

Improved model of lattice gas in the adsorption of carbon monoxide and oxygen

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ABSTRACT

The adsorption and subsequent oxidation of carbon monoxide (CO) on a platinum (Pt) surface has been studied using computational methods. The Monte Carlo method is used to this end through the lattice model. This study focuses on the improvement of this first theoretical model (ZGB) proposed for the oxidation of CO. In this work, four different models are revised in detail with the objective of establishing a comparison between the obtained results on the oxidation of CO on the Pt with an orientation (111) surface. The variance between the models lies on the nature of the sticking coefficient of the CO and oxygen (O₂) molecules on Pt (111). This adsorption depends on the initial concentration of CO in the gas phase and the number of vacant sites on the platinum surface. The results obtained in these simulations show that the first model, the ZGB model, differs considerably from the other models, and thus the results with the second and third model have a better adjustment to the adsorption of the CO and O₂ molecules, since they take into account the gas concentration, the sticking coefficient and the interaction with the neighboring particles. In this sense, the oxidation reaction occurs in a wider theoretical range around 0.5 mole fraction of CO and 0.2 mole fraction of O atomic, and the poisoning of the platinum catalytic surface can be inhibited if the concentration of carbon monoxide is included as a control parameter.

Keywords: Gas adsorption; ZGB model; Gas lattice; Carbon monoxide oxidation.

Modelo mejorado de gas lattice en la adsorción de monóxido de carbono y oxígeno

RESUMEN

La adsorción y posterior oxidación del monóxido de carbono (CO) en una superficie de platino (Pt) se ha estudiado utilizando métodos computacionales. El método de Monte Carlo se utiliza para este fin a través del modelo de red. Este estudio se centra en la mejora de este primer modelo teórico (ZGB) propuesto para la oxidación de CO. En este trabajo, se revisan en detalle cuatro modelos diferentes con el objetivo de establecer una comparación entre los resultados obtenidos sobre la oxidación de CO en el Pt con una superficie de orientación (111). Esta adsorción depende de la concentración inicial de CO en la fase gaseosa y el número de sitios vacantes en la superficie del Pt. La variación entre los tres modelos radica en la naturaleza del coeficiente de pegado de las moléculas de CO y oxígeno (O₂) en Pt [111]. Esta adsorción depende de la concentración inicial de CO en la fase gaseosa y del número de sitios vecinos disponibles. Los resultados obtenidos en estas simulaciones

muestran que el primer modelo, el modelo ZGB, difiere considerablemente de los otros modelos y, por lo tanto, los resultados con el segundo y tercer modelo tienen un mejor ajuste en la adsorción de las moléculas de CO y O₂, ya que toman en cuenta la concentración de gas, el coeficiente de pegado y la interacción con las partículas vecinas. En este sentido, la reacción de oxidación ocurre en un rango de alrededor 0.5 fracción molar de CO y 0.2 de O atómico, y el envenenamiento de la superficie catalítica de platino puede inhibirse si se incluye la concentración de monóxido de carbono como parámetro de control.

Palabras clave: Adsorción de gas; Modelo ZGB; Gas lattice; Oxidación de monóxido de carbono.

1. Introducción

The CO is a small but dangerous gas, which makes it impossible for humans to detect it, thus endangering the health and well-being of the population due to the high toxicity and environmental damage [1]. CO has a great significance since it is a byproduct of the partial oxidation of carbon-containing products into the environment [2, 3]. Additionally, the increasing use of vehicles has caused a subsequent increase in the concentration of CO, reaching drastic levels that severely affect the quality of the air [4-6]. For the above, the study of the oxidation of the carbon monoxide has a great interest in catalytic chemical reactions in the scientific community and the industry, since they are crucial to comprehend the key components of the catalytic process at a nanometric scale from a theoretical [7-9] and experimental [10-14] approach.

One of the main theoretical tools used in the studies of the oxidation reaction of CO on a solid surface are the gas lattice models [15-17]. This type of model represents the surface of the catalyst and the atoms of the adsorbed molecules as a network in whose cells one atom per cell is located. In general, and for simplicity reasons, the cells are arranged in a regular grid that is dependent on the coordination number of the metal. The gas molecules maintain the mass, the momentum, and the energy [18]. The adsorption of the gas is done on the metal in a cell, and the interaction between particles occupying the neighboring cells is based on the assumption that the associated energy is constant for both particles and that there is no energetic interaction between them [19, 20].

The first gas lattice model used for the simulation of the oxidation of CO was the ZGB model [21]. In this simplified model, the solid catalytic surface was represented using a reticular network, and the gas molecule was simulated as a point that was adsorbed on an available site of the surface. Other models propose to study the movement of oxygen atoms in neighboring sites (diffusion). In the models proposed in this work, a chemisorption is carried out, for which the movement of oxygen atoms to neighboring sites is not taken into account. Also, this model considers that the particles of different nature adsorbed on adjacent sites will react and desorption would be instantaneous following a Langmuir-Hinshelwood mechanism, leaving two sites vacant [4]. This first approach does not properly represent the adsorption process due to the strong assumptions and idealizations [22].

In addition, the ZGB model does not consider the energetic interactions, and the poisoning of the solid surface is not observed. This phenomenon occurs when, for a given concentration of the gas phase in the atmosphere, the solid surface is occupied mostly by a single gas species [23-25]. Therefore, the results obtained for high concentrations of CO were produced in a surface covered completely by oxygen molecules, and for high concentrations of CO the surface was covered with the same CO molecule. This poisoning

phenomenon is not observed for any oxygen concentration. In the case of CO molecule, the coating of the surface occurs when concentrations are above 50% in the gas phase, likewise, it considers, in addition to the surface, the interstitial sites of the subsurface [26]. This represents a wider range for the oxidation reaction to take place, since at lower concentrations of CO the closest neighbors are more active for the production of CO₂. Thus, the rapid diffusion of oxygen between the surface and the subsurface would eliminate the poisoning of the surface due to the adsorption mechanism. In spite of this, the model does not accurately represent the phenomenon [27].

On the other hand, the interactions between neighboring molecules have not been taken into account much before, and this interaction is key to understanding and modelling in a more effective way the catalytic reaction for the oxidation of the CO [28]. The model that first considered the neighboring interactions focused on three aspects: the coordination number of the lattice, the density, and the distribution of the active sites that intervene on the catalytic process. All these aspects allowed to obtain transition probabilities with a higher precision [29–31]. The range of production of carbon dioxide increases when the interaction between particles of the same species hinders the adsorption and the interaction between particles of different species favors the reaction and desorption of the molecules [32].

In the same way, a relevant factor is the inactive phase on the surface, where inert sites and impurities are located. The remaining sites are usually occupied with oxygen molecules. Monte Carlo simulations have been used to evaluate the different relations between the parameters as a function of the concentration of impurities. Results show that the presence of impurities on the catalytic surface alters the critical behavior of the system, presenting different phases and a different range in the production of CO₂ [33]. Alternatively, other studies on the oxidation of CO have included the spatial diffusion of the oxygen atoms and the CO molecules that are adsorbed on the platinum surface. This approximation considers two different ways in which the diffusion of the atoms occurs, and two different combinations of the diffusion/adsorption process, generating several possible models. These are analyzed by time-dependent Monte Carlo simulations and stable state Monte Carlo simulations, showing continuous and discontinuous phase transitions of the molecules and atoms that take place on the catalyst. This implies that the diffusion problem can be used in a superficial reaction model and can be solved as a simple statistical optimization concept [34].

Conversely, Monte Carlo simulations have also been used to determine the sticking coefficient taking into account the inert sites on the surface. This study allows to obtain a schematic of the possible phase transitions using color maps as a function of the adsorption velocities of the CO and the density of inert sites. Results are evidence of the weak influence due to the inclusion of inert sites on the catalytic surface, and highlight the importance of refining the points of phase transition, leaving some values of the density of the inert sites and using larger reticular surfaces [35].

Finally, the latest approaches to the theoretical evaluation of CO oxidation using the gas network model have shown that crucial factors are the nature of neighboring sites and vacancies on the catalytic surface. These factors play the main role in helping to describe the experimentally observed phase transitions theoretically [7, 36]. For the above, in this work a series of molecular simulations are developed using the Monte Carlo method to describe the adsorption of carbon monoxide and molecular oxygen on a catalytic Pt (111) surface taking into account the main factors that affect the oxidation. The proposed models consider the effect of the interaction between neighboring molecules on the surface, and a variable sticking coefficient is used for

the molecules covering the surface, which is taken from previous experimental studies, whereby better theoretical results are expected.

2. Materials and methods

The process of carbon monoxide oxidation follows equation 1. Four different models of monolayer chemical adsorption were studied. Of these, the reference model (ZGB) does not take into account the adhesion coefficient, nor the interactions between adsorbed atoms or molecules, the others consider the following modifications in the parameters: i) a variable adhesion coefficient for carbon monoxide carbon and a fixed adhesion coefficient for the oxygen molecule, which corresponds to the concentration of atomic oxygen on the surface after adsorption. ii) a variable coefficient for both gas molecules. iii) a variable coefficient for gas molecules, and furthermore has the restriction that the adsorption of an oxygen molecule can only occur if three neighboring sites are unoccupied. With the four models a more precise approximation for the oxidation of CO is obtained, and the oxygen poisoning of the catalyst for lower concentrations of CO, and CO poisoning for higher concentrations can be eliminated. This could increase the size of the reactive window in the production of CO₂.



In order to obtain a variable sticking coefficient that successfully shows the effect of the concentration of the adsorbed molecules and provides an adsorption probability for a molecule in the gas phase, previous studies indicate that the adsorption probability as a function of the degree of coverage of the surface are used [37]. For carbon monoxide, the adsorption probability is given by:

$$\frac{S_c(CO)}{S_0} = \left(1 + \frac{\theta_{CO}/\theta_z}{1-\theta_{CO}/\theta_z} k\right)^{-1} \quad (2)$$

where S_c is the instant adsorption probability; θ_{CO} is the CO concentration; θ_z is the saturation concentration at which a total coverage of the surface is obtained, S_0 is the initial adsorption probability; and finally, k describes the degree of mobility of the precursors. In these simulations, S_0 is considered to be 0.8, k takes a value of 0.55, and θ_z is 0.53, which are optimum values for the CO oxidation, and guarantee the convergence of the system. For the degree of coverage of the O atomic, and considering the experimental results [37] a parametrization is proposed using the Newton method [38], obtaining a seventh grade polynomial that gives the variable sticking coefficient given by:

$$S_c(O_2) = 46.22\theta_0^6 - 70.03\theta_0^5 + 12.98\theta_0^4 + 31.68\theta_0^3 + 6.24\theta_0^2 - 0.71\theta_0 + 0.06 \quad (3)$$

where θ_0 is the concentration of oxygen and S_c is the sticking coefficient of the oxygen molecule.

The corresponding simulations for each of the four models were programmed using Fortran language [39]. A Pt (111) surface was generated, with a size of 128 cells in the x direction and 256 cells in the y direction. Monte Carlo method [40] was used to evaluate the oxidation of CO. In this method, a molecule from the gas phase is randomly selected and, depending on the model, an adsorption event is attempted considering the corresponding restrictions. If the attempt is successful, the neighbor sites are assessed for occupancy of a

molecule of a different nature. That is, if there are two neighbors that are CO and CO₂, the CO₂ formation reaction occurs. This means that the site occupied by the CO molecule and the O atom remain free, therefore two vacant sites are formed on the surface. A total of 8×10^7 cycles were performed in the equilibrium phase, followed by the same amount of cycles in the production stage where results were computed. The concentration of CO varies from 0 to 1, with a step of 0.01, in order to generate the phase diagrams for the oxidation process.

3. Results and analysis

ZGB model does not take into account the coverage of the surface with a sticking coefficient thus the gas molecules and the interactions between adsorbed atoms are not considered. In this way, the oxidation of the CO molecule occurs in a very small range of concentrations of CO in the gas phase, only between 0.63 and 0.66 as can be seen in Figure 1. This implies an abrupt phase transition for the CO and O concentrations, causing oxygen poisoning below 0.63 and carbon monoxide poisoning above 0.66. These results show that this method does not accurately describe the catalytic oxidation of CO, since the experimental range of oxidation was observed between 0.39 and 0.53 [29, 33, 41]. The lack of computational capability when this model was first proposed was probably the reason behind the simplistic approach to the problem, reaching an equilibrium state sooner than expected.

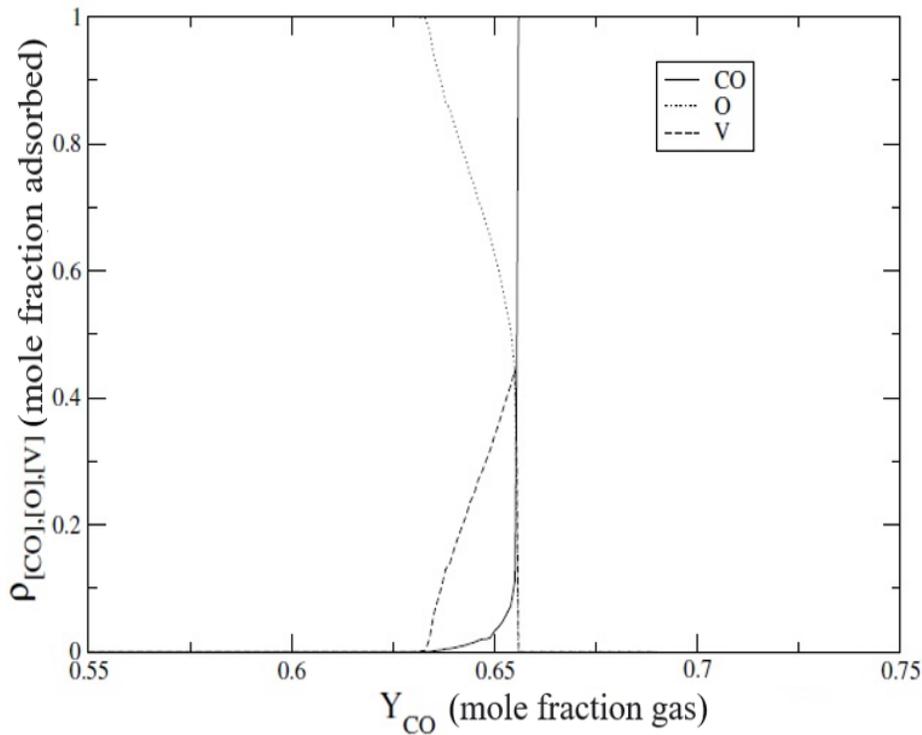


Figure 1. ZGB model. The Y_{CO} axis depicts the CO concentration on the gas phase and the ρ axis shows the molecule density on the surface (ρ [CO]; [O]; [V]). Where [CO], [O] and [V] are CO, O atomic and vacancies concentration at surfaces, respectively.

The results for the second model are shown in Figure 2. In this model, the main difference of this model with respect to the ZGB reference model is the way in which the gas molecule is selected. For each event, the

verification that the sticking coefficient is lower than the fixed value (0.025 or 0.05) is made, since the sticking coefficient of the CO molecule is different for each concentration (Equation 2). If the conditions are met, the adsorption event takes place. Also, if any of the neighbors have different natures, the reaction occurs and immediate desorption follows, this creates two vacancies. From Figure 2 can be observed that this model drastically reduces the oxygen poisoning for a fixed sticking coefficient for the oxygen molecule of 0.025. For low concentrations of CO, however, poisoning with oxygen is still observed. This behavior is still not consistent with the real adsorption process, since the poisoning with oxygen is not observed at a laboratory level and the superficial oxide is even more reactive to the oxidation of CO [42]. The range of production of CO is notoriously larger and the variable sticking coefficient allows to prevent the poisoning of the surface by this molecule. Therefore, the production of CO₂ occurs continuously in a reactivity range of 0.06 until 1.00 for Y_{CO} .

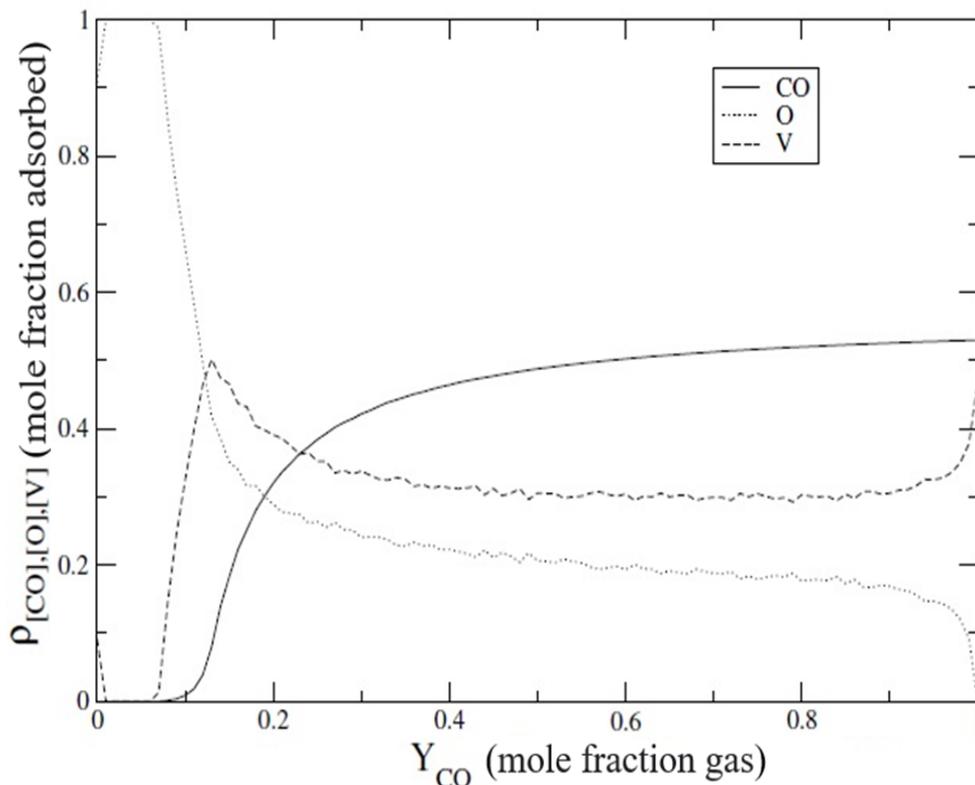


Figure 2. Model with variable sticking coefficient for CO and a fixed value of 0.025 for O₂. The Y_{CO} axis depicts the CO concentration on the gas phase and the ρ axis shows the molecule density on the surface (ρ [CO]; [O]; [V]). Where [CO], [O] and [V] are CO, O atomic and vacancies concentration at surfaces, respectively.

For the case where the fixed sticking coefficient of 0.05 for the oxygen molecule was used, clearly avoids the poisoning of carbon monoxide at high concentrations as well as fixed sticking coefficient of 0.025, but it sees a slight increase in the degree of oxygen poisoning is observed at 0.05 as it is exhibited in Figure 3. This model is able to describe the oxidation process more accurately than the ZGB model and is consistent with previous findings that state that the catalytic activity of the system increases significantly with respect to stationary values. Most experimental and theoretical studies corroborate an increase in the desorption rates [43]. The range of reactivity for a $SC(O_2) = 0.05$ is between 0.13 and 1.

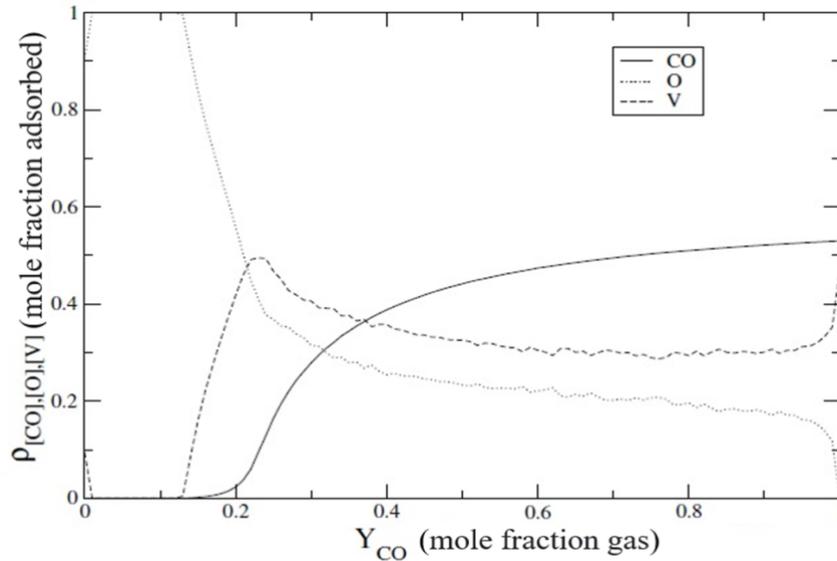


Figure 3. Model with variable sticking coefficient for CO and a fixed value of 0.05 for O₂. The Y_{CO} axis depicts the CO concentration on the gas phase and the ρ axis shows the molecule density on the surface (ρ [CO]; [O]; [V]). Where [CO], [O] and [V] are CO, O atomic and vacancies concentration at surfaces, respectively.

Figure 4 presents the results for the model with variable sticking coefficients for the CO (Equation 2) and the O₂ (Equation 3). The results observed are quite similar to the ones obtained by the model with a fixed coefficient of 0.025. CO and oxygen poisoning are reduced for values of Y_{CO} smaller than 0.05. This means that oxygen poisoning is not avoided and persists in the model, which is still a mistake. The reactive window where the production of CO₂ is achieved is in the range of 0.05 and 1.

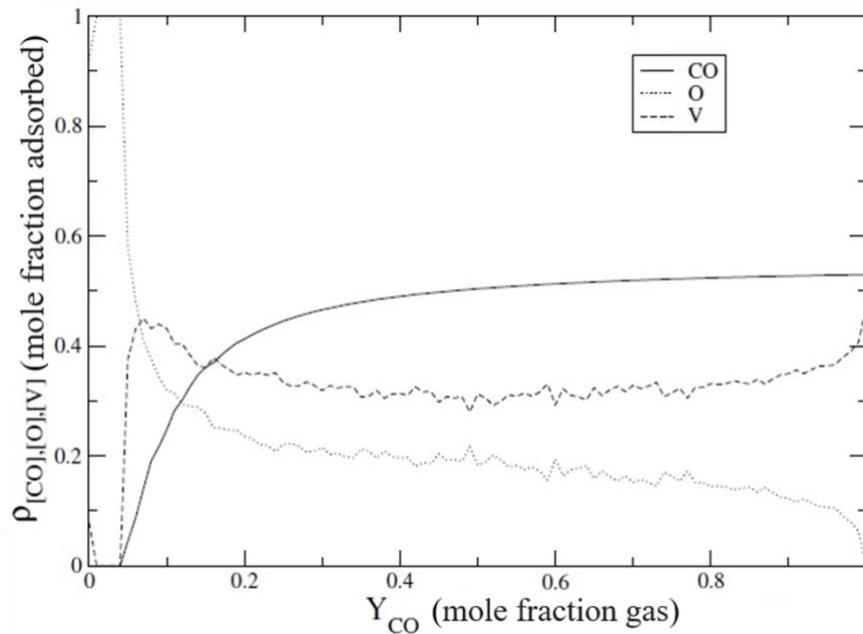


Figure 4. Model with variable sticking coefficient for CO and O₂. The Y_{CO} axis depicts the CO concentration on the gas phase and the ρ axis shows the molecule density on the surface (ρ [CO]; [O]; [V]). Where [CO], [O] and [V] are CO, O atomic and vacancies concentration at surfaces, respectively.

The results for the last model are shown in Figure 5. These results consider the random choice of an oxygen molecule. Furthermore, for adsorption to take place, one of the three available sites on the surface must be selected. If this actually occurs, the molecule is adsorbed and the presence of a neighboring CO is verified, in which case the reaction and subsequent desorption of CO₂ occurs. For this model, surface oxygen poisoning is completely avoided due to the restrictions placed on the oxygen adsorption event. This model is more accurate in describing the interactions that take place between oxygen atoms, as previous studies have shown that these interactions are highly repulsive. [37, 42, 44]. The phase diagram that results from using this model is a more accurate representation of the catalytic reaction of the oxidation of carbon monoxide, and a reactive window is observed for all CO concentrations.

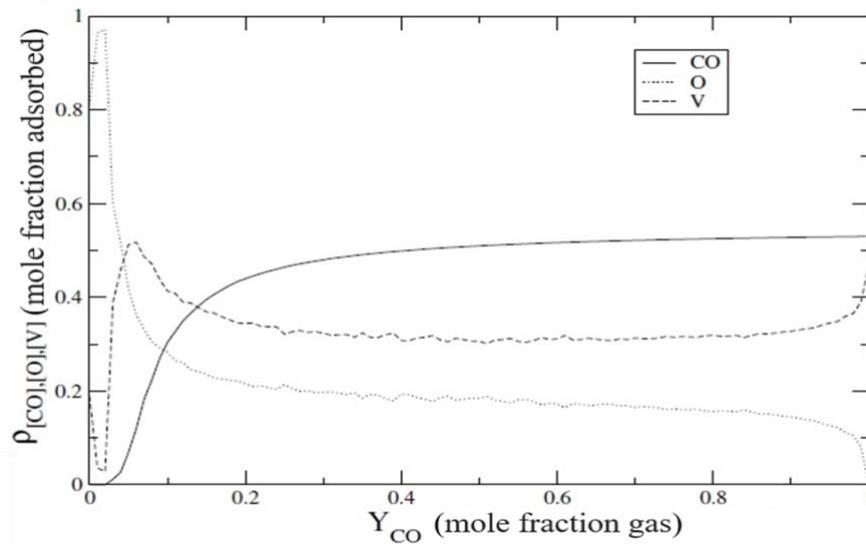


Figure 5. Model with variable sticking coefficient for CO and O₂ and three available neighbors for adsorption of O₂. The Y_{CO} axis depicts the CO concentration on the gas phase and the ρ axis shows the molecule density on the surface (ρ [CO]; [O]; [V]). Where [CO], [O] and [V] are CO, O atomic and vacancies concentration at surfaces, respectively.

The relationship between the adsorbed oxygen and the vacancies observed in the post-ZGB models could be explained considering that these models take into account the interactions between neighbors and the sticking coefficients of each of the gas molecules, which allows a representation of the adsorption and subsequent oxidation taking into account the nature of the neighboring atoms and the concentration of the gasses. If the chemical environment of adsorption is not taken into account, theoretical poisoning would occur, which would generate a monolayer of either CO or oxygen atoms on the surface.

4. Conclusions

The studies carried out after the publication of the ZGB model have tried to explain and describe more precisely the real process that takes place in the CO oxidation reaction. The parameters that have been key in improving this model are the interaction between neighboring particles, diffusion, the adhesion coefficient and surface modification.

The analysis of the models confirms that the interaction between neighboring particles is crucial for the oxidation reaction to be observed in a wider range of CO concentration and, therefore, prevent catalyst

poisoning by either of the two species of gasses. In this sense, although diffusion is a relevant parameter in the improvement of the ZGB model, the type of interactions that take place on the surface with the adsorbed molecules define better results for the study.

Of the four models analyzed here, the fourth model presents the best results since it manages to inhibit carbon monoxide and oxygen poisoning. In addition, this yields the optimal concentrations of gasses that favor the oxidation of CO and although there are more complex models, which take into account energy parameters, the model presented with the gas lattice approximation manages to phenomenologically describe the oxidation process of carbon monoxide, which can be used for experimental applications in processes that seek to reduce the production of carbon monoxide in combustion reactions.

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