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Refining emission rate estimates using a coupled receptor–dispersion modeling approach

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ABSTRACT

Receptor modeling techniques like chemical mass balance are used to attribute pollution levels at a point to different sources. Here we analyze the composition of particulate matter and use the source profiles of sources prevalent in a region to estimate quantitative source contributions. In dispersion modeling on the other hand the emission rates of various sources together with meteorological conditions are used to determine the concentrations levels at a point or in a region. The predictions using these two approaches are often inconsistent. In this work these differences are attributed to errors in emission inventory. Here an algorithm for coupling receptor and dispersion models is proposed to reduce the differences of the two predictions and determine the emission rates accurately. The proposed combined approach helps reconcile the differences arising when the two approaches are used in a stand-alone mode. This work is based on assuming that the models are perfect and uses a model-to-model comparison to illustrate the concept.

1. Introduction

The classical approaches of dispersion modeling and receptor modeling which have been extensively used in the past are complementary in nature. In most studies these have been used independently. Dispersion models are used to predict concentrations in a region given the emission rates and meteorological conditions. This is used to determine concentrations from point sources, line sources, and area sources prevailing in a region (Seinfeld and Pandis, 1998). Here the convection diffusion equation is solved taking into account the dispersion due to turbulence in terms of a dispersion coefficient. Receptor modeling techniques like chemical mass balance on the other hand can be used to determine contributions of sources to pollution levels at a point. Here we analyze the composition of particulate matter and use the profiles of sources prevalent in a region to determine their contributions to pollution levels. Receptor modeling techniques such as Chemical Mass Balance and Positive Matrix Factorization based on statistical methods have been used extensively in the past (Yatkin and Bayram, 2008).

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 estimates of emission rates of various sources together with meteorological conditions are used to estimate the 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. In addition the meteorological conditions measured at a point may not be representative of that prevailing in a region and this can result in erroneous predictions. Several authors have proposed the use of hybrid or combined approaches to resolve differences or inaccuracies using individual approaches. Qin and Oduyemi (2003) used a dispersion model to predict contributions of vehicle emissions. This was incorporated along with a receptor model. Kumar et al. (2004) combined factor analysis_multiple regressions with dispersion modeling to predict concentrations and estimate apportionment factors to match monitored data.

In this paper a coupled receptor–dispersion modeling approach is proposed which uses emission inventory estimates and receptor concentrations to arrive at a more accurate value of emissions contributing to the pollution levels at a point or in a region. In the context of using coupled receptor–dispersion models Haupt (2005) has proposed an approach based on genetic algorithms to overcome the limitations of the individual approaches combining their benefits. The approach was based on analysis of simulated data "measured" over a period of time.

In this paper estimates of emission rates of various sources are assumed to be known from an emission inventory study.

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The dispersion model is used to compute the concentration of the pollutants from these sources at a point. In the context of particulate matter (PM) this represents the source contributions arising from the dispersion modeling approach. The contributions can also be estimated using a receptor model from a speciation analysis of samples of PM collected using CMB. This step requires additional information i.e., the source profile of various sources. The contributions predicted by the dispersion model are often found to be at variance from those measured at a receptor. The predictions using the two different methods are reconciled to accurately determine the emission rates. The proposed combined approach helps reduce the differences by considering receptor and dispersion modeling simultaneously.

The emission rates are varied using an optimization technique. Two possible objective functions are proposed in this paper. In the first approach the error in the receptor concentrations R^{Dis} of varies species in PM predicted by the dispersion modeling approach and the experimentally measured concentrations R^{Exp} is minimized. This yields the optimization problem.

$$\underset{Q}{\text{Minimize}} J_1 = \left\| R^{Exp} - R^{Dis}(Q) \right\| \tag{1a}$$

Here the emission rates of the different sources Q are found such that the difference between the experimental values of the receptor concentrations R^{Exp} and that predicted from dispersion modeling R^{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 source contributions of the dispersion models are matched with those of the receptor model.

$$\underset{Q}{\text{Minimize}} J_2 = \left\| S^{Dis}(Q) - S^{CMB} \right\| \tag{1b}$$

Here S^{Dis}, S^{CMB} represent the source contributions from dispersion and receptor models.

When the objective function contains the details of only the deviations in the predicted or experimental receptor concentrations or source contributions as in (1a, b) the optimization scheme may converge to multiple solutions corresponding to local minima. To be able to discriminate between these solutions and obtain a physically realistic solution the deviation of the emission rates from the inventory estimates is included in the objective function. This helps us gravitate towards a unique physically realistic solution to the optimization problem. The two objective functions (1a, b) then are modified as

$$\underset{Q}{\text{Minimize}} J_3 = \left\| Q - Q^{est} \right\| + \left\| R^{Exp} - R^{Dis}(Q) \right\| \tag{2a}$$

$$\underset{Q}{\text{Minimize}} J_4 = \left\| Q - Q^{est} \right\| + \left\| S^{Dis}(Q) - S^{CMB} \right\| \tag{2b}$$

In this work we demonstrate the algorithm proposed on a synthetic data set. Here errors are introduced in the data set to make it realistic. The flow chart for the optimization algorithms based on the objective functions J_3, J_4 is shown in Figs. 1 and 2.

2. Validation of the proposed algorithm

2.1. Case of distinct source profiles

The algorithm is applied on a synthetic data set for validation. For the sake of simplicity all sources are assumed different in the sense that they all have distinct source profiles. The focus in this paper is to demonstrate the methodology being proposed. For this the situation where all emissions come from point sources is considered. For the purposes of illustration the short term model which uses a steady state Gaussian plume representation to model emissions from sources such as stacks and isolated vents is used (Petersen and Rumsey, 1987; Touma et al., 1995). The locations of

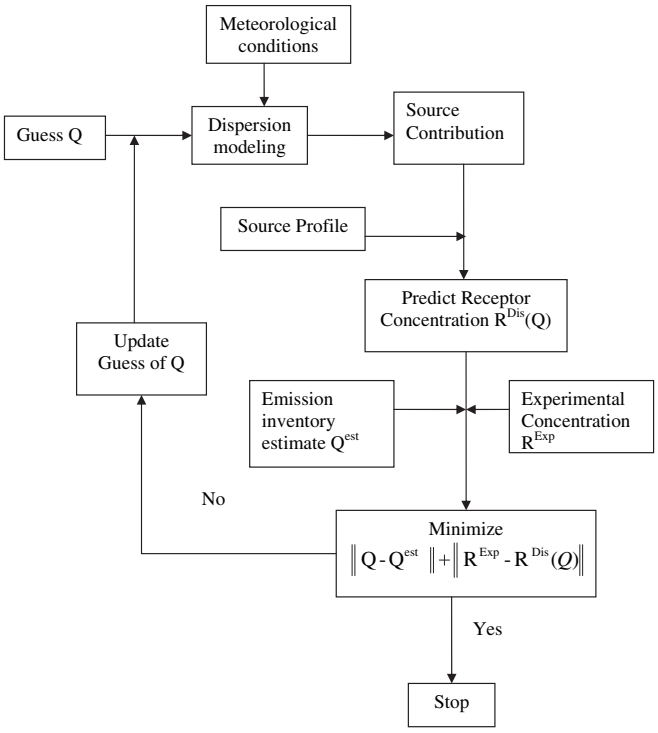

Fig. 1. Flow chart depicting the algorithm based on objective function J_3.

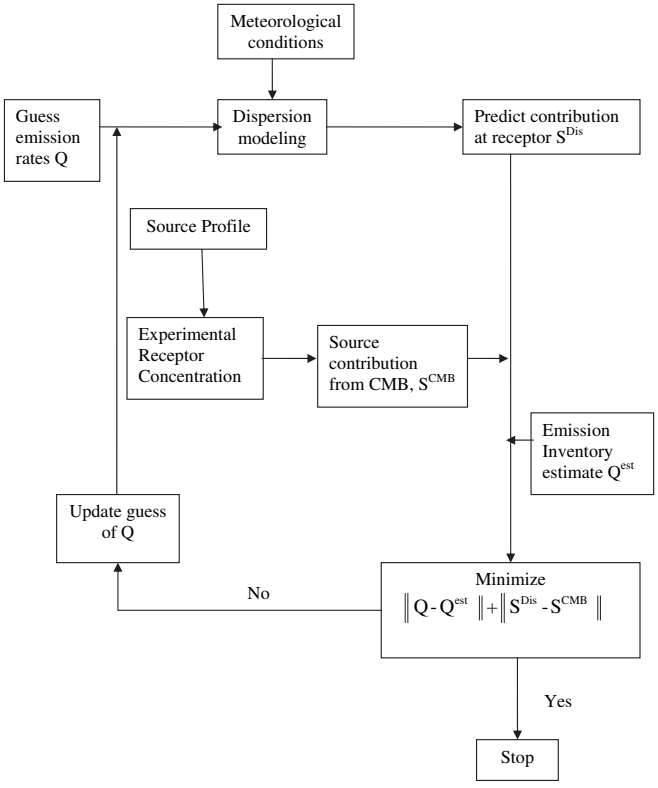

Fig. 2. Flow chart depicting the algorithm based on objective function J_4.