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Numerical Simulation of Methanol Gasification at different pressures

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Research Program: Gasification

Introduction

Gasification of biomass is as old as our planet, earth. Forest fires, formation of blue hallow in a swamp are two common examples of gasification of biomass. Early modern large-scale application of gasification was mainly for city streets and wealthy people's houses lightening (Britain 19th century). Even though gasification is as aged as combustion technologies, it didn't develop with industrialization as combustion due to low prices and fulsome supply of fossil fuels such as oil and natural gas [1]. In recent decades, gasification has come into interest and is getting more and more widespread. Greenhouse gas emission reduction, gas and oil prices instabilities and interest in more reliable fuel supply, and in renewable and locally available energy sources can be considered as most effective factors that has put an upsurge in gasification. Gasification converts fuels into useful and convenient gases and chemicals. Like most other chemical reactions, it requires a medium for reaction which can be a gas or supercritical water. Unlike combustion, gasification packs energy into chemical bonds rather than breaking them to produce energy. It augments the hydrogen-to-carbon (H/C) ratio to produce a gaseous fuel with high energy density. Along lots of experimental attempts, an abundant numerical simulation has been done [2], because a simulation can assist the designer or plant engineer to practically optimize the operation or the design of the plant using available data for a pilot plant or the current plant. Thermodynamic equilibrium, kinetic, computational fluid dynamics (CFD), and artificial neural network models are common gasifier simulation models. In this paper we have presented the CFD model combined with equilibrium to simulate the methanol gasification.. There are many similarities between modeling of combustion and gasification, for instance the spraying, evaporation, and so on, but combustion usually occurs in lean conditions unlike gasification which takes place under rich condition of fuel. By making a rich mixture of fuel during the gasification process we can harvest more CO and H2 as syngas products. The global reaction can be written as follow:

$$Fuel + O_2 \rightarrow CO + H_2 \quad (1)$$

Numerical simulation:

In this paper we simulated the gasification of methanol in a gasifier at different pressures. Methanol is being sprayed at the top of the reactor as well as air. The interaction between methanol and air makes the methanol droplets to evaporate and move along the reactor while it gradually with air and converts to desired syngas (CO and H2). The spraying, evaporation, and momentum equations are solved using KIVA. We presented the CTC model [3] to predict the product different species mole fraction along the reactor. An ideal state at the outlet occurs when the entire products mole fraction meet their equilibrium condition values. In CTC model the time rate of change of the partial density of species m, due to conversion from one chemical species to another, is given by:

$$\frac{dY_m}{dt} = -\frac{Y_m - Y_m^*}{\tau_c} \quad (2)$$

where Y_m is the mass fraction of species m, Y_m^* is the local instantaneous thermodynamics equilibrium

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value of the mass fraction, and τ_c is assumed to be the same for the entire species considered necessary to predict thermodynamics equilibrium temperatures accurately. An important aspect of this model is to formulate properly the characteristic time, $\tau_c$which is the sum of a laminar timescale and a turbulent timescale:

$$^2{}_c = ^2{}_l + f^2{}_t \quad (3)$$

assuming an equilibrium state concentration of fuel equal to zero, the following laminar timescale is obtained:

$$^2{}_l = A^{-1}[CH_3OH]^{0.75}[O_2]^{-1.5}\exp(\frac{E}{RT}) \quad (4)$$

We didn't not consider the turbulent effects of timescale in this study due to its insignificant effect of the final result (f=0). Two well-known equilibrium reactions were used to find the products thermodynamic equilibrium mole fraction at each time step. Using the global reaction, mass balance and the abovementioned equilibrium we are able to find the equilibrium mass faction of products instantaneously and exert them in CTC model to find species mass and mole fraction at each time step.

Results:

Tables. 1-2 show the comparison between the experimental data and equilibrium results for different pressure at fixed temperature. As we desire to capture more gaseous products with high energy density, the rich condition has been considered which leads to more CO and H2 products unlike combustion. It can be seen there is a good agreement between experiment data and equilibrium approach, so we can assert that thermodynamic equilibrium is a reasonable approach in modeling the gasifier. The reason why we are using CTC model can be attributed to the fact that the whole reactions and gasification evolves gradually along the reactor to reach to the ideal condition which is equilibrium state. The results show that as the gasifier works in higher pressure the desired syngas products experience a slight reduction in mole fraction.

Table.1 : comparison of products mole fraction between experimental data and equilibrium approach, P=1 atm, T=850 Celsius, Phi=0.25 (air to fuel ratio)

Species	Experiment (mole fraction)%	Equilibrium (mole fraction) %
H2	56	59.8
CO	33.9	30.5
CH4	1.26	0
CO2	8.6	9.64

Table.2 : comparison of products mole fraction between experimental data and equilibrium approach, P=7.8 atm, T=850 Celsius, Phi=0.25 (air to fuel ratio)

Species	Experiment (mole fraction)%	Equilibrium (mole fraction) %
H2	54.9	57.9
CO	35.5	29.6
CH4	0.9	1.84
CO2	8.6	10.7

Table.3 shows the comparison between the numerical simulation and experimental data. Here a good agreement can be seen between tow data sets.

Table.3 : comparison of products mole fraction between experimental data and equilibrium approach, P=7.8 atm, T=850 Celsius, Phi=0.25 (air to fuel ratio)

Species	KIVA (mole fraction)%	Equilibrium (mole fraction) %
H2	54.79	56
CO	28.78	33.9
CO2	8.3	8.6

Fig 1. shows the methanol spraying and evaporation near the inlet. It shows that methanol droplets with contact to air evaporate and some of them hit the gasifier wall which evaporate as they move along the wall (wall temperature is fixed at 850 Celsius).

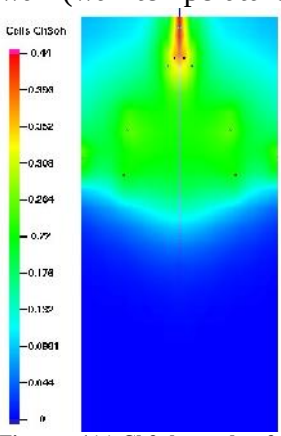

Figure 1(a).Ch3oh mole fraction contours and liquid droplets at t=0.05s, φ=0.25 and P=1 atm

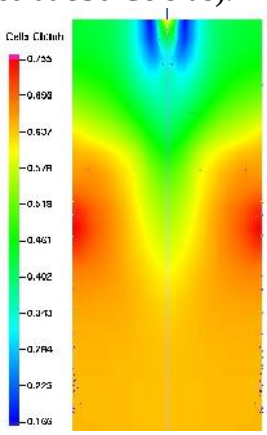

Figure 1(b).Ch3oh mole fraction contours and liquid droplets at t=4s, φ=0.25 and P=1 atm

References

[1] Prabir basu, 2010, Biomass gasification and Pyrolysis, Elsevier, USA

[2] A. Gomez-Barea, B. leckner, 2010, Modeling of biomass gasification in fluidized bed, Progress in Energy and Combustion Science

[3] S. Kong, Z. Han, R.D. Reitz, 1995, The Development and Application of a Diesel Ignition and Combustion Model for Multidimensional Engine Simulations, SAE Paper 950278, Journal of Engines

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