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Supplementary material

SUPPLEMENTARY MATERIAL TO

Evaluation of optimization methods for solving the receptor model for chemical mass balance

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SOME DETAILS OF THE CMB WITH A GENETIC ALGORITHM (CMB–GA)[1]

The main routine has a program for the genetic algorithm and the other subroutine is for the calculation of the objective function based on simulation in MATLAB. This starts execution by assigning the maximum number of generations. To commence with, the first initial population is created in the zeroth generation from two different sets of chromosomes having *p* individuals. For each set of chromosomes, objective functions are calculated from the subroutine. The function calls once for each set. In each call, it creates a binary population based on the bounds provided in the FieldD. FieldD is a field descriptor that is constructed using the matrix replication function, *rep*, to build the matrix 'FieldD', describing the representation and interpretation of the chromosomes. It describes number of variable (*Nvar*), each Gray coded using 20 (*Preci*) bits over the interval [lb, ub]. An initial population is then created with the function *crtbp* thus, producing a matrix, Chrom′, of Nind′ uniformly distributed random binary strings of length $Nvar \times Preci$. This is decoded to phenotypic values then it is passed to the subroutine for objective function calculation. The subroutine returns the objective function values of an array of size *p*. These returned values are arranged in ascending order. This is repeated for next set of chrome, the return values from the subroutine are again sorted then stored in an array. The first half of the first set and second half of the second set will be the initial population for the first generation.

The selected individuals recombine to generate the offspring by crossover and mutation. Mutation is randomly applied with a low probability, typically in the range of 0.001 and 0.05. The parent chromes will be replaced with the child, once the offspring are created. Then the objective function calculation performed

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again and fitness values are assigned to them. This process continues until all the parameter values converge. If the parameter values and the objective function value became the same over 1000 generations, the program is terminated. The objective function can be expressed as:

$$\text{Objective function} = \left\| (c_{\text{pre}} - c_{\text{exp}})^2 \right\| \tag{5}$$

where c_{exp} and c_{pre} are the concentrations of the species determined experimentally by Chow *et al.*[2] and those predicted by the model, respectively. The above results multiplied with the source profile can enable the source contributions to be obtained directly. The subroutine calculates the objective functions for 'P' individuals. Each individual contains *Nvar*, no tuning parameters. For an individual run, the respective parameters are positioned in their respective index of the tuned parameter.[3] The converged solution for a 1000 generations, a stall limit of infinity, a population matrix size of 50×300 and the basic mass equation were used as the selection functions and a tolerance limit of 0.00001 that gave an estimation of a source contribution and the calculated species concentration (c_{pre}).

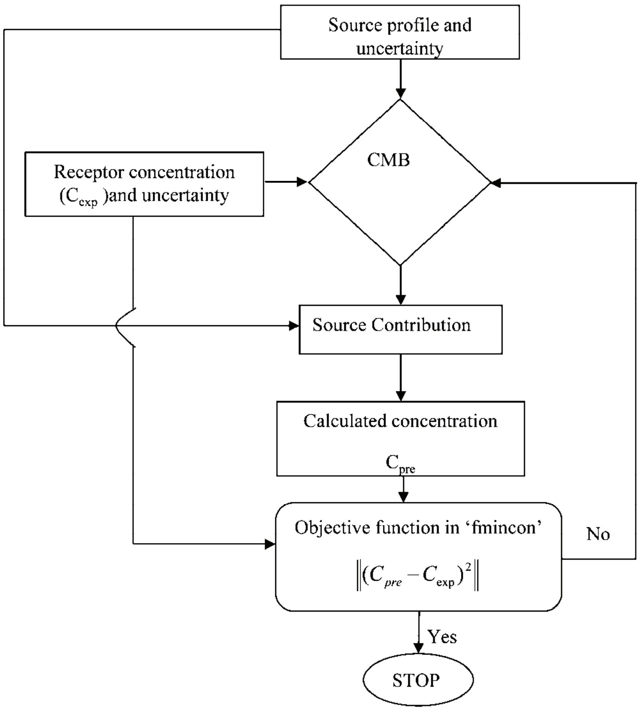

Fig. S-1. Execution of the CMB source contribution by the *fmincon* solver in MATLAB.

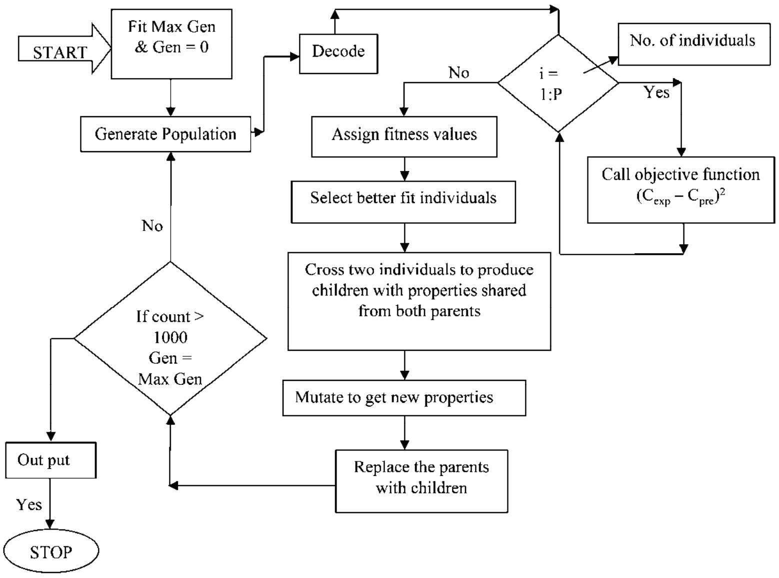

Fig. S-2. Execution of the genetic algorithm code.

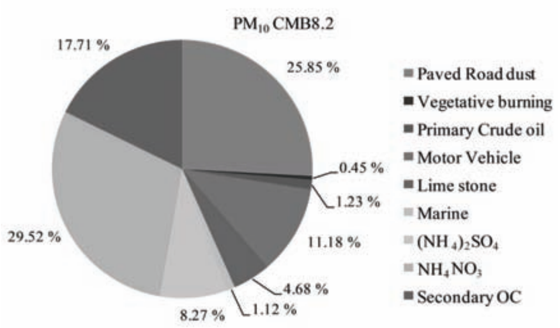

Fig. S-3a. Source contributions obtained for the PM_{10} Fresno data using CMB8.2.

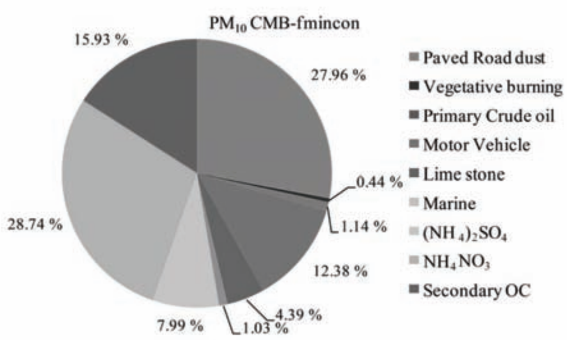

Fig. S-3b. Source contributions obtained for the PM_{10} Fresno data using CMB–fmincon.

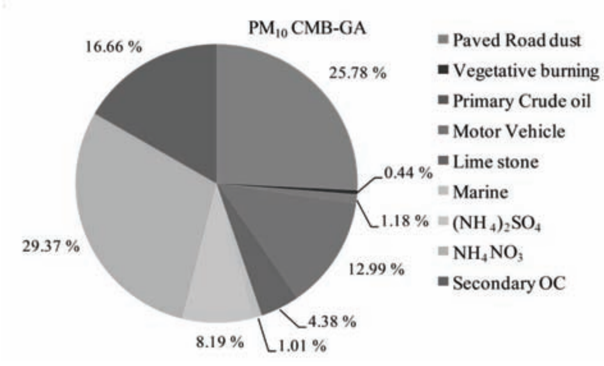

Fig. S-3c. Source contributions obtained for the PM_{10} Fresno data using CMB–GA.

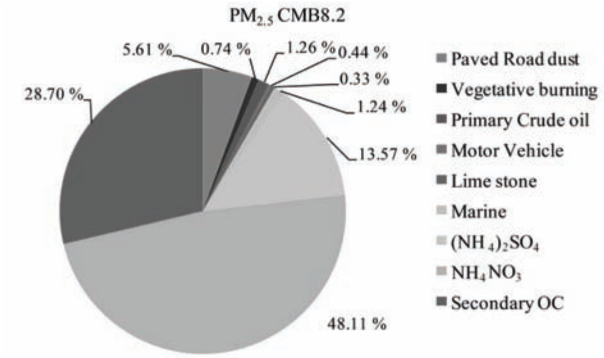

Fig. S-3d. Source contributions obtained for the $PM_{2.5}$ Fresno data using CMB8.2.

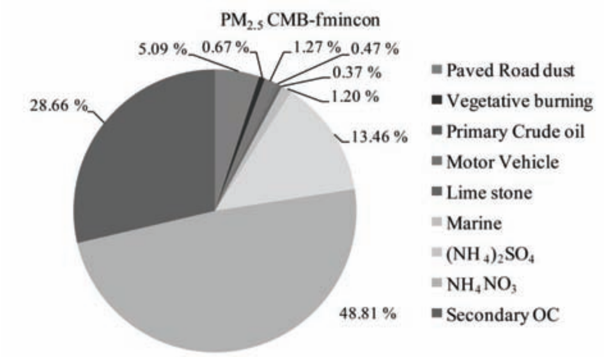

Fig. S-3e. Source contributions obtained for the $PM_{2.5}$ Fresno data using CMB–fmincon.

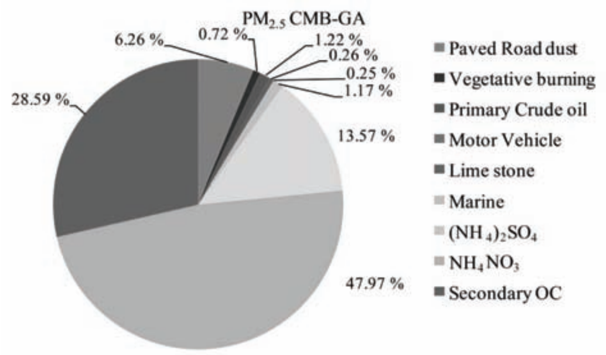

Fig. S-3f. Source contributions obtained for the $PM_{2.5}$ Fresno data using CMB–GA.

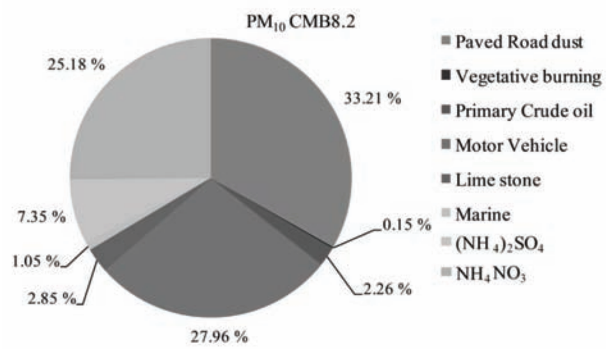

Fig. S-4a. Source contributions obtained for the PM_{10} Bakersfield data using CMB8.2.

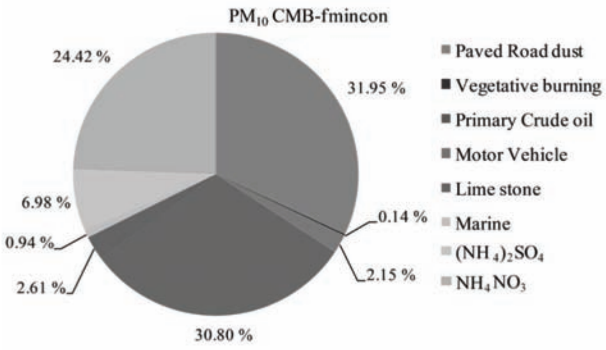

Fig. S-4b. Source contributions obtained for the PM_{10} Bakersfield data using CMB–fmincon.

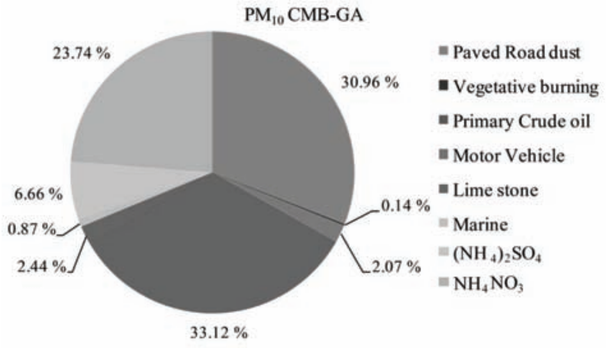

Fig. S-4c. Source contributions obtained for the PM_{10} Bakersfield data using CMB–GA.

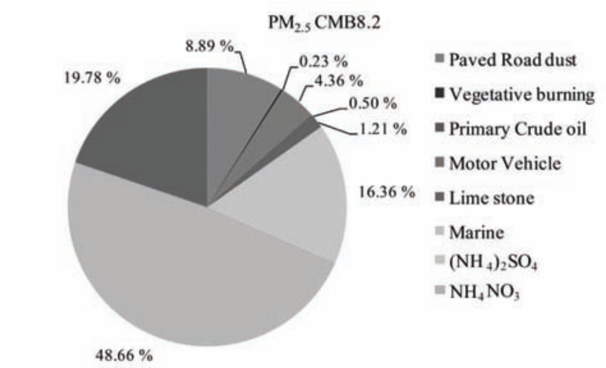

Fig. S-4d. Source contributions obtained for the $PM_{2.5}$ Bakersfield data using CMB8.2.

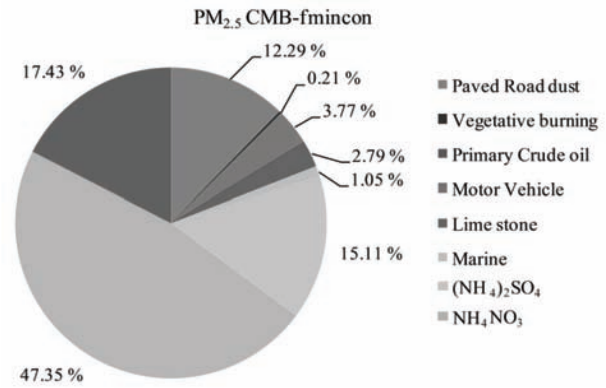

Fig.S-4e. Source contributions obtained for the $PM_{2.5}$ Bakersfield data using CMB–fmincon.

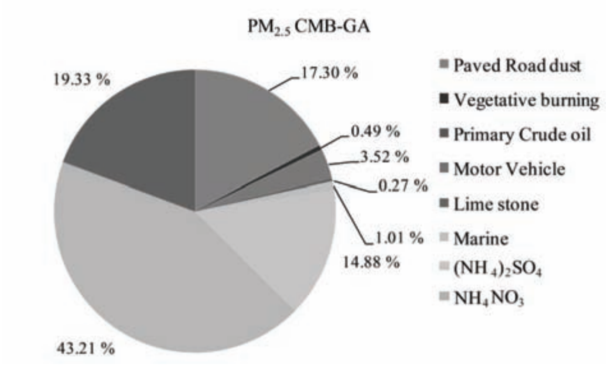

Fig. S-4f. Source contributions obtained for the PM$_{2.5}$ Bakersfield data using CMB–GA.

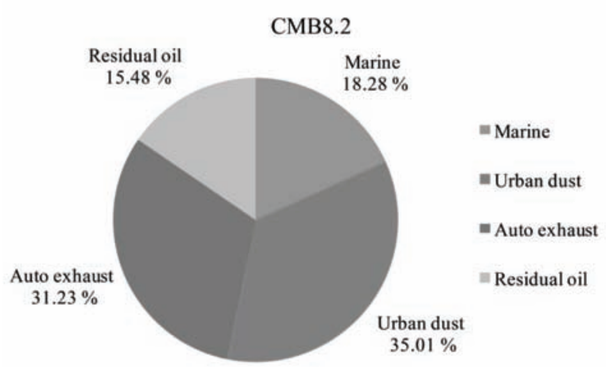

Fig. S-5a. Source contributions obtained for the PM$_{10}$ Portland, Oregon data using CMB8.2.

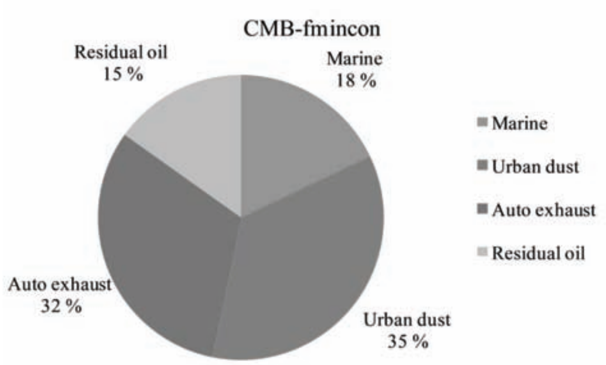

Fig. S-5b. Source contributions obtained for the PM$_{10}$ Portland, Oregon data using CMB–fmincon.

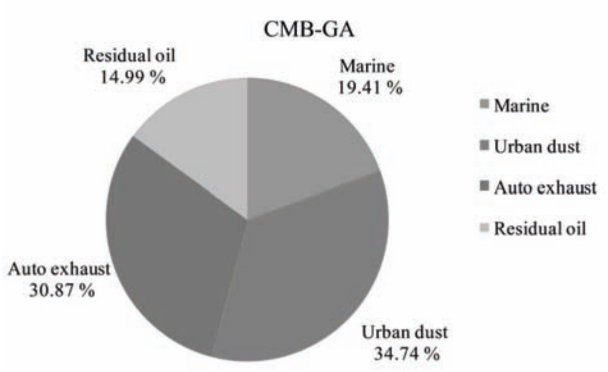

Fig. S-5c. Source contributions obtained for the PM_{10} Portland, Oregon data using CMB–GA.

REFERENCES

1. A. Chipperfield, P. Fleming, H. Pohlheim, C. Fonseca, *Genetic Algorithm TOOLBOX User’s Manual*, Version 1.2, University of Sheffield, Sheffield, UK
2. J. C. Chow, J. G. Watson, D. H. Lowenthal, P. A. Solomon, K. L. Magliano, S. D. Ziman, L. W. Richard, *Aerosol Sci. Technol*. **18** (1993) 105
3. S. E. Haupt, G. S. Young, C. T. Allen, *J. Appl. Meteorol*. **45** (2006) 476.