+, and Cl-containing species during gas cooling were investigated. This study is part of our ongoing research to develop a tool for predicting the fate of inorganics in the downstream processing equipment of a steam/oxygen pressurized fluidized-bed gasification system from feedstock to the end product. In our previous study,29 experimental and modeling work of biomass gasification and inorganics condensation has been performed. Results from the developed model have been compared with the experimental results, and a reasonable agreement is achieved. In this work, the developed model is further improved on the method of obtaining the composition of main gas components. The composition of main gas components is measured using online gas chromatography in our previous study. In this study, the composition of main gas components is calculated on the basis of a semiempirical model developed using Aspen Plus. In this way, effects of various parameters on the system involving inorganics can be directly investigated.

2. METHODOLOGIES

2.1. Overall Model Description. The developed process model is based on the following assumptions: the process is at a steady state; all reactions associated with inorganic elements reach equilibrium; there is no pressure loss along the process stream; reactions involving major elements such as C, H, O, N, S, and Cl occur first, followed by reactions involving minor elements (Al, Ca, Fe, K, Mg, Na, P, Si, and Ti).

The methodology for process model development is depicted in Figure 1. Overall, fates of major elements and minor elements are modeled separately. The composition of gaseous species, involving major elements, is predicted using a semiempirical model. The parameters for gaseous species, formed by major elements, serve as input data for the chemical equilibrium model for minor elements. The condensation of gaseous inorganics during gas cooling is calculated on the basis of an equilibrium model. The developed process model can predict the release and condensation of inorganics under nearly actual process conditions.

2.2. Semiempirical Model for Major Elements. At large, a biomass gasification process includes several steps such as drying, devolatilization, and gasification (oxidation and gasification).23,30 The drying and devolatilization steps occur instantaneously under the environment of high temperature and intense heat transfer. Then, in the presence of the injected gasification agent, both homogeneous and heterogeneous gasification reactions occur. Therein, exothermic oxidation reactions provide the heat for endothermic reduction reactions. One point to note is that there are no obvious boundaries for the above-mentioned three steps because of the boundary overlap.
In an actual gasification process, the carbon in biomass is not completely converted and the gas residence time in the gasifier is also limited. Because of the presence of these nonequilibrium factors, the yields of H₂ and CO are overpredicted and the yields of CO₂, light hydrocarbons, tars, and char are underpredicted by the global thermodynamic equilibrium calculations. In terms of nitrogen, experimental results by de Jong et al. show that the primary N-containing component is NH₃. The experimental measurements, performed by Zhou et al., also imply that NH₃ and N₂ are two dominant components derived from the nitrogen in the fuel, whereas equilibrium models predict that most of the nitrogen in the fuel is released in the form of N₂. Therefore, reactions involving nitrogen are far from equilibrium under real gasification conditions. In the present study, a semiempirical model is used to predict the composition of major gaseous species from gasifier using empirical correlations to predict the yields of nonequilibrium species. These empirical correlations, shown in Table 1, are fitted with experimental data from pressurized steam/O₂-blown fluidized-bed gasification with forest residues and crushed wood pellets as feedstock.

Table 1. Correlations for Nonequilibrium Substances Used in the Aspen Plus Gasifier Model

| Substance | Conversion Correlation |
|-----------|------------------------|
| C         | 0.0155 × T + 86.068%   |
| CH₄       | -0.003 × T + 7.074 mol/kg |
| C₂H₂      | -0.00004 × T + 0.06454 mol/kg |
| C₂H₆      | -0.002 × T + 2.987 mol/kg |
| C₂H₄      | -0.001 × T + 1.196 mol/kg |
| C₆H₆      | -0.000155 × T + 0.150921 mol/kg |
| C₂H₂O     | 0.27 mol/kg |
| C₆H₁₀     | 0.3 mol/kg |
| NH₃       | 0.04154 mol/kg |

*T represents gasifier freeboard temperature, in degree Celsius.

The correlations shown in Table 1 are valid only for a gasification process using a similar feedstock (crushed wood pellets and forest residues) and a similar gasifier type and configuration. Furthermore, these correlations are valid only within the range of the data used for fitting the model parameters.

The semiempirical model for the major elements is established using five blocks, as depicted in Figure 2. A Ryield block is used to model the biomass drying and devolatization processes, where biomass (CH₄O₂ClNₓSₙ(ash))(H₂O)ₙ is decomposed into C, H, O, N, S, Cl, ash, and H₂O according to ultimate and proximate analyses. This is fulfilled by a programed FORTRAN subroutine.

\[
\begin{align*}
\text{CH}_x\text{O}_y\text{Cl}_z\text{N}_a\text{S}_b(\text{ash})(\text{H}_2\text{O})_c & = \varphi \text{C} + \frac{\alpha}{2} \text{H}_2 + \frac{\beta}{2} \text{O}_2 + \frac{\gamma}{2} \text{Cl}_2 + \frac{x}{2} \text{N}_2 + \delta \text{S} + \varepsilon \text{ash} \\
& + (1 - \varphi) \text{C} + \varphi \text{H}_2\text{O} + Q
\end{align*}
\]

wherein \(\varphi\) means the percentage of carbon participating in the actual gasification process; the carbon conversion is estimated using empirical correlations (see Table 1). The unconverted carbon \((1 - \varphi)\text{C}\) is separated out using a Sep block. Q represents the heat energy used for decomposing the biomass, which is derived from the gasification section.

A RGibbs block is adopted to model the gasification section, predicting the chemical composition of the product gas based on the principle of Gibbs free energy minimization. The possible products, specified in the Gibbs block, include H₂, CO, CO₂, H₂O, CH₄, C₂H₄, C₂H₆, C₂H₂, C₂H₆, C₁₀H₈, N₂, NH₃, HCN, HCl, H₂S, COS, and ash components. In Aspen Plus, ash is generally regarded as an unconventional inert component and therefore it does not participate in chemical and phase equilibriums. To study the fate of the actual ash components and to avoid a doubling input of the ash content, inert ash \(\varepsilon\) is first removed by using a Sep block with a subsequent addition of various ash components in the gasification section. Because the removed inert ash takes a part of heat away, to sustain the energy balance of the system, the heat carried by the inert ash is supplemented to the gasification section. Because the release of inorganic elements during gasification is modeled in SimuSage, these added ash components are still set as nonreacting components in Aspen Plus.

2.3. Model for Studying the Fate of Inorganics during Gasification and Gas Cooling. Figure 3 depicts the schematic diagram of a model for studying the fate of inorganics during both gasification and gas cooling. The release of minor elements during biomass gasification is modeled using TPbGttBalance and TPbPhaseSplitter. Gas cooling is modeled using TPbHeatExch with TPbGttBalance. TPbPhaseSplitter is used to model separation of the condensed phase from the gas phase. The parameters of gaseous species, calculated by Aspen Plus, serve as input data for SimuSage. Because TPbGttBalance performs complete equilibrium calculations based on the parameters of inlet streams and reaction conditions, nonequilibrium factors cannot be taken into account. Therefore, nonequilibrium species, including CH₄, C₂H₂, C₂H₆, C₂H₄, C₂H₆, C₄H₁₀, C₂H₄, C₂H₆, and NH₃, are removed before the SimuSage calculations. To consider the potential effects of CH₄ and other hydrocarbons on the fate of inorganics during both gasification and gas cooling, formations of CH₄, C₂H₂, C₂H₆, C₂H₄, C₂H₆, C₁₀H₈, and C₁₀H₆ are taken into account during SimuSage calculations. This leads to the formation of minor amounts of CH₄ (around 0.001 vol % level) and other...
light hydrocarbons (less than 0.001 vol % level). In view of the large volume of major gas species, the minor amounts of the formed CH₄ and light hydrocarbons can be neglected.

The thermodynamic database used in SimuSage comprises 17 elements (C, H, O, N, P, S, Cl, Al, Ca, Fe, Mg, Si, Ti, Mn, K, Na, and Zn), 100 pure liquids, 677 pure solids, 144 gaseous species, and 18 solution phases (15 solid solution phases and 3 liquid solution phases). A more comprehensive description of this customized thermodynamic database can be found in our previous study.29

2.4. Model Parameters. Because of ash component analysis data not being given in the study fitting empirical correlations,33 a wood with similar proximate, ultimate and heating value data is used as feedstock for calculations.

Table 2 presents the proximate analysis, the ultimate analysis, the high heating value, and the ash analysis of wood. The ash content in wood is measured by ashing the wood at 750 °C. The elements in wood contain C, H, O, N, S, Cl, Al, Ca, Fe, K, Mg, Mn, Na, P, Si, and Ti.

Table 3 shows the gasifier operating parameters. Table 4 shows the feeding conditions of wood and the gasification agent.

For calculating the flow rate of oxygen and steam, the fuel is based on the dry and ash-free basis.

| Material | Temperature (°C) | Pressure (MPa) |
|----------|------------------|----------------|
| wood     | 20               | 0.25           |
| oxygen   | 200              | 0.25           |
| steam    | 200              | 0.25           |

Table 4. Feeding Conditions of Wood and the Gasification Agent

For a given gasification temperature, the flow rate of oxygen is calculated based on the energy balance.

A mixture of 30 wt % sand (SiO₂) and 70 wt % limestone (CaCO₃) is used as the bed material. The amount of bed material is set as 0.055 kg/kg wet biomass, which is within the experimentally used range of the ratio of the bed material feed rate to the biomass feed rate.36

3. MODEL VALIDATION

In terms of the semiempirical model for the major elements, the predicted composition of main product gas components including H₂, CO, CO₂, and H₂O in the wet gas is compared with the wet gas composition measured for the experiments using similar feedstock composition, as illustrated in Figure 4. For the modeling case using a gasification temperature of 823 °C, the mass ratio of steam to fuel is set as 0.50 to be consistent with the experimental operating conditions. Figure 4 shows that for the concentrations of H₂, CO, CO₂, and H₂O, the averaged relative error between the calculated and measured values is 19%. The relative error is defined as the ratio of the absolute value of the difference between the calculated value and measured value to the measured value. The relative errors predicted by the complete thermodynamic equilibrium model are 55.6% for the molar fraction of CO₂, 84% for the molar fraction of CO, and 111.1% for the molar fraction of H₂. Compared with the composition predicted by the complete

Figure 3. Model established using SimuSage for studying the release and condensation of inorganics.

Table 2. Wood Composition Analysis

| Proximate Analysis (%) (mass) | Ultimate Analysis (%) (mass) | HHV (MJ/kg) |
|------------------------------|-------------------------------|-------------|
| Mass | FC | Vd | Ad | Cd | Hd | Nd | CLd | Sd | Od | HHV |
|------|----|----|----|----|----|----|------|----|----|------|
| 6.600 | 17.560 | 81.240 | 1.200 | 49.520 | 6.000 | 0.090 | 0.005 | 0.010 | 43.175 | 19.394 |

Table 3. Operating Conditions of the Steam/O₂-Blown Fluidized-Bed Gasifier

| Condition | Pressure (MPa) | Heat Loss (%) | Oxygen to Fuel Ratio (kg/kg) | Steam to Fuel Ratio (kg/kg) |
|-----------|---------------|--------------|-----------------------------|-----------------------------|
| Pressure  | 0.25          | 7            | 0.54                        | 0.54                        |

All tables are used to provide detailed information about the wood composition, operating conditions, and feeding conditions. The tables include proximate and ultimate analysis data, along with ash analysis and operating parameters. The tables also show the conditions used for calculating the flow rates of oxygen and steam, which are based on the dry and ash-free basis.
thermodynamic equilibrium model, the composition of main product gas components predicted using the developed semiempirical model has been much closer to the experimentally measured composition. Additionally, the experimental data is expected to have an error of around 5%. Judging by the results, reasonably good agreement between the measured values and the values predicted by the model developed using Aspen Plus has been achieved. One point should be noted that the experimental data used for comparison are derived from the gasification experiments using a similar feedstock. On condition that good experimental data are collected for fitting empirical correlations, the predicted composition would be more accurate.

In the case of the model for studying the fate of inorganics during both gasification and gas cooling, the predicted elemental compositions of the condensed phase under different cooling temperatures are in general consistent with the elemental compositions identified using scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM/EDS). This demonstrates that this model, developed using
SimuSage, is valid for the investigation of the release and condensation of inorganics.

In summary, the model established by combining Aspen Plus and SimuSage is valid and can be used to investigate the release

Figure 6. Relationship between cooling temperature and accumulated mass of each condensate under different gasification temperatures (885 °C, 870 °C, 855 °C, and 840 °C): (a) with bed material addition and (b) without bed material addition.
of inorganics during gasification and the condensation of inorganics during gas cooling.

4. MODEL APPLICATION

The developed model is applied to investigate the condensation of Na, K, and Cl-containing species during gas cooling from four initial gasification temperatures (885 °C, 870 °C, 855 °C, and 840 °C) to 350 °C. The four gasification temperatures are within the range of the data used for fitting the empirical correlations. The developed model is valid to be used to investigate the effects of gasification temperature. Other model parameters (wood composition and gasification conditions) are the same as given in Section 2.4. The equilibrium calculation and experimental measurement performed by Scott Q. Turn showed that only a part of bed material actually participates in the elemental partition during gasification.8 The study by Porbatzki et al. also indicated that the releases of inorganic species such as KCl(g), HCl(g), and H2S(g) are strongly affected by other elements (e.g., Si and Ca) in the fuel. Additionally, because of the poor mixing of the bed material and biomass in the gasifier, not all biomass can interact with the bed material during gasification. Therefore, two boundary cases including with and without addition of bed material in the gasifier are modeled in the present study. This could help have a comprehensive understanding on the effects of gasification temperature. The calculation threshold for all cases is set as 1 × 10−6.

Figure 5 quantitatively presents the proportion of Na, K, and Cl remained in the gas phase (Rg) after gas cooling. Rg is defined as eq 1.

\[
R_g = \frac{n_{g\text{-e}}}{n_{g}}
\]

where \(n_{g\text{-e}}\) is the initial amount of element in the gas phase, equal to the amount of each element released into the gas phase during gasification, and \(n_{g}\) represents the amount of element remained in the gas phase after gas cooling.

For the case without addition of bed material during gasification, the trends between the cooling temperature and the proportion of each element (Na, K, and Cl) remained in the gas phase are the same as those for the case with the addition of bed material. Therefore, the only relationships between the cooling temperature and \(R_g\) of Na, K, and Cl in the case of addition of bed material are presented in Figure 5.

Overall, regardless of the gasification temperature, proportions of Na, K, and Cl remained in the gas phase decrease with the cooling temperature until being constant. Additionally, the three elements have different condensation rates. For the investigated four gasification temperatures, the sodium-related species are first condensed out of the gas phase, followed by potassium- and chlorine-related species. The different condensation rates of Na and K have also been observed in the study by Froment et al.17 Because gaseous alkalis are primarily condensed in the form of carbonates and only a little amount of gaseous alkalis is condensed as chlorides (see Figure 6), the fraction of Cl remained in the gas phase is higher than the fractions of Na and K during gas cooling. Under the specified calculation threshold (1 × 10−6), the sodium- and potassium-related species can be completely condensed out of the gas phase after 660 °C and 410 °C, respectively (see Figure 5).

There are nearly no Na- and K-containing species in the gas phase, as the cooling temperature is lower than 410 °C. However, chlorine remains in the gas phase in the form of HCl(g). In short, gas cooling is beneficial for removing alkalis in the product gas but not useful for removing some chlorine-containing species such as HCl(g).

Figure 6 shows that for both cases with and without addition of bed material, the amount of condensate increases with the increase of gasification temperature. This can be explained that for these investigated gasification temperatures more volatile elements can be released into the gas phase at a higher gasification temperature;17,19 more gaseous inorganics are consequently condensed out of the gas phase during gas cooling for the case using a higher gasification temperature.

Figure 6 depicts that for both the cases with and without addition of bed material under all investigated gasification temperatures Na and K in the condensed phases are mainly present in the forms of chlorides, hydroxides, and carbonates. For some gasification temperatures, minor amounts of K2S(l) and Na2S(l) are also formed in the condensed phase (see Figure 6). The presence of S, K, and Na in the condensates is also observed using SEM/EDS in the inorganics condensation experiments.29 For the case with addition of bed material, potassium carbonates (K2CO3(ss) and K2CO3(s)) and...
potassium chloride (KCl(ss)) are main condensates (see Figure 6a). For the case without addition of bed material, K_2CO_3(ss) and KCl(ss) are dominant condensates followed by K_3CO_3(l) (see Figure 6b). The cooling calculations performed by Froment et al. also indicated that K_2CO_3(s) is the main condensate followed by KCl(s), whereas no liquid condensates are predicted to be present. This difference in the mass distribution of condensates between our and Froment’s studies can be attributed to the thermodynamic database. Because solution phases are not taken into account in the database used by Froment et al., no formation of melt and solid solution phases can be predicted during condensation calculations in their study.

Regardless of the gasification temperature and bed material, two temperature ranges are present within which no salt melt is formed during gas cooling. The two temperature ranges are separately distributed in a low-temperature zone (less than 660 °C) and a high-temperature zone (higher than 685 °C, less than T_m). T_m represents the maximum temperature of the corresponding temperature range. Within the temperature range from 660 °C to 685 °C, the salt melt is formed during gas cooling.

Figure 7 shows the high-temperature range without melt formation during gas cooling for each gasification temperature. For the case without addition of bed material, the theoretical high-temperature ranges without melt formation are within 685–835 °C, 685–835 °C, 685–810 °C, and 685–785 °C for gasification temperatures 885 °C, 870 °C, 855 °C, and 840 °C, respectively. For the case with addition of bed material, the corresponding high-temperature ranges are 685–885 °C, 685–860 °C, 685–855 °C, and 685–840 °C. For a specific gasification temperature, the temperature range without salt melt formation is wider for the case with addition of bed material compared with the case without addition of bed material. Furthermore, with the increasing gasification temperature, the high-temperature range without salt melt formation becomes successively wider.

Because no salt melt can be formed within the temperature ranges shown in Figure 7, high-temperature filters can be operated within these temperature ranges to avoid ash deposition and corrosion. One point should be noted that steam and tars may be condensed as the gas phase as the gas temperature is decreased. For this point, water saturation temperature and tar dew point are calculated. The saturated temperature of water at 2.5 bar is calculated to be 127.4 °C. The tar dew points are calculated using a complete tar dew point model developed by Energy Research Centre of the Netherlands (ECN). A detailed description of the tar dew point model can be found elsewhere. The calculated tar dew point is around 72 °C, which is obviously lower than the given temperature ranges shown in Figure 7. Actually, except for the two tar model compounds (C_6H_6 and C_{10}H_8) used in the present study, other tar compounds with much higher boiling points are also present in the gasification product gas. Despite this, the measured tar dew point is reported to be lower than 370 °C, which is also below the high-temperature ranges given in Figure 7. Therefore, there is no possibility of forming liquid condensed water and condensed tars under these temperature ranges where no salt melt can be formed. To remove the fine ash and other particles from the raw product gas without causing filter failure, the operating temperature of high-temperature filters can be fixed within these predicted temperature ranges. It should be noted that the given temperature ranges without forming the salt melt are merely theoretical ranges. The detailed temperature ranges and the possibility of applying the temperature ranges of not forming salt melt still need to be experimentally demonstrated.

5. CONCLUSIONS

A model is established to investigate the release and condensation of inorganics for a wood steam/oxygen-blown fluidized-bed gasification process. In the established model, fates of major elements (C, H, O, N, S, and Cl) and minor elements (Al, Ca, Fe, K, Mg, Mn, Na, P, Si, Ti, and Zn) are modeled separately. The composition of gaseous species, involving major elements, is predicted using Aspen Plus on a semiempirical model. The model established using Aspen Plus consists of five sections including biomass decomposition, ash separation, ash heat recovery, unconverted carbon separation, and gasification. The release of minor elements and the condensation of inorganics are predicted using SimuSage. The release of minor elements during biomass gasification is modeled using TPbGtBalance and TPbPhaseSplitter. The gas cooling is modeled using TPbHeatExch with TPbGtBalance. TPbPhaseSplitter is used for modeling the separation of condensed phase from the gas phase. The combination of Aspen Plus with SimuSage is achieved by manually inputting the stream parameters calculated from Aspen Plus into SimuSage. On the basis of this established model, effects of gasification temperature on the condensation of Na+, K+, and Cl-containing species during gas cooling are studied. From the obtained results, the following conclusions can be made. The process model established by combining Aspen Plus and SimuSage is valid and can be used to investigate the release of inorganics during gasification and condensation of inorganics during gas cooling. Under the investigated gasification conditions, regardless of the bed material, there are two temperature ranges within which no salt melt is formed during gas cooling. As gasification temperature increases, the high-temperature range without salt melt formation becomes successively wider.

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