



# Prediction of biomass-generated syngas using extents of major reactions in a continuous stirred-tank reactor



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## ABSTRACT

Syngas, the main gasification product, is a well-known intermediate for making fuels, chemicals and power. The objective of this study was to develop and validate reaction kinetics-based gasification model using extents of major reactions in a CSTR (continuous stirred-tank reactor) to predict syngas composition and yield. The model was studied by varying biomass and air flowrates from 2.9 to 4.2 dry kg/h and 4.5–10 kg/h, respectively, with temperature from 801 to 907 °C. Results showed significant improvement in the predictions of syngas composition and yield, and gasification efficiency. The extents of gasification reactions indicated that at ERs (equivalence ratios) below 0.32, the water gas reaction contributed the most to the syngas CO and H<sub>2</sub> yields. The char oxidation reaction was also the dominating reaction contributing to CO yield at ERs below 0.40. At ERs above 0.29, the Boudouard and methane oxidation reactions were the most dominating reactions contributing to the CO yield while the water gas shift reaction contributed to the H<sub>2</sub> yield. The developed model corrected one of the key underlying assumptions that biomass decomposes into elemental forms (C, H, O, N and S), however, gasification temperature, carbon conversion efficiency and tar yield were assumed to be given.

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## 1. Introduction

Biomass, such as grass, plants and crop residues, is a sustainable and renewable energy feedstock. Many research efforts have successfully demonstrated generation of fuels and power from biomass [1–6]. However, biomass is categorized as a low-grade energy fuel and has limited uses as a direct feedstock for generating liquid fuels and chemicals. Gasification, a thermochemical conversion process, converts the low-grade solid biomass under high temperature into gaseous fuel called syngas. The biomass-generated syngas consists mainly of CO, H<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub> (if air is used as an oxidizing agent), and impurities such as tar, H<sub>2</sub>O, NH<sub>3</sub> and H<sub>2</sub>S. Syngas is a well-known intermediate for making biofuels, biochemical and biopower through various conversion processes. However, these conversion processes require syngas with different concentrations of H<sub>2</sub>, CO, and CO<sub>2</sub> [7] as well as H<sub>2</sub>/CO ratios from 0.4 to 4 [7–9]. To maximize the product (fuels, chemicals or power) yields; it is necessary that biomass gasification matches the needs

of downstream conversions in terms of gas composition, levels of impurities, and yield of the syngas. The biomass-generated syngas quality and yield, on the other hand, rely heavily on several factors such as the properties of biomass, gasifier operating conditions, and complex chemical reactions that occur during the gasification.

With the advent of latest computational techniques and sophisticated simulation tool, such as Aspen™ Plus, the biomass gasification process can be modeled and the syngas composition and yield can be predicted more reliably. Several Aspen™ Plus gasification modeling studies [10–14] using RGibbs (Gibbs equilibrium reactor) are available for different biomass feedstocks. However, little information is available on kinetics modeling of biomass gasification using extents of major reactions in a continuous stirred-tank reactor (CSTR).

When using the Gibbs equilibrium reactor modeling approach, one of the primary assumptions many researchers make is that the gasification reactions reach equilibrium, which does not happen due to short residence time (i.e. space time) [10,15]. In addition, the gasification involves several homogenous and heterogenous reactions R(1)–R(7) [16] and the kinetics of these reactions play a significant role on syngas composition and yield. Equilibrium modeling approaches do not consider the influence of these influential reactions. As a result, large deviations between the

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## Nomenclature

### Latin letters

$C_C, C_{CH_4}, C_{CO}, C_{CO_2}, C_{H_2}, C_{H_2O}, C_{O_2}$  concentrations of C, CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, O<sub>2</sub>, respectively, in the inlet material stream, mol/m<sup>3</sup>

$f$  dampering factor

$F_0C, F_0CH_4, F_0CO, F_0CO_2, F_0H_2, F_0H_2O, F_0N_2, F_0O_2$  initial molar flowrates of C, CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub> and O<sub>2</sub>, respectively, entering into the CSTR, mol/s

$F_0T$  total initial molar flowrate of materials entering into the CSTR, mol/s

$FC, FCH_4, FCO, FCO_2, FH_2, FH_2O, FN_2, FO_2$  final molar flowrates of C, CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub> and O<sub>2</sub>, respectively, leaving the CSTR, mol/s

FT total final molar flowrate of materials leaving the CSTR, mol/s

$k_1, k_2, k_3, k_4$  rate constants for reaction R(1)

$k_5, k_6, k_7$  rate constants for reaction R(2)

$k_8, k_9, k_{10}, k_{11}, k_{12}$  rate constants for reactions R(3)–R(7), respectively

$K_{eq}$  equilibrium constant of R(3)

$M_C$  carbon molar weight, g/mol

$R$  the ideal gas constant, J/(mol K)

$r_1, r_2, r_3, r_4, r_5, r_6, r_7$  rate equations for reactions R(1)–R(7), respectively, mol/(m<sup>3</sup>s)

$r_C, r_{CH_4}, r_{CO}, r_{CO_2}, r_{H_2}, r_{H_2O}, r_{O_2}$  net reaction rates for C, CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, O<sub>2</sub>, respectively, mol/(m<sup>3</sup>s)

$T$  absolute temperature, K

$P_0, P$  initial and final pressures in the reactor, Pa

$V_R$  volume of the reactor, m<sup>3</sup>

$v_0, v$  inlet and outlet volumetric flowrate of materials through the CSTR, m<sup>3</sup>/s

$X$  carbon conversion

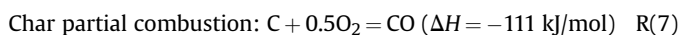
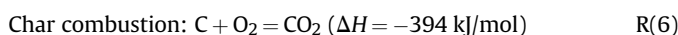
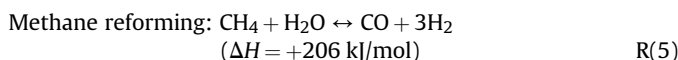
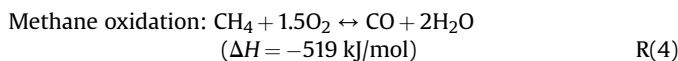
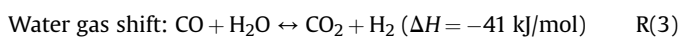
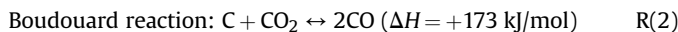
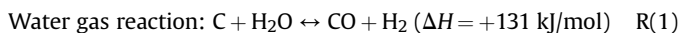
### Greek letters

$\zeta_1, \zeta_2, \zeta_3, \zeta_4, \zeta_5, \zeta_6, \zeta_7$  extents of reactions R(1)–R(7), respectively, mol/s

$\rho_{char}$  char density, kg/m<sup>3</sup>

$\tau$  space time, s

predicted and experimental values of the syngas composition have been found while using the equilibrium modeling approach.



By including kinetics of the major reactions, the CSTR based reaction kinetics gasification model can more reliably predict the syngas composition for the given biomass feedstock, gasification conditions, and type of oxidizing agent. Nikoo and Mahinpey [17] developed an Aspen™ Plus gasification model using RCSTR (CSTR reactor) model for pine sawdust. Simulations were performed assuming reactor temperatures of 700–900 °C. The authors, however, considered only five gasification reactions which may have led to the deviations between experimental and predicted gas compositions. The authors reported mean error deviations of 0.18–0.34 for H<sub>2</sub>, 0.09–0.11 for CO, 0.20–0.30 for CO<sub>2</sub> and 0.16–0.27 for CH<sub>4</sub> on % volume basis. Authors also assumed that the volatile reactions followed Gibbs equilibrium that is unlikely to happen because of the fast volatile reactions leading to the deviations observed between experimental and simulation data. Moreover, most of the previous biomass gasification models use RYield reactor of Aspen™

Plus to decompose biomass (a non-conventional material) into conventional elemental components such as C, H, O, N, S and ash. This is done because properties of non-conventional materials are not available in Aspen™ Plus database whereas properties of conventional components are. However, the above decomposition of biomass into several elemental components can only occur in extreme reaction conditions far beyond the conditions during gasification. Hence, the currently available models of biomass gasification are inadequate to simulate reaction mechanisms of biomass gasification and reliably predict syngas needed for production of fuels and chemicals.

The novelty of present study lies in the development of a gasification model using a modeling approach based on extents of major gasification reactions and the fundamental design of CSTR. The model incorporated extensive gasification condition, such as seven major gasification reactions, their kinetics parameters, reactor volume and space time that are not possible in Gibbs equilibrium based gasification model studied by several researchers. Also, this model incorporates a novel biomass decomposition approach of converting the biomass into products such as C, H<sub>2</sub>O, CO, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub> and tar that are feasible during biomass gasification [18]. The specific objectives of this study were to develop kinetics-based gasification model using extents of major reactions in a CSTR to predict syngas composition and yield, and to validate model prediction with the experimental results obtained on our fluidized-bed gasifier.

## 2. Materials and methods

### 2.1. Biomass feedstock and gasification conditions

Kanlow switchgrass was gasified in a lab-scale fluidized-bed gasifier with air as an oxidizing agent. The higher heating value of the switchgrass was 18.83 MJ/kg dry biomass. The details of the

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