

## INFLUENCE OF HYDROGEN ADDITION ON THE STERIC FACTOR OF NATURAL GAS/HYDROGEN MIXTURES

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**Abstract:** Currently, the intense consumption of fossil fuels has caused an increase in greenhouse gases emissions into the atmosphere. For this reason, alternative energy sources are being considered as partial or total substitutes for these fuels. Hydrogen ( $H_2$ ) is the most promising fuel gas due to its different production routes such as steam reforming of methane, gasification and electrolysis of water. Thus, several investigations have focused on the possibility of mixing hydrogen with natural gas (NG) as an alternative for the generation of clean energy. On the other hand, chemical kinetic is one of the most important fundamentals that is closely related to the ignition and extinction of the flame. In this context, the identification of detailed pathways that convert reactants to products has made it possible to advance the field of combustion. However, the reactants are not converted directly into products, but intermediate products are obtained. Thus, the set of elementary reactions used to describe the global reaction is called chemical kinetic mechanisms. Most of the elementary reactions relevant to combustion are bimolecular, i.e., two molecules collide and react to become two different molecules. This event can be evaluated taking into account two very important factors, that is; 1) activation energy and 2) steric factor, both factors are part of the collision theory. The objective of this work was to evaluate the prediction of collision theory in the combustion process of hydrogen/natural gas mixtures through the steric factor. Besides, a detailed mathematical model was provided for the calculation of the adiabatic flame temperature under lean stoichiometric conditions, as well as its effect on the steric factor. The results showed that by adding  $H_2$  to the NG/ $H_2$  mixture, the steric factor decreases. On the other hand, as the equivalence ratio increases, the steric factor decreases, therefore, increasing the adiabatic flame temperature there is a decrease in the steric factor.

**Keywords:** *Steric factor, Collision theory, Hydrogen, Natural gas, Mixtures.*

### 1. INTRODUCTION

To combat climate change through the reduction of greenhouse gas emissions, renewable and sustainable fuels are needed to replace fossil fuels with relatively high carbon content (Midilli and Dincer, 2008). Thus, arises the need to implement a new energy vector that provides the same energy value and contributes to reducing  $CO_2$  emissions (Messaoudani et al., 2016). One such potential fuels is hydrogen, which is considered as a promising energy carrier because of the high energy density on mass base, and its carbon-free property (Zhao et al., 2019). With the development of hydrogen production and storage technologies, compressed hydrogen can be used as a very competitive energy storage strategy to serve the areas that electricity grid cannot reach (Zhao et al., 2019). Hydrogen can be generated from different sources, including fossil fuels, renewable fuels, or electrolysis of water. It implies that it would be produced in large quantities and would certainly need to be transported from the place of production to the end-user (Messaoudani et al., 2016). Pipelines are the cheapest and safest way to transport hydrogen over long distances with minimal energy loss. One of the most important barriers that interrupt hydrogen to be broadly utilized is the present lack of hydrogen infrastructure (Messaoudani et al., 2016). Experience indicates that implementing a new technology does not essentially require drastic change; it can be realized by small modifications to existing methods and infrastructure (Messaoudani et al., 2016).

Conventional hydrogen production method using fossil fuels include 1) steam reformation of natural gas, 2) partial oxidation of residual oil and 3) coal gasification (Steinberg and Cheng, 1989). However, to reduce the carbon intensity linked to energy use, renewable methods for generating hydrogen are of interest, which also help address energy security concerns for regions that are highly depend on energy import (Sheffield, 2007).

## Nomenclature

n: number of moles  
V: Volume of vessel [ $\text{cm}^3$ ]  
 $v_x$ : velocity of the particle in the “x” direction [ $\text{cm s}^{-1}$ ]  
T: Temperature of the process [K]  
P: Pressure [kPa]  
F: Force [kN]  
N: normalization constant  
m: mass of the particle [g]  
 $\langle v \rangle$ : relative velocity of a particle [ $\text{cm s}^{-1}$ ]  
 $V_{\text{col}}$ : Volume of collision [ $\text{cm}^3 \text{ collision}^{-1}$ ]  
Z: collision frequency  
 $p$ : steric factor  
 $f$ : successful collision fraction  
[A]: concentration of substance A [ $\text{mol cm}^{-3}$ ]  
[B]: concentration of substance B [ $\text{mol cm}^{-3}$ ]  
 $N_{\text{AV}}$ : Avogadro’s number  
 $E_a$ : activation energy [ $\text{kcal kmol}^{-1}$ ]  
A: pre-exponential factor [ $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ]  
 $\sigma$ : diameter [cm]  
 $\bar{R}$ : universal gas constant  
 $\mu$ : reduced mass [g]  
k: constant of reaction rate [ $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ]  
 $\Delta T$ : time interval [s]  
 $v_R$ : reaction rate [ $(\text{cm}^3)^{1-x-y} \text{ mol}^{-(1-x-y)} \text{ s}^{-1}$ ]; units agree with Eq. (21).  
Q: thermal power [kW]  
 $\dot{W}$ : shaft power [kW]  
 $v$ : system speed [ $\text{m s}^{-1}$ ]  
g: gravity [ $\text{m s}^{-2}$ ]  
z: system height [m]  
 $\Phi$ : equivalence ratio  
 $\alpha$ : normalized excess air  
h: specific enthalpy [ $\text{kJ kg}^{-1}$ ]  
H: enthalpy [kJ]  
 $\bar{h}$ : molar enthalpy [ $\text{kJ kmol}^{-1}$ ]

## Subscript

T: Total  
A: molecule A  
B: molecule B  
AB: molecule A and B  
bi: bimolecular  
ref: reference  
CV: control volume  
out: outlet  
in: inlet  
react: reactants  
prod: products  
col: collision

There may be several additional advantages to using a mixture of hydrogen and natural gas compared to pure natural gas. It is well known that lean operation significantly reduces  $NO_x$  emissions (Middha et al., 2011). The use of hydrogen significantly increases the flame speed in poor conditions, making that regime practically accessible. It also reduces the ignition energy of the fuel (the ignition energy of hydrogen is an order of magnitude less than that of methane, while the laminar burning rate is an order of magnitude greater) (Middha et al., 2011). The use of hydrogen also speeds up the combustion of methane and increases the efficiency of catalysis at lower exhaust temperatures (Middha et al., 2011).

Today, most pipeline gas is consumed by combustion devices, either to generate electricity in power plants or to provide heat in industrial, commercial, and residential applications. Due to the significantly variable combustion properties between hydrogen and natural gas (e.g., wide flammability range and high flame speed of hydrogen), it is not practical to replace natural gas with hydrogen directly (Zhao et al., 2019). However, this difference in properties also plays a very important role in the safety of the mixture, i.e., hydrogen/natural gas combines the positive safety properties of hydrogen (strong buoyancy, high diffusivity) and methane (much lower flame speeds and narrower flammability limits as compared to hydrogen) (Middha et al., 2011).

As mentioned above, the combustion process is closely linked to the future use of hydrogen/natural gas mixtures in different areas. Combustion is the result of dynamic events that occur between the particles that make up a substance, that is, atoms, molecules, and radical species. Several physical-chemical phenomena would not be understood without the further introduction of time-dependent principles. Thus, thanks to the study of the chemical reaction rate, it is possible to know the burning efficiency of any fuel to heat production and/or work while minimizing the formation of incomplete combustion products. However, this topic has many factors to take into account that complicate its understanding. The objective of this work is to show a simplified and organized procedure, focused on collision theory, to determine the probability of a successful reaction, which is estimated from the geometric factor also called the steric factor.

## 2. METHOD AND MATERIALS

The method to be used in this work is the deductive method, that is, to show the content from premises. Thus, starting from the first conceptions of the theory of kinetic gases, continuing with the collision frequency and ending with the collision theory, the expressions that will allow the calculation of the steric factor in a chemical reaction, especially in natural gas/hydrogen mixtures, will be deduced. The kinetic theory and the collision theory have the following postulates in common (Dunaway and Siddique, 2021; Fleming, 2021):

- 1) The particles that make up a gas obey Newton's laws and travel in a straight line unless they collide with another particle or with the vessel wall.
- 2) The particles are so small compared to the average distance between them.
- 3) All particles are solid, hard spheres.
- 4) Molecular collisions are perfectly elastic so kinetic energy is conserved.
- 5) The reaction of interest is between just two particles.
- 6) Gas particles do not interact with other particles except through collision.
- 7) A collision occurs when the distance between the centers of two particles is less or equal to the sum of their radius.
- 8) The kinetic energy of the particles in a gas sample is proportional to the temperature.

The investigation of the pressure exerted by gas inside a vessel led to the formulation of the kinetic theory, which states that an elastic fluid is made up of a very large number of small particles in rapid motion colliding with each other as well with the vessel walls. To find the expression for gas pressure as a function of particle velocity, five main features of the system were considered:

- a) Volume of collision
- b) Avogadro's Law
- c) The momentum of each particle (considering the direction of the velocity of each particle, i.e.,  $V_x$  and  $-V_x$ )
- d) The total force ( $F_t$ ) of the particles colliding with the vessel wall ( $F_T = n_{col}F_i$ )
- e) Definition of pressure ( $P = F A^{-1}$ )

Putting together all these points, Eq. (1) is obtained:

$$P = \frac{n_T m}{V} v_x^2 \quad (1)$$

Due to the dynamics of the particles, the velocity  $v_x$  can acquire infinite values that can be represented by a distribution of molecular velocities. Therefore, the velocity distribution function, known as the Maxwell-Boltzmann distribution, is given by Eq. (2):

$$f(v_x) = N \exp\left(\frac{-mv_x^2}{2k_B T}\right) \quad (2)$$

The normalization constant (N) can be derived from the probability distribution function, defined by Eq. (3):

$$\int_{-\infty}^{\infty} f(v_x) dv_x = 1 \quad (3)$$

Introducing Eq. (2) into Eq. (3) and solving the integral, it is obtained  $N = (m/2\pi k_B T)^{1/2}$ . Finally, the Maxwell-Boltzmann distribution is written as follows:

$$f(v_x) = \sqrt{\frac{m}{2\pi k_B T}} \exp\left(\frac{-mv_x^2}{2k_B T}\right) \quad (4)$$

However, in reality a particle has not only a distribution of speeds but also a distribution of directions. In 1860, James Clerk Maxwell proposed a general form for the velocity distribution that consisted of converting from Cartesian coordinates  $(x, y, z)$  to spherical coordinates  $(v, \theta, \phi)$ , obtaining the following expression (Fleming, 2021):

$$f(v) = Nv^2 \exp\left(\frac{mv^2}{2k_B T}\right) \quad (5)$$

Again, introducing Eq. (5) into Eq. (3) and solving the integral, the new normalization constant (N) is found:

$$N = 4\pi \sqrt{\left(\frac{m}{2\pi k_B T}\right)^3} \quad (6)$$

Nevertheless, the velocity acquired by a particle can take on infinite values with a given probability from which a mean would be chosen to represent the average velocity ( $\bar{v}$ ) of the particle inside the system. Thus, the average velocity of a particle can be calculated from Eq. (7):

$$\bar{v} = \int_{-\infty}^{\infty} v f(v) dv \quad (7)$$

Note that by setting the endpoints of the integral to infinity, time is implicitly included. Introducing Eqs. (5) and (6) into Eq. (7) and solving the integral, we have:

$$\bar{v} = \left(\frac{8k_B T}{\pi m}\right)^{1/2} \quad (8)$$

In a system of particles,  $m$  is called the reduced mass, it is usually represented as  $\mu$  and is defined as follows (Dunaway and Siddique, 2021):

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (9)$$

On the other hand, the distribution of velocities and directions of a particle is closely linked to the encounter frequency between particles, that is, the collision frequency ( $Z_i$ ), which is defined, in a given system, as the average number of collisions per unit of time (Dunaway and Siddique, 2021). It is expressed mathematically as follows:

$$Z_i = \frac{n}{t} = \frac{\text{number of collisions}}{\text{unit of time}} \quad (10)$$

Note that the number of collisions is related to the number of particles in the system. In 1857, Rudolf Clausius introduced the "mean free path" concept, which states that the distance traveled between collisions is large, therefore the particle will move in a time interval  $\Delta t$ , sweeping the cylindrical volume (of collision) with radius  $d$  (Turns, 2000). Based on this, Eq. (10) can be rewritten as Eq. (11):

$$Z_i = \frac{(\text{collision volume})(\text{concentration})}{\text{time interval}} \quad (11)$$

If we consider that a particle A is in collision with each particle B, being the particles B static, then A will have a relative velocity  $\langle v \rangle$  (Dunaway and Siddique, 2021). Therefore, Eq. (11) will be written as follows:

$$Z_i = \frac{(V_{col}) \left( \frac{n_B}{V_{col}} \right)}{\Delta t} \quad (12)$$

Furthermore, the cylindrical collision volume would be given by Eq. (13):

$$V_{col} = (\pi d^2) \langle v \rangle \Delta t \quad (13)$$

Substituting Eq. (13) in Eq. (12), we have:

$$Z_i = \pi d^2 \langle v \rangle \left( \frac{n_B}{V_{col}} \right) \quad (14)$$

where,  $Z_i$  represents the collision frequency of particle A with all particles B. However, we are interested in the collision frequency associated with all the A and B particles, so the term  $(n_A/V_{col})$  is added to Eq. (14), resulting in Eq. (15):

$$Z_{AB} = \pi d^2 \langle v \rangle \left( \frac{n_A}{V_{col}} \right) \left( \frac{n_B}{V_{col}} \right) \quad (15)$$

If the colliding particles have different sizes (hence, different radius), we have  $d = r_A + r_B$ ,  $d$  is both the radius of the collision cylinder and distance between the centers of the colliding spheres. Therefore,  $d = \sigma_{AB}$  and  $2\sigma_{AB} = \sigma_A + \sigma_B$ . Substituting  $d = \sigma_{AB}$  and the average velocity of the particle (Eq. 8) in Eq. (15), we have:

$$Z_{AB} = \pi \sigma_{AB}^2 \left( \frac{8k_B T}{\pi m} \right)^{1/2} [A][B] \quad (16)$$

where,  $k_B$  is the Boltzmann constant,  $k_B = 1.381 \times 10^{-23} \text{ J K}^{-1}$ . Eq. (16) states the frequency of collisions between particles A and B. However, there is a particular collision that will result in a reaction. This phenomenon is addressed by the collision theory, which involves two important aspects (Clark, 2021):

- a) Correct orientation for collision
- b) Sufficient kinetic energy to break interatomic bonds.

The first condition is given by the orientation factor or also called the steric factor, denoted by  $p$ , which indicates the probability that two particles react in the collision as long as the direction and spatial arrangement are appropriate. The second condition is determined by the energy barrier, which must be overcome to start the chemical reaction. This energy barrier is called the activation energy, denoted by  $E_a$ , which indicates the energy required to break interatomic bonds in a collision. Therefore, only a fraction ( $f$ ) of the colliding particles will have a successful collision with the potential to start a reaction. This fraction is defined as follows (Zhao, 2020):

$$f = \exp(-E_a/\bar{R}T) \quad (17)$$

On the other hand, the reaction rate ( $v_R$ ) is proportional to both the collision frequency ( $Z_{AB}$ ) and the fraction of successful collisions ( $f$ ). However, there is another parameter that links both factors, that is, the collision orientation, geometric factor or steric factor ( $p$ ). Thus, we have the following expression:

$$v_R = Z_{AB} p f \quad (18)$$

Besides, the instantaneous speed is directly proportional to the number of atoms or Avogadro's number ( $N_{AV}$ ), that is:

$$v_R = -\frac{1}{N_{AV}} \frac{d[A]}{dt} \quad (19)$$

where,  $[A]$  is the concentration of substance A, the negative sign indicates consumption of A. The other equation involving the rate of consumption of A is the law of mass action, which is expressed by Eq. (20):

$$\frac{d[A]}{dt} = -k_{bi}[A]^x[B]^y \quad (20)$$

where,  $k_{bi}$  is the rate constant, which is specified for each temperature.

All ultimate bimolecular reactions are globally second-order relative to each reactant, that is,  $x = 1$  and  $y = 1$ . Substituting Eq. (19) in Eq. (20), we get:

$$-N_{AV} v_R = -k_{bi}[A]^x[B]^y \quad (21)$$

Finally, introducing Eq. (18) into Eq. (21), we have Eq. (22):

$$k_{bi}(T) = pN_{AV}\sigma_{AB}^2 \left( \frac{8\pi k_B T}{\mu} \right)^{1/2} \exp(-E_a/\bar{R}T) \quad (22)$$

Equation (22) can be rewritten as follows:

$$k_{bi}(T) = A \exp(-E_a/\bar{R}T) \quad (23)$$

where;  $A = Z'_{AB} p$  and;

$$Z'_{AB} = N_{AV}\sigma_{AB}^2 \left( \frac{8\pi k_B T}{\mu} \right)^{1/2}. A \text{ is called pre-exponential coefficient.}$$

Equation (23) is known as the Arrhenius Equation (Lower, 2021). From Eq. (22), it can be seen that the pre-exponential factor (A) is not strictly constant but depends on  $T^{1/2}$ . For this reason, the Arrhenius Equation is modified to an expression with three parameters (Turns, 2000):

$$k_{bi}(T) = A (T^*)^b \exp(-E_a/\bar{R}T) \quad (24)$$

where;  $T^* = 298(T/T_{ref})$  being  $T_{ref} = 298$  K. Thus, equaling Eqs (22) and (24), the steric factor can be obtained.

It is seen that Eqs. (22) and (24) need some parameters to estimate the value of the steric factor (p). These parameters are shown in Tab. 1 with the corresponding reactions for each fuel considered, that is, natural gas and hydrogen. Also, Tab. 2 shows the diameters for each chemical species considered in the reaction.

Table 1. Factors to take into account in solving equations (22) and (24).

Natural gas (Dagaut, 2002)			
Number	Reaction	A	b
R1	$H + O_2 + M \rightarrow HO_2 + M$	$2.80 \times 10^{18}$	-0.9
R2	$H + O_2 \rightarrow O + OH$	$2.65 \times 10^{16}$	-0.7
R3	$H + CH_3(+M) \rightarrow CH_4(+M)$	depend on pressure	
R4	$OH + HO_2 \rightarrow O_2 + H_2O$	$1.45 \times 10^{13}$	0
R5	$HO_2 + CH_3 \rightarrow OH + CH_3O$	$3.78 \times 10^{13}$	0
R6	$CH_3 + O_2 \rightarrow O + CH_3O$	$2.80 \times 10^{18}$	0
R7	$CH_3 + O_2 \rightarrow OH + CH_2O$	$2.31 \times 10^{12}$	0
R8	$CH_3 + CH_3(+M) \rightarrow C_2H_6(+M)$	depend on pressure	
R9	$HCO + H_2O \rightarrow H + CO + H_2O$	$1.55 \times 10^{18}$	-1
Hydrogen (Turns, 2000)			
Number	Reaction	A	b
R1	$H_2 + O_2 \leftrightarrow OH + H$	$1.7 \times 10^{13}$	0
R2	$OH + H_2 \leftrightarrow H_2O + H$	$1.17 \times 10^{13}$	1.3
R3	$O + OH \leftrightarrow O_2 + H$	$3.61 \times 10^{14}$	-0.5
R4	$O + H_2 \leftrightarrow OH + H$	$5.06 \times 10^4$	2.67
R5	$OH + OH \leftrightarrow O + H_2O$	$6.0 \times 10^8$	1.3

Table 2. Diameters of the chemical species considered in each reaction from Tab. 1 (reactants only) (Turns, 2000).

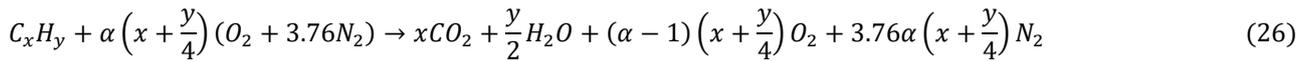
Element	Diameter ( $10^{-8}$ cm)
H	2.708
O <sub>2</sub>	3.467
HO <sub>2</sub>	3.564
O	3.050
OH	3.147
H <sub>2</sub> O	2.641
CH <sub>3</sub>	3.743
HCO	3.705
CH <sub>2</sub> O	3.720
H <sub>2</sub>	2.827

Once the steric factor value for each reaction (see Tab. 1) is found, the average steric factor ( $P_{av.}$ ) can be calculated using Eq. (25):

$$P_{av.} = \frac{\sum_{i=1}^n p_i}{\sum_{i=1}^n n_i} \quad (25)$$

where,  $n$  is the total number of reactions and  $p_i$  is the steric factor for each reaction.

On the other hand, Eq. (26) will be used to evaluate the adiabatic flame temperature under different conditions of excess air and hydrogen concentrations.



where,  $\alpha$  is the normalized excess air,  $(x + y/4)$  is the stoichiometric oxygen coefficient for the combustion reaction, and the coefficients  $x$  and  $y$  depend on the carbon and hydrogen content of natural gas and hydrogen. The normalized excess air ( $\alpha$ ) is related to the equivalence ratio ( $\Phi$ ) through Eq. (27) (Turns, 2000):

$$\alpha = \frac{1}{\Phi} \quad (27a)$$

or

$$\% \text{ stoichiometric air} = \frac{100\%}{\Phi} \quad (27b)$$

The maximum temperature of the reaction can be estimated from the calculation of the adiabatic flame temperature. Thus, considering the energy conservation equation (Eq. 28), it is possible to calculate the temperature of the flame at constant pressure.

$$\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m} \left[ (h_{out} - h_{in}) + \frac{1}{2}(v_{out}^2 + v_{in}^2) + g(z_{out} - z_{in}) \right] \quad (28)$$

Taking into account that the process is adiabatic, that is, the system does not do work and does not generate heat for the surroundings, Eq. (29) is obtained (Turns, 2000):

$$H_{react.}(T_i, P) = H_{prod.}(T_{ad}, P) \quad (29a)$$

or, equivalently on a molar basis per kmol of the mixture.

$$n_{react.} \bar{h}_{react.}(T_i, P) = n_{prod.} \bar{h}_{prod.}(T_{ad}, P) \quad (29b)$$

### 3. RESULTS AND DISCUSSIONS

In this section, the different results obtained for the steric factor of natural gas/hydrogen mixtures under lean stoichiometric conditions will be presented. Thus, this section will be split into two parts. First, results of the adiabatic flame temperature evaluated between 5 and 25% of excess air will be presented, as well as the influence of the addition of H<sub>2</sub> on natural gas/hydrogen mixtures. Second, results of the influence of the addition of H<sub>2</sub> on the steric factor evaluated at different flame temperatures will also be presented.

Figure 1 shows that for a constant air/fuel ratio (or constant  $\alpha$ ), the adiabatic flame temperature increases as the hydrogen concentration increases. This is because hydrogen has a higher heating value than natural gas, so the energy generation will be greater. On the other hand, the adiabatic flame temperature decreases as the equivalence ratio decreases. This is because a larger amount of air acts as a diluent that compensates for the increase in H<sub>2</sub> in the hydrogen/natural gas mixture.

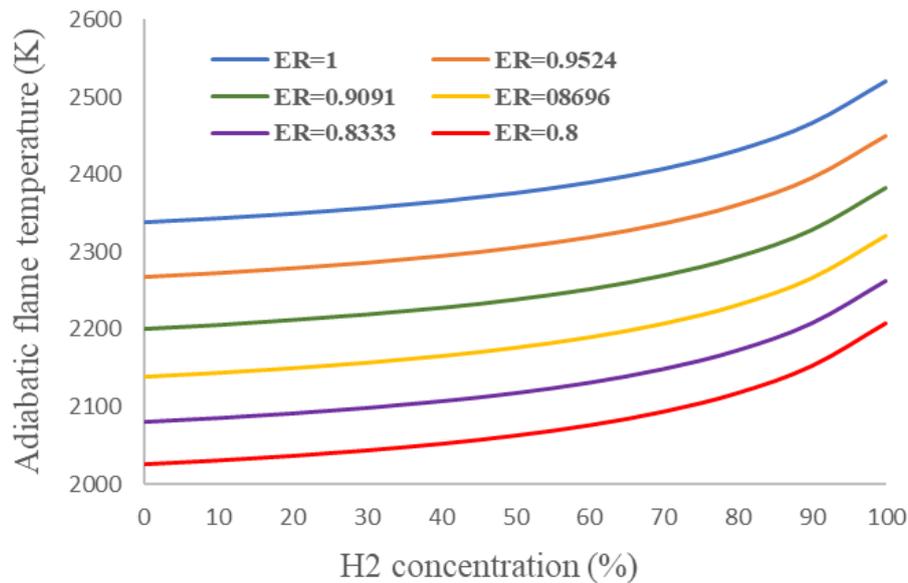


Figure 1. Variation of adiabatic flame temperature (AFT) as a function of hydrogen concentration at a fixed Equivalence Ratio (ER).

Figure 2 shows that the steric factor decreases as the equivalence ratio increases. There are two possible interpretations for this result; a) at the start of the reaction, and b) during the reaction.

#### a) At the start the reaction

The steric factor is related to the influence of an external factor (passage of an electric current, for example) and not only to the collisions between molecules. Therefore, the greater influence of an external factor on the reaction, the lower value the steric factor will take. The flammability limits are the phenomena of the greatest evidence for this statement (Rios Escalante et al., 2022, 2018). Combustion is a process that involves three important factors: an ignition source, an oxidizer, and fuel. In addition, it is known that a chemical reaction achieves maximum energy generation under stoichiometric conditions ( $\Phi = 1$ ). On the other hand, there are fuel concentrations limits for a reaction to occur. These limits are called flammability limits and fall into two categories: Lower Flammability Limits (LFL) and Upper Flammability Limits (UFL). The first refers to a higher concentration of oxidant than fuel ( $\Phi < 1$ ) and the second refers to a higher concentration of fuel than oxidant ( $\Phi > 1$ ).

Thus, the decrease in the concentration of the oxidant, in the LFL, implies an approximation to the stoichiometric conditions, which means a greater influence of an energy source on the reaction of the mixture and, therefore, a lower value of the steric factor. On the contrary, the increase in the concentration of the oxidant, in the LFL, implies a distance from the stoichiometric conditions, which means a lesser influence of the energy source on the reaction of the mixture and, therefore, a higher value of the steric factor.

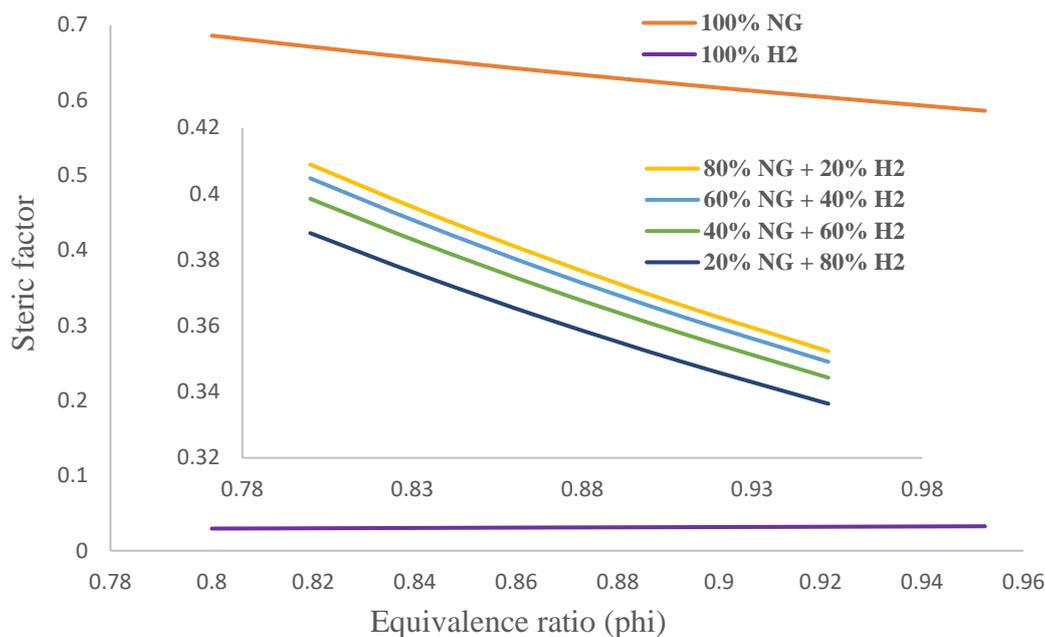


Figure 2. Variation of steric factor as a function of Equivalence ratio (ER) for different concentrations of hydrogen.

#### b) During the reaction

From the results, it can be seen that the steric factor reaches values higher than unity, as is the case of reactions R1 and R9 (for natural gas). This is mainly due to the presence of three particles in the reaction (M in R1 and H<sub>2</sub>O in R9), which considerably increases the probability of a successful collision and is evidenced by the high value of the pre-exponential factor of both reactions. When the probability of a successful collision is very high (sometimes exceeding the unity), it means that an effective collision has occurred, due to the high degree of dissociation involving a greater number of particles. Note that the collision frequency decreases since, despite the fact that the temperature of the system increases, the particles formed in the reaction are different, therefore, the probability of a successful collision increases because both are in an inverse relationship according to Eq. (23). Thus, the more complex the molecule, the higher its steric factor. For example, hydrogen reaches its elemental state H (hydrogen ion) fastest than natural gas since the last is made up of a greater number of chemical species. In this way, a higher collision frequency between elemental species (the same species) will be produced, obtaining a lower value of the steric factor. Therefore, the steric factor of hydrogen will be lower than the steric factor of natural gas. Consequently, by adding hydrogen to the natural gas/hydrogen mixtures, the steric factor decreases.

On the other hand, according to Turns (2000), when dissociation is not considered in the calculation of adiabatic flame temperature, its value is overestimated. It means that, as the adiabatic flame temperature increases, the influence of dissociation is negligible, therefore, a higher collision frequency (between the same molecules) will occur, and a lower value of the steric factor will be obtained. This work did not include the dissociation of chemical species in the reaction.

## 4. CONCLUSIONS

The influence of hydrogen addition on the steric factor of natural gas/hydrogen mixtures was evaluated. The deductive method was applied to reach general conclusions from the premises. The results showed that the steric factor strongly depends on the molecular structure of the fuel. The more complex the structure, the higher the value of the steric factor. On the other hand, the steric factor also indicates the influence of an energy source, that is, the greater the influence of an energy source, the lower the value of the steric factor. Conversely, the lower the influence of an energy source, the higher the steric factor values.

## 5. ACKNOWLEDGMENT

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## 7. RESPONSABILIDADE AUTORAL

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