

## Effects of Hydrogen Addition on the Entropy Generation of Biogas Conventional Combustion

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### Article history

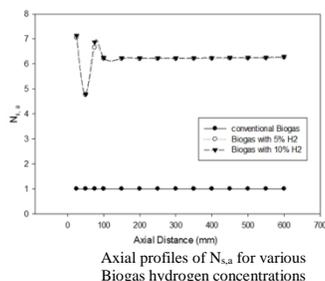
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### Graphical abstract



### Abstract

Biogas has a great potential to be applied for heat and power generation throughout the world due to its availability from various resources. However, one of the most important barriers of biogas utilization development is its low calorific value. In order to increase the performance of biogas in industrial application, hydrogen enriched biogas could be substituted. In this paper a set of numerical simulations were conducted to estimate the variation of entropy generation in hydrogen enriched biogas flames due to hydrogen addition to the fuel. Reynolds Averaged Navier Stokes with a second order turbulence closure and laminar flamelet combustion model was applied to compute energy fields and flow in the flame. It was found that hydrogen enrichment resulted in an augmentation in the entropy generation rate of the biogas conventional flame. Such increase could be attributed to the increase in irreversibilities due to biogas flame temperature rise.

**Keywords:** Entropy; biogas; hydrogen; flame

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### 1.0 INTRODUCTION

Energy crisis and the increasing rate of pollutant generation have encouraged scientists to find alternative fuels to guarantee the secure energy generation and people health.<sup>1-5</sup> Experimental studies illustrate that biogas shows its compatibility with current combustion systems and biogas could be applied as an alternative fuel to solve a part of the future fossil fuel shortage. Therefore, a comprehensive knowledge of the available technologies is needed for biogas users.<sup>6</sup> Moreover, general knowledge of the chemical characteristics and combustion properties of the biogas is needed for efficient combustion process. Generally, the selection of the best system for biogas conversion into thermal energy for lighting, transportation, heating and power generation is the main goal of biogas production.<sup>7</sup> It was pointed out that by biogas utilization the net emission of greenhouse gases such as CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O reduced drastically compared to methane.<sup>8</sup> The most important advantages of biogas production is collecting the organic waste materials and generating irrigation water and fertilizer concomitantly. Unlike other biomass sources, biogas does not have any geographical limitations.<sup>9</sup> Landfills and old waste deposits, municipal solid waste (MSW), rising main sewers, coal mining, rice paddies, anaerobic digestions, cattle ranching and agricultural products are the main sources of biogas in the

world.<sup>10-18</sup> Furthermore, since food industries are developed due to the increasing rate of world population, animal husbandry has become one of the most important sources of biogas in the world.<sup>19</sup> More than 15% of global methane generation is attributed to biogas emission from ruminants, thus biogas capturing from livestock dung and energy generation from biogas have become important.<sup>20</sup> The sustainable strategies in the managing of waste water sources can intensify the possibility of biogas generation from waste materials.<sup>21</sup> Compared to natural gas by 90–95% methane, depends on feedstock the rate of methane in biogas is 40–65%. Therefore, biogas is a low calorific value (LCV) gaseous fuel. Generally, the collected biogas is cleaned and its impurities like water and sulfuric gases are eliminated. The biogas cleaning and upgrading methods and combustion improvement technologies are designed based on biogas composition. In general 55–65% of biogas is constituted by methane. The lower heating value of methane is 34,300 kJ/m<sup>3</sup> and the lower heating value of biogas is about 13,720–27,440 kJ/m<sup>3</sup>. In biogas heating value calculation, the heating value of the whole species is considered. The heating value of non-combustible components like CO<sub>2</sub> is taken into consideration. Also, the impacts of water vapour on lower heating value, air–fuel ratio, biogas flammability limits and flame temperature should be taken into account. In biogas modelling, usually CO<sub>2</sub> and CH<sub>4</sub> are considered because

more than 98% of biogas is a combination of them and other species like water vapour and hydrogen sulphide (H<sub>2</sub>S) are eliminated. Practically removal of these corrosive gases is necessary due to their negative impact on equipment especially burner and boiler in furnace.

## 2.0 HYDROGEN ADDITION TO BIOGAS

Hydrogen which is considered as a clean fuel due to low emission formation has a great potential to be applied as a major fuel in the future.<sup>23, 24</sup> However, due to high diffusivity and flammability of hydrogen, safety in storage and transport of hydrogen is encountered some problems.<sup>25</sup> The effects of hydrogen addition on the combustion of gaseous fuel are radical because the combustion properties of these flames depend heavily on the characteristics of the gaseous fuel and flame circumstances. Hydrogen enrichment of various gaseous fuels such as CH<sub>4</sub>, propane (C<sub>3</sub>H<sub>8</sub>) and natural gas was investigated during the last decade. Ignition of hydrogen-enriched fuel mixtures under the lean flammability limits causes the fuel saving goals. In hydrogen-enriched fuel the Arrhenius reaction rate is intensified due to augmentation of the flame temperature, therefore high reaction rate of hydrogen is recorded and the rate of required oxygen in the lean mixture rises. Due to the low computational cost fast chemistry models are superior in the simulation of hydrogen-enriched fuel combustion.<sup>26</sup> The conserved scalar model was applied to model a non-premixed turbulent combustion of mixture of methane and hydrogen by Ilbas.<sup>27</sup> An unacceptable accuracy was reported by Mardani when similar flame with eddy dissipation concept (EDC) was modeled.<sup>28</sup> It was reported that for simulation of hydrogen-enriched methane combustion, the steady laminar flamelet model has better prediction in terms of minor species.<sup>29,30</sup> Yilmaz compared the results of flamelet method with equilibrium model when Probability Density Function (PDF) was calculated for mass fraction of species.<sup>31</sup> It was reported that mixture fraction and temperature illustrate better results within the reaction zone could be achieved. Hossain pointed out that just major species could be predictable by flame sheet model.<sup>29</sup> Although accurate results for water vapor mass fraction and flame temperature could be obtained by flame sheet model, unaccepted prediction of CO<sub>2</sub> is one of the weak points of this method. Various chemical reaction mechanisms were applied by different researchers in their modeling method and it was reported that chemical reaction mechanism modeling method is very important in laminar flamelet model. For example in simulation was done by Ilbas only seven species were used.<sup>27</sup> Yilmaz applied GRI mechanism with 18 species.<sup>31</sup> Ravikanti used GRI2.11 and reported that the results are in good agreement with the reduced DRM-22 mechanism results.<sup>30</sup> In the combustion modeling was done by Frassoldati, 600 reactions were applied and 48 species were taken into account.<sup>32</sup>

## 3.0 ENTROPY GENERATION

Hydrogen enrichment is one of the potential methods which were introduced for improving biogas combustion for heat and power generation. Hydrogen addition to the biogas enables the combustion system to work at very lean circumstances which improves the efficiency of combustion system.<sup>33-35</sup> However, the temperature of hydrogen-enriched biogas flame increases significantly in some regions.<sup>36</sup> This condition causes a mitigation in the reversibility work of combustion system which could expunge the fuel economy achievements. For a given

thermodynamic system, the lost work can be calculated by formula (1).

$$\dot{W}_{rev} - \dot{W} = T_0 \dot{S}_{gen} \quad (1)$$

$\dot{W}_{rev}$  is the reversible work,  $\dot{W}$  is the actual work and  $\dot{S}_{gen}$  is the total entropy generated in the combustion system. Generally, entropy is produced due to various factors depending on the characteristics of combustion system such as chemical reactions, heat transfer and viscous dissipation. In formula (2) illustrates the local entropy generation in a two dimensional radial axisymmetric domain when the heat and mass irreversibilities is considered in the thermodynamic system.<sup>37,38</sup>

$$\dot{S}_{gen} = \frac{k}{r^2} \left[ \left( \frac{\partial T}{\partial x} \right)^2 + \left( \frac{\partial T}{\partial r^2} \right)^2 \right] + \frac{\mu}{T} \Psi \quad (2)$$

The first and second terms on the right side of formula refer to heat transfer entropy generation ( $\dot{S}_{ht}$ ) and viscous dissipation entropy generation ( $\dot{S}_v$ ) respectively and  $\Psi$  is viscous dissipation parameter defined by formula (3).

$$\Psi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial r} \right)^2 + \left( \frac{v}{r} \right)^2 \right] + \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial x} \right)^2 + \left( \frac{\partial w}{\partial r} - \frac{w}{r} \right)^2 \quad (3)$$

The axial, radial and swirl velocity of various components is demonstrated by u, v and w respectively.

## 4.0 SIMULATION

In this simulation, pure biogas is considered as a combination of 40% CO<sub>2</sub> and 60% methane and the effects of 5% and 10% hydrogen addition to this combination when the rate of CO<sub>2</sub> is constant are investigated. Based on Shih investigation,<sup>39</sup> realizable k-ε simulation yields more acceptable results for shear flows. Therefore, the standard k-ε model is applied to model combustion with the laminar flamelet combustion model in present study. Furthermore, the main reason for this decision is that the turbulence kinetic energy dissipation is computed differently in realizable and standard k-ε model and the flamelet model employs dissipation to count for deviation from equilibrium this difference in dissipation formulation affects the modeling of combustion differently. Therefore, performance of realizable k-ε model with flamelet model could be investigated biogas-enriched conventional flames. Following transportation equations are modeled k and ε in the standard k-ε model. For turbulent kinetic energy k:

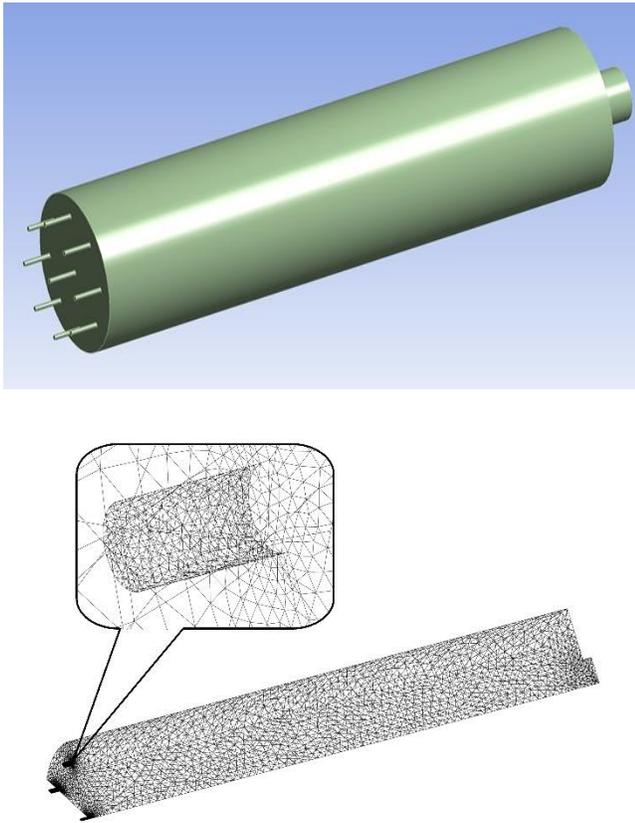
$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + P_k + P_b - \rho \epsilon - Y_M + S_k \quad (4)$$

For dissipation ε:

$$\frac{\partial}{\partial t} (\rho \epsilon) + \frac{\partial}{\partial x_i} (\rho \epsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (P_k + C_{3\epsilon} P_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon \quad (5)$$

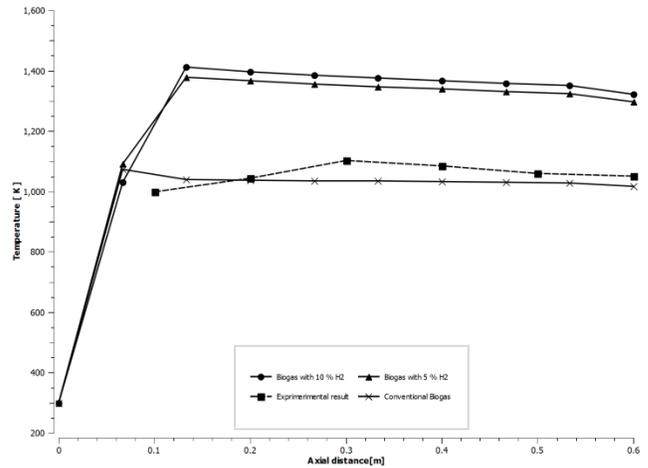
The laminar flamelet turbulent combustion is applied to model the interaction turbulence and chemical reaction. The GRI3.0 chemical reaction mechanisms were employed to calculate the chemical species.<sup>40</sup> In this study attention is given to the variations of the local entropy generation rates due to hydrogen enrichment of biogas conventional flame. ANSYS Fluent 14 is applied to carry on the simulation and computational

work.<sup>42</sup> CFD model of the chamber for this numerical study is based on the geometry of the experimental flameless combustion carried out by SE Hosseini.<sup>6</sup> The inside diameter and the length of the chamber are 150 mm and 600 mm respectively. The 5 mm central inlet of the burner is considered for the inlet of the hydrogen enriched biogas mixture and the other inlets are considered for the oxidizer entrances. The emissions are exhausted through a central hole with 50 mm diameter. Convergence rate and scalar properties can be modified by mesh refinement and grid resolution. The chamber geometry is not very complicated, therefore calculations speed increase due to lower meshing nodes and elements. The quantity of mesh grids directly impacts on the solution duration. Since the chamber model is symmetrical, just an eighth part of the model is solved. Figure 1 shows the schematic of the furnace and a part of the furnace which has been meshed.



**Figure 1** Schematic of the furnace and its mesh

For validation, comparisons between this numerical solution of the reacting flow and experimental measurements presented by Hosseini are compared.<sup>6</sup> Figure 2 demonstrates numerical and experimental results of the temperature distribution along the furnace. This figure confirms that the numerical results are in good agreement with experimental records and the simulation settings are reliable. Indeed Figure 3 depicts the radial distribution of temperature in four various sections of the chamber.



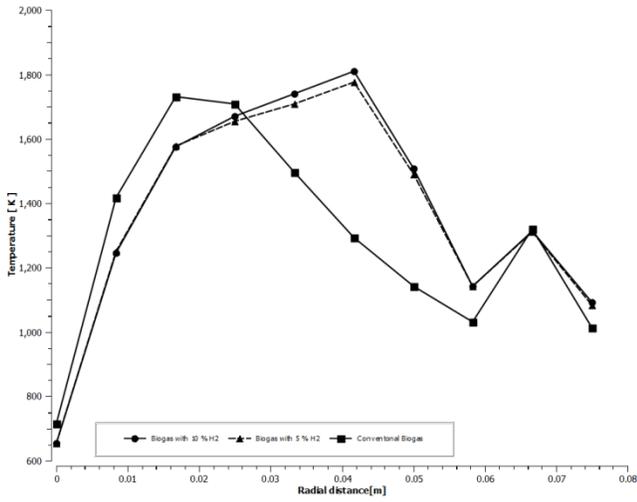
**Figure 2** Numerical and experimental results of the temperature distribution along the furnace

## 5.0 ENTROPY GENERATION

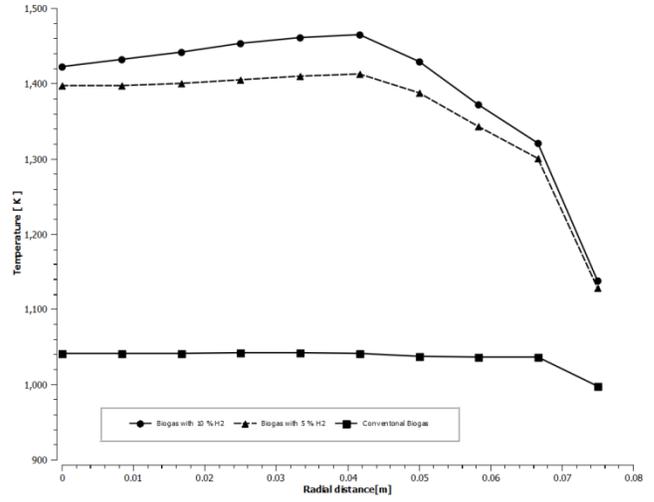
Figure 4 demonstrates the entropy generation in the chamber in biogas conventional combustion and hydrogen-enriched biogas traditional combustion when 5% and 10% hydrogen is added respectively. Since high entropy generation intensifies irreversibility, exergy loss is higher in traditional combustion of hydrogen-enriched biogas when 10% hydrogen is added. SK Som stipulated that the most irreversibility in a conventional combustion system is related to the internal heat transfer within the combustor between the products and reactants.<sup>43</sup> Entropy generation in hydrogen-enriched biogas with 10% could be attributed to higher temperature inside the chamber.

### 5.1 Entropy Augmentation Number

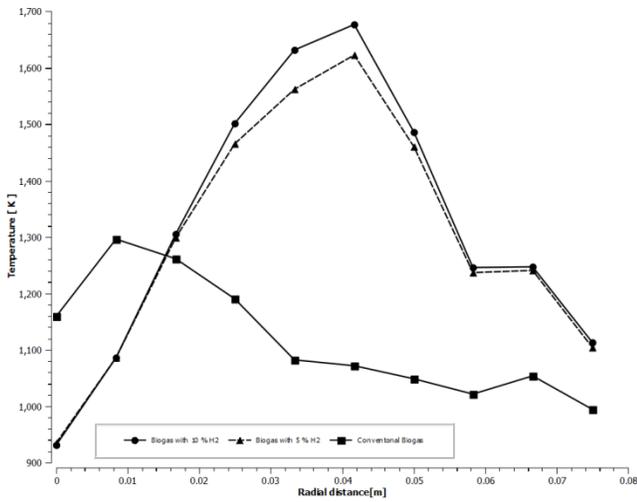
The entropy augmentation number  $N_{s,a}$  is the dimensionless ratio of local entropy generation in two specific cases ( $\frac{\dot{S}_{gen,i}}{\dot{S}_{gen,1}}$ ) which  $\dot{S}_{gen,1}$  and  $\dot{S}_{gen,i}$  are the local entropy generation in biogas conventional flame (without hydrogen enrichment) and in hydrogen-enriched biogas flame (with hydrogen enrichment), respectively. When  $N_{s,a}$  is less than unity, it can be concluded that the addition of hydrogen resulted in a reduction of entropy, hence an enhancement of the system exergy. Figure 5 displays axial profiles of  $N_{s,a}$  for various biogas hydrogen concentrations. From this figure it can be seen that the hydrogen addition causes substantial increase of  $N_{s,a}$  in some whole of the chamber.



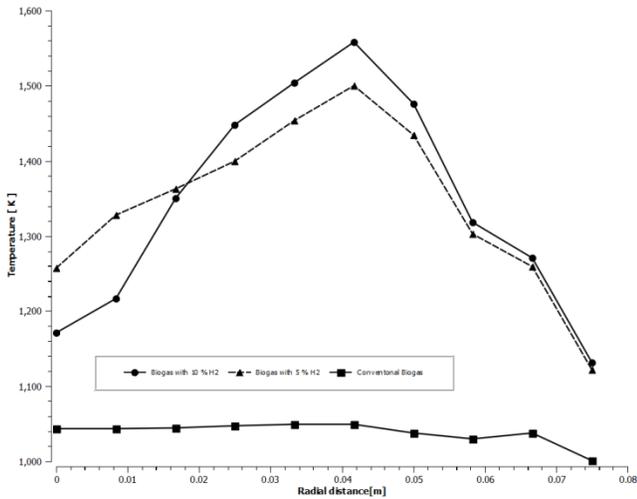
(a) Radial distribution of temperature  $x=25$  mm



(d) Radial distribution of temperature  $x=100$  mm

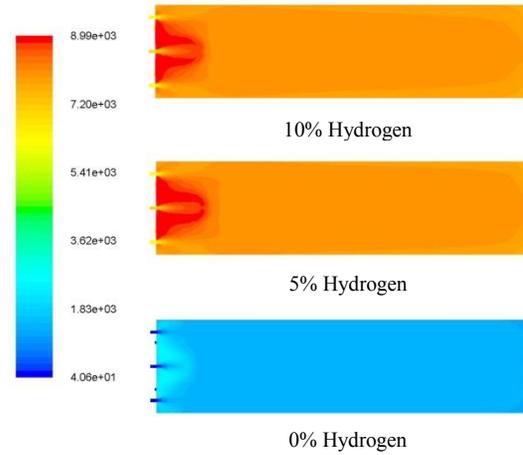


(b) Radial distribution of temperature  $x=50$  mm

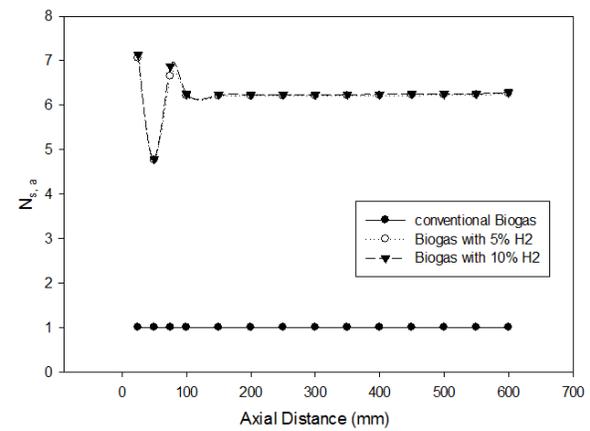


(c) Radial distribution of temperature  $x=75$  mm

**Figure 3** Radial temperature distribution along the furnace in various sections



**Figure 4** Entropy generation in the chamber in hydrogen-enriched biogas traditional combustion



**Figure 5** Axial profiles of  $N_{s,a}$  for various biogas hydrogen concentrations

## 6.0 CONCLUSION

Numerical simulations of the entropy generation in turbulent hydrogen-enriched biogas flame have been conducted. Pure biogas and biogas consist of 5% and 10% hydrogen were modeled. It was found that the entropy generation rate increases due to hydrogen enrichment. Such increase was attributed as rises in the entropy augmentation number. Future investigations should prepare more detailed insights on the characteristics of entropy generation patterns and extend the analysis to cover a wider range of hydrogen concentration.

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