

# COMPUTER SIMULATION STUDY OF CO-O<sub>2</sub> CATALYTIC REACTION ON BODY CENTERED CUBIC LATTICE: COMPARATIVE STUDY. MONTE CARLO SIMULATION

\* A.U.Qaisrani, M.Khalid,  
\* Q.N.Malik & Q.N.Chohan.  
\*\* K.M.Khan

\*Department of Physics, Gomal University, D.I.Khan

\*\*Nuclear Physics Division, PINSTECH, Nilore, Islamabad

## Abstract:

The effect of different lattice sizes in monomer-dimer surface, sub-surface catalytic reaction is studied by computer simulation using Monte Carlo method. This reaction system has been studied on the surface and subsurface of body centered cubic structure, which extends to only two layers in the z-direction. The different cases have been studied for two different lattice sizes and results are compared.

## 1- Introduction

The process mentioned above is not only important for pollution control, but also serves as a model catalytic reaction. After extensive study it has been established fact that reaction mechanism is of a Langmuir-Hinshelwood (L-H) type in which the reactants go through reaction after adsorption [1,2]. Ziff, Gulari, first introduced it and Bars had [3] as a computer simulation model and is known as ZG model. [3] used the L-H type mechanism. In this model only simple square lattice was used. A CO-O<sub>2</sub> molecule is selected at random to come to the surface. If the selected molecule is O<sub>2</sub>, then two nearest neighbouring (nn) vacant sites are chosen from the lattice to adsorb it in atomic form. While CO can be adsorbed on one vacant site in the molecular form.

It is worth mentioning here that if the randomly selected site or one of the two nn sites is occupied the molecule bounces off the surface. This process is repeated. Whenever a molecule is adsorbed, all nn sites are scanned to produce CO(g) and all CO-O pairs are removed from the surface, which constitutes L-H reaction step. The reaction probability of CO is taken, as YCO and O<sub>2</sub> molecule is 1-YCO.

Khan et al.[4] have studied catalytic oxidation of CO on the surface and subsurface of a simple cubic structure. In this structure each surface site, has four nn sites on the surface and one nn on the subsurface. In order to study the subsurface impact they studied various reaction