Analysis and Simulation of the Automobile Pollution Control

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Abstract: - The development in the area of computer technologies has opened many computer applications/simulations. The computer simulation has provided an inexpensive approach to study the physical systems. These systems were very difficult and expensive to study through the two standard methods that are theory and experiment. Computer simulation has received an equal importance to that of these two standards. Researcher had applied computer simulation approach to study the physical systems. Green house effects and depletion of ozone layer are two well-known effects of air pollution. The exhausts of the million of vehicles plying the road consist mostly of oxides of poisonous gases. These oxides are more harmful in the presence of sunlight and water vapors, which after reactions produce photochemical smoke. This smoke attacks the respiratory systems of children and adults severely. It is estimated that about 60 % of nitrogen oxides contaminated air in Pakistan are emitted from the exhausts of automobiles. In most of the developed countries the use of catalysors in the exhaust system of the cars has become standard. The material coated on the catalysors act as catalysts in oxidizing the poisonous gases to non-poisonous gases. The threat of air pollution is consequently reduced considerably.
The current paper presents the computer simulation approach to understand the mechanism involved in the catalytic oxidation of NO. This simulation approach provides a basic concept of controlling of the automobile pollution. The proposed simulation model though is simple and has some limitations. It does not consider temperature effects and the calculations were restricted to limited lattice size. The crystal surface represented by a lattice was assumed to be a perfect one, which is not possible in actual practice. Apart from its limitations, the proposed model shows some very interesting results, which could help explain some of the intricacies of the actual process. It would also be interesting to expand this work to consider the other important reactions.

Key-Words: - Air Pollution, Poisonous Gases, Oxides, NO, CO, Chemical Smoke, Computer Simulation

1 Introduction

The two most well known effects of air pollution are Green house effect and depletion of ozone layer. While elsewhere in the world people are worrying about these problems, in Azad Kashmir and Pakistan scientists have yet to do comprehensive and meaningful research in this field. However, in the absence of any real data one can only guess the extent of damage caused in the main cities of Pakistan by air pollution.

Think about Lahore, a typical industrial city of Pakistan has witnessed a substantial decline in the air quality. During winter more than half the population goes down with sore eyes, throat irritation, lung infections and asthma. Apart from more than thousands of medium-sized industries, there are over a million vehicles especially motorcycles and Rickshaws plying the roads of Lahore? The exhausts of these vehicles [5] consist mostly of oxides of carbon, nitrogen and hydrocarbons. Carbon monoxide [1, 2] is known for its toxic effects on living beings. Carbon monoxide remains one of the most important causes of accidental and suicidal poisoning deaths. It reduces the oxygen-carrying capacity of the blood by binding to hemoglobin for car boxy hemoglobin (the affinity of hemoglobin for carbon monoxides being 200-300 times greater than for oxygen).

But their more insidious aspect is due to the fact that in the presence of sunlight and water vapors they react with the hydrocarbons to produce photochemical smoke [3, 4]. This smoke attacks the respiratory system of children and adults. Another aspect of these emissions is their reaction to produce ozone. The ozone corrodes rubber damages crops. In Pakistan, it is estimated that 60% of nitrogen oxide contaminated air is emitted from the exhausts of automobiles.

In most of the developed countries the use of catalysors [6] in the exhaust system of the vehicles has become standard. These catalysors have a

surface, which is surfaced with a combination of Rhodium and Platinum. These elements act as catalysts in oxidizing carbon monoxide (CO) to carbon dioxide (CO_2), while at the same time reducing the oxides of nitrogen to harmless nitrogen gas (N_2). The threat of air pollution is consequently reduced considerably [7].

2. Problem Statement And Proposed Solution

While the use of these catalysors [6] is on the increase in developed countries very little is known both experimentally as well as theoretically about the way reactions occur on the surface. An experimental study of these reactions involves working under ultra high vacuums and on very clean surfaces. The actual reactions on the other hand take place at atmospheric pressures and rough surfaces. Because of these differences in the nature of catalyst material and in pressure regimes, it is not certain if one can apply the information obtained experimentally to the actual conditions. Since the reactions on the surface are extremely complex, theoretical studies are also in their starting stages.

Ever changing the accession of the computers, the computer simulation technique has assumed and importance equal to that of theory and experiment. Certain physical systems, which are hard to study by these regular methods, are now being probed by computer simulation. We have utilized the computer simulation technique to understand the mechanism involved in the catalytic oxidation of NO. The catalytic oxidation of CO had already been explored by researchers [2], for our study we have chosen the simple two-component NO-CO system. For simplicity, we shall first develop one-dimensional model, then extend it to a more realistic two-dimensional model.

2 Chemical Reactions

In reality the reactions taking place on the surface of the catalyst are extremely complicated. For our study we have chosen the two simple components CO and NO. The simple catalytic reaction that falls in this category is the reduction of nitrogen oxide (NO) by carbon monoxide (CO). The surface will act as a catalyst and it will reduce the energy required for dissociation of Nitrogen from NO and helps in the formation of carbon dioxide by an easy combination of CO with O.

The reaction is as follow: -

CO-NO reaction:

$$CO\ (g) + S \rightarrow CO - S$$

$$NO\ (g) + 2S \rightarrow N - S + O - S$$

$$N - S + N - S \rightarrow N2\ (g) + 2S$$

$$CO - S + O - S \rightarrow CO_2\ (g) + 2S$$

A "(g)" signifies that the reactant is in the gaseous form. An "S" denotes a surface site. In this reaction CO molecule strikes the surface site and gets adsorbed on it only if the surface site is vacant. A NO molecule on the other hand on adsorption decomposes into its constituents (this is the role of the catalytic surface to help in dissociation of NO). A CO can combine with an O to form a CO2 gas molecule, which desorbs easily from the surface. There is an additional step where N combines with another N to form N_2, which desorbs from the surface.

4 Proposed Model and Computer Simulation

For computer simulation of the above reaction we propose the following model:

Consider a reservoir containing the two gases (reactants) in a given proportion. The reservoir is in contact with the catalytic surface. The surface is modeled by a square lattice (or linear lattice), each lattice site represents a possible site for the adsorption of reactants. For generality in what follows we will denote the two reacting species by X and Y_2 (X represents CO and Y_2 represents NO). The simulation starts by picking one reactant randomly with a probability, which is proportional to its concentration in the reservoir. Generating a random number RN lying between 0 and 1 does this. If RN < CX (where CX is the concentration of X species in the reservoir, it lies between 0 and 1) then an X atom is selected other-wise Y_2 is selected. A site on the lattice is also selected at random. This is again done by generating a random number RN such that 1<= RN <= LSZ2 (here LSZ2 is the number of site in the lattice). If the site selected is already occupied then the trial ends as the selected reactants bounces back from the surface. If however, the selected site is empty then either of the following two possibilities can occur.

(i) If initially X has been selected then this sticks to the empty site. The nearest neighbor of this particular site is scanned in a random fashion for the possibility of the presence of

(i.a) a Z (assume if Y_2 is dissociated then it forms Z-Y or N-O i.e. Z=N and Y=O) atom. If Z is present then X will bounce back.

(i.b) a Y atom. If Y is present

then XY (CO_2) is formed which is desorbed from the lattice surface leaving behind two empty sites.

(ii) If initially Y_2 has been selected then we need another empty site neighboring the selected for its adsorption, as Y_2 disassociates on striking the surface. The selection of the second sight next to the previously selected is also made randomly. If this random selection leads to an occupied site then the trial ends, however, if the adjacent selected site is empty the Y_2 is adsorbed onto the two sites in its disassociated form i.e. Z-Y. The nearest neighbors of Z and Y atoms are scanned in a random fashion. And

(ii.a) if the neighbors of Y atom are scanned in a random way to detect the presence of X. If X is located then XY (CO_2) is formed which desorbs leaving behind two empty sites.

(ii.b) if the neighbors of Z atom are scanned in a random way to detect the presence of Z. If Z is located then ZZ (N_2) is formed which desorbs leaving behind two empty sites.

Because the simulation involves a number of random processes it is also called Monte Carlo simulation. The number of trials equal to the total number of sites constitutes one Monte Carlo cycle; this will be a measure of our time. During one Monte Carlo cycle each site on the lattice has the probability of being selected once for the reaction.

5 Proposed Linear Lattice Surface Model

Consider first, a hypothetical linear lattice. We have assumed the first lattice site has as one of its neighbors the last site and vice versa (called Periodic boundary conditions). It is to insure that the lattice is an infinite one. Rest of the simulation proceeds as we have already described in the previous section

5.1 Program Variables and Their Definitions

A list of the major variables that are used in the program is given below.

- x represents the seed code for random number generation.
- cx is the concentration of X (lying between 0 and 1)
- lsz size of the linear lattice (maximum size=1600)
- ntim time measured in Monte Carlo cycles
- lat(i) specifies the location of the site i
- jpa(i) is the right neighbor of site i
- jma(i) is the left neighbor of site i
- ix counter to measure number of X atoms on a lattice
- iy counter to measure number of Y atoms on a lattice
- iz counter to measure number of Z atoms on a lattice
- ixy counter to measure the production of XY
- icx fractional coverage of X (lies between 0 and 1, obtained by dividing ix by lsz)
- icz fractional coverage of Z (lies between 0 and 1, obtained by dividing iz by lsz)
- icy fractional coverage of Y (lies between 0 and 1, obtained by dividing iy by lsz)
- icxy production of XY per Monte Carlo cycle
- sk defines the skip value for the printer

5.2 Results

The concentration of X (CX) was varied from 0 to 1 in steps of 0.01. The fractional coverage of X and Y as well as the production rate of XY was monitored as a function of time (Monte Carlo cycles). When the system achieved equilibrium, these values stabilize. It is seen that for CX < 0.4, the final state of the lattice is a poisoned one, the poisoning being due to X specie. For CX > 0.4 the poisoning is due to Y_2. In each case the coverage is 1 (except when CX = 0) and there is no production of XY. At CX = 0.4 the lattice does not poison. This is the only value for which we get continuous production of XY. The results are shown in Fig. 1. The poisoning time increases as we approach the point CX =0.4 from either side. Typical at CX = 0.2 and 0.39 the poisoning times are about 100 and 3000 Monte Carlo cycles respectively. For a linear lattice therefore we conclude that the final state of the system is always a poisoned one, except at the

point CX = 0.4 at which the reactions can proceed continuously.

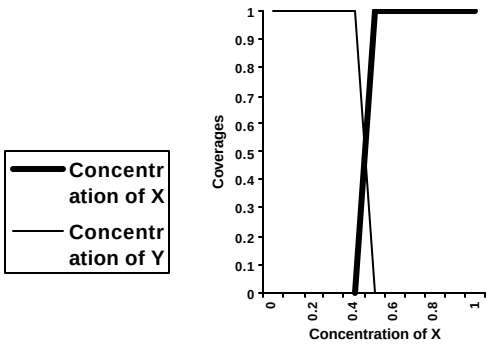

Figure 1: One Dimensional Lattice Coverage Vs. Feed Concentration of X.

5.3 Test of the Program

Considering some limiting cases for which the results are known or can be easily visualized tested the program.

(i) CX = 0, almost 85-90% of the lattice is covered by Y. Its random distribution on the linear lattice leaves some single vacancies.

(ii) At CX = 1, the lattice is entirely covered by X atoms.

(iii) We changed the program slightly so that both X and Y are mono atomic i.e. occupy single sites. Due to symmetry we expect the transition from X poisoned to Y poisoned to take place at CX = 0.5. This is exactly what we get. This also is a test for the program for X adsorption.

(iv) When the lattice status is obtained an X is never found sitting next to a Y.

6 Two Dimensional Lattice Surface Model

The program for one-dimensional lattice is straight forwardly extended to two dimensions. We consider a 40 * 40 square lattice. This means that there are 1600 sites on the surface. Each site now has 4 nearest neighbor sites rather than 2 as for linear case. The program is modified accordingly i.e. LAT (i) is replaced by LAT (i, j). Periodic boundary conditions are imposed in two directions. Program description remains the same as the previous section except that 4 neighbors are scanned to see whether XY is produced or not.

6.1 Program Variables and Their Definitions

The program variables are almost the same as those for one-dimensional program, with the addition of the following:

- lsz2 square of the lattice size (isz * lsz)
- lat(i,j) specifies the location of a site i,j.

6.2 Results

The concentration of (CX) was varied from 0 to 1 in steps of 0.1. The final equilibrium coverage of X and Y were noted. It is seen that for CX < 0.39 the lattice gets poisoned with X atoms i.e. coverage of X is 1 and that of Y is 0. For CX > 0.53 the lattice is again poisoned but this time by Y atoms. For the range 0.39 <= CX <= 0.53 the lattice does not get

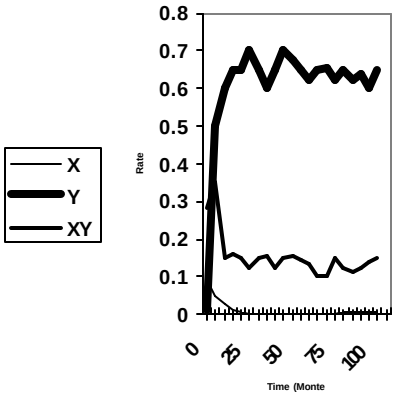

Figure 2: Coverages and Production Rate

poisoned, at least for 5000 Monte Carlo cycles. Within this range the coverages stabilize after some time to a certain mean value. Fig. 2 represents a typical graph showing how the coverages vary as Monte Carlo time in this region.

After ignoring the initial region we take a reading of coverages after every 10 Monte Carlo cycles. An average is obtained at the end of 5000 Monte Carlo cycles. If we ignore the initial 500 Monte Carlo cycles then each value of coverage is an average over 450 readings.

The production rate of XY is shown in Fig.3.

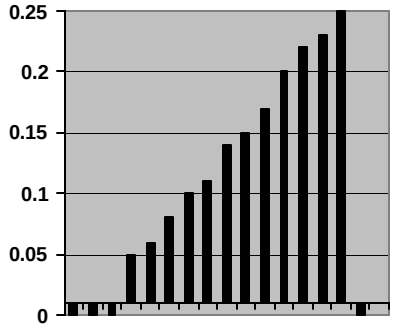

Figure 3: Production of XY

6.3 Test of the program

The program was tested in the following way:

(i) For CX= 1, the lattice is poisoned by X.

(ii) For CX = 0, the lattice is about 85-90% covered by Y with single vacancies distributed randomly.

(iii) For the case LAT (i,j) $\rightarrow$LAT(i) we generate the results of the one-dimensional lattice.

(iv) When Z-Y is replaced by monoatomic Y we get a reactive state only at CX = 0.5 (by symmetry). For CX < 0.5 the lattice is poisoned by X and for CX > 0.5 it is poisoned by Y.

(v) When the status of the lattice is obtained an X will never be found sitting next to a Y.

7 Proposed Model Limitations

The model we have presented is extremely simple. It ignores the following important points

(i) Diffusion of atoms on the surface

(ii) Desorption of atoms (molecules) other than XY

(iii) Temperature effect

(iv) Calculations were restricted to lattice containing 1600 sites with a maximum time of 5000 Monte Carlo cycles.

(v) The crystal surface represented by a lattice is assumed to be perfect; in actual practice this is never true.

8 Future Work

We are planning to implement the computer simulation approach in different areas of science i.e. medical, and other relevant areas. In human body there are a number of different reactions, which are taking place in the presence of different environments. It is very time consuming and involves a lot of financial resources to study and get certain results in these systems. We are interested in implementing computer simulation approach to get the desired results by reducing the overall costs (time and finance etc.) involved in studying these typical physical systems.

9 Conclusions

In spite of the severe limitations of the model we have shown that simulations in two dimensions give a range of feed concentration for which a steady production of XY (CO_2) can be maintained. This is an interesting result and could help explain some of the intricacies of the actual process. It would be interesting to expand this work to consider the some other important chemical reaction like the one, which we have discussed in this paper. A more realistic model could also be constructed by incorporating the process that we have ignored and discussed above in previous section.

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