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Energy Evaluation of Synthesis Gas in a Turbocharger System Employing CFD Tools

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ABSTRACT

Renewable energy sources derived from biomass, such as synthesis gases, represent an opportunity to take advantage of available waste resources and contribute to global energy rationing. This study developed an analysis with computational fluid dynamics (CFD) to estimate the energy behavior of synthesis gases through a turbocharger system. The synthesis gas used to drive the turbocharger turbine was extracted from the gasification of biomass from the Colombian Caribbean. The application of models for rigid body motion, as well as models of momentum, turbulence, energy, and conservation transport of species, suggest that the energy potential available by the turbine ranges from 0.4 kW to 5.2 kW of power generation, concerning mass flow rates entering the simulated system. The main findings of the study were temperature profiles, speed profiles, rotational speed variation, torque, and mechanical power generated in the turbocharger. It is emphasized that the synthesis gas studied presents a good behavior to generate energy through a turbine system of a turbocharger device.

1. Introduction

The transition from conventional energy transformation methods to the use of renewable energies invites us to venture into new ways of generating energy through increasingly cleaner sources [1-3]. As is the use of biomass material, which, being a residue of agro-industrial processes, can be used for energy generation as indicated in previous studies [4, 5]. What leads to studies to generate new forms of energy transformation, is how biomass presents in its composition a high potential in its volatile material, and its fewer polluting emissions are based on a fuel that will have a high content of H_2 and not based on hydrocarbon chains that increase the carbon footprint in its emissions.

Biomass has been used as an element of study by various researchers, such as Raheem *et al.,* [6] in their study of gasification of residual material such as algae to obtain synthesis gas, in which they used various catalysts to increase the production of H_2 as a biofuel product of said gasification, thus reducing the ash content and tar product of gasification. Consequently Situmorang *et al.,* [7] in their

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study show an energy panorama focused on the gasification of biomass material, indicating that this process is the best way to directly replace the generation of energy through fossil fuels. In other studies, Cao *et al.,* [8] and Diallo *et al.,* [9] carried out a study of the technologies focused on the production of hydrogen from synthesis gas extracted from biomass material, highlighting the importance of the use of biomass for its generation potential as clean energy and its production of H_2 as biofuel. How and See Ref. [10] analyzed the potential of lignocellulosic sweet melon bark biomass for the generation of synthesis gases and then producing bioethanol.

Safarian *et al.,* [11] in their study detailed the importance of the models used to simulate gasification systems where the characteristic aspects of each model and the projection of results to be obtained are specified. Kumar and Paul [12] developed a study using Computational Fluid Dynamics (CFD) for a wood biomass gasifier system, in which they performed validations through theoretical models, simulations, and experimental procedures. Where small differences were obtained with the simulated predictions.

Likewise, various studies have been developed applying CFD tools to analyze behaviors, that can hardly be measured or instrumented experimentally, so in works developed such as those of Ref. [13-17] they applied simulations by CFD means of estimating the energy performance of a turbocharger turbine system, comparing output variables at different mass flow rates among other factors.

While few studies[18, 19] simulated a turbocharger compressor system's geometric and energetic effects, comparing the yields obtained from these processes. The study of rotors based on meshing movement requires several design stages. For this reason, the use of computational tools such as ANSYS in its rigid body motion module provides the tools to study the energy behavior of these systems [20-23].

Considering the previous studies mentioned, an energy analysis is carried out for a turbocharger system using CFD techniques, when selecting synthesis gases as biofuels. The results of this study are presented with three selected biomasses from the Colombian Caribbean. The variables studied in this device are the operating temperature, the rotation speed of the turbocharger turbine shaft, the torque, and the power obtained according to the mass flow implemented. This article contributes to the literature related to the computational study of turbochargers when biofuels are used in internal combustion engines.

2. Materials and Method

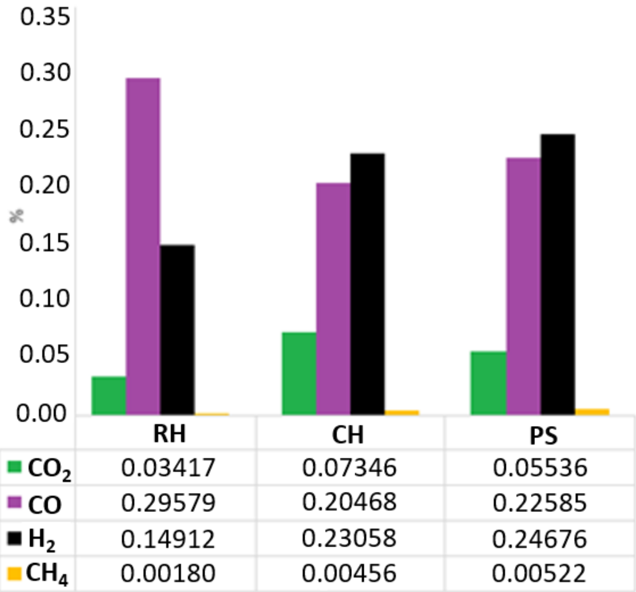
The purpose of the study focuses on the use of biofuels in a turbocharger device, of which the measurement of energy behavior encompasses the use of CFD computational tools, associating reaction and combustion models for biofuels obtained from synthesis gas from the gasification of certain biomasses, in turn applying energy models, and rigid body behavior models to simulate the movement of a turbine. It is necessary to present the composition characteristics of the biomass to be studied to estimate the energy potentials [24, 25].

Table 1 shows the Proximate and Ultimate analyses of the selected biomasses from which, as a product of their gasification, the synthesis gas that will be used in the modeling of this study is obtained. These data were obtained from Ref. [26]. The selected biomasses are presented by the following acronyms, Rice Husk (RH), Coconut Husk (CH), and Palm Shell (PS).

Table 1
Proximate and ultimate analysis of the selected biomasses

	Proximate analysis		
	PS	CH	RH
Volatile	0.7274	0.7145	0.6233
Fixed carbon	0.1687	0.1528	0.1587
Ash content	0.0247	0.0126	0.1703
Moisture	0.0792	0.1201	0.0476
	Ultimate analysis		
	PS	CH	RH
C	0.4860	0.4540	0.4980
H	0.0999	0.0905	0.0700
O	0.4047	0.4537	0.4240
N	0.0086	0.0016	0.0020
S	0.0007	0.0003	0.0060

The physicochemical properties of the synthesis gas obtained from the gasification of the previously selected biomasses are presented below in Figure 1.



	RH	CH	PS
🟩 CO_2	0.03417	0.07346	0.05536
🟪 CO	0.29579	0.20468	0.22585
■ H_2	0.14912	0.23058	0.24676
🟨 CH_4	0.00180	0.00456	0.00522

Fig. 1. Synthesis gas production in percentages

As can be seen in the figure, the content of H_2 and CO present the highest percentages of the volatile material produced in the gasification of the selected biomasses, being similar in production for CH and PS. Once the chemical composition of the volatile material of the synthesis gas is known, the models used in the simulation are related. These models are based on the momentum conservation equations, the turbulence model that adjusts to the fluid-dynamic and energy transport behavior of the system, and the energy and species conservation models indicated by the studies [27-32].

Momentum equation:

$$\frac{\partial}{\partial t}\left(\rho\vec{V}\right)+\vec{V}.\nabla\left(\rho\vec{V}\right)=-\nabla p+\nabla.\bar{\bar{\tau}}+\overrightarrow{F_b'} \quad (1)$$

Eq. (1) is a vector equation with directions x, y and z. Where $\vec{V}$ is the velocity vector, *p* is the pressure acting on the fluid, $\overline{\overline{\tau}}$ is the viscous stress tensor, and $\overrightarrow{F_b'}$ is body force per unit volume.
Turbulence model equation:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_j}\left(\rho k u_j\right)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k \tag{2}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_j}\left(\rho\varepsilon u_j\right)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k+C_{3\varepsilon}G_b\right)-\rho C_{2\varepsilon}\frac{\varepsilon^2}{k}+S_\varepsilon \tag{3}$$

Eq. (2) and Eq. (3) presents the *k*-*ε* turbulence model for diffusion *k* and dissipation *ε* of the flow regime, where G_k contains the kinetic energy generation due to velocity gradients, G_b contains the kinetic energy generation due to buoyancy, and Y_M presents the contribution of fluctuating compressible dilatation to the overall rate of dissipation. $C_{1\varepsilon}$, $C_{3\varepsilon}$, $C_{2\varepsilon}$ are constants, S_k and S_ε are user-defined source terms, μ_t is the eddy viscosity, μ is the viscosity of the fluid, σ_k and σ_ε are the turbulent Prandtl numbers for *k* and ε respectively. u_j represents the velocity component in the corresponding direction. The elements described for the *k*-*ε* turbulence model were obtained from [33-37]. The species conservation model is presented in Eq. (4).

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla(\rho\vec{v}Y_i)=-\nabla J_i+R_i+S_i \tag{4}$$

Where R_i is the rate of production of species *i* in each chemical reaction, S_i is the rate of creation by addition of the dispersed phase, J_i is the diffusive flux of species *i*, and Y_i is the mass fraction for each species *i*. For the energy conservation model, the following components are presented in Eq. (5).

$$\frac{\partial}{\partial t}(\rho E)+\nabla(\rho\vec{v}E+p\vec{v})=\nabla\left(k\nabla T-\sum_j h_j\vec{J}_j+\overline{\tau}\vec{v}\right)+s_h \tag{5}$$

Where *ρ* is the density of the flowing substance, *E* is the energy of the substance, $\vec{v}$ is the velocity of the substance, *k* is the effective conductivity, and S_h includes the heat of the chemical reaction. Once the thermochemical models associated with the study phenomenon have been described, the mechanical components to be evaluated are defined, such as the turbine extracted from a turbocharger system, as shown in Figure 2.

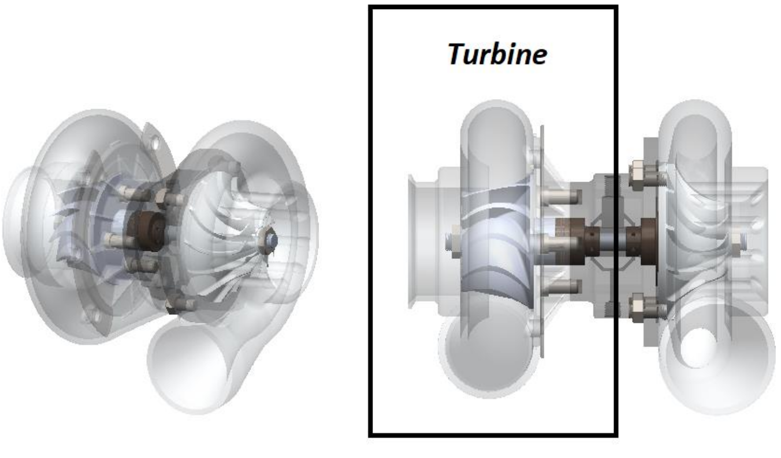


Fig. 2. Turbocharger system

The dimensions used for the body of the selected turbine are presented in Figure 3, which contains the geometry of the spiral casing, and rotor.

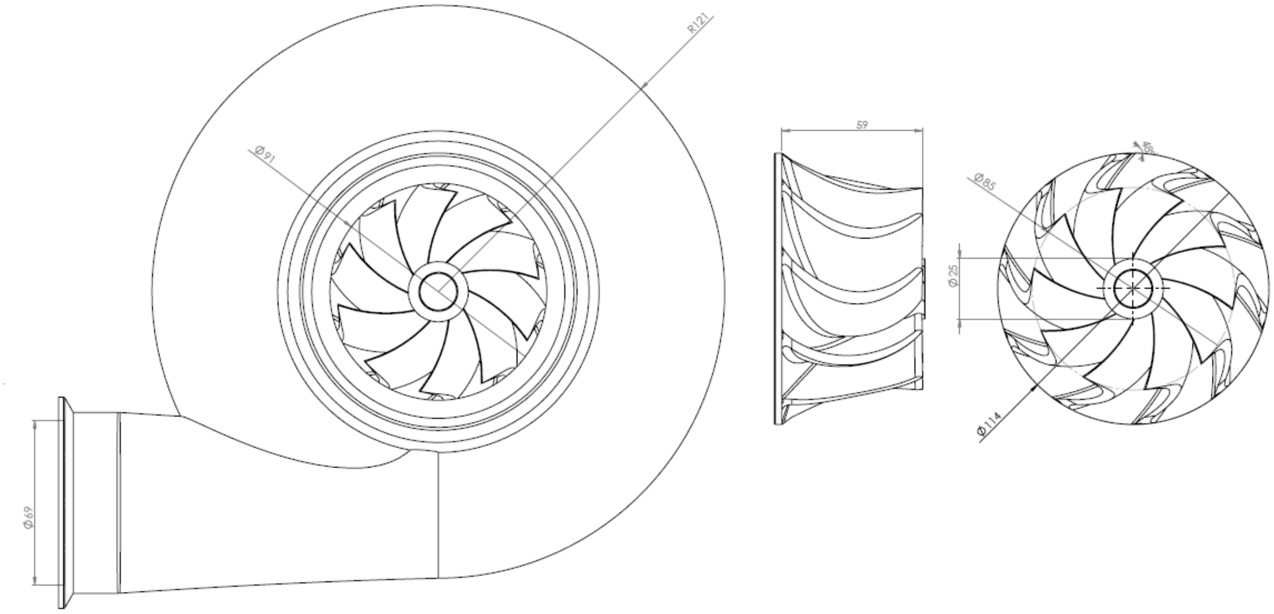


Fig. 3. Turbine dimension drawing in units of mm

Following the selection of the solids and their geometric characteristics, these are loaded into the CFD modeling software, and the models for the motion of a rigid body, in this case, the turbine rotor, are applied.

Eq. (6) – (8) are presented for the motion of a rigid body undergoing translation and rotation, the rate of change generated by linear momentum *P* and π which is equal to the force and torque which are *F* and m respectively. In addition to the rotational movement conditioned to polar coordinates.

$$\frac{\partial P}{\partial t} = F \tag{6}$$

$$\frac{\partial \pi}{\partial t} = m \tag{7}$$

$$\dot{\theta} \times I\dot{\theta} + I\ddot{\theta} = m \tag{8}$$

For this case of rotational movement, the variable I is established, which is the moment of inertia, and is defined in Eq. (9).

$$I = \begin{bmatrix} \int[(y-y_G)^2+(z-z_G)^2]dm & -\int[(x-x_G)(y-y_G)]dm & -\int[(x-x_G)(z-z_G)]dm \\ -\int[(x-x_G)(y-y_G)]dm & \int[(x-x_G)^2+(z-z_G)^2]dm & -\int[(y-y_G)(z-z_G)]dm \\ -\int[(x-x_G)(z-z_G)]dm & -\int[(y-y_G)(z-z_G)]dm & \int[(x-x_G)^2+(y-y_G)^2]dm \end{bmatrix} \tag{9}$$

For the proper use of Eq. (6)-(9), it is necessary to know the mass of the mobile element of the turbine, that is, the shaft and rotor assembly, in addition to its moments of inertia (see Table 2)

Table 2
Physical properties of the turbine shaft system

Moments of inertia and mass		
967.33 *g*		
Ixx = 0.1651 kg m^2	Ixy = 0.0195 kg m^2	Ixz = 0.0413 kg m^2
Iyx = 0.0195 kg m^2	Iyy = 0.1489 kg m^2	Iyz = 0.0618 kg m^2
Izx = 0.0413 kg m^2	Izy = 0.0618 kg m^2	Izz = 0.0441 kg m^2

3. Results

Once the solution criteria have been established and the meshing movement mechanisms have been activated through the models according to the movement of a rigid body, the temperature profiles of the behavior of the combusted gas are obtained by using for this study a relation 61:1 for the mass flows of air and fuel for all the mixtures that pass through the pipelines and drive the turbine.

In addition, the dynamic fluid behavior is obtained, such as the velocity profiles of the gases through the system, the rotational speed of the turbine, as well as the behavior of the torque force applied to it. Figure 4 and Figure 5 below show the profile and graph of the temperature behavior of the gases combusted through the system.

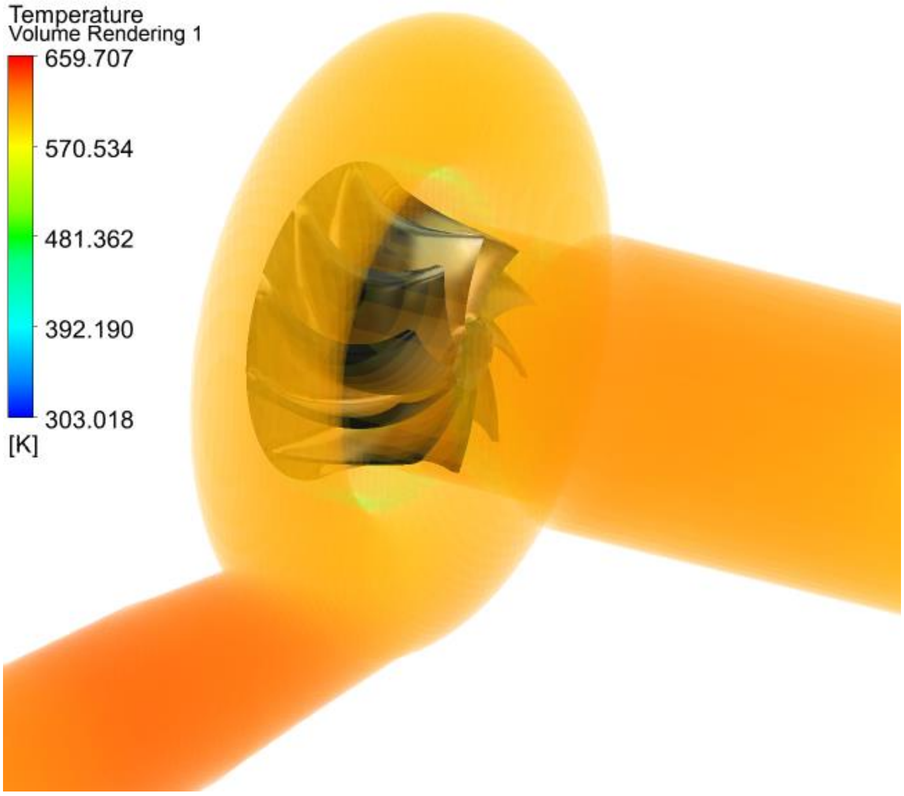


Fig. 4. Flue gas temperature profile through the turbine system

It can be seen from the temperature profile that the behavior of the combustion gases remains stable throughout the turbine system for a given mass flow. Therefore, when graphing this behavior at different ranges of mass flow for each type of substance evaluated, the following behavior is obtained in Figure 5.

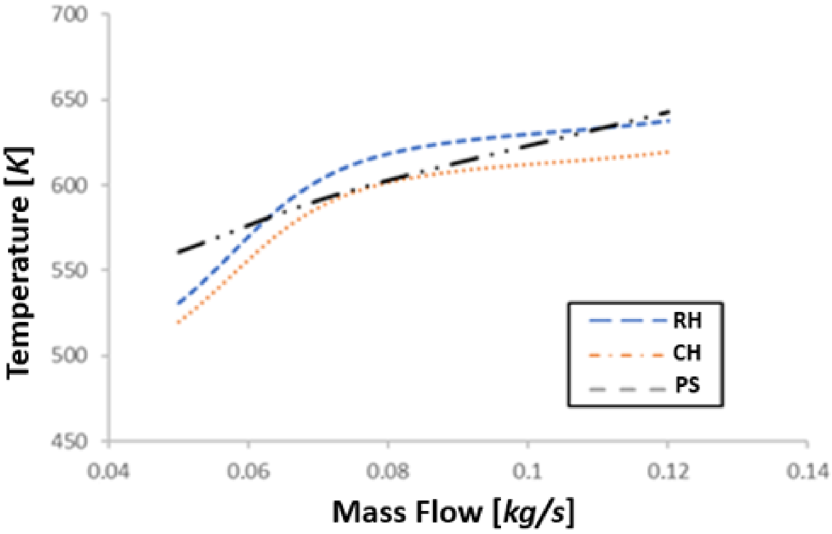


Fig. 5. Behavior of temperature concerning mass flow

As shown in the previous figure, the thermal behavior of each group of synthesis gas is compared for the applied mass flow rate, presenting differences in terms of temperatures reached; however, the PS has a behavior that tends to linearity, obtaining a temperature of 643 *K* for the value of 0.12 *kg/s* of mass flow evaluated. Estos comportamientos de temperatura presentados por los gases de síntesis estudiados pueden corroborarse en trabajos completos como los siguientes [38, 39], en donde se detalla los potenciales caloríficos según la mezcla de gases de síntesis obtenidos y los rangos de temperatura de operación. For fluid dynamic behavior, the velocity profiles through the system are presented below in Figure 6 by means of contour schemes for two view sections.

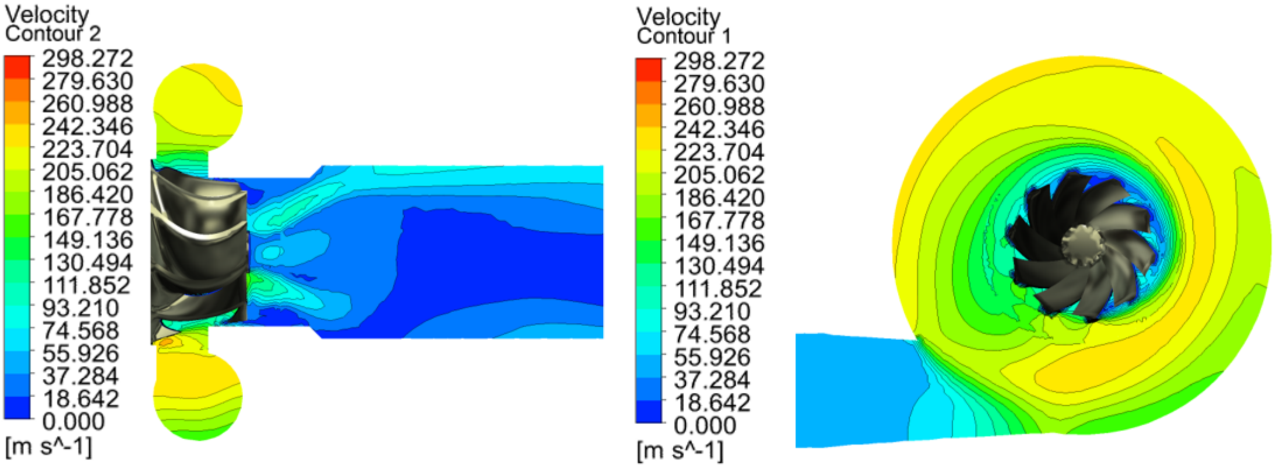


Fig. 6. Fluid dynamic behavior of combustion gases

It can be noted that the tangential speeds reached in the turbine runner are between the ranges of 100 *m/s* to 206 *m/s*, values similar to those obtained in the study by Borovkov *et al.,* [14] for mass flow rates used. Presenting rotation speeds between the ranges of 16000 *rpm* to 40400 *rpm* for the mass flow values implemented. See Figure 7 below.

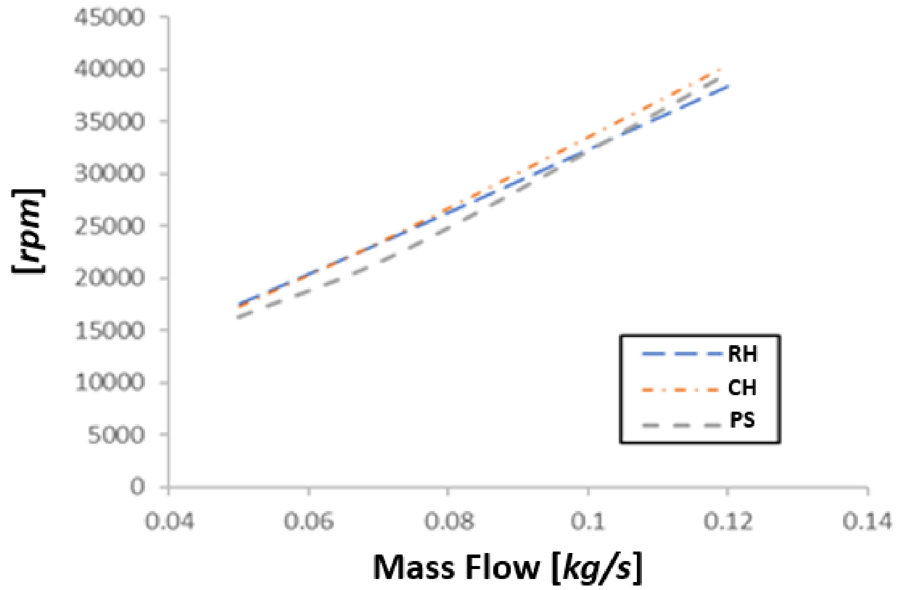


Fig. 7. Rotational speeds at different mass flow rates

In addition to the thermal and fluid dynamic behavior, the simulated mechanical aspects are obtained, such as the reactive torque of the turbine rotor, and the power generated by the gas group. Figure 8 shows the behavior of torque and power for mass flow.

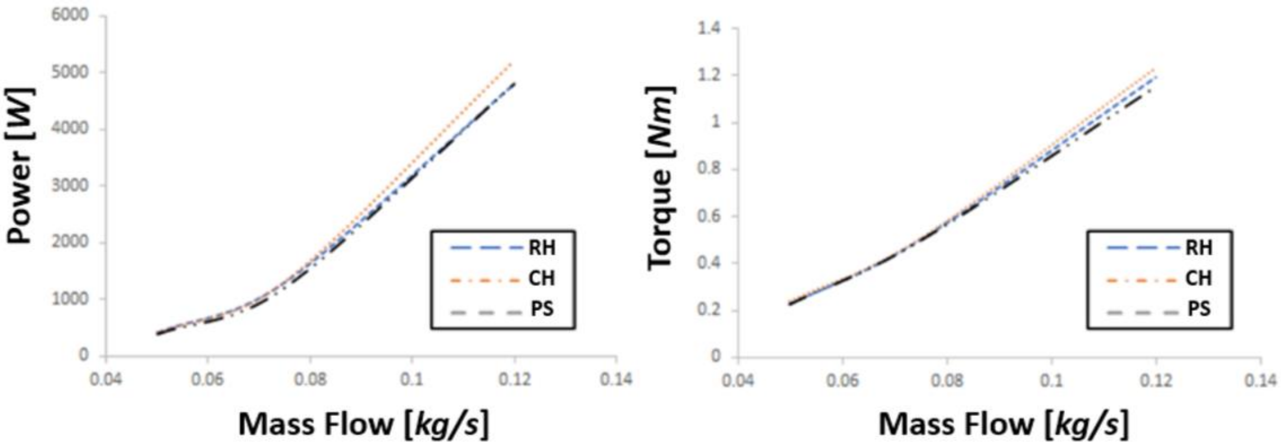


Fig. 8. Power and torque at different mass flow rates

As could be observed for the mass flow rates used and according to the calorific power of each one of the gasified synthesis gases, the behaviors of the torque and the power generated in the system were obtained, these ranges being useful for a heating system. energy extraction by turbo compressor. Generation ranging from 0.4 *kW* to 5.2 *kW* of power generation.

4. Conclusions

Simulations using CFD tools allow studies where experimental methods require a lot of instrumentation and sometimes it is difficult to obtain certain readings. This study simulated the dynamic and energetic fluid behavior of synthesis gas burning in a turbocharger, to analyze operating temperature ranges, rotational speeds, torque, and turbine shaft power.

For this, a reaction mechanism and a combustion model of synthesis gases were proposed, to estimate the energy potential, when using the volatile material for a certain mixture of combustible air. It is highlighted that the biomasses used Rice Husk, Coconut Husk, and Palm Shell, presented a similar energy potential on the turbine studied with values ranging from 0.4 kW to 5.2 kW.

According to the potentials obtained, it is suggested that the use of syngas as a fuel used for power generation through a turbine of a turbocharger system is viable and applicable. Therefore, it is recommended to carry out experimental studies through the data presented in the study and compare it with another diversity of biomass material.

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