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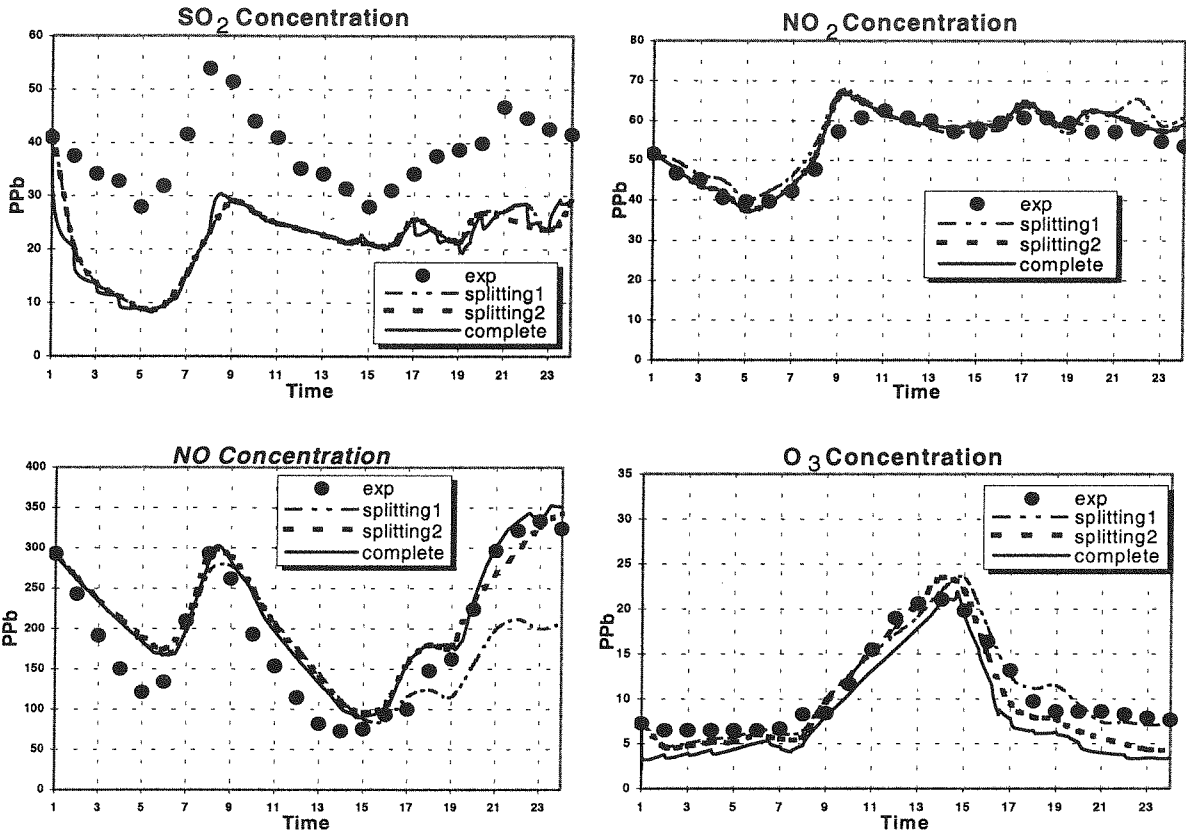
Figure (6) Fatemi daily variation of pollutants (1-D simulation model).
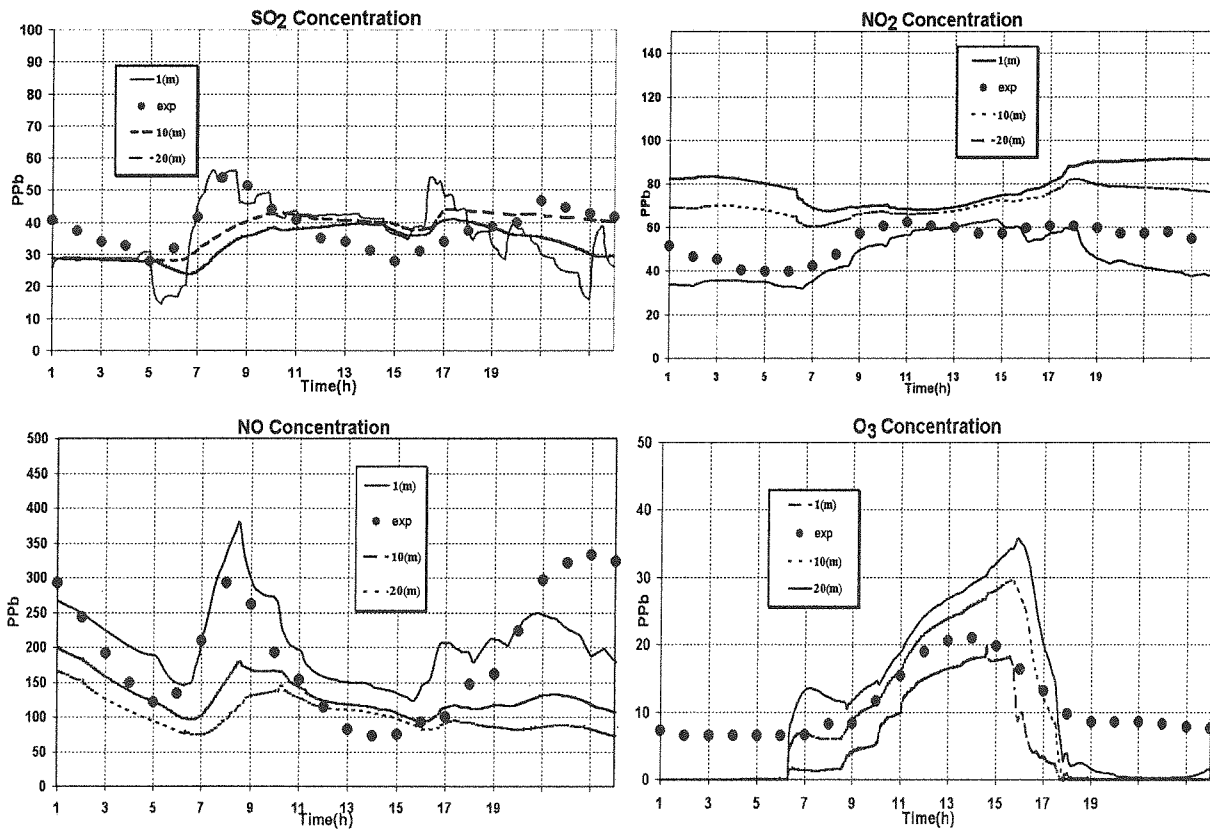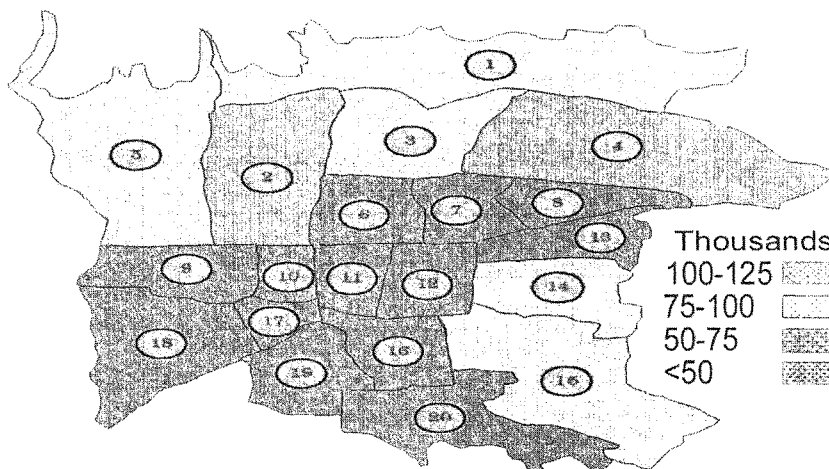

Figure (7) Fatemi daily variation of pollutants at 3 vertical height (3-D simulation model).

Distribution of Vehicle Fleet in
Municipality of Tehran

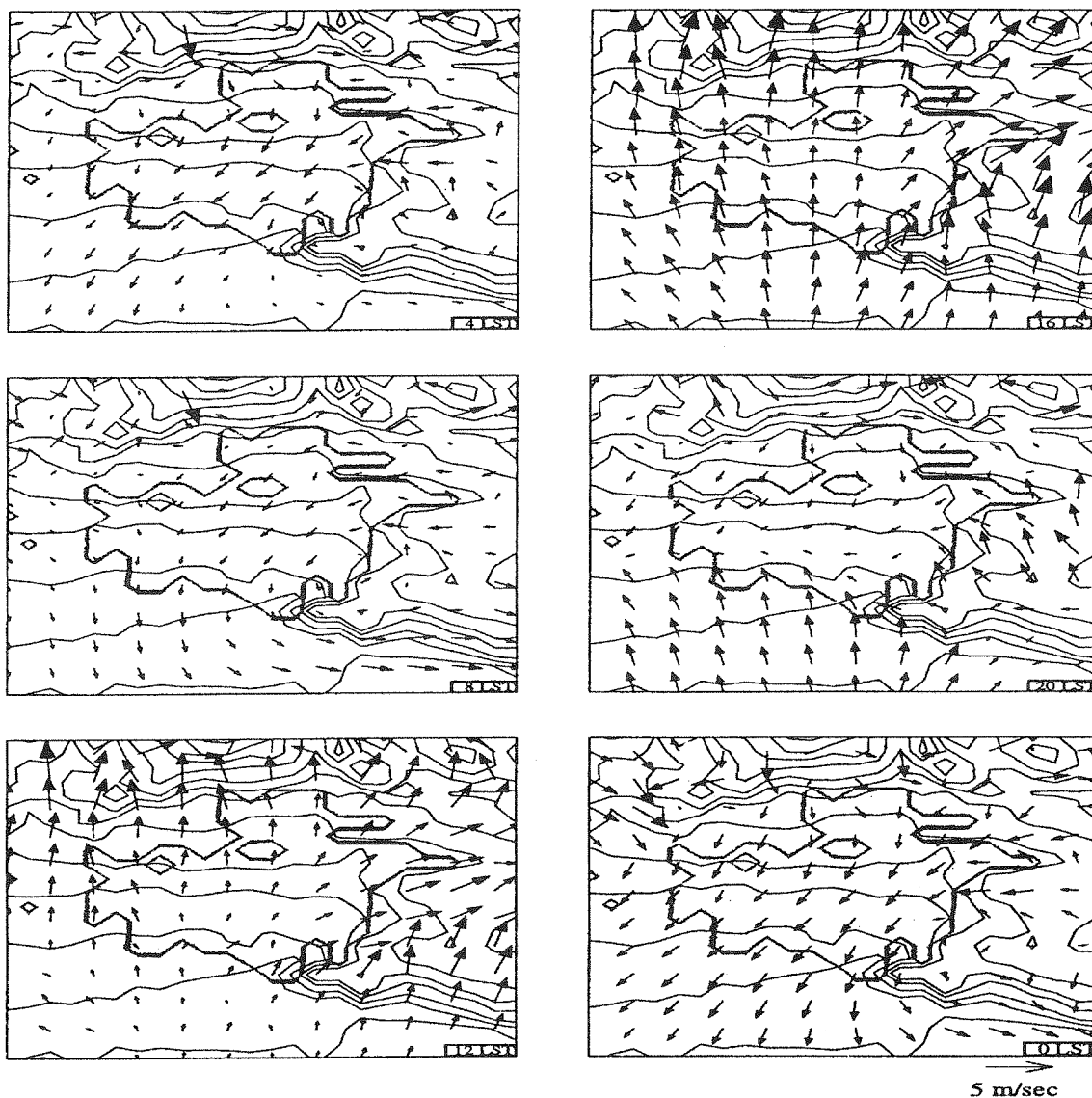Figure (4)-areas of Greater Tehran (AQCC).

5 m/sec

Figure (5) horizontal cross wind field at level 10 meters for urban area at local time with MEMO run.
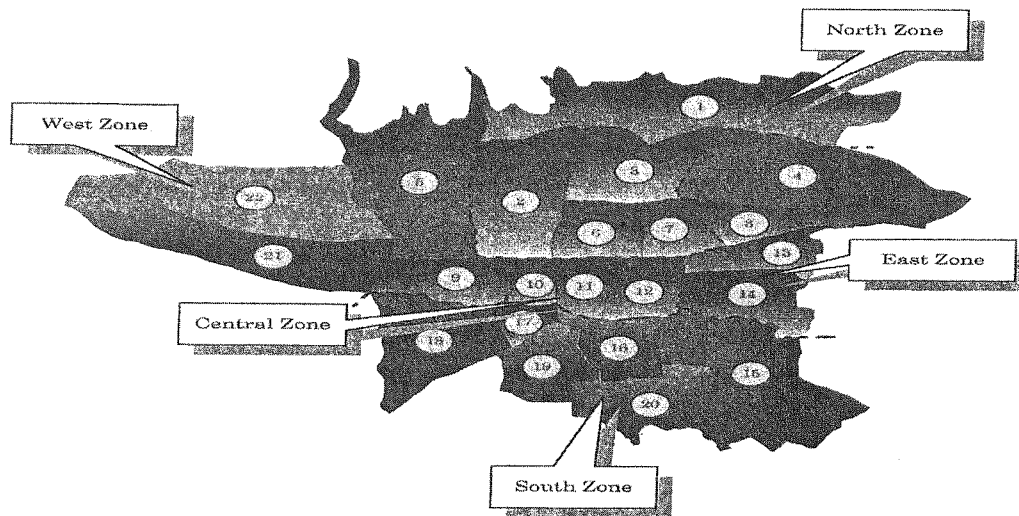
Figure (1) the concept of 5 zone and 22 districts of Tehran (AQCC).
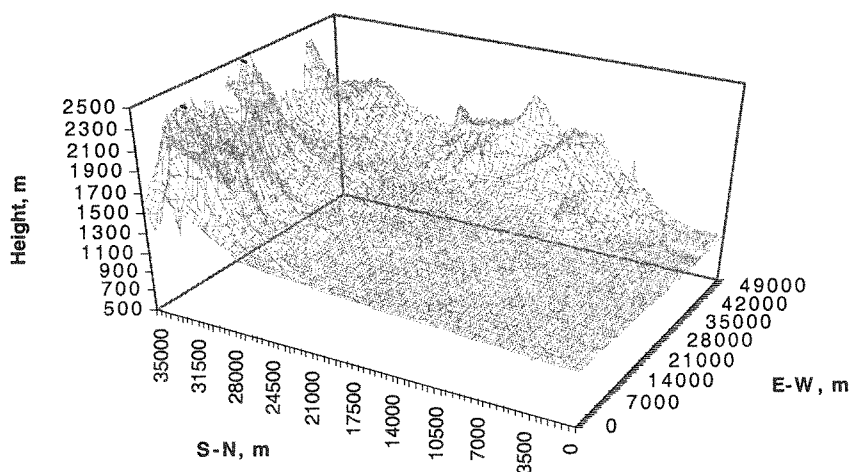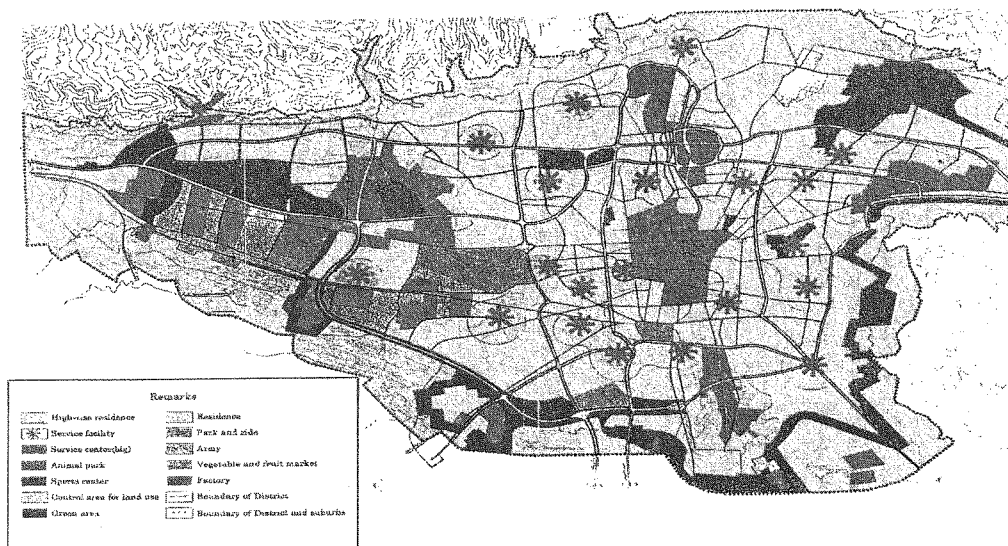

Figure (2) Topography of Tehran.

Figure (3) land use plan.

non splitting method by one-tenth of previous time step (splitting 2), therefore the results of splitting method are slightly less accurate than non splitting method but the results are acceptable.

Subsequently we would like to solve 3-D model for grater Tehran, but because of large network and high run time with existed computer which require long CPU time, therefore we must decrease number of grid point of the network (coarsen grid) or solve this model for partial urban area.

In this paper we have presented model for partial urban and compared with experimental data (fig 4). Fortunately, the simulation model predictions are comparable with the trend of the experimental data, and with further development of the model in near future, this computer simulation can be used effectively to predict pollution level for large urban area as a result of exact and actual input data (meteorology, topography, emission data). This model can provide a reliable tool for the decision makers to suggest solutions to the severe air pollution problem in Tehran.

Conclusion

Fig .6 shows that the increasing number of reactions and species has improved the results of the model. The non splitting model is capable of predicting the variation of concentration of pollutant with time by using over 114 reactions and 48 components. The splitting model is a little less accurate than non splitting model with the same time step, but is more adapted with less time step. 3-D simulation model with less CPU time in present computers with above description resulted in good prediction (Fig.7). 3-D simulation model could be improved by using the benefits of a three-dimensional hydrodynamic model (wind velocity field), real topography, and representative meteorological data.

<div align="center">

Nomenclature

</div>

$\langle\,\rangle$	Mean of variable in time and space	S	Volume emission of pollutants, $Kgmol/m^3/s$ Sink/source
[]	Operator	T	Time, s
A	Advection	U	Wind velocity vector, m/s
C	Concentration, $Kgmol/m^3$ (ppm or ppb)	U	Component of wind velocity, m/s
D	Molecular Diffusion Coeff., m^2/s Dispersion	v_d	Deposition velocity, m/s
E	Surface emission of pollutants, $Kgmol/m^2/s$	X	Vector of direction
G	Gas-phase chemistry	x, y	Horizontal direction, m
K	Eddy diffusivity, m^2/s	Z	Vertical direction, m
R	Rate of Reaction of species, $Kgmol/m^3/s$		

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Subscripts

</div>

0	Surface or lower boundary	dis.	Dispersion
1,...,N	Number of species	I	ith specie or direction
adv.	Advection	J	jth direction
ch.	Chemical Reaction	Max	upper boundary
D	Deposition	si.	Sink/source
Z	Vertical direction		

<div align="center">

Greek Letters

</div>

λ	Wet scavenge coefficient
Δ	Gradient

$$\langle C^1(t + Dt)\rangle = [A(Dt)]\langle C(t)\rangle$$
$$\langle C^2(t + Dt)\rangle = [D(Dt)]\langle C^1(t + Dt)\rangle$$
$$\langle C^3(t + Dt)\rangle = [S(Dt)]\langle C^2(t + Dt)\rangle \tag{13}$$
$$\langle C(t + Dt)\rangle = [G(Dt)]\langle C^3(t + Dt)\rangle$$

At symmetric series operator we have used:

$$\langle C(t + Dt)\rangle = [A(Dt/2)][D(Dt/2)][S(Dt/2)][G(Dt)]$$
$$[S(Dt/2)][D(Dt/2)][A(Dt/2)]\langle C(t)\rangle \tag{14}$$

The latest operator which is recommended [6] can work quite well and has probably the best performance.

Chemical Reactions and System Identifications

In the previous work [4], we eliminated the NMHCs species, rapid reactants and intermediate species that have been changed rapidly. In present model we add non-methane chemistry class and chemical equations belonging to them [10, 8]. The present model includes all classes and their related reactions. we checked this reactions with carbon band mechanism 4 (CBM4) and SAPREC97[2] based on about experience the best reaction terms are selected to run photochemical simulation model.

Results

we have compared the non splitting Eulerian model and splitting methods with the previous model [4]. In order to study the effect of the large number of reactions on the type and concentration of pollutants, the three-dimensional model primary is reduced to one dimension, with variable grid spaces increasing from surface to mixing layer height. In this one-dimensional Eulerian model, the number of reactions and species from about 50 and 21 increases to 108 and 48 respectively. One-dimensional dispersion model, including chemical reactions is solved by Crank-Nicolson method in the vertical direction, with variable grid size (total 43). K_{zz}, the vertical eddy diffusion coefficient, is used to consider the effect of dispersion [9].

Fig 3 shows the daily variation of the concentrations of NO, NO_2, SO_2, CO, and O_3 close to the surface during one working day and compare them with articles [4]. Based on the number and amount of emissions from each vehicle, daily variations of the pollutants are estimated for the working days and used as the dominant moving pollutant sources. Average data for three months (Municipality of Tehran, et al. 1997 that is closely to daily variation of the concentrations) was available to compare the predictions of model and actual data. Appreciable closeness between the predictions and the experimental data is obtained. The discrepancy between the experimental results and the simulation predictions can be attributed to the fact that data averaged over three months was used, the exact meteorological conditions were not employed and the model was one-dimensional. The experimental and predicted results show trends corresponding to the morning (6-7 AM) and evening (4-5 PM and 8 PM) traffic peak in all the Fig 4.

In order to study the validity of solving the model by the splitting method, it has been compared with non splitting method. The results are shown in Fig. 6 for NO, NO_2, CO, SO_2, and O_3 components respectively. These figures show that the accuracy of splitting method (splitting 1) is less than the non splitting method. The results of splitting method shall be near

$$\frac{\partial \langle C_i \rangle}{\partial y} = 0 \quad : y = 0, y = y_{max} \tag{7}$$

$$\frac{\partial \langle C_i \rangle}{\partial t} + u_j \frac{\partial \langle C_i \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} K_{jj} \frac{\partial \langle C_i \rangle}{\partial x_j}$$
$$+ R_i\left(\langle C_1 \rangle, ..., \langle C_N \rangle, T\right) + S_i(X, t) - v_d \langle C_i \rangle \quad : z = 0 \tag{8}$$

$$\frac{\partial \langle C_i \rangle}{\partial z} = 0 \quad : z = z_{max} \tag{9}$$

Surface removal velocity (v_d) is function of pollutant and land species [10].

Initial concentration for pollutant species in simulation is obtained from previous computer run assuming zero concentration at start.

For wet scavenge condition we add $- l_i \langle C_i \rangle$ to right side of main equation that (CAMx, ver. 3.00, Dec2000):

$$l_i = 3 * 10^{10} k_i R \tag{10}$$
$R = Rainfall$ \qquad k= Henry's law solubility

The numerical method used in this study is the finite difference method in which the expansion of equations and their solving have been carried out using the Crank-Nicolson, under-relaxation iteration and time adaptive method that were coupled with nonlinear reaction. These equations were solved by two way, bi conjugate and ADI method.

Operator Splitting

Operator splitting is the most popular technique for the solution of equation (3) . The basic idea is, instead of solving the full equation at once, to solve independently the part of the problem corresponding to the various processes and then couple the various changes resulting from the separate partial calculations, therefore chemical transport models are characterized by advection operator, diffusion operator, gas-phase chemistry operator, aerosol operator, and sink/source operator. We used the symmetric series splitting operator scheme for the solution of the atmospheric model equation. Therefore equation (4) at parallel form is:

$$\frac{\partial \langle C_i \rangle}{\partial t} = \frac{\partial \langle C_i \rangle}{\partial t}\bigg|_{dis.} + \frac{\partial \langle C_i \rangle}{\partial t}\bigg|_{ch.} + \frac{\partial \langle C_i \rangle}{\partial t}\bigg|_{si.} + \frac{\partial \langle C_i \rangle}{\partial t}\bigg|_{adv.} + \frac{\partial \langle C_i \rangle}{\partial t}\bigg|_{uns.} \tag{11}$$

$$\langle C(x, y, z, t) \rangle = \langle C(x, y, z, t) \rangle +$$
$$\left[[A(Dt)] + [D(Dt)] + [G(Dt)] + [S(Dt)] + [W(Dt)] \right] \langle C(x, y, z, t) \rangle \tag{12}$$

that:

[A]: Advection operator \qquad [G]: Gas-phase chemistry operator
[D]: Diffusion operator \qquad [S]: Sink / Source operator
[W]: Wet scavenge operator

For example, the advection operator is U. $\langle C_i \rangle$. Another approach, which can work well, is series operator:

It must be noted that only a well-tested and well-calibrated simulation model can provide accurate answers to the questions relating to the future of air pollution and its control in Tehran. Air pollution in mountainous city, with high radiation, greatly depends on photochemical reactions and often the amount of ozone in such conditions is high. The atmospheric features of the mountainous city of Tehran (dry and warm climate), together with its specific topography require special investigation of these phenomena. especially, the presence of the strong inversion layers at most times of the year, and weak local winds result in little dispersion of pollutants on large scales.

The purpose of initiating this study has been the investigation of the mechanisms for diffusion, transfer and reaction of pollutants and an attempt will be made to consider all the meteorological situations as well as the effect of the variation in height and the existing reactions across Tehran. In present paper, however, most part of the chemical reactions present in the atmosphere, emission source, removal (wet & dry), diffusion and convection of pollutants will be considered in the context of a 3-dimensional model. The topographic map of Tehran, which is surrounded from two sides by mountains, is shown in Fig.2.

Chemical-Dispersion Model Equations

The flow of air in the atmosphere, however, is turbulent. Due to the random nature of the turbulent flow, these equations cannot be solved directly [7]. This problem can be solved by average spatial and temporal from mass balance Equation, defining eddy diffusion coefficient and disregarding the molecular diffusion (being insignificant compared to the eddy diffusion coefficient) as follows:

$$D_i \frac{\partial^2 \langle C_i \rangle}{\partial x_j^2} \quad \frac{\partial}{\partial x_j}\langle u_j C_i \rangle \tag{1}$$

$$\langle u_j C_i \rangle = - K_{jk} \frac{\partial \langle C_i \rangle}{\partial x_k} \qquad : \qquad j = 1,2,3 \tag{2}$$

$$\frac{\partial \langle C_i \rangle}{\partial t} + u_j \frac{\partial \langle C_i \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} K_{JJ} \frac{\partial \langle C_i \rangle}{\partial x_j} + R_i\left(\langle C_1 \rangle,...,\langle C_N \rangle, T\right) + S_i(X,t) \tag{3}$$

$$\frac{\partial \langle C_i \rangle}{\partial t} + \bar{u}\frac{\partial \langle C_i \rangle}{\partial x} + \bar{v}\frac{\partial \langle C_i \rangle}{\partial y} + \bar{w}- \frac{K_{zz}}{z}\frac{\partial \langle C_i \rangle}{\partial z}$$
$$= K_{xx}\frac{\partial^2 \langle C_i \rangle}{\partial x^2} + K_{yy}\frac{\partial^2 \langle C_i \rangle}{\partial y^2} + K_{zz}\frac{\partial^2 \langle C_i \rangle}{\partial z^2} + S_i(x,y,z,t) + R_i(\langle C_1 \rangle,...,\langle C_n \rangle) \tag{4}$$

$$C = C_{initial} \quad : t = 0 \tag{5}$$

$$\frac{\partial \langle C_i \rangle}{\partial x} = 0 \quad : x = 0, x = x_{max} \tag{6}$$

Splitting and Non Splitting are Pollution Models Photochemical Reactions in the Urban Areas of Greater Tehran Area

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Abstract

During the past years, one of the most important problems has been air pollution in urban areas. In this regard, ozone, as one of the major products of photochemical reactions, has great importance. The term 'photochemical' is applied to a number of secondary pollutants that appear as a result of sun-related reactions, ozone being the most important one. So far various models have been suggested to predict these pollutants. In this paper, we developed the model that has been introduced by Dabir, et al. [4]. In this model more than 48 chemical species and 114 chemical reactions are involved. The results of this development, showed good to excellent agreement across the region for compounds such as O_3, NO, NO_2, CO, and SO_2 with regard to VOC and NMHC. The results of the simulation were compared with previous work [4] and the effects of increasing the number of components and reactions were evaluated. The results of the operator splitting method were compared with non splitting solving method. The result showed that splitting method with one-tenth time step collapsed with non splitting method (Crank-Nicolson, under-relaxation iteration method without splitting of the equation terms). Then we developed one dimensional model to 3-D and results were compared with experimental data.

Keywords

O_3, NO_x, CO, SO_2, Photochemical Reaction, 3-D Eulerian Model, Splitting Model, Secondary Reaction.

Model Description

Computer simulation and mathematical modeling of the phenomena of air pollution are still considered as a developing branch of science. In the course of the recent decades the complexity and size of the computer models, as well as the development of computers, have been enhanced rapidly. The scales and sizes of the networks used for air pollution models have been presented by Seinfeld [9].

In spite of these developments, some areas like Tehran (fig. 1) still need special consideration with regards to their specific conditions (unique meteorology, topography, being surrounded from two sides by mountains (fig. 2) [1,8], various land use (fig. 3), emission sources profile (fig, 4), and low wind velocity (fig. 5). Air pollution models are the on¹⁻ practical and objective tools that can answer the problem of air pollution in the city of ᵀ