

Mathematical Modeling of Conversion CO To CO₂ in Batch Mode CO₂ Laser System.

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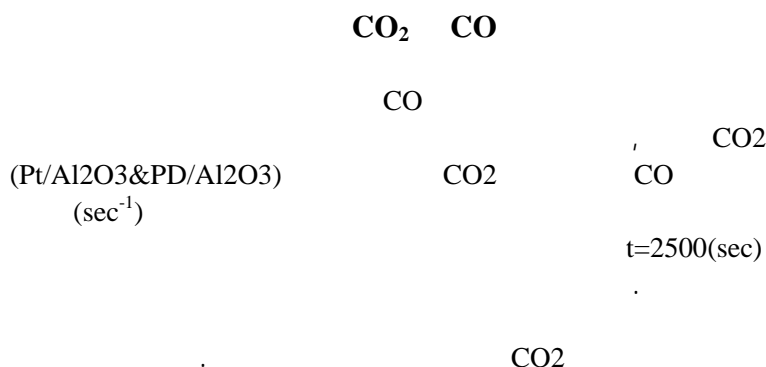
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Abstract

The oxidation of carbon monoxide CO over supported noble metal catalyst is an important part of the catalytic control in sealed-off TEA CO₂ laser system. In this model, the activities of supported noble metal catalysts (Pt/Al₂O₃ and Pd/Al₂O₃) separately in removal CO as CO₂ gas phase are studied at isothermal conditions. A batch equation is used in this model to study the effect of reaction rate parameter k (sec⁻¹) on conversion processes at contact time $t = 2500$ (sec) and to control the path of gases from and the reactor cavity to indicate the effect of contact time. These results are confirming that the dissociated gases are removed by using catalysts to regenerate CO₂ molecules during the electrical discharge.

Key word: CO, CO oxidation catalysts, Noble Metal Reducible Oxide (NMOR), Pt/Al₂O₃, Pd/Al₂O₃.



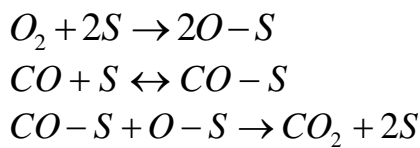
1-Introduction

CO oxidation catalysts have a long history of applications, so it is instructive to first consider the special requirements of the laser application. The removal of CO as CO₂ is accomplished via catalytic converter with the supported noble-metals Pt and Pd (i.e. Pt/Al₂O₃ and Pd/Al₂O₃ catalysts). The gas-solid form is a most important type of heterogeneous [1]. In this regard, numerous studies of the kinetics as well as investigations of the effects of supports and additives on

the kinetics of this reaction over supported catalysts have been reported.

Catalysts that have been tried as CO oxidation catalysts for sealed-off CO₂ lasers, include the following: Pt/SnO₂, Pd/SnO₂, Cu/CuO, Pt, Pd/SnO₂, Rh/SnO₂, Ru/MnO, Pt/MnO, Au/Fe₂O₃ and Au/MnO₂ [2]. These materials fall into a class of catalysts called "*Noble Metal Reducible Oxide*" (NMRO) catalysts. This class includes noble metals, which are dispersed over a metal oxide [3,4,5].

During oxidation of CO by O2, whether in the gas-phase (*homogeneous*) or over a catalyst surface (*heterogeneous*), two basic steps must occur: dissociation of the O2 molecule and formation of O-CO bond. These two steps usually occur in separate events. Over the surface of a catalyst, O2 must adsorb and dissociate and CO must adsorb next to and react with an O atom and replenish CO2 [6,7,8] as shown:



Where "S" is a site or area on the metal surface that can adsorb one CO molecule or one O atom.

In literature, there are many authors investigated the conversion of CO to CO2 experimentally in CO2 laser system [9,10]. On the other hand, there were few mathematical models in literature that describe the reaction kinetics for such system [11].

Therefore in this paper we report the behavior of first-order differential equation of CO oxidation over supported noble metal catalysts such as (Pt/Al2O3, Pd/Al2O3) and investigate the effect of reaction rate constant k (sec^{-1}) on CO2 regeneration at the same contact time from experimental results are used to test such model under isothermal conditions (see table 1)[12].

2- Numerical modeling of Conversion CO to CO2 by Using Batch Equation in CO2 Laser Systems.

1-Model assumption

For motivation a batch equation is used with analytical solutions for this purpose we assume the following:

- Batch operation system

- Reaction volume is constant (i.e. $dv/dt=0$)
- First-order reaction kinetics, $r = -kC_{CO}$

$$\frac{dC_{CO}}{dt} = -kC_{CO} \quad (1)$$

Notice that the time rate of change of component CO is only a function of the concentration of CO. Then equation (1) can be solved for isothermal operation, since C_{CO} and t are separable, to find:

$$\ln \frac{C_{CO}}{C_0} = -kt \quad (2)$$

$$C_{CO} = C_0 e^{-kt} \quad (3)$$

Where: -

C_0 is the initial condition for the concentration of CO ($mol.cm^{-3}$)

C_{CO} is the concentration of CO at any time ($mol.cm^{-3}$)

k is the rate constant (sec^{-1})

t is the space time (sec)

Also, the equation (2) for constant volumetric flow rate (Q) is useful in determining the space-time t for reaction rates that depend only on the concentration of one species.

Equation (3) can be represented as a function of conversion (x) for constant volume as shown:

$$C_{CO} = C_0(1 - x) \quad (4)$$

Using equation (3) together with equation (4), the conversion of CO at any time can be represented by:

$$x = 1 - e^{-kt} \quad ..(5)$$

Where: -

x is conversion of CO to CO₂ gas phase.

t is contact time (sec) .

k is the reaction rate constant (sec⁻¹).

3-Results and Discussion:

The simulation result of determining the activity of pt/Al₂O₃ and pd/Al₂O₃ in oxidizing the carbon monoxide, CO gas phase in sealed-off CO₂ laser system, is shown in figures (1) and (2), respectively. From these figures it was found that the activity of pt/Al₂O₃ in conversion of CO to CO₂ is more efficient than using pd/Al₂O₃ as a function of contact time t . From these figures, on the other hand, one can note that the conversion is increased approximately exponentially with increasing the reaction rate constant k (sec⁻¹) at the same contact time. These results are confirming that the removal of CO by using pt/Al₂O₃ catalyst is more efficient due to the thermal effects and trend of both CO and Pt to connect together as shown in figure (1). While removing CO with pd/Al₂O₃ catalyst is less active because of the trend of Pd surface to connect with O₂ for the harmony of electronic distributions of both O₂ and Pd as shown in figure (2). As shown from the results above the k is not truly a constant, but is merely independent of the concentration of the species involved in the reaction. It's almost always strongly dependent on temperature as shown in figures. This assumption is valid in most laboratory and industrial reaction and seems to work quite well.

4-Conclusions

The activity of supported noble metal catalysts such as (Pt/Al₂O₃ and Pd/Al₂O₃) depends on reaction rate parameter k (sec⁻¹) for each temperature at the same contact time. The different catalysts have different effects on alternative reaction paths. Also, the use of each catalyst (Pt/Al₂O₃ and Pd/Al₂O₃) had overcome the most important factor previously limiting the life of such lasers, i.e. the generation of O₂ and CO by the dissociation of CO₂ during operation and improved the activity of Pt/Al₂O₃ is more efficient than Pd/Al₂O₃ in removal of CO gas phase.

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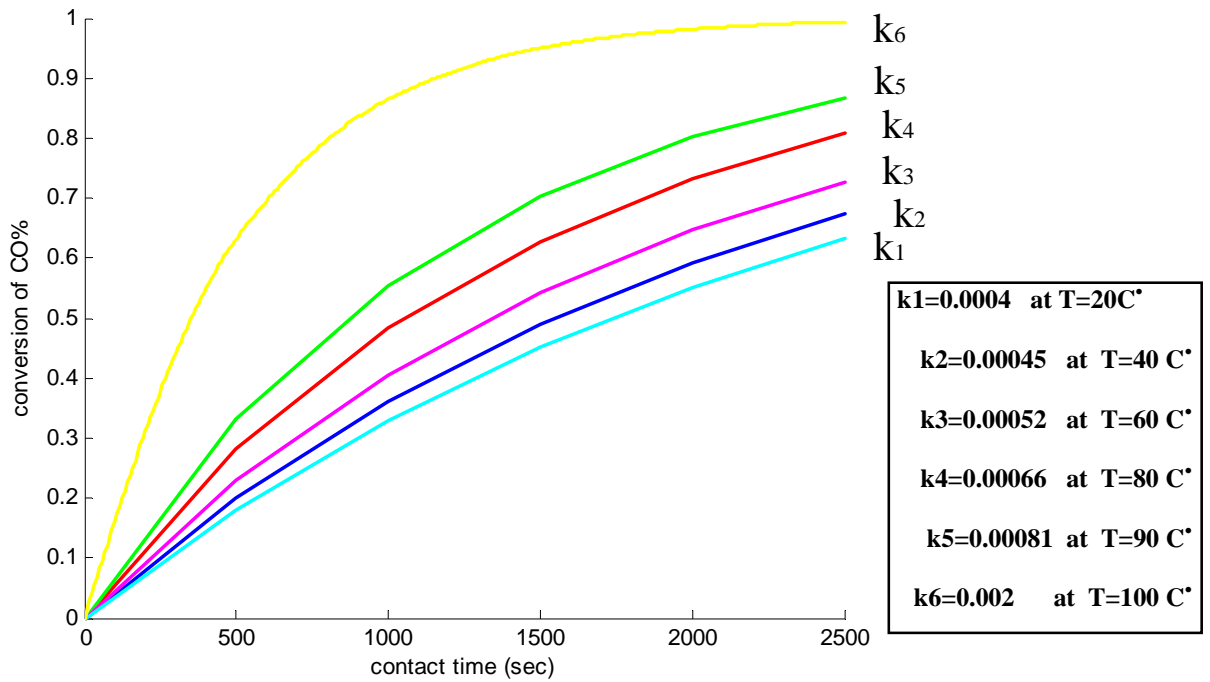


Figure 1: Conversion of CO to CO₂ with pt/Al₂O₃ catalyst as a function of contact time for different rate

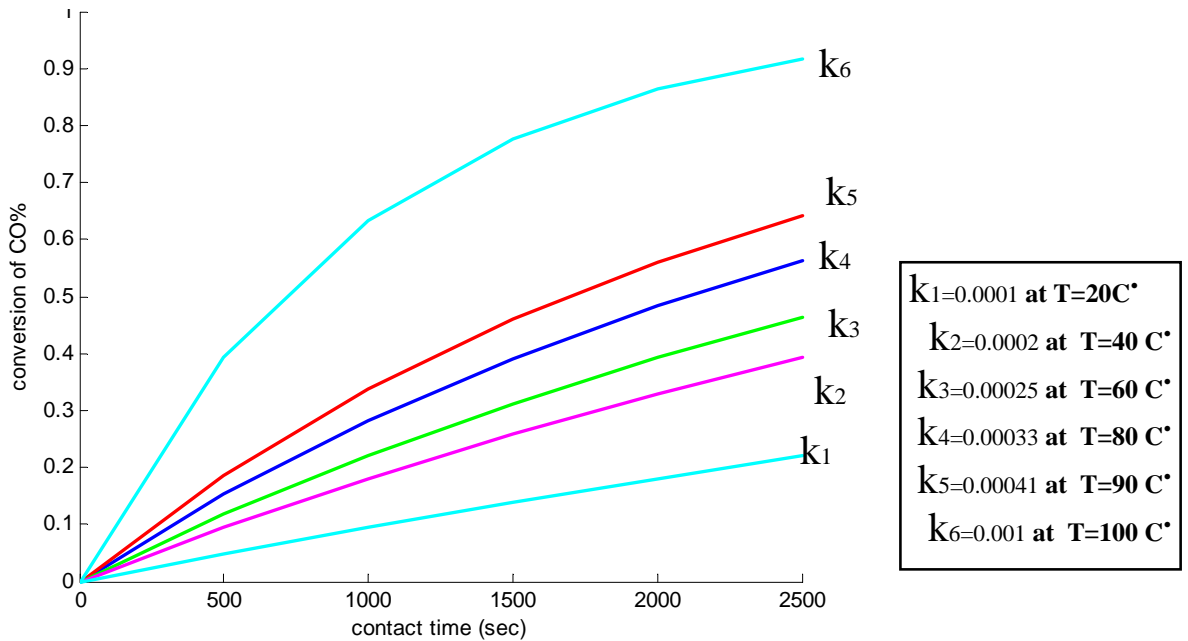


Figure 2: Conversion of CO to CO₂ with pd/Al₂O₃ catalyst as a function of contact time for different rate

Table (1): Catalysts properties [12].

<i>Catalyst properties</i>	Pt/Al₂O₃ catalyst	Pd/Al₂O₃ catalyst	Al₂O₃
Density $g.cm^{-3}$	1.12	1.13	1.113
Macroscopic volume $cm^3.g^{-1}$	0.66	0.64	1.08
Microscopic volume $cm^3.g^{-1}$	0.45	0.43	0.56
BET surface area $cm^2.g^{-1}$	17×10^5	16.9×10^5	18.9×10^5
Impregnation depth on Al ₂ O ₃ cm	3.9×10^{-2}	2.3×10^{-2}	X

