Coupled Receptor-Dispersion model evaluation for the assessment of area source emission rate

N Anu, M S G Nandagopal, V Aneesh and N Selvaraju*
Department of Chemical Engineering, National Institute of Technology Calicut, Kozhikode-673601, Kerala, India

Received 30 August 2014; revised 12 January 2015; accepted 26 March 2015

Atmospheric pollution is a major disaster in the current century. The geometry of pollutants emission from various sources has been categorised as point, area and volume. Particulate matters (PM_{10} & PM_{2.5}), gaseous pollutants and volatile organic carbons (VOCs) are the significant pollutants from various source types due to natural as well as anthropogenic activities. These pollutants once entered into the atmosphere get transport due to the meteorological aspects and other reasons. Hence the cause effect of these significant species may adversely generate negative impacts on the environment called receptors. The current research work focused on the prediction of emission rate (Q, unit/sec) from an area source through a combined receptor-dispersion (shear) model analysis. The Shear model coupled with chemical mass balance receptor model will produce better emission rate estimation from an area source such as agricultural land. For this vertical mixing height (z) in the dispersion model has been considered as 2 m and the area has been divided to 100 strips of width 10 m. Shear model predicts the concentration of pollutants which is emitted from an area source. Chemical mass balance receptor model can estimate the contribution of these sources at far distance say 1000 m from the source of emission. The results obtained from these distinct approaches have been cordially assessed for refining dispersion model parameter such as emission rate (Q, unit/sec) using coupled receptor-dispersion (area source) model. The observation was adequate for error in the emission rate increases as receptor concentration varies for 20%, 40%, 60% and 80% in both objective functions J_3 and J_4 considered. The results obtained were clearly suggests the individuals to make use of the coupled model approach for a better pollutant emission management at the location.

Keywords: Air pollution, Receptor model, Shear model, Emission rate, Receptor concentration.

Introduction
Atmospheric pollutants (Particulate matters and gases) emitted from different sources may disperse and deposit at various locations due to meteorological aspects, emission rate from sources etc. Open field burning^1, mining^2 and solid waste dump yard^3 act as sources of ground level pollutant emission to the atmosphere. Hazardous air pollutants due to the partial burning of biomass and solid waste causes severe health problems in human being and damage to the building structures, which leads to the discrepancy of an aesthetic environment^4,5,6. Atmospheric stability due to wind turbulence, temperature, elevation etc. leads to the bulk transport and its dilution of atmospheric pollutants. Transportation and dilution of pollutants at a far distance from the generation site has better solution for the public health impacts and implementation of emission regulation policies. Dispersion model such as ADMS and AERMOD on local scale performance can predict long-term mean concentration of pollutants at the downwind distance. The dispersion equations used in the model to compute averaged mean concentrations for different averaging periods are assumed to apply to short-term peaks during an averaging period^7. In general the ground level sources are those emission from mobile sources, small point sources (small production plants, gasoline stations, and waste treatment sites), and area sources like solvent use, agricultural activities^8, stockpiles and lime stone quarries^9. Ainsile^10 developed a source area model for population exposure to develop strong intense pollution maps due to the dispersion and advection properties of pollutants at various stability criteria. It has been reported that approximately 78% of the collected municipal solid waste (MSW) in China has been disposed during 2010, mainly practiced through landfill, composting and incineration. The characteristics of air pollutants and greenhouse gases discharge vary substantially among different MSW disposal methods due to global warming
warrants particular attention throughout the world, a series of air pollutants (including greenhouse gases, odorous gases, PCDD/Fs, heavy metals, PM,) discharged from waste disposal and treatment processes have become one of the new significant emerging air pollution sources, which arousing great concerns about their adverse effects on surrounding ambient air quality and public health. These emissions discussed above have the general property that generate from a ground level area can disperse and transport through air and deposit somewhere (known as receptor).

There might be so many pollutant sources from an area with distinct emission characteristics and rate which have to be optimized through the evaluation of the receptor concentrations. In coupled receptor-dispersion model the error between receptor concentration data from field study and that one predicted by area source model by various objective functions evaluation

**Gauss dispersion model**

Gauss developed a model to predict the concentration of pollutants emitted from a point source at a downwind distance when the input parameters available. The input parameters are emission rate \( Q \), average wind velocity \( u_0 \), standard deviation in the horizontal \( \sigma_h \) and vertical \( \sigma_v \), distance, height of the point source \( h \), height of the receptor \( h_r \) where the pollutants get settled. The modified forms of this dispersion model for a line source and area source were also performed to evaluate the effect of these sources cause pollution at various locations in and around by varying the consequent variables in the model. Due to the mathematical difficulties associated with line and area source models formulated from the Gauss dispersion model to evaluate the long term mean dispersion concentration in specific locations such as runways and terminal areas, complex numerical integration method has been developed to predict the receptor concentration. Burning biomass waste, households, e-waste etc. causes the transport of particulate matter and gaseous pollutants. Based on the wind turbulence and direction they might dilute and transport to long distance, which can reduce the strength of the pollutants or odor at the source itself. Modified Gauss dispersion model for area source pollutant concentration in the atmosphere has been developed to determine the dispersion characteristics of pollutants from a low level (ground level) emission sources such as agricultural land. Selvaraju and Pushpavanam have observed two distinct objective models combined with modified assumptions to estimate the emission rate from various point sources at the downwind locations (receptors). The same approach has been evaluated through an accurately predicted concentration from an area source model coupled with chemical mass balance receptor model to estimate the optimum emission rate by minimizing the error between source contribution as well as receptor concentration estimates from both the models. Anu et al. carried out an optimization approach using genetic algorithm in CMB model for the refined source contribution estimation. In the current research work coupled receptor-dispersion (Shear) model approach has been illustrated which uses the information of emission inventory estimates as well as receptor concentrations to arrive at a more accurate value of emission rates which contribute to ground level pollution and reflect the pollution levels at downwind location.

**Materials and Methods**

**Area source model**

General form of area source model for dispersion of atmospheric particles has been derived based on the Gaussian plume dispersion model with the assumption that the effective height in the vertical direction \( z \) as zero. The concentration of pollutants dispersed in air has been better explained by the Shear model than any other area source models such as Smith model and Parker model. In Shear model, according to the height near the ground level changes the wind velocity also change, that cause shear force between the atmospheric layers. Hence change in wind velocity near the ground level become significant while calculating the dispersion and transport of pollutants. The area source model used to obtain the total concentration \( C(x,z) \) at a downwind distance \( x \) due the \( i \) number of strips of width \( X \) at a height \( z \) above the ground is termed as Shear model, which is given by Equation 1.

\[
C(x,z) = \sum_{i=1}^{Q} \frac{u_i e^{-(i-1)B \exp(B \cdot x)+D (i/\Gamma(z/2))^{\gamma(z/2)}}}{\Gamma(s) A} \text{ for } z>0 \quad \ldots (1)
\]

Where, \( C \) = downwind concentration (unit/m³), \( Q \) = emission rate of pollutants (units/s), \( A = \Gamma(s) \), \( \Gamma(s) = \text{gamma function of } s \), \( B = -u_i z^i / (a_i \times K_i) \), \( D = \Gamma(s,(-B/x)) \), \( a = (m-n+2) \), \( x = \text{downwind distance} \).
distance (m), \( z \) = vertical distance (m), \( n \) = exponent of power law velocity profile, \( m \) = exponent of eddy diffusivity profile, where \( m = 1 - n \), \( s \) = stability parameter based on \( m \) and \( n \), \( s = (m+1) \), \( u_1 \) = wind velocity at a reference height \( z_1 \) (m/s), and \( K_1 \) = diffusivity constant at a reference height \( z_1 \). An area source configuration was considered based on low or ground level releases with no significant plume rise (for example contaminated site, mining site, solid waste dump yard etc) with five emission sources namely S1, S2 S3, S4 and S5 shown in Fig.1.

The various stability criteria by Pasquill are given in Table 1 and atmospheric stability criteria for simulating the model were assumed to be 'stable'. The predicted concentration from the area source model has been back calculated using MATLAB 2008a. The concentration predicted can be used as receptor concentration and combined with chemical mass balance receptor model. The emission rate \( (Q, \text{unit/sec}) \) can be made refined using a combine approach of receptor model and area source dispersion model to predict the concentration more accurately.

### Receptor model

Receptor model such as chemical mass balance (CMB) on the other hand can be used to determine contributions of sources to pollution levels in a location. The data of speciation analysis of particulate matters collected and the profiles (composition) of sources prevalent in a region are used to determine source contributions to pollution levels in that particular location (receptor). Receptor modeling techniques such as CMB, positive matrix factorization (PMF) and Unmix are based on statistical methods and have been used extensively in the past\(^{21,22}\). CMB needs knowledge of prevalent sources in a region and their source profiles. The success of CMB is determined by the accuracy of the source profiles and the receptor concentrations. In dispersion modeling emission rate of various sources together with meteorological conditions are used to estimate the concentration (contributions) at a point. The actual emissions may be significantly different from the estimated emissions and this can give rise to significant differences between the dispersion model predictions and experimentally measured values of concentration levels\(^{23}\). In addition the meteorological conditions measured at a point may not be representative of that existing in a region and this can result in erroneous predictions. Hence, the use of hybrid or combined approaches to determine the differences or inaccuracies in the results generated through the individual approaches. Qin and Oduyemi\(^{24}\) used a dispersion model to predict contributions of vehicle emissions incorporated along with PMF receptor model. Kumar \textit{et al.}\(^{25}\) combined factor analysis-multiple regressions with dispersion modeling to predict concentrations and estimate apportionment factors to match monitored data.

![Fig. 1—Location of distinct emission sources (S1, S2, S3, S4 and S5) relative to receptor location and wind direction in an area.](image)

<table>
<thead>
<tr>
<th>Surface wind speed, m/s</th>
<th>Strong Day time insolation</th>
<th>Moderate</th>
<th>Slight Night time conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Thin overcast or ( \geq \frac{1}{2} ) cloudiness(^*)</td>
</tr>
<tr>
<td>&lt;2</td>
<td>A</td>
<td>A-B</td>
<td>B</td>
</tr>
<tr>
<td>2</td>
<td>A-B</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>4</td>
<td>B</td>
<td>B-C</td>
<td>C</td>
</tr>
<tr>
<td>6</td>
<td>C</td>
<td>C-D</td>
<td>D</td>
</tr>
<tr>
<td>&gt;6</td>
<td>C</td>
<td>D</td>
<td>D</td>
</tr>
</tbody>
</table>


* Applicable to heavy overcast day or night

\(^*\) The degree of cloudiness is defined as that fraction of the sky above the local apparent horizon that is covered by clouds.
Coupled Receptor-Dispersion (Area source) model

Defining objective functions

To obtain the minimum emission rate from a source there must an objective function to be defined, which has been attained from the difference between receptor concentration from experimental analysis and that predicted by the dispersion model should be minimum. Hence the first objective function to minimize this error has been defined by the Equation 2.

\[
\text{Minimize } Q_1 = \| R_{\text{Exp}} - R_{\text{Dis}}(Q) \| \quad \cdots (2)
\]

Here the emission rates of the different sources ‘Q’ are found such that the difference between the experimental values of the receptor concentrations ‘R_{\text{Exp}}’ and that predicted from dispersion modeling ‘R_{\text{Dis}}’ is minimized. The latter is dependent on ‘Q’ the emission rates of different sources.

A second choice for the objective function is to find ‘Q’ such that the difference between source contributions from the dispersion model and that of the receptor model has been minimized and given as Equation 3.

\[
\text{Minimize } Q_2 = \| S_{\text{Dis}}(Q) - S_{\text{CMB}} \| \quad \cdots (3)
\]

Where,

\( S_{\text{Dis}} \) is the source contribution from dispersion model

\( S_{\text{CMB}} \) represent the source contributions from receptor model

When the objective function contains the details of only the deviations in the predicted or experimental receptor concentrations or source contributions as in Equations 2 and 3 the optimization scheme may converge to multiple solutions corresponding to local minima. To discriminate between these solutions and obtain a physically realistic elucidation the deviation of the emission rates from emission inventory estimates is included in the objective function. This helps us to gravitate towards a unique physically realistic solution in the optimization problem. Thus the two objective functions then are modified as Equations 4 and 5.

\[
\text{Minimize } Q_3 = \| Q - Q_m \| + \| R_{\text{Exp}} - R_{\text{Dis}}(Q) \| \quad \cdots (4)
\]

\[
\text{Minimize } Q_4 = \| Q - Q_m \| + \| S_{\text{Dis}}(Q) - S_{\text{CMB}} \| \quad \cdots (5)
\]

Execution of the model

The above defined objective functions were implemented in the MATLAB 2008a to obtain the converged emission rate from an area source coupled with CMB model. For this the emission rate from various points in an area has been assumed. The parameters for the area source model were, exponent of power law velocity profile for Stable atmospheric condition \( m = 0.7 \), diffusivity constant at a reference height \( z_1 \) for Stable condition \( K_1 = 0.993 \), vertical distance \( z = 2 \text{ m} \), wind velocity at a reference height \( u_1 = 1 \text{ m/s} \), Strips width \( X = 10 \text{ m} \) and the number of strips has been taken as 100 so that the downwind distance \( x \) will be 1000 m.

Algorithm for execution of the model using the objective functions \( J_3 \) and \( J_4 \) has been shown in Fig. 2 and Fig.3. It was assumes an initial guess of the emission rates to validate the algorithm. To carry out the multivariable optimization, MATLAB subroutine ‘fminsearch’ has been used in the model execution. Both the objective functions \( J_3 \) and \( J_4 \) are analyzed. For \( J_3 \) and \( J_4 \) the base values of ‘Q’ were used to find concentrations \( R_{\text{Exp}} \) (contributions \( S_{\text{CMB}} \)) and ‘Q’ was iterated upon. It was found that the
algorithm converges to the base value of emission rates used in generating the synthetic data set for different choices of initial guess ‘$Q$’. This was true for both objective function $J_3$ and $J_4$.

**Results and Discussion**

The default values of the emission rates were assumed initially and receptor concentrations have been generated for a particular meteorology conditions by Equation 1 to illustrate the performance of the algorithm. The receptor concentrations are then made realistic by adding or subtracting a random error to the ideal values generated. A uniform distribution of random error has been used for this. This represents a realistic experimental data which would contain errors. The percentage of error in this data set was changed to different levels from 20 to 80 percent. This means that when the error level is 20 % the values lie within ±20 % of the base value. The algorithm was then used to estimate the emission rates of the different sources by minimizing the error using the two different objective functions as Equations 3 and 4. The base value of ‘$Q$’ used to generate the data set ‘$R$’ is the same as the converged value when there is no error. When perturbations are imposed, the emission rates to which the algorithm converges are shown in the Table 2 and 3. It was observed that as the error percentage increases, the emission rates estimated deviate significantly from the base values.

**Conclusion**

In the current research work coupled receptor-dispersion (Shear) model approach has been illustrated which uses the information of emission inventory estimates as well as receptor concentrations to arrive at a more accurate value of emission rates which

<table>
<thead>
<tr>
<th>Variation in R</th>
<th>Q converged</th>
<th>Error Q</th>
<th>Objective Function $J_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.2000</td>
<td>0.0000</td>
<td>0.3824</td>
</tr>
<tr>
<td>20%</td>
<td>0.4877</td>
<td>0.0742</td>
<td>0.6291</td>
</tr>
<tr>
<td>40%</td>
<td>0.5885</td>
<td>0.1364</td>
<td>1.0382</td>
</tr>
<tr>
<td>60%</td>
<td>0.6417</td>
<td>0.2763</td>
<td>1.7649</td>
</tr>
<tr>
<td>80%</td>
<td>0.7047</td>
<td>0.5831</td>
<td>2.0412</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variation in R</th>
<th>Q converged</th>
<th>Error Q</th>
<th>Objective Function $J_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.2000</td>
<td>0.0000</td>
<td>0.5537</td>
</tr>
<tr>
<td>20%</td>
<td>0.0853</td>
<td>0.0860</td>
<td>0.8176</td>
</tr>
<tr>
<td>40%</td>
<td>0.1254</td>
<td>0.1122</td>
<td>1.1100</td>
</tr>
<tr>
<td>60%</td>
<td>0.1543</td>
<td>0.2166</td>
<td>1.6134</td>
</tr>
<tr>
<td>80%</td>
<td>0.1669</td>
<td>0.2957</td>
<td>2.0830</td>
</tr>
</tbody>
</table>
References


