Numerical Analysis of Heterogeneous Oxidation Reaction on Multi-stage Air Inlet Downdraft Gasifier

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Abstract. Gasification technology is one of the thermochemical conversion methods that can be a solution to overcome the negative municipal solid waste (MSW) impact. Syngas application from gasification on the internal combustion engine has problems with tar content. One method for reducing tar content is by means of a multi-stage air inlet in the reduction zone to initiate heterogeneous oxidation reactions. In this study a three-dimensional computational fluid dynamic model was used to simulate gasification reactions. The simulation was carried out using a one-phase model with k epsilon turbulence model, P1 radiation model, devolatilization model using kobayashi model, MSW fuel modeled as a discrete phase that moves in the continuous phase, and the reactions that occur are volumetric and particle surface reaction in which the interaction of turbulence-chemistry using finite-rate/eddy-dissipation. The ratio of air used is 10%, 20%, 30%, and 40% between oxidation and reduction. Based on the simulation results, there is an increase in syngas composition, especially CO because there is a heterogeneous oxidation reaction between carbon in the reduction zone with oxygen which also triggers a rise in temperature in the oxidation zone. CO₂ concentration decreases due to an increase in the rate of boudouard reaction. But when the amount of air continues to increase there is a decrease in temperature in the oxidation zone because the amount of air for the oxidation reaction decreases, the simulation results obtained can be used to optimize the downdraft gasifier by adding air input to the reduction zone.

1. Introduction
An increase in the population in the world has a negative impact on the amount of municipal solid waste that continues to grow. Based on data on world population growth, an increase in the world's population, especially in urban areas, in 2020 reaches 66% [1]. This number will increase the population of the world's population which in 2015 7 million people. The handling of municipal solid waste currently varies from accumulation in final landfills, incinerator combustion, methane gas harvesting, and using thermochemical processes namely gasification technology. when compared to direct combustion,
gasification has advantages because in addition to producing heat that can be converted into energy, this technology also produces gas (syngas). Direct MSW combustion has a negative impact on the environment because it causes CO and CO2 emissions, while landfill accumulation also causes CH4 emissions and affects the quality of groundwater due to liquid waste deposits (leachate) [2, 3]. Therefore, from the various methods of handling MSW above, the most environmentally friendly is Gasification. with gasification technology, solid waste is converted into energy in the form of gas (syngas) [4]. The gasification reaction occurs through several stages, namely drying, pyrolysis, partial oxidation, and reduction. The resulting syngas consists of combustible gas components (CO, H2, CH4) and non-combustible (CO2, O2, N2, H2O), besides, gasification also produces residues in the form of ash and tar. This syngas can be used for both thermal and power applications. for the power application itself, including being used as fuel on diesel fuel motors with dual fuel mode. However, to be able to be used on the syngas diesel engine that is produced, it must meet the minimum standards of tar 100 mg / Nm3 [4, 5]. Several studies have been carried out to reduce the tar content in syngas by using primary and secondary methods. The primary method reduces the tar content in situ in the gasifier. while the secondary method decreases the tar content after leaving the gasifier using various methods including cyclone, water scrubber and dry filter [6].

The primary method that has been carried out by several researchers is to modify the structure of the gasifier with multilevel air input. In the condition of one level, the air for gasification enters the partial oxidation zone while in the multilevel condition the air enters the zone of pyrolysis, oxidation, and reduction. To input air in the pyrolysis zone, a study was conducted by Sudarmanta and arif [7-10] which modifies the gasification of an airway into two airways. Bentzen [11] air entering the pyrolysis zone and gave bulkhead using the grate to separate pyrolysis and partial oxidation zone. Bui [12] adding air to the pyrolysis zone to determine the effect of air input to the performance of gasification. Martinez dan galindo [13, 14] vary the percentage of air input in the pyrolysis and oxidation zone to obtain the optimum ratio. From the various studies reported that there was an increase in gasification performance in the form of an increase in the volumetric gas percentage especially CO and also a pyrolysis zone temperature increase, besides that the tar content could also be reduced to 80% compared to a single air input. In addition to input pyrolysis air, shi and nerijus [15, 16] conduct experiments with air input in all three zones namely pyrolysis, oxidation, and reduction. The results of his research report that when air is put into the reduction zone, the air will tend to react with carbon compared to gas. Therefore, heterogeneous reactions in the reduction zone occur in an oxidative environment. In addition, because the air in the reduction zone oxidizes a small amount of carbon, an increase in temperature increases the CO2 and H2O reduction reaction rate to be more intensive. In addition, the amount of unoxidized residual charcoal is also reduced because it has reacted with oxygen from the air. However, from various studies there has been no numerical research for multilevel air input using a computational fluid dynamic (CFD) model.

Numerical modeling is needed because not all phenomena in the gasification process can be measured through experiments. other than that, for the purpose of numerical modeling optimization is needed before physical modification or optimization is carried out. Various CFD gasification modeling studies have been conducted by several researchers including Gupta and Simone [17, 18] modeling the gasification reaction to find out the temperature distribution along the gasifier. therefore, the purpose of this study is to analyze the effect of air input in the reduction zone on operating conditions (temperature distribution, pressure, and speed) and gasification performance (syngas composition, low heating value, and cold gas efficiency).

2. Material and Method

2.1. Computation model
The type of gasifier used in this numerical analysis is the downdraft gasifier. This gasifier design uses two air inputs, namely the oxidation zone and the reduction zone. 3-dimensional modeling is done to simplify the form of the gasifier by making a fluid domain only on the inside of the gasifier. Figure 1 shows a picture showing the domain of this simulation where air enters the oxidation and reduction zone through five 10° slope nozzles. The fuel used is MSW pellets with a composition of 60% organic waste and 40% non-organic. The diameter is 6 mm with an average length of 10-15 mm. fuel characterization is done using the ultimate test, proximate, and bomb calorimeter to determine the composition of the fuel. The 3D model is meshed by using a mixture of tetrahedral and hexahedral models. The number of elements is 839,159. To obtain accurate simulation results, a grid independency analysis was conducted.

2.2. Numerical Model
Numerical simulation analysis was carried out using FLUENT 15 version of student software. The equations involved in this simulation are flow equations, turbulence, species transport, energy, and radiation. The turbulence model used is realizable k-ε. The transport equation for the species involved in the simulation used the species transport equation model so that the mass fraction and mole fraction for species can be calculated. The chemistry interactions between species are modeled with the finite-rate/eddy-dissipation model. The fuel is modeled into a particle in the form of spherical and combusting particle. The fuel particle is modeled as a discrete phase that moves in the continuous phase and is injected into the surface area above the gasifier. fuel decomposition in the pyrolysis process is modeled with Kobayashi (two competing rates). Radiation heat transfer that occurs in the gasifier is modeled with the P-1 model. Because the gasifier used is downdraft and syngas move down the gasifier, the gravitational force is activated in the direction of the Y axis. The initiation of combustion is done by patching a temperature of 1000°C in the oxidation region.

![Figure 1. Geometry and Meshing model](image)

| Analysis      | Contents | % mass |
|---------------|----------|--------|
| Fixed carbon  | 20.19    |        |
| Proximate     | Volatile | 65.78  |
|               | Moisture | 9.82   |
4.21
Carbon       47.265
Ultimate
Hydrogen     6.7
Oxygen       45.545
Nitrogen     0.49
Calorific Value $1.348 \times 10^8$ (J/kg)

2.3. Reaction Model

The stages of the gasification reaction simulation are modeled according to the sequence of stages of gasification starting from drying, pyrolysis, oxidation, and reduction. The first pellet fuel through drying process is modeled with material droplets. Furthermore, it will undergo an evaporation process into hot steam because the temperature of the particle is lower than its intake temperature (law 1 and law 6 thermodynamics) [19].

$$T_p < T_{vap} T_p$$  (1)

$$m_p \leq (1 - f_v,0) m_p,0$$  (2)

Decomposition modeling uses the Kobayashi model where the decomposition process is controlled by two devolatilization kinetic parameters (R1 and R2) with two different temperatures. Decomposition occurs when the fuel particle temperature reaches the evaporation temperature so that the particle mass does not exceed its non-volatile mass [19].

$$\mathcal{R}_1 = A_1 e^{-(E_1/RT_p)}$$  (3)

$$\mathcal{R}_2 = A_2 e^{-(E_2/RT_p)}$$  (4)

$$\frac{m_p(t) - m_u}{(1 - f_w,0) m_{p,0}} = \int t \left( m_0 R_1 + m_0 R_2 \right) \exp \left( -\int t R_1 + R_2 dt \right) dt$$  (5)

When the decomposition process has occurred and produces a solid product in the form of charcoal, then there will be particle surface reaction which consumes the fraction fb [19].

$$m_p < (1 - f_v,0) (1 - f_w,0) m_{p,0}$$  (6)

$$m_p > (1 - f_v,0) - f_{comb} (1 - f_w,0) m_{p,0}$$  (7)

The surface reaction rate is determined by kinetic and diffusion rate based on a kinetic/diffusion-limited theory by Baum and Street [19].

$$D_0 = C_s \left[ (T_p + T_\infty)/2 \right]^{\alpha_s}$$  (8)

With kinetic rate:

$$\mathcal{R} = C_s e^{-(E_r/RT_p)}$$  (9)
The rate of reaction of partial fuel combustion occurs very quickly and is influenced by temperature and turbulence. The rate of chemical reactions that occur in the gasification stage is calculated using an Arrhenius rate and turbulence mixing rate using the finite-rate/eddy-dissipation model. The kinetic parameters and reactions involved in the gasification stage are presented in table 2.

### Table 2. Kinetic parameter for homogeneous and heterogeneous reactions [17]

| Heterogeneous reactions | Kinetic parameter, A (kg/m²/s/Pa⁰.⁵), E (J/kmol) |
|-------------------------|-----------------------------------------------|
| C(s) + 0.5O₂ → CO (R1)  | A₁ = 0.052, E₁ = 6.1 x 10⁷                   |
| C(s) + CO₂ → 2CO (R2)   | A₂ = 0.0732, E₂ = 1.125 x 10⁸                 |
| C(s) + H₂O → CO + H₂ (R3)| A₃ = 0.0782, E₃ = 1.15 x 10⁸                |
| Homogeneous reactions   |                                               |
| CO + 0.5O₂ → CO₂ (R4)    | A₄ = 2.239 x 10¹², E₄ = 1.674 x 10⁸           |
| H₂ + 0.5O₂ → H₂O (R5)    | A₅ = 6.8 x 10¹⁵, E₅ = 1.67 x 10⁸             |
| CH₄ + 0.5O₂ → CO + 2H₂ (R6)| A₆ = 4.4 x 10¹¹, E₆ = 1.25 x 10⁸         |
| CO + H₂O ↔ CO₂ + H₂ (R7) | A₇ = 2.34 x 10¹⁰, E₇ = 2.883 x 10⁸             |
| CH₄ + H₂O → CO + 3H₂ (R8)  | A₈ = 8.7 x 10⁷, E₈ = 2.51 x 10⁸             |

2.4. Simulation process
The computational process is carried out using a 3-dimensional model which is analyzed using the finite volume method. The air ratio or equivalent ratio used is 0.4. while the comparison made is for the single stage condition or input air in the oxidation zone and multi stage or input air in the oxidation and reduction zone. The ratio used in this study are 10%, 20%, 30%, and 40%. The boundary conditions used in this numerical analysis are presented in table 3.
Table 3. Boundary condition [20]

| Boundary condition                        | value   |
|------------------------------------------|---------|
| MSW particle inlet temperature (°C)      | 30      |
| MSW flow rate (kg/s)                     | 0.00374 |
| Air inlet flow rate stage 1 (kg/s)       | 0.003366|
| Air inlet flow rate stage 2 (kg/s)       | 0.000374|
| MSW particle density (kg/m³)             | 370     |
| MSW HHV (KJ/kg)                          | 13415   |

3. Result and Discussion

In Figure 2 and Figure 3 shows the simulation results of temperature distribution along the gasifier with the difference in air ratio between reduction and oxidation zones from 10% to 40%. When the air ratio at the right level from a single state becomes a level starting from 10% to 40% what happens is an increase in temperature in the reduction zone. While the temperature in the oxidation, pyrolysis, and drying zones decreases. The increase in temperature in the reduction zone occurs because of a partial oxidation reaction between carbon and oxygen contained in the air. This oxidation reaction produces a certain amount of heat resulting in an increase in temperature. While the decrease in temperature in the oxidation zone occurs due to a decrease in the amount of air. As a result, the amount of oxidized charcoal decreases and the rate of oxidation reaction decreases. Therefore, there is a decrease in temperature in the pyrolysis and drying zone because both of them require heat. However, when viewed by the overall temperature distribution, the decrease in temperature in the oxidation, pyrolysis and drying zones does not exceed the minimum temperature limit in the zone. Instead the reduction zone to get additional heat energy can affect the reactivity of the gasification reaction (R2, R7, and R8).

In addition to affecting change in the temperature distribution, inclusion of air in the reduction zone also leads to changes in volumetric percentage of flammable gas. when the temperature in the reduction zone rises, there is an increase in the endothermal reaction rate R2 therefore in figure 3 when the percentage of air by 10% is added to the reduction zone, the percentage of volumetric CO increases. Besides that, H₂ also increases because there is an increase in the reaction rate of R7 due to the increase in temperature.
Increase in CO, H$_2$, and CH$_4$ respectively from 24.3% to 24.82%, 13.04% to 14.2%, and 1.61% to 1.76%, while CO$_2$ decreased from 20.23% to 1.82%. However, when the amount of air continues, the composition of CO, H$_2$, CH$_4$ and CO$_2$ decreases. This happens because more carbon is consumed so the number of reactants for the reaction R2 and R3 decreases.

When compared with the experimental results, the temperature distribution in this numerical simulation is greater. If in the experiment the highest temperature is 1,300°C, in numerical simulations it reaches 1,700°C. This is because in the numerical simulation the gasifier wall is assumed to be adiabatic while in the experiment there is a lot of heat loss. The same thing with composition and LHV is also greater than numerical simulation results compared to experiments. But overall both temperature and syngas composition have the same trend of increase and decrease as the experiment. However, further experimentation needs to be done to reduce the difference to smaller ones.

Figure 3. Temperature profile

Figure 4. a) Comparison of Low Heating Value from Numerical and Experimental Analysis, b) Syngas Composition and LHV
Changes in the low heating value (LHV) as an indicator of the performance of gasification is affected by the volumetric percentage of flammable gas. When viewed from the pattern of increase and decrease, the optimum LHV is obtained when the amount of air input in the reduction zone is 10%. Although there was an increase in the rate of carbon consumption which affected the rate of fuel consumption, but because the percentage of volumetric flammable gas decreased, LHV also decreased. Comparison between the results of experiments with numerical analysis is presented in Figure 4.

4. Conclusion
The 3D model was created to simulate the gasification of MSW pellets by adding air inlet on the pyrolysis zone ranging from 10% to 40%. The simulation results revealed that the addition of air in the reduction zone was able to improve gasification performance in the form of an increase in temperature in the reduction zone and a decrease in temperature in the oxidation, pyrolysis and drying zones which are still above the minimum temperature value. In addition, there is also an increase in the volumetric gas percentage, especially CO. Low heating value and cold gas efficiency also increased. Henceforth, with this numerical model it can be used as a reference to optimize gasification performance by adding air to the reduction zone.

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