

# CMBGC-Iteration 1.0

## User Guide

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# CMBGC-Iteration 1.0

Chemical mass balance gas constraint-Iteration model (CMBGC-Iteration) is an extension to the more traditional CMB model and can be applied to estimate the contribution of sources to particulate matter, using gas phase species concentration constraints.

In this model, the uncertainties of ambient dataset and source profiles are involved in the iterative solution.

# CMBGC-Iteration 1.0

**CMBGC-Iteration**

Loading  Run  Save

**PM concentration**

| PM  | Mean | SD | Max | Min |
|-----|------|----|-----|-----|
|     |      |    |     |     |
|     |      |    |     |     |
| III |      |    |     |     |

**Ambient species concentration**

Species select  All  non

|     | Species | Mean | SD | Max |
|-----|---------|------|----|-----|
|     |         |      |    |     |
|     |         |      |    |     |
|     |         |      |    |     |
|     |         |      |    |     |
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|     |         |      |    |     |
|     |         |      |    |     |
|     |         |      |    |     |
| III |         |      |    |     |

**Source contribution**

| Source | Mean | Uncerta... | % |
|--------|------|------------|---|
| 1      |      |            |   |
| 2      |      |            |   |
| 3      |      |            |   |
| 4      |      |            |   |

Contribution plot   
Convergence

PM(%)   
R2  Chi2

**MPIN**

|     |  |  |  |  |  |  |  |
|-----|--|--|--|--|--|--|--|
|     |  |  |  |  |  |  |  |
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|     |  |  |  |  |  |  |  |
|     |  |  |  |  |  |  |  |
|     |  |  |  |  |  |  |  |
| III |  |  |  |  |  |  |  |

**Modeled species information**

| Species | fitting | Measure | Un_M | Calculate | Un_C | C/M |
|---------|---------|---------|------|-----------|------|-----|
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
| III     |         |         |      |           |      |     |

**Modeled gas information**

| Gas          | Fitting              | Measure | Calculate | C/M |
|--------------|----------------------|---------|-----------|-----|
|              |                      |         |           |     |
|              |                      |         |           |     |
|              |                      |         |           |     |
|              |                      |         |           |     |
|              |                      |         |           |     |
|              |                      |         |           |     |
| Bound of C/M | <input type="text"/> |         |           |     |

# CMBGC-Iteration 1.0

- **RUNNING ENVIRONMENT :**

Win XP、Win7、Win8 (32 bit or 64 bit system)

Before running the program, **Matlab (2009 or higher) should be** install firstly.

# CMBGC-Iteration 1.0

- **Download address:**

<http://russellgroup.ce.gatech.edu/node/16>

or

[http://env.nankai.edu.cn/air/list/?110\\_1.html](http://env.nankai.edu.cn/air/list/?110_1.html)

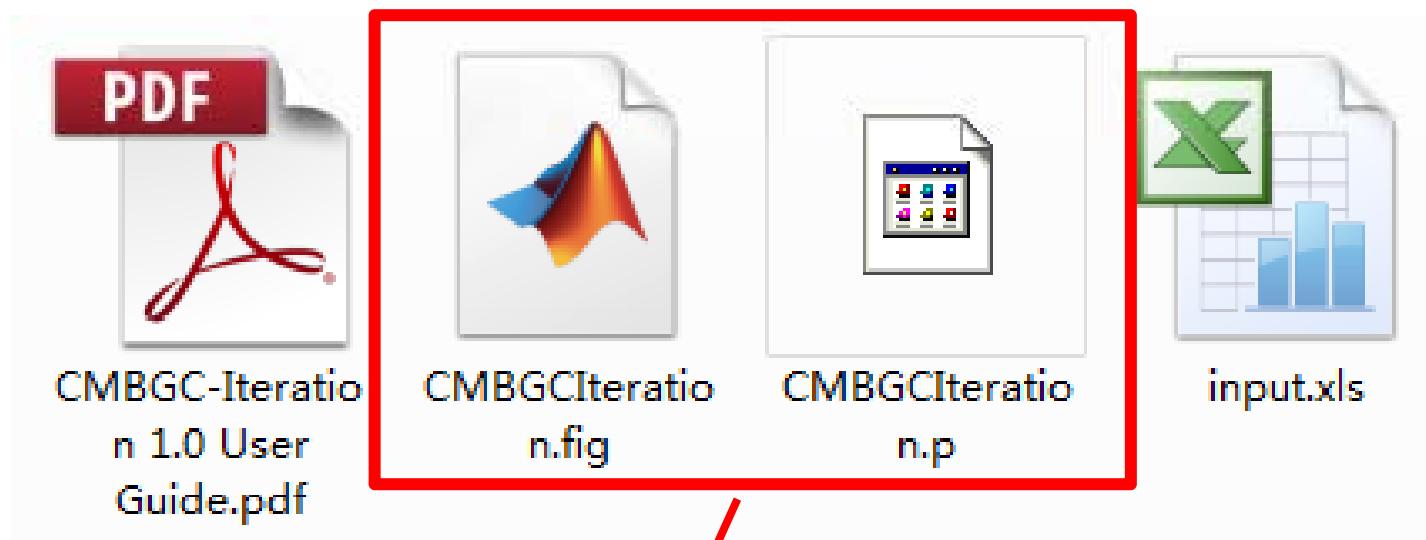
# CMBGC-Iteration 1.0



**Extract the CMBGC-Iteration.zip  
file**

# CMBGC-Iteration 1.0

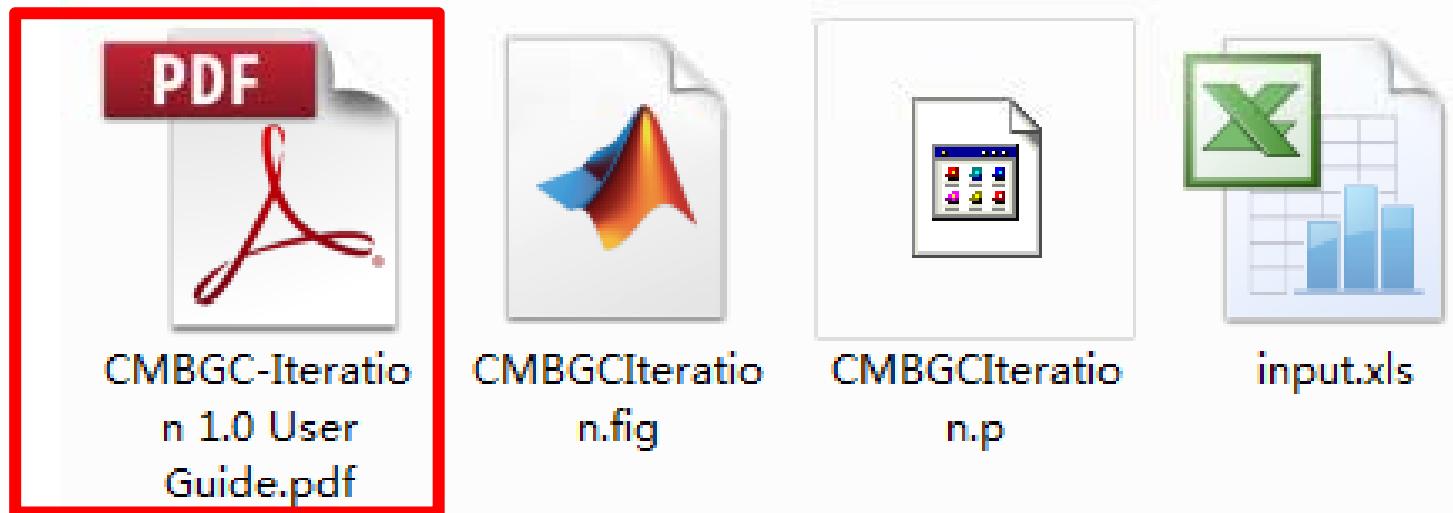
Four files in CMBGC-Iteration.zip



Matlab program files

# CMBGC-Iteration 1.0

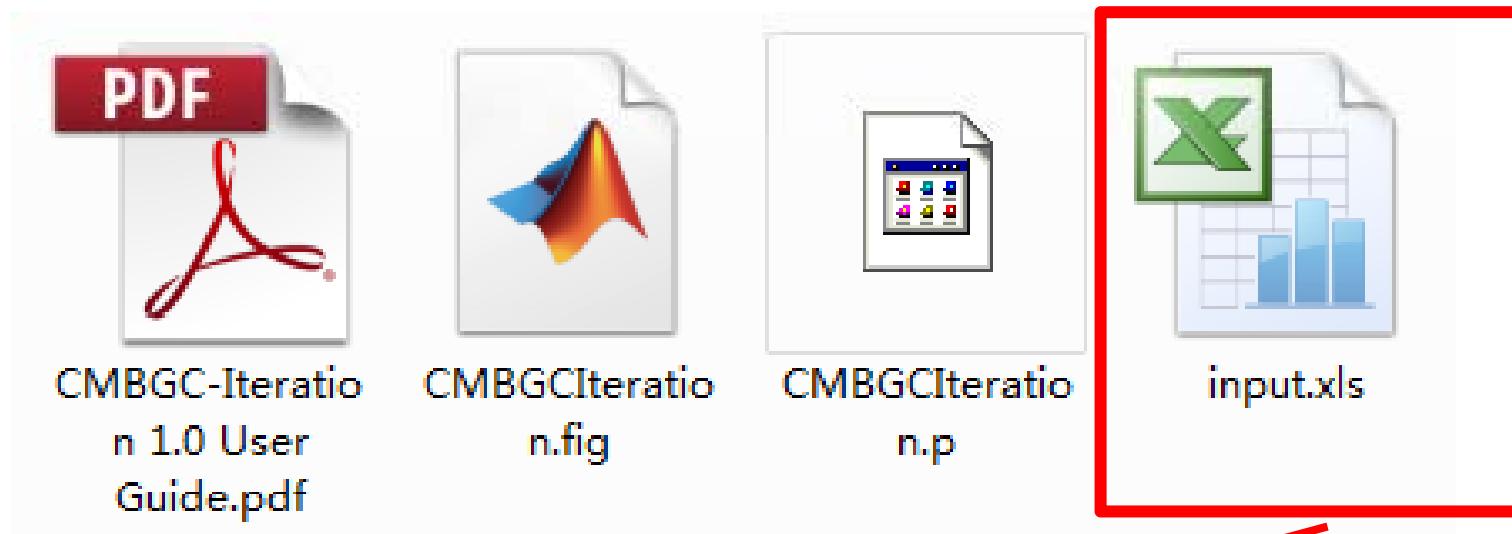
Four files in CMBGC-Iteration.zip



User Guide for CMBGC-Iteration

# CMBGC-Iteration 1.0

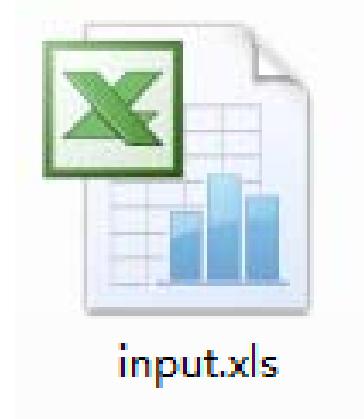
Four files in CMBGC-Iteration.zip



Example of input file

# CMBGC-Iteration 1.0

- Input file



**Input file of CMBGC-Iteration 1.0 is .xls file**

(User can modify the name of input file)

# CMBGC-Iteration 1.0

## Input file

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N        | O      | K |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|----------|--------|---|
| 1  | Date     | PM2.5 | S02      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu       | Fe     | K |
| 2  | 2006/1/5 | 4     | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133  | 0.0539 |   |
| 3  | 2006/1/8 | 7.2   | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271  | 0.0704 |   |
| 4  | #####    | 5.9   | 3.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147  | 0.0641 |   |
| 5  | #####    | 3.7   | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076  | 0.0397 |   |
| 6  | #####    | 10.8  | 2.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216  | 0.0708 |   |
| 7  | #####    | 5.8   | 7.8528   | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573 | 0.00215  | 0.0577 |   |
| 8  | #####    | 7.9   |          |          |          |       |       |        |        |        |         | 0.00254 | 0.0603 | 0.00089  | 0.0934 |   |
| 9  | 2006/2/1 | 9.9   |          |          |          |       |       |        |        |        |         | 0.0043  | 0.0294 | 0.0014   | 0.0436 |   |
| 10 | 2006/2/4 | 6.3   | 1        |          |          |       |       |        |        |        |         | 0.00117 | 0.0577 | 0.00343  | 0.0767 |   |
| 11 | 2006/2/7 | 10.5  | 2.9448   | 586.915  | 149.8924 | 1.44  | 2.37  | 0.807  | 1.547  | 2.613  | 0.0027  | 0.00306 | 0.0828 | 0.00284  | 0.111  |   |
| 12 | #####    | 12.5  | 2.9448   | 331.1935 | 39.64846 | 2.38  | 1.91  | 1.29   | 0.7839 | 2.8191 | 0.0027  | 0.00362 | 0.0398 | 0.00251  | 0.0414 |   |
| 13 | #####    | 12.4  | 0.26     | 167.0083 | 18.68926 | 3.44  | 0.752 | 1.17   | 0.598  | 2.602  | 0.0359  | 0.00485 | 0.0695 | 0.000325 | 0.0358 |   |
| 14 | #####    | 14.7  | 0.26     | 428.2052 | 21.62643 | 4.39  | 2.89  | 2.22   | 0.3588 | 2.0672 | 0.0027  | 0.00298 | 0.0106 | 0.00146  | 0.0106 |   |
| 15 | #####    | 17.1  | 0.26     | 267.2133 | 53.57082 | 3.55  | 3.16  | 2.29   | 0.7943 | 2.4067 | 0.0027  | 0.00323 | 0.0116 | 0.00171  | 0.0292 |   |
| 16 | #####    | 9.2   | 0.26     | 243.355  | 39.3458  | 1.37  | 1.5   | 0.88   | 0.5343 | 2.1467 | 0.0027  | 0.00192 | 0.0149 | 0.00129  | 0.0204 |   |
| 17 | #####    | 9     | 0.810034 | 331.1935 | 29.50704 | 3.24  | 1.06  | 1.17   | 0.507  | 1.443  | 0.0154  | 0.00516 | 0.0292 | 0.000325 | 0.0345 |   |
| 18 | 2006/3/6 | 17.6  | 0.9816   | 434.2217 | 57.65673 | 6.76  | 1.55  | 2.56   | 1.0972 | 3.0568 | 0.0027  | 0.00602 | 0.0446 | 0.00294  | 0.0529 |   |
| 19 | 2006/3/9 | 6.6   | 0.26     | 200.41   | 43.58304 | 1.38  | 0.457 | 0.477  | 0.5967 | 1.1523 | 0.0363  | 0.00187 | 0.0617 | 0.0011   | 0.0677 |   |
| 20 | #####    | 18.8  | 0.9816   | 184.2278 | 29.50704 |       |       |        |        |        |         |         | 021    |          |        |   |
| 21 | #####    | 12.2  | 7.1984   | 496.2533 | 47.97161 |       |       |        |        |        |         |         | 503    |          |        |   |
| 22 | #####    | 0.42  | 0.569043 | 510.5683 | 12.78739 |       |       |        |        |        |         |         | 227    |          |        |   |
| 23 | #####    | 0.42  | 0.26     | 291.0717 | 17.78128 |       |       |        |        |        |         |         | 189    |          |        |   |
| 24 | #####    | 8.9   | 0.951855 | 484.1073 | 81.26421 |       |       |        |        |        |         |         | 752    |          |        |   |
| 25 | #####    | 13.4  | 0.26     | 348.3317 | 13.09005 |       |       |        |        |        |         |         | 276    |          |        |   |
| 26 | 2006/4/2 | 14.3  | 0.26     | 408.2887 | 16.09601 |       |       |        |        |        |         |         | 451    |          |        |   |
| 27 | 2006/4/5 | 11    | 0.343333 | 114.52   | 26.33142 | 1.41  | 1.03  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444 | 0.00106  | 0.0356 |   |
| 28 | 2006/4/9 | 9     | 0.26     | 252.8983 | 20.05123 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352 | 0.0014   | 0.0426 |   |

Six worksheets in input file

Do not change the names of  
six worksheets!

# CMBGC-Iteration 1.0

## Input file

|    | A        | B     | C                                | D        | E        | F     | G     | H      | I      | J      | K       | L       | M       | N        | O       | K      |  |
|----|----------|-------|----------------------------------|----------|----------|-------|-------|--------|--------|--------|---------|---------|---------|----------|---------|--------|--|
| 1  | Date     | PM2.5 | SO2                              | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca      | Cu       | Fe      | K      |  |
| 2  | 2006/1/5 | 4     | 0.26                             | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888  | 0.00133  | 0.0539  |        |  |
| 3  | 2006/1/8 | 7.2   | 6.2168                           | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104   | 0.00271  | 0.0704  |        |  |
| 4  | #####    | 5.9   | 3.817333                         | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957  | 0.00147  | 0.0641  |        |  |
| 5  | #####    | 3.7   | 0.6544                           | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511  | 0.00076  | 0.0397  |        |  |
| 6  | #####    | 10.8  | 2.508533                         | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434  | 0.00216  | 0.0708  |        |  |
| 7  | #####    | 5.8   | 7.8528                           | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573  | 0.00215  | 0.0577  |        |  |
| 8  | #####    | 7.9   | 0.6544                           | 390.4091 | 51.11927 | 0.844 | 0.215 | 0.304  | 0.6097 | 1.5893 | 0.075   | 0.00254 | 0.0603  | 0.00089  | 0.0934  |        |  |
| 9  | 2006/2/1 | 9.9   | 2.835733                         | 501.025  | 41.54009 | 2.98  | 0.515 | 1.01   | 0.7631 | 1.8539 | 0.0027  | 0.0043  | 0.0294  | 0.0014   | 0.0436  |        |  |
| 10 | 2006/2/4 | 6.    |                                  |          |          |       |       |        |        |        |         | 0.00117 | 0.0577  | 0.00343  | 0.0767  |        |  |
| 11 | 2006/2/7 | 10.   |                                  |          |          |       |       |        |        |        |         | 0.00306 | 0.0828  | 0.00284  | 0.111   |        |  |
| 12 | #####    | 12.   | Concentration of ambient dataset |          |          |       |       |        |        |        |         |         | 0.00362 | 0.0398   | 0.00251 | 0.0414 |  |
| 13 | #####    | 12.4  | 0.26                             | 167.0083 | 18.68926 | 3.44  | 0.752 | 1.17   | 0.598  | 2.602  | 0.0359  | 0.00485 | 0.0695  | 0.000325 | 0.0358  |        |  |
| 14 | #####    | 14.7  | 0.26                             | 428.2022 | 21.62643 | 3.39  | 2.89  | 2.22   | 0.3588 | 2.0672 | 0.0027  | 0.00298 | 0.0106  | 0.00146  | 0.0106  |        |  |
| 15 | #####    | 17.1  | 0.26                             | 267.2133 | 53.57082 | 3.55  | 3.16  | 2.29   | 0.7943 | 2.4067 | 0.0027  | 0.00323 | 0.0116  | 0.00171  | 0.0292  |        |  |
| 16 | #####    | 9.2   | 0.26                             | 247.355  | 39.3458  | 1.37  | 1.5   | 0.88   | 0.5343 | 2.1467 | 0.0027  | 0.00192 | 0.0149  | 0.00129  | 0.0204  |        |  |
| 17 | #####    | 9     | 0.810034                         | 331.1935 | 29.50704 | 3.24  | 1.06  | 1.17   | 0.507  | 1.443  | 0.0154  | 0.00516 | 0.0292  | 0.000325 | 0.0345  |        |  |
| 18 | 2006/3/6 | 17.6  | 0.9816                           | 434.2217 | 57.65673 | 6.76  | 1.55  | 2.56   | 1.0972 | 3.0568 | 0.0027  | 0.00602 | 0.0446  | 0.00294  | 0.0529  |        |  |
| 19 | 2006/3/9 | 6.6   | 0.26                             | 200.41   | 43.58304 | 1.38  | 0.457 | 0.477  | 0.5967 | 1.1523 | 0.0363  | 0.00187 | 0.0617  | 0.0011   | 0.0677  |        |  |
| 20 | #####    | 18.8  | 0.9816                           | 184.2278 | 29.50704 | 7.16  | 1.57  | 2.15   | 0.5278 | 2.2982 | 0.0027  | 0.00583 | 0.0435  | 0.000325 | 0.021   |        |  |
| 21 | #####    | 12.2  | 7.1984                           | 496.2533 | 47.97161 | 1.5   | 0.757 | 0.612  | 1.0127 | 4.5363 | 0.0027  | 0.00437 | 0.0584  | 0.00107  | 0.0503  |        |  |
| 22 | #####    | 0.42  | 0.539043                         | 510.5683 | 12.78739 | 2.83  | 1.31  | 1.52   | 0.4186 | 2.7534 | 0.0027  | 0.00387 | 0.0181  | 0.000325 | 0.0227  |        |  |
| 23 | #####    | 0.42  | 0.26                             | 291.0717 | 17.78128 | 2.76  | 1.24  | 1.1    | 0.2964 | 1.0816 | 0.0027  | 0.00134 | 0.0182  | 0.00082  | 0.0189  |        |  |
| 24 | #####    | 8.9   | 0.951855                         | 484.1073 | 81.26421 | 1.16  | 2.49  | 1.03   | 0.9126 | 2.1794 | 0.0027  | 0.00251 | 0.205   | 0.00192  | 0.0752  |        |  |
| 25 | #####    | 13.4  | 0.26                             | 348.3317 | 13.09005 | 5.38  | 0.298 | 1.94   | 0.3471 | 1.4599 | 0.0027  | 0.00413 | 0.04    | 0.001    | 0.0276  |        |  |
| 26 | 2006/4/2 | 14.3  | 0.26                             | 408.2887 | 16.09601 | 5.14  | 0.759 | 1.7    | 0.4238 | 2.2122 | 0.00659 | 0.00635 | 0.043   | 0.00104  | 0.0451  |        |  |
| 27 | 2006/4/5 | 12    | 0.545333                         | 114.52   | 26.33142 | 4.41  | 1.05  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444  | 0.00106  | 0.0356  |        |  |
| 28 | 2006/4/9 | 9     | 0.26                             | 252.8983 | 20.05122 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352  | 0.0014   | 0.0426  |        |  |



# CMBGC-Iteration 1.0

## Input file

Concentration of ambient dataset

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N        | O      | P |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|----------|--------|---|
| 1  | Date     | PM2.5 | S02      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu       | Fe     | P |
| 2  | 2006/1/5 | 4     | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133  | 0.0539 |   |
| 3  | 2006/1/8 | 7.2   | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271  | 0.0704 |   |
| 4  | #####    | 5.9   | 3.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147  | 0.0641 |   |
| 5  | #####    | 3.7   | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076  | 0.0397 |   |
| 6  | #####    | 10.8  | 2.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216  | 0.0708 |   |
| 7  | #####    | 5.8   | 7.8528   | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573 | 0.00215  | 0.0577 |   |
| 8  | #####    | 7.9   | 0.6544   | 390.4091 | 51.11927 | 0.844 | 0.215 | 0.304  | 0.6097 | 1.5893 | 0.075   | 0.00254 | 0.0603 | 0.00089  | 0.0934 |   |
| 9  | 2006/2/1 | 9.9   | 2.835733 | 501.025  | 41.54009 | 2.98  | 0.515 | 1.01   | 0.7631 | 1.8539 | 0.0027  | 0.0043  | 0.0294 | 0.0014   | 0.0436 |   |
| 10 | 2006/2/4 | 6.3   | 1.934748 | 796.8683 | 105.477  | 0.711 | 0.63  | 0.247  | 1.1401 | 2.4669 | 0.0027  | 0.00117 | 0.0577 | 0.00343  | 0.0767 |   |
| 11 | 2006/2/7 | 10.5  | 2.9448   | 586.915  | 149.8924 | 1.44  | 2.37  | 0.807  | 1.547  | 2.613  | 0.0027  | 0.00306 | 0.0828 | 0.00284  | 0.111  |   |
| 12 | #####    | 12.5  | 2.9448   | 331.1    |          |       |       |        |        |        |         |         | 398    | 0.00251  | 0.0414 |   |
| 13 | #####    | 12.4  | 0.26     | 167.0    |          |       |       |        |        |        |         |         | 695    | 0.000325 | 0.0358 |   |
| 14 | #####    | 14.7  | 0.26     | 428.2    |          |       |       |        |        |        |         |         | 106    | 0.00146  | 0.0106 |   |
| 15 | #####    | 17.1  | 0.26     | 267.2133 | 53.57082 | 3.55  | 3.16  | 2.29   | 0.7943 | 2.4067 | 0.0027  | 0.00323 | 0.0116 | 0.00171  | 0.0292 |   |
| 16 | #####    | 9.2   | 0.26     | 243.355  | 39.3458  | 1.37  | 1.5   | 0.88   | 0.5343 | 2.1467 | 0.0027  | 0.00192 | 0.0149 | 0.00129  | 0.0204 |   |
| 17 | #####    | 9     | 0.810034 | 331.1935 | 29.50704 | 3.24  | 1.06  | 1.17   | 0.507  | 1.443  | 0.0154  | 0.00516 | 0.0292 | 0.000325 | 0.0345 |   |
| 18 | 2006/3/6 | 17.6  | 0.9816   | 434.2217 | 57.65673 | 6.76  | 1.55  | 2.56   | 1.0972 | 3.0568 | 0.0027  | 0.00602 | 0.0446 | 0.00294  | 0.0529 |   |
| 19 | 2006/3/9 | 6.6   | 0.26     | 200.41   | 43.58304 | 1.38  | 0.457 | 0.477  | 0.5967 | 1.1523 | 0.0363  | 0.00187 | 0.0617 | 0.0011   | 0.0677 |   |
| 20 | #####    | 18.8  | 0.9816   | 184.2278 | 29.50704 | 7.16  | 1.57  | 2.15   | 0.5278 | 2.2982 | 0.0027  | 0.00583 | 0.0435 | 0.000325 | 0.021  |   |
| 21 | #####    | 12.2  | 7.1984   | 496.2533 | 47.97161 | 1.5   | 0.757 | 0.612  | 1.0127 | 4.5363 | 0.0027  | 0.00437 | 0.0584 | 0.00107  | 0.0503 |   |
| 22 | #####    | 0.42  | 0.569043 | 510.5683 | 12.78739 | 2.83  | 1.31  | 1.52   | 0.4186 | 2.7534 | 0.0027  | 0.00387 | 0.0181 | 0.000325 | 0.0227 |   |
| 23 | #####    | 0.42  | 0.26     | 291.0717 | 17.78128 | 2.76  | 1.24  | 1.1    | 0.2964 | 1.0816 | 0.0027  | 0.00134 | 0.0182 | 0.00082  | 0.0189 |   |
| 24 | #####    | 8.9   | 0.951855 | 484.1073 | 81.26421 | 1.16  | 2.49  | 1.03   | 0.9126 | 2.1794 | 0.0027  | 0.00251 | 0.205  | 0.00192  | 0.0752 |   |
| 25 | #####    | 13.4  | 0.26     | 348.3317 | 13.09005 | 5.38  | 0.298 | 1.94   | 0.3471 | 1.4599 | 0.0027  | 0.00413 | 0.04   | 0.001    | 0.0276 |   |
| 26 | 2006/4/2 | 14.3  | 0.26     | 408.2887 | 16.09601 | 5.14  | 0.759 | 1.7    | 0.4238 | 2.2122 | 0.00659 | 0.00635 | 0.043  | 0.00104  | 0.0451 |   |
| 27 | 2006/4/5 | 14    | 0.545333 | 114.52   | 26.33142 | 4.41  | 1.05  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444 | 0.00106  | 0.0356 |   |
| 28 | 2006/4/9 | 9     | 0.26     | 252.8983 | 20.05123 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352 | 0.0014   | 0.0426 |   |

First line: title line

# CMBGC-Iteration 1.0

## Input file

Concentration of ambient dataset

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N        | O      | K |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|----------|--------|---|
| 1  | Date     | PM2.5 | SO2      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu       | Fe     | K |
| 2  | 2006/1/5 | 4     | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133  | 0.0539 |   |
| 3  | 2006/1/8 | 7.2   | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271  | 0.0704 |   |
| 4  | #####    | 5.9   | 3.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147  | 0.0641 |   |
| 5  | #####    | 3.7   | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076  | 0.0397 |   |
| 6  | #####    | 10.8  | 2.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216  | 0.0708 |   |
| 7  | #####    | 5.8   | 7.8528   | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573 | 0.00215  | 0.0577 |   |
| 8  | #####    | 7.9   | 0.6544   | 390.4091 | 51.11927 | 0.844 | 0.215 | 0.304  | 0.6097 | 1.5893 | 0.075   | 0.00254 | 0.0603 | 0.00089  | 0.0934 |   |
| 9  | 2006/2/1 | 9.9   | 2.8      |          |          |       |       |        |        | 539    | 0.0027  | 0.0043  | 0.0294 | 0.0014   | 0.0436 |   |
| 10 | 2006/2/4 | 6.3   | 1.9      |          |          |       |       |        |        | 669    | 0.0027  | 0.00117 | 0.0577 | 0.00343  | 0.0767 |   |
| 11 | 2006/2/7 | 10.5  | 2        |          |          |       |       |        |        | 613    | 0.0027  | 0.00306 | 0.0828 | 0.00284  | 0.111  |   |
| 12 | #####    | 12.5  | 2        |          |          |       |       |        |        | 191    | 0.0027  | 0.00362 | 0.0398 | 0.00251  | 0.0414 |   |
| 13 | #####    | 12.4  |          |          |          |       |       |        |        | 602    | 0.0359  | 0.00485 | 0.0695 | 0.000325 | 0.0358 |   |
| 14 | #####    | 14.7  |          |          |          |       |       |        |        | 672    | 0.0027  | 0.00298 | 0.0106 | 0.00146  | 0.0106 |   |
| 15 | #####    | 17.1  |          |          |          |       |       |        |        | 667    | 0.0027  | 0.00323 | 0.0116 | 0.00171  | 0.0292 |   |
| 16 | #####    | 9.2   |          |          |          |       |       |        |        | 467    | 0.0027  | 0.00192 | 0.0149 | 0.00129  | 0.0204 |   |
| 17 | #####    | 9     | 0.8      |          |          |       |       |        |        | 443    | 0.0154  | 0.00516 | 0.0292 | 0.000325 | 0.0345 |   |
| 18 | 2006/3/6 | 17.6  | 0        |          |          |       |       |        |        | 568    | 0.0027  | 0.00602 | 0.0446 | 0.00294  | 0.0529 |   |
| 19 | 2006/3/9 | 6.6   | 0.26     | 200.41   | 43.58304 | 1.38  | 0.457 | 0.477  | 0.5967 | 1.1523 | 0.0363  | 0.00187 | 0.0617 | 0.0011   | 0.0677 |   |
| 20 | #####    | 18.8  | 0.9816   | 184.2278 | 29.50704 | 7.16  | 1.57  | 2.15   | 0.5278 | 2.2982 | 0.0027  | 0.00583 | 0.0435 | 0.000325 | 0.021  |   |
| 21 | #####    | 12.2  | 7.1984   | 496.2533 | 47.97161 | 1.5   | 0.757 | 0.612  | 1.0127 | 4.5363 | 0.0027  | 0.00437 | 0.0584 | 0.00107  | 0.0503 |   |
| 22 | #####    | 0.42  | 0.569043 | 510.5683 | 12.78739 | 2.83  | 1.31  | 1.52   | 0.4186 | 2.7534 | 0.0027  | 0.00387 | 0.0181 | 0.000325 | 0.0227 |   |
| 23 | #####    | 0.42  | 0.26     | 291.0717 | 17.78128 | 2.76  | 1.24  | 1.1    | 0.2964 | 1.0816 | 0.0027  | 0.00134 | 0.0182 | 0.00082  | 0.0189 |   |
| 24 | #####    | 8.9   | 0.951855 | 484.1073 | 81.26421 | 1.16  | 2.49  | 1.03   | 0.9126 | 2.1794 | 0.0027  | 0.00251 | 0.205  | 0.00192  | 0.0752 |   |
| 25 | #####    | 13.4  | 0.26     | 348.3317 | 13.09005 | 5.38  | 0.298 | 1.94   | 0.3471 | 1.4599 | 0.0027  | 0.00413 | 0.04   | 0.001    | 0.0276 |   |
| 26 | 2006/4/2 | 14.3  | 0.26     | 408.2887 | 16.09601 | 5.14  | 0.759 | 1.7    | 0.4238 | 2.2122 | 0.00659 | 0.00635 | 0.043  | 0.00104  | 0.0451 |   |
| 27 | 2006/4/5 | 14    | 0.545333 | 114.52   | 26.33142 | 4.41  | 1.05  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444 | 0.00106  | 0.0356 |   |
| 28 | 2006/4/9 | 9     | 0.26     | 252.8983 | 20.05123 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352 | 0.0014   | 0.0426 |   |

Dataset

Number of samples should  
greater than one

# CMBGC-Iteration 1.0

## Input file

Concentration of ambient dataset

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N        | O      | K |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|----------|--------|---|
| 1  | Date     | P12.5 | SO2      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu       | Fe     | K |
| 2  | 2006/1/5 | 4     | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133  | 0.0539 |   |
| 3  | 2006/1/8 | 7.2   | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271  | 0.0704 |   |
| 4  | #####    | 5.9   | 3.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147  | 0.0641 |   |
| 5  | #####    | 3.7   | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076  | 0.0397 |   |
| 6  | #####    | 10.8  | 2.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216  | 0.0708 |   |
| 7  | #####    | 5.8   | 7.8528   | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573 | 0.00215  | 0.0577 |   |
| 8  | #####    | 7.9   | 0.6544   | 390.40   |          |       |       |        |        |        |         |         | 03     | 0.00089  | 0.0934 |   |
| 9  | 2006/2/1 | 9.9   | 2.835733 | 501.0    |          |       |       |        |        |        |         |         | 94     | 0.0014   | 0.0436 |   |
| 10 | 2006/2/4 | 6.3   | 1.934748 | 79.86    |          |       |       |        |        |        |         |         | 77     | 0.00343  | 0.0767 |   |
| 11 | 2006/2/7 | 10.5  | 2.9448   | 586.915  | 149.8924 | 1.44  | 2.37  | 0.807  | 1.547  | 2.613  | 0.0027  | 0.00306 | 0.0828 | 0.00284  | 0.111  |   |
| 12 | #####    | 12.5  | 2.9448   | 331.1935 | 39.64846 | 2.38  | 1.91  | 1.29   | 0.7839 | 2.8191 | 0.0027  | 0.00362 | 0.0398 | 0.00251  | 0.0414 |   |
| 13 | #####    | 12.4  | 0.26     | 167.0083 | 18.68926 | 3.44  | 0.752 | 1.17   | 0.598  | 2.602  | 0.0359  | 0.00485 | 0.0695 | 0.000325 | 0.0358 |   |
| 14 | #####    | 14.7  | 0.26     | 428.2052 | 21.62643 | 3.39  | 2.89  | 2.22   | 0.3588 | 2.0672 | 0.0027  | 0.00298 | 0.0106 | 0.00146  | 0.0106 |   |
| 15 | #####    | 17.1  | 0.26     | 267.2133 | 53.57082 | 3.55  | 3.16  | 2.29   | 0.7943 | 2.4067 | 0.0027  | 0.00323 | 0.0116 | 0.00171  | 0.0292 |   |
| 16 | #####    | 9.2   | 0.26     | 243.355  | 39.3458  | 1.37  | 1.5   | 0.88   | 0.5343 | 2.1467 | 0.0027  | 0.00192 | 0.0149 | 0.00129  | 0.0204 |   |
| 17 | #####    | 9     | 0.810034 | 331.1935 | 29.50704 | 3.24  | 1.06  | 1.17   | 0.507  | 1.443  | 0.0154  | 0.00516 | 0.0292 | 0.000325 | 0.0345 |   |
| 18 | 2006/3/6 | 17.6  | 0.9816   | 434.2217 | 57.65673 | 6.76  | 1.55  | 2.56   | 1.0972 | 3.0568 | 0.0027  | 0.00602 | 0.0446 | 0.00294  | 0.0529 |   |
| 19 | 2006/3/9 | 6.6   | 0.26     | 200.41   | 43.58304 | 1.38  | 0.457 | 0.477  | 0.5967 | 1.1523 | 0.0363  | 0.00187 | 0.0617 | 0.0011   | 0.0677 |   |
| 20 | #####    | 18.8  | 0.9816   | 184.2278 | 29.50704 | 7.16  | 1.57  | 2.15   | 0.5278 | 2.2982 | 0.0027  | 0.00583 | 0.0435 | 0.000325 | 0.021  |   |
| 21 | #####    | 12.2  | 7.1984   | 496.2533 | 47.97161 | 1.5   | 0.757 | 0.612  | 1.0127 | 4.5363 | 0.0027  | 0.00437 | 0.0584 | 0.00107  | 0.0503 |   |
| 22 | #####    | 0.42  | 0.569043 | 510.5683 | 12.78739 | 2.83  | 1.31  | 1.52   | 0.4186 | 2.7534 | 0.0027  | 0.00387 | 0.0181 | 0.000325 | 0.0227 |   |
| 23 | #####    | 0.42  | 0.26     | 291.0717 | 17.78128 | 2.76  | 1.24  | 1.1    | 0.2964 | 1.0816 | 0.0027  | 0.00134 | 0.0182 | 0.00082  | 0.0189 |   |
| 24 | #####    | 8.9   | 0.951855 | 484.1073 | 81.26421 | 1.16  | 2.49  | 1.03   | 0.9126 | 2.1794 | 0.0027  | 0.00251 | 0.205  | 0.00192  | 0.0752 |   |
| 25 | #####    | 13.4  | 0.26     | 348.3317 | 13.09005 | 5.38  | 0.298 | 1.94   | 0.3471 | 1.4599 | 0.0027  | 0.00413 | 0.04   | 0.001    | 0.0276 |   |
| 26 | 2006/4/2 | 14.3  | 0.26     | 408.2887 | 16.09601 | 5.14  | 0.759 | 1.7    | 0.4238 | 2.2122 | 0.00659 | 0.00635 | 0.043  | 0.00104  | 0.0451 |   |
| 27 | 2006/4/5 | 14    | 0.545333 | 114.52   | 26.33142 | 4.41  | 1.05  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444 | 0.00106  | 0.0356 |   |
| 28 | 2006/4/9 | 9     | 0.26     | 252.8983 | 20.05123 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352 | 0.0014   | 0.0426 |   |

concentration un\_con profile un\_pro source\_gas parameter

# CMBGC-Iteration 1.0

## Input file

Concentration of ambient dataset

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N        | O      | K |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|----------|--------|---|
| 1  | Date     | PM2.5 | S02      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu       | Fe     | K |
| 2  | 2006/1/5 | 4     | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133  | 0.0539 |   |
| 3  | 2006/1/8 | 7.2   | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271  | 0.0704 |   |
| 4  | #####    | 5.9   | 1.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147  | 0.0641 |   |
| 5  | #####    | 3.7   | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076  | 0.0397 |   |
| 6  | #####    | 10.8  | 1.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216  | 0.0708 |   |
| 7  | #####    | 5.8   | 7.8528   | 334.0167 | 73.84904 | 0.770 | 0.801 | 0.171  | 0.875  | 0.915  | 0.0027  | 0.00133 | 0.0570 | 0.00133  | 0.0577 |   |
| 8  | #####    | 7.9   | 0.6544   | 390.4091 | 51.11927 | 0.    | 0.    | 0.     | 0.     | 0.     | 0.      | 0.      | 0.     | 0.       | 0.     |   |
| 9  | 2006/2/1 | 9.9   | 1.835733 | 501.025  | 41.5409  | 2     | 2     | 2      | 2      | 2      | 2       | 2       | 2      | 2        | 2      |   |
| 10 | 2006/2/4 | 6.3   | 1.934748 | 796.8683 | 105.477  | 0.    | 0.    | 0.     | 0.     | 0.     | 0.      | 0.      | 0.     | 0.       | 0.     |   |
| 11 | 2006/2/7 | 10.5  | 2.9448   | 586.915  | 149.8924 | 1     | 1     | 1      | 1      | 1      | 1       | 1       | 1      | 1        | 1      |   |
| 12 | #####    | 12.5  | 2.9448   | 331.1935 | 39.64846 | 2     | 2     | 2      | 2      | 2      | 2       | 2       | 2      | 2        | 2      |   |
| 13 | #####    | 12.4  | 0.26     | 167.0083 | 18.68926 | 3     | 3     | 3      | 3      | 3      | 3       | 3       | 3      | 3        | 3      |   |
| 14 | #####    | 14.7  | 0.26     | 428.2052 | 21.62643 | 3     | 3     | 3      | 3      | 3      | 3       | 3       | 3      | 3        | 3      |   |
| 15 | #####    | 17.1  | 0.26     | 267.2133 | 53.57082 | 3     | 3     | 3      | 3      | 3      | 3       | 3       | 3      | 3        | 3      |   |
| 16 | #####    | 9.2   | 0.26     | 243.355  | 39.3458  | 1     | 1     | 1      | 1      | 1      | 1       | 1       | 1      | 1        | 1      |   |
| 17 | #####    | 9     | 0.810034 | 331.1935 | 29.50704 | 3     | 3     | 3      | 3      | 3      | 3       | 3       | 3      | 3        | 3      |   |
| 18 | 2006/3/6 | 17.6  | 0.9816   | 434.2217 | 57.65673 | 6     | 6     | 6      | 6      | 6      | 6       | 6       | 6      | 6        | 6      |   |
| 19 | 2006/3/9 | 6.6   | 0.26     | 200.41   | 43.58304 | 1     | 1     | 1      | 1      | 1      | 1       | 1       | 1      | 1        | 1      |   |
| 20 | #####    | 18.8  | 0.9816   | 184.2278 | 29.50704 | 7     | 7     | 7      | 7      | 7      | 7       | 7       | 7      | 7        | 7      |   |
| 21 | #####    | 12.2  | 7.1984   | 496.2533 | 47.97161 | 1     | 1     | 1      | 1      | 1      | 1       | 1       | 1      | 1        | 1      |   |
| 22 | #####    | 0.42  | 0.569043 | 510.5683 | 12.78739 | 2.83  | 1.31  | 1.52   | 0.4186 | 2.7534 | 0.0027  | 0.00387 | 0.0181 | 0.000325 | 0.0227 |   |
| 23 | #####    | 0.42  | 0.26     | 291.0717 | 17.78128 | 2.76  | 1.24  | 1.1    | 0.2964 | 1.0816 | 0.0027  | 0.00134 | 0.0182 | 0.00082  | 0.0189 |   |
| 24 | #####    | 8.9   | 0.951855 | 484.1073 | 81.26421 | 1.16  | 2.49  | 1.03   | 0.9126 | 2.1794 | 0.0027  | 0.00251 | 0.205  | 0.00192  | 0.0752 |   |
| 25 | #####    | 13.4  | 0.26     | 348.3317 | 13.09005 | 5.38  | 0.298 | 1.94   | 0.3471 | 1.4599 | 0.0027  | 0.00413 | 0.04   | 0.001    | 0.0276 |   |
| 26 | 2006/4/2 | 14.3  | 0.26     | 408.2887 | 16.09601 | 5.14  | 0.759 | 1.7    | 0.4238 | 2.2122 | 0.00659 | 0.00635 | 0.043  | 0.00104  | 0.0451 |   |
| 27 | 2006/4/5 | 14    | 0.545333 | 114.52   | 26.33142 | 4.41  | 1.05  | 1.55   | 0.6682 | 2.7858 | 0.0027  | 0.00414 | 0.0444 | 0.00106  | 0.0356 |   |
| 28 | 2006/4/9 | 9.3   | 0.26     | 252.8983 | 20.05123 | 2.99  | 1.16  | 1.16   | 0.3922 | 1.9419 | 0.0027  | 0.00236 | 0.0352 | 0.0014   | 0.0426 |   |

Second column: PM column – concentration of PM (unit: ug/m<sup>3</sup>)

PM column should be list after of Date column

# CMBGC-Iteration 1.0

## Input file

Concentration of ambient dataset

|    | A        | B     | C        | D        | E        | F     | G     | H      | I      | J      | K       | L       | M      | N       | O      | K     |
|----|----------|-------|----------|----------|----------|-------|-------|--------|--------|--------|---------|---------|--------|---------|--------|-------|
| 1  | Date     | PM2.5 | S02      | CO       | NOx      | SO4   | NO3   | NH4    | EC     | OC     | Al      | Br      | Ca     | Cu      | Fe     | K     |
| 2  | 2006/1/5 |       | 0.26     | 367.4183 | 48.87959 | 0.288 | 0.516 | 0.0611 | 0.5252 | 1.4088 | 0.00547 | 0.00096 | 0.0888 | 0.00133 | 0.0539 |       |
| 3  | 2006/1/8 | 7.    | 6.2168   | 522.8087 | 72.80349 | 0.72  | 0.653 | 0.18   | 0.7592 | 2.5848 | 0.0027  | 0.00372 | 0.104  | 0.00271 | 0.0704 |       |
| 4  | #####    | 5.    | 3.817333 | 434.2217 | 78.61594 | 1.15  | 0.459 | 0.367  | 0.8658 | 1.8702 | 0.0027  | 0.00132 | 0.0957 | 0.00147 | 0.0641 |       |
| 5  | #####    | 3.    | 0.6544   | 510.5683 | 49.40925 | 0.626 | 0.247 | 0.207  | 0.403  | 1.317  | 0.0027  | 0.00027 | 0.0511 | 0.00076 | 0.0397 |       |
| 6  | #####    | 10.   | 2.508533 | 534.4267 | 96.77554 | 1.75  | 2.82  | 1.11   | 1.0413 | 2.5097 | 0.0027  | 0.00217 | 0.0434 | 0.00216 | 0.0708 |       |
| 7  | #####    | 5.    | 7.8528   | 334.0167 | 73.84904 | 0.579 | 0.391 | 0.174  | 0.975  | 2.215  | 0.0027  | 0.00166 | 0.0573 | 0.00215 | 0.0577 |       |
| 8  | #####    | 7.    | 0.6544   | 390.4091 | 51.11927 | 0.844 | 0.211 | 0.304  | 0.6097 | 1.5893 | 0.075   | 0.00254 | 0.0603 | 0.00089 | 0.0934 |       |
| 9  | 2006/2/1 | 9.    | 2.835733 | 501.025  | 41.54009 | 2.98  | 0.515 | 1.01   | 0.7631 | 1.8539 | 0.0027  | 0.0043  | 0.0294 | 0.0014  | 0.0436 |       |
| 10 | 2006/2/4 | 6.    | 1.934748 | 796.8683 | 105.477  |       |       |        |        |        |         |         |        |         |        | 0767  |
| 11 | 2006/2/7 | 10.   | 2.9448   | 586.915  | 149.8924 |       |       |        |        |        |         |         |        |         |        | 0.111 |
| 12 | #####    | 12.   | 2.9448   | 331.1935 | 39.64846 |       |       |        |        |        |         |         |        |         |        | 0414  |
| 13 | #####    | 12.   | 0.26     | 167.0083 | 18.68926 |       |       |        |        |        |         |         |        |         |        | 0358  |
| 14 | #####    | 14.   | 0.26     | 428.2052 | 21.62643 |       |       |        |        |        |         |         |        |         |        | 0106  |
| 15 | #####    | 17.   | 0.26     | 267.2133 | 53.57082 |       |       |        |        |        |         |         |        |         |        | 0292  |
| 16 | #####    | 9.    | 0.26     | 243.355  | 39.3458  |       |       |        |        |        |         |         |        |         |        | 0204  |
| 17 | #####    |       | 0.810034 | 331.1935 | 29.50704 |       |       |        |        |        |         |         |        |         |        | 0345  |
| 18 | 2006/3/6 | 17.   | 0.9816   | 434.2217 | 57.65673 |       |       |        |        |        |         |         |        |         |        | 0529  |
| 19 | 2006/3/9 | 6.    | 0.26     | 200.41   | 43.58304 |       |       |        |        |        |         |         |        |         |        | 0677  |
| 20 | #####    | 18.   | 0.9816   | 184.2278 | 29.50704 |       |       |        |        |        |         |         |        |         |        | 0.021 |
| 21 | #####    | 12.   | 7.1984   | 496.2533 | 47.97161 |       |       |        |        |        |         |         |        |         |        | 0503  |
| 22 | #####    | 0.4   | 0.569043 | 510.5683 | 12.78739 |       |       |        |        |        |         |         |        |         |        | 0227  |
| 23 | #####    | 0.4   | 0.26     | 291.0717 | 17.78128 |       |       |        |        |        |         |         |        |         |        | 0189  |
| 24 | #####    | 8.    | 0.951855 | 484.1073 | 81.26421 |       |       |        |        |        |         |         |        |         |        | 0752  |
| 25 | #####    | 13.   | 0.26     | 348.3317 | 13.09005 |       |       |        |        |        |         |         |        |         |        | 0276  |
| 26 | 2006/4/2 | 14.   | 0.26     | 408.2887 | 16.09601 |       |       |        |        |        |         |         |        |         |        | 0451  |
| 27 | 2006/4/5 | 1     | 0.545333 | 114.52   | 26.33142 |       |       |        |        |        |         |         |        |         |        | 0356  |
| 28 | 2006/4/9 | 9.    | 0.26     | 252.8983 | 20.05123 |       |       |        |        |        |         |         |        |         |        | 0426  |

Gases columns: concentration of ambient gases (unit: ug/m<sup>3</sup>)

Gases columns should be list after of PM column

User can modify the number of gas categories

# CMBGC-Iteration 1.0

## Input file

# Concentration of ambient dataset

# CMBGC-Iteration 1.0

## Input file

|    | A        | B           | C   | D  | E   | F   | G     | H     | I      | J     | K        | L      | M       | N      |          |
|----|----------|-------------|-----|----|-----|-----|-------|-------|--------|-------|----------|--------|---------|--------|----------|
| 1  | Date     | PM2.5       | SO2 | CO | NOx | SO4 | NO3   | NH4   | EC     | OC    | Al       | Br     | Ca      | Cu     |          |
| 2  | 2006/1/5 | 0.533333333 |     | 0  | 0   | 0   | 0.021 | 0.032 | 0.0043 | 0.156 | 0.190392 | 0.003  | 0.00026 | 0.0064 | 0.00034  |
| 3  | 2006/1/8 | 0.741333333 |     | 0  | 0   | 0   | 0.052 | 0.04  | 0.013  | 0.169 | 0.266566 | 0.0045 | 0.00038 | 0.0075 | 0.00034  |
| 4  | #####    | 0.656833333 |     | 0  | 0   | 0   | 0.083 | 0.026 | 0.026  | 0.182 | 0.219606 | 0.0045 | 0.00026 | 0.0069 | 0.00034  |
| 5  | #####    | 0.513833333 |     | 0  | 0   | 0   | 0.045 | 0.015 | 0.015  | 0.143 | 0.180834 | 0.0045 | 0.00045 | 0.0038 | 0.00034  |
| 6  | #####    | 0.975333333 |     | 0  | 0   | 0   | 0.12  | 0.14  | 0.078  | 0.182 | 0.266502 | 0.0045 | 0.00029 | 0.0033 | 0.00034  |
| 7  | #####    | 0.650333333 |     | 0  | 0   | 0   | 0.042 | 0.021 | 0.012  | 0.182 | 0.24747  | 0.0045 | 0.00028 | 0.0042 | 0.00034  |
| 8  | #####    | 0.786833333 |     | 0  | 0   | 0   | 0.061 | 0.012 | 0.021  | 0.156 | 0.199925 | 0.0066 | 0.00031 | 0.0044 | 0.00034  |
| 9  | 2006/2/1 | 0.916833    |     |    |     |     |       |       |        |       |          | 0.0045 | 0.0004  | 0.0023 | 0.00034  |
| 10 | 2006/2/4 | 0.682833    |     |    |     |     |       |       |        |       |          | 0.0045 | 0.00026 | 0.0042 | 0.00035  |
| 11 | 2006/2/7 | 0.955833    |     |    |     |     |       |       |        |       |          | 0.0045 | 0.00033 | 0.006  | 0.00034  |
| 12 | #####    | 1.085833    |     |    |     |     |       |       |        |       |          | 0.0045 | 0.00038 | 0.003  | 0.00034  |
| 13 | #####    | 1.079333    |     |    |     |     |       |       |        |       |          | 0.0035 | 0.00043 | 0.0051 | 0.000542 |
| 14 | #####    | 1.228833333 | 0   | 0  | 0   | 0   | 0.24  | 0.2   | 0.16   | 0.143 | 0.220002 | 0.0045 | 0.00034 | 0.0012 | 0.00034  |
| 15 | #####    | 1.384833333 | 0   | 0  | 0   | 0   | 0.25  | 0.22  | 0.16   | 0.169 | 0.257532 | 0.0045 | 0.00035 | 0.0013 | 0.00034  |
| 16 | #####    | 0.871333333 | 0   | 0  | 0   | 0   | 0.098 | 0.092 | 0.062  | 0.156 | 0.238356 | 0.0045 | 0.00027 | 0.0014 | 0.00034  |
| 17 | #####    | 0.858333333 | 0   | 0  | 0   | 0   | 0.23  | 0.062 | 0.083  | 0.156 | 0.191484 | 0.003  | 0.00045 | 0.0023 | 0.000542 |
| 18 | 2006/3/6 | 1.417333333 |     | 0  | 0   | 0   | 0.48  | 0.1   | 0.18   | 0.195 | 0.30515  | 0.0045 | 0.00051 | 0.0034 | 0.00034  |
| 19 | 2006/3/9 | 0.702333333 |     | 0  | 0   | 0   | 0.099 | 0.026 | 0.034  | 0.156 | 0.172439 | 0.0036 | 0.00026 | 0.0045 | 0.00034  |
| 20 | #####    | 1.495333333 | 0   | 0  | 0   | 0   | 0.51  | 0.087 | 0.15   | 0.156 | 0.247501 | 0.0045 | 0.00049 | 0.0033 | 0.000542 |
| 21 | #####    | 1.066333333 | 0   | 0  | 0   | 0   | 0.11  | 0.039 | 0.043  | 0.182 | 0.401203 | 0.0045 | 0.00041 | 0.0043 | 0.00034  |
| 22 | #####    | 0.546666667 | 0   | 0  | 0   | 0   | 0.2   | 0.088 | 0.11   | 0.156 | 0.276236 | 0.0045 | 0.00037 | 0.0017 | 0.000542 |
| 23 | #####    | 0.546666667 | 0   | 0  | 0   | 0   | 0.2   | 0.08  | 0.078  | 0.143 | 0.163017 | 0.0045 | 0.00025 | 0.0017 | 0.00034  |
| 24 | #####    | 0.851833333 | 0   | 0  | 0   | 0   | 0.083 | 0.15  | 0.073  | 0.182 | 0.247622 | 0.0045 | 0.00029 | 0.015  | 0.00034  |
| 25 | #####    | 1.144333333 | 0   | 0  | 0   | 0   | 0.38  | 0.016 | 0.14   | 0.143 | 0.190628 | 0.0045 | 0.00039 | 0.0031 | 0.00034  |
| 26 | 2006/4/2 | 1.202833333 |     | 0  | 0   | 0   | 0.36  | 0.041 | 0.12   | 0.156 | 0.239145 | 0.003  | 0.00053 | 0.0033 | 0.00034  |
| 27 | 2006/4/5 | 1.183333333 |     | 0  | 0   | 0   | 0.31  | 0.066 | 0.11   | 0.169 | 0.286122 | 0.0045 | 0.0004  | 0.0034 | 0.00034  |
| 28 | 2006/4/8 | 0.912933333 |     | 0  | 0   | 0   | 0.21  | 0.078 | 0.082  | 0.143 | 0.219988 | 0.0045 | 0.0003  | 0.0027 | 0.00034  |

Uncertainties of ambient dataset  
(Unit: ug/m<sup>3</sup>)



# CMBGC-Iteration 1.0

## Input file

Uncertainties of ambient dataset  
(Unit: ug/m<sup>3</sup>)

|    | A        | B           | C   | D  | E   | F     | G     | H      | I     | J        | K      | L       | M      | N        |
|----|----------|-------------|-----|----|-----|-------|-------|--------|-------|----------|--------|---------|--------|----------|
| 1  | Date     | PM2.5       | SO2 | CO | NOx | SO4   | NO3   | NH4    | EC    | OC       | Al     | Br      | Ca     | Cu       |
| 2  | 2006/1/5 | 0.533333333 | 0   | 0  | 0   | 0.021 | 0.032 | 0.0043 | 0.156 | 0.190392 | 0.003  | 0.00026 | 0.0064 | 0.00034  |
| 3  | 2006/1/8 | 0.741333333 | 0   | 0  | 0   | 0.052 | 0.04  | 0.013  | 0.169 | 0.266566 | 0.0045 | 0.00038 | 0.0075 | 0.00034  |
| 4  | #####    | 0.65        |     |    |     |       |       |        |       |          |        |         |        |          |
| 5  | #####    | 0.51        |     |    |     |       |       |        |       |          |        |         |        |          |
| 6  | #####    | 0.97        |     |    |     |       |       |        |       |          |        |         |        |          |
| 7  | #####    | 0.65        |     |    |     |       |       |        |       |          |        |         |        |          |
| 8  | #####    | 0.78        |     |    |     |       |       |        |       |          |        |         |        |          |
| 9  | 2006/2/1 | 0.910000000 | 0   | 0  | 0   | 0.21  | 0.021 | 0.012  | 0.19  | 0.219877 | 0.0045 | 0.0004  | 0.0023 | 0.00034  |
| 10 | 2006/2/4 | 0.682833333 | 0   | 0  | 0   | 0.051 | 0.036 | 0.017  | 0.195 | 0.267329 | 0.0045 | 0.00026 | 0.0042 | 0.00035  |
| 11 | 2006/2/7 | 0.955833333 | 0   | 0  | 0   | 0.1   | 0.12  | 0.057  | 0.221 | 0.286328 | 0.0045 | 0.00033 | 0.006  | 0.00034  |
| 12 | #####    | 1.085833333 | 0   | 0  | 0   | 0.17  | 0.11  | 0.091  | 0.169 | 0.285971 | 0.0045 | 0.00038 | 0.003  | 0.00034  |
| 13 | #####    | 1.079333333 | 0   | 0  | 0   | 0.24  | 0.039 | 0.083  | 0.156 | 0.266989 | 0.0035 | 0.00043 | 0.0051 | 0.000542 |
| 14 | #####    | 1.228833333 | 0   | 0  | 0   | 0.24  | 0.2   | 0.16   | 0.143 | 0.228882 | 0.0045 | 0.00034 | 0.0012 | 0.00034  |
| 15 | #####    | 1.384833333 | 0   | 0  | 0   | 0.25  | 0.22  | 0.16   | 0.169 | 0.257532 | 0.0045 | 0.00035 | 0.0013 | 0.00034  |
| 16 | #####    | 0.871333333 | 0   | 0  | 0   | 0.098 | 0.092 | 0.062  | 0.156 | 0.238356 | 0.0045 | 0.00027 | 0.0014 | 0.00034  |
| 17 | #####    | 0.858333333 | 0   | 0  | 0   | 0.23  | 0.062 | 0.083  | 0.156 | 0.191484 | 0.003  | 0.00045 | 0.0023 | 0.000542 |
| 18 | 2006/3/6 | 1.417333333 | 0   | 0  | 0   | 0.48  | 0.1   | 0.18   | 0.195 | 0.30515  | 0.0045 | 0.00051 | 0.0034 | 0.00034  |
| 19 | 2006/3/9 | 0.702333333 | 0   | 0  | 0   | 0.099 | 0.026 | 0.034  | 0.156 | 0.172439 | 0.0036 | 0.00026 | 0.0045 | 0.00034  |
| 20 | #####    | 1.495333333 | 0   | 0  | 0   | 0.51  | 0.087 | 0.15   | 0.156 | 0.247501 | 0.0045 | 0.00049 | 0.0033 | 0.000542 |
| 21 | #####    | 1.066333333 | 0   | 0  | 0   | 0.11  | 0.039 | 0.043  | 0.182 | 0.401203 | 0.0045 | 0.00041 | 0.0043 | 0.00034  |
| 22 | #####    | 0.546666667 | 0   | 0  | 0   | 0.2   | 0.088 | 0.11   | 0.156 | 0.276236 | 0.0045 | 0.00037 | 0.0017 | 0.000542 |
| 23 | #####    | 0.546666667 | 0   | 0  | 0   | 0.2   | 0.08  | 0.078  | 0.143 | 0.163017 | 0.0045 | 0.00025 | 0.0017 | 0.00034  |
| 24 | #####    | 0.851833333 | 0   | 0  | 0   | 0.083 | 0.15  | 0.073  | 0.182 | 0.247622 | 0.0045 | 0.00029 | 0.015  | 0.00034  |
| 25 | #####    | 1.144333333 | 0   | 0  | 0   | 0.38  | 0.016 | 0.14   | 0.143 | 0.190628 | 0.0045 | 0.00039 | 0.0031 | 0.00034  |
| 26 | 2006/4/2 | 1.202833333 | 0   | 0  | 0   | 0.36  | 0.041 | 0.12   | 0.156 | 0.239145 | 0.003  | 0.00053 | 0.0033 | 0.00034  |
| 27 | 2006/4/5 | 1.183333333 | 0   | 0  | 0   | 0.31  | 0.066 | 0.11   | 0.169 | 0.286122 | 0.0045 | 0.0004  | 0.0034 | 0.00034  |
| 28 | 2006/4/8 | 0.912933333 | 0   | 0  | 0   | 0.21  | 0.078 | 0.082  | 0.143 | 0.219988 | 0.0045 | 0.0003  | 0.0027 | 0.00034  |

# CMBGC-Iteration 1.0

## Input file

Uncertainties of ambient dataset  
(Unit: ug/m<sup>3</sup>)

|    | A        | B          | C   | D  | E   | F     | G     | H      | I     | J        | K      | L       | M       | N        |
|----|----------|------------|-----|----|-----|-------|-------|--------|-------|----------|--------|---------|---------|----------|
| 1  | Date     | PM2.5      | SO2 | CO | NOx | SO4   | NO3   | NH4    | EC    | OC       | Al     | Br      | Ca      | Cu       |
| 2  | 2006/1/5 | 0.53333333 | 0   | 0  | 0   | 0.021 | 0.032 | 0.0043 | 0.156 | 0.190392 | 0.003  | 0.00026 | 0.0064  | 0.00034  |
| 3  | 2006/1/8 | 0.74133333 | 0   | 0  | 0   | 0.052 | 0.04  | 0.013  | 0.169 | 0.266566 | 0.0045 | 0.00038 | 0.0075  | 0.00034  |
| 4  | #####    | 0.65683333 | 0   | 0  | 0   | 0.083 | 0.026 | 0.026  | 0.182 | 0.219606 | 0.0045 | 0.00026 | 0.0069  | 0.00034  |
| 5  | #####    | 0.51383333 | 0   | 0  | 0   | 0.045 | 0.015 | 0.015  | 0.143 | 0.180834 | 0.0045 | 0.00045 | 0.0038  | 0.00034  |
| 6  | #####    | 0.97533333 | 0   | 0  | 0   | 0.12  | 0.14  | 0.078  | 0.182 | 0.266502 | 0.0045 | 0.00029 | 0.0033  | 0.00034  |
| 7  | #####    | 0.65033333 | 0   | 0  | 0   | 0.042 | 0.021 | 0.012  | 0.182 | 0.24747  | 0.0045 | 0.00028 | 0.0042  | 0.00034  |
| 8  | #####    | 0.78683333 | 0   | 0  | 0   | 0.061 | 0.012 | 0.021  | 0.156 | 0.199925 | 0.0066 | 0.00031 | 0.0044  | 0.00034  |
| 9  | 2006/2/1 | 0.91683333 | 0   | 0  | 0   | 0.21  | 0.027 | 0.072  | 0.169 | 0.219877 | 0.0045 | 0.0004  | 0.0023  | 0.00034  |
| 10 | 2006/2/4 | 0.68283333 | 0   | 0  | 0   |       |       |        |       |          |        |         | 0.00035 |          |
| 11 | 2006/2/7 | 0.95583333 | 0   | 0  | 0   |       |       |        |       |          |        |         | 0.00034 |          |
| 12 | #####    | 1.08583333 | 0   | 0  | 0   |       |       |        |       |          |        |         | 0.00034 |          |
| 13 | #####    | 1.07933333 | 0   | 0  | 0   |       |       |        |       |          |        |         | 0.00542 |          |
| 14 | #####    | 1.22883333 | 0   | 0  | 0   |       |       |        |       |          |        |         | 0.00034 |          |
| 15 | #####    | 1.38483333 | 0   | 0  | 0   | 0.23  | 0.22  | 0.16   | 0.169 | 0.207532 | 0.0045 | 0.00035 | 0.0013  | 0.00034  |
| 16 | #####    | 0.87133333 | 0   | 0  | 0   | 0.098 | 0.092 | 0.062  | 0.156 | 0.238356 | 0.0045 | 0.00027 | 0.0014  | 0.00034  |
| 17 | #####    | 0.85833333 | 0   | 0  | 0   | 0.23  | 0.062 | 0.083  | 0.156 | 0.191484 | 0.003  | 0.00045 | 0.0023  | 0.000542 |
| 18 | 2006/3/6 | 1.41733333 | 0   | 0  | 0   | 0.48  | 0.1   | 0.18   | 0.195 | 0.30515  | 0.0045 | 0.00051 | 0.0034  | 0.00034  |
| 19 | 2006/3/9 | 0.70233333 | 0   | 0  | 0   | 0.099 | 0.026 | 0.034  | 0.156 | 0.172439 | 0.0036 | 0.00026 | 0.0045  | 0.00034  |
| 20 | #####    | 1.49533333 | 0   | 0  | 0   | 0.51  | 0.087 | 0.15   | 0.156 | 0.247501 | 0.0045 | 0.00049 | 0.0033  | 0.000542 |
| 21 | #####    | 1.06633333 | 0   | 0  | 0   | 0.11  | 0.039 | 0.043  | 0.182 | 0.401203 | 0.0045 | 0.00041 | 0.0043  | 0.00034  |
| 22 | #####    | 0.54666666 | 0   | 0  | 0   | 0.2   | 0.088 | 0.11   | 0.156 | 0.276236 | 0.0045 | 0.00037 | 0.0017  | 0.000542 |
| 23 | #####    | 0.54666666 | 0   | 0  | 0   | 0.2   | 0.08  | 0.078  | 0.143 | 0.163017 | 0.0045 | 0.00025 | 0.0017  | 0.00034  |
| 24 | #####    | 0.85183333 | 0   | 0  | 0   | 0.083 | 0.15  | 0.073  | 0.182 | 0.247622 | 0.0045 | 0.00029 | 0.015   | 0.00034  |
| 25 | #####    | 1.14433333 | 0   | 0  | 0   | 0.38  | 0.016 | 0.14   | 0.143 | 0.190628 | 0.0045 | 0.00039 | 0.0031  | 0.00034  |
| 26 | 2006/4/2 | 1.20283333 | 0   | 0  | 0   | 0.36  | 0.041 | 0.12   | 0.156 | 0.239145 | 0.003  | 0.00053 | 0.0033  | 0.00034  |
| 27 | 2006/4/5 | 1.18333333 | 0   | 0  | 0   | 0.31  | 0.066 | 0.11   | 0.169 | 0.286122 | 0.0045 | 0.0004  | 0.0034  | 0.00034  |
| 28 | 2006/4/8 | 0.91293333 | 0   | 0  | 0   | 0.21  | 0.078 | 0.082  | 0.143 | 0.219988 | 0.0045 | 0.0003  | 0.0027  | 0.00034  |

Uncertainties of gases can be set as zeros

# CMBGC-Iteration 1.0

## Input file

Uncertainties of ambient dataset  
(Unit: ug/m<sup>3</sup>)

|    | A        | B           | C   | D  | E   | F     | G     | H      | I     | J        | K      | L       | M      | N       |
|----|----------|-------------|-----|----|-----|-------|-------|--------|-------|----------|--------|---------|--------|---------|
| 1  | Date     | PM2.5       | SO2 | CO | NOx | SO4   | NO2   | MDL    | EC    | OC       | AL     | Pm      | Cs     | Cu      |
| 2  | 2006/1/5 | 0.533333333 | 0   | 0  | 0   | 0.021 | 0.032 | 0.0043 | 0.156 | 0.190392 | 0.003  | 0.00026 | 0.0064 | 0.0003  |
| 3  | 2006/1/8 | 0.741333333 | 0   | 0  | 0   | 0.052 | 0.04  | 0.013  | 0.169 | 0.266566 | 0.0045 | 0.00038 | 0.0075 | 0.0003  |
| 4  | #####    | 0.656833333 | 0   | 0  | 0   | 0.083 | 0.026 | 0.026  | 0.182 | 0.219606 | 0.0045 | 0.00026 | 0.0069 | 0.0003  |
| 5  | #####    | 0.513833333 | 0   | 0  | 0   | 0.045 | 0.015 | 0.015  | 0.143 | 0.180834 | 0.0045 | 0.00045 | 0.0038 | 0.0003  |
| 6  | #####    | 0.975333333 | 0   | 0  | 0   | 0.12  | 0.14  | 0.078  | 0.182 | 0.266502 | 0.0045 | 0.00029 | 0.0033 | 0.0003  |
| 7  | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0042 | 0.0003  |
| 8  | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0044 | 0.0003  |
| 9  | 2006/1   |             |     |    |     |       |       |        |       |          |        |         | 0.0023 | 0.0003  |
| 10 | 2006/1   |             |     |    |     |       |       |        |       |          |        |         | 0.0042 | 0.0003  |
| 11 | 2006/1   |             |     |    |     |       |       |        |       |          |        |         | 0.006  | 0.0003  |
| 12 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.003  | 0.0003  |
| 13 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0051 | 0.00054 |
| 14 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0012 | 0.0003  |
| 15 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0013 | 0.0003  |
| 16 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0014 | 0.0003  |
| 17 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0023 | 0.00054 |
| 18 | 2006/1   |             |     |    |     |       |       |        |       |          |        |         | 0.0034 | 0.0003  |
| 19 | 2006/1   |             |     |    |     |       |       |        |       |          |        |         | 0.0045 | 0.0003  |
| 20 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0033 | 0.00054 |
| 21 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0043 | 0.0003  |
| 22 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0017 | 0.00054 |
| 23 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0017 | 0.0003  |
| 24 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.015  | 0.0003  |
| 25 | #####    |             |     |    |     |       |       |        |       |          |        |         | 0.0031 | 0.0003  |
| 26 | 2006/4/2 | 1.202833333 | 0   | 0  | 0   | 0.36  | 0.041 | 0.12   | 0.156 | 0.239145 | 0.003  | 0.00053 | 0.0033 | 0.0003  |
| 27 | 2006/4/5 | 1.183333333 | 0   | 0  | 0   | 0.31  | 0.066 | 0.11   | 0.169 | 0.286122 | 0.0045 | 0.0004  | 0.0034 | 0.0003  |
| 28 | 2006/4/8 | 0.812933333 | 0   | 0  | 0   | 0.21  | 0.078 | 0.082  | 0.143 | 0.219988 | 0.0045 | 0.0003  | 0.0027 | 0.0003  |

Daily uncertainties of species can be measured or calculated as:

$$Un_{ij} = \sqrt{a \cdot x_{ij}^2 + b \cdot (MDL)^2}$$

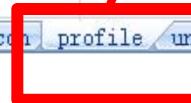
Un is the uncertainties of species, a is the error fractions, b is the coefficient of MDL (can be set as 0.5), MDL is the Minimum Detectable Limits of species.

# CMBGC-Iteration 1.0

## Input file

|    | A      | B      | C      | D      | E      | F      | G      | H      | I      | J      | K      | L      | M      | N      | O     |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|
| 1  | SID    | SO4    | N03    | NH4    | EC     | OC     | Al     | Br     | Ca     | Cu     | Fe     | K      | Mn     | Pb     | Se    |
| 2  | LDGV   | 0.0133 | 0      | 0      | 0.2355 | 0.5486 | 0.0019 | 0      | 0.0118 | 0.0004 | 0.012  | 0.0001 | 0.0001 | 0.0006 |       |
| 3  | HDDV   | 0.0046 | 0.002  | 0      | 0.7351 | 0.1981 | 0      | 0      | 0.0006 | 0      | 0.0002 | 0.0001 | 0      | 0      |       |
| 4  | SDUST  | 0.001  | 0.001  | 0      | 0.006  | 0.044  | 0.095  | 0      | 0.018  | 0.0003 | 0.053  | 0.0092 | 0.0016 | 0.0001 |       |
| 5  | BURN   | 0.0239 | 0.0024 | 0.0165 | 0.1575 | 0.6441 | 0.0011 | 0.0008 | 0.004  | 0      | 0.0007 | 0.0573 | 0      | 0      |       |
| 6  | CFPP   | 0.2874 | 0.0069 | 0.0179 | 0.0138 | 0.2718 | 0.053  | 0.0003 | 0.1655 | 0.0009 | 0.0361 | 0.0052 | 0.0012 | 0.0006 | 0.005 |
| 7  | AMSLF  | 0.727  | 0      | 0.273  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 8  | AMBSLF | 0.835  | 0      | 0.156  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 9  | AMNITR |        |        |        |        |        |        |        |        |        |        |        | 0      | 0      | 0     |
| 10 | SOC    |        |        |        |        |        |        |        |        |        |        |        | 0      | 0      | 0     |
| 11 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 12 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 13 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 14 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 15 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 16 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 17 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 18 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 19 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 20 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 21 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 22 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 23 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 24 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 25 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 26 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 27 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |

Profiles of source categories  
(Unit: g/g)



# CMBGC-Iteration 1.0

## Input file

Profiles of source categories  
(Unit: g/g)

|    | A      | B      | C      | D      | E      | F      | G      | H      | I      | J      | K      | L      | M      | N      | O     |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|
| 1  | SID    | SO4    | N03    | NH4    | EC     | OC     | Al     | Br     | Ca     | Cu     | Fe     | K      | Mn     | Pb     | Se    |
| 2  | EDSV   | 0.0100 | 0      | 0      | 0.2055 | 0.5100 | 0.0010 | 0      | 0.0110 | 0.0001 | 0.010  | 0.0001 | 0.0001 | 0.0000 | 0     |
| 3  | HDDV   | 0.0046 | 0.002  | 0      | 0.7351 | 0.1981 | 0      | 0      | 0.0006 | 0      | 0.0002 | 0.0001 | 0      | 0      | 0     |
| 4  | SDUST  | 0.001  | 0.001  | 0      | 0.006  | 0.044  | 0.095  | 0      | 0.018  | 0.0003 | 0.053  | 0.0092 | 0.0016 | 0.0001 | 0     |
| 5  | BURN   | 0.0239 | 0.0024 | 0.0165 | 0.1575 | 0.6441 | 0.0011 | 0.0008 | 0.004  | 0      | 0.0007 | 0.0573 | 0      | 0      | 0     |
| 6  | CFPP   | 0.2874 | 0.0069 | 0.0179 | 0.0138 | 0.2718 | 0.053  | 0.0003 | 0.1655 | 0.0009 | 0.0361 | 0.0052 | 0.0012 | 0.0006 | 0.005 |
| 7  | AMSLF  | 0.727  | 0      | 0.273  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 8  | AMBSLF | 0.835  | 0      | 0.156  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 9  | AMNITR | 0      | 0.775  | 0.225  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 10 | SOC    | 0      | 0      | 0      | 0      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0     |
| 11 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 12 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 13 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 14 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 15 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 16 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 17 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 18 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 19 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 20 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 21 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 22 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 23 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 24 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 25 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 26 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 27 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |

Title Line

The sequence of species should  
be the same to that in  
“concentration” worksheet

# CMBGC-Iteration 1.0

## Input file

Profiles of source categories  
(Unit: g/g)

|    | A      | B      | C      | D      | E      | F      | G      | H      | I      | J      | K      | L      | M      | N      | O     |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-------|
| 1  | SID    | SO4    | N03    | NH4    | EC     | OC     | Al     | Br     | Ca     | Cu     | Fe     | K      | Mn     | Pb     | Se    |
| 2  | LDGV   | 0.0133 | 0      | 0      | 0.2355 | 0.5486 | 0.0019 | 0      | 0.0118 | 0.0004 | 0.012  | 0.0001 | 0.0001 | 0.0006 |       |
| 3  | HDDV   | 0.0046 | 0.002  | 0      | 0.7351 | 0.1981 | 0      | 0      | 0.0006 | 0      | 0.0002 | 0.0001 | 0      | 0      |       |
| 4  | SDUST  | 0.001  | 0.001  | 0      | 0.006  | 0.044  | 0.095  | 0      | 0.018  | 0.0003 | 0.053  | 0.0092 | 0.0016 | 0.0001 |       |
| 5  | BURN   | 0.0239 | 0.0024 | 0.0165 | 0.1575 | 0.6441 | 0.0011 | 0.0008 | 0.004  | 0      | 0.0007 | 0.0573 | 0      | 0      |       |
| 6  | CFPP   | 0.2874 | 0.0069 | 0.0179 | 0.0138 | 0.2718 | 0.053  | 0.0003 | 0.1655 | 0.0009 | 0.0361 | 0.0052 | 0.0012 | 0.0006 | 0.005 |
| 7  | AMSLUF | 0.727  | 0      | 0.273  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |       |
| 8  | AMBSLF | 0.835  | 0      | 0.156  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |       |
| 9  | AMNITR | 0      | 0.773  | 0.225  | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |       |
| 10 | SOC    | 0      | 0      | 0      | 0      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |       |
| 11 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 12 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 13 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 14 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 15 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 16 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 17 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 18 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 19 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 20 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 21 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 22 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 23 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 24 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 25 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 26 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |
| 27 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |       |

Source name column

User can change the order or  
number of source categories

# CMBGC-Iteration 1.0

## Input file

Profiles of source categories  
(Unit: g/g)

|    | A      | B               | C               | D               | E      | F      | G      | H               | I              | J              | K      | L      | M              | N      | O              |
|----|--------|-----------------|-----------------|-----------------|--------|--------|--------|-----------------|----------------|----------------|--------|--------|----------------|--------|----------------|
| 1  | SID    | SO <sub>4</sub> | NO <sub>2</sub> | NU <sub>4</sub> | EC     | OC     | A1     | P <sub>CO</sub> | C <sub>1</sub> | C <sub>2</sub> | Fe     | V      | W <sub>1</sub> | Ph     | C <sub>3</sub> |
| 2  | LDGV   | 0.0133          | 0               | 0               | 0.2355 | 0.5486 | 0.0019 | 0               | 0.0118         | 0.0004         | 0.012  | 0.0001 | 0.0001         | 0.0006 |                |
| 3  | HDDV   | 0.0046          | 0.002           | 0               | 0.7351 | 0.1981 | 0      | 0               | 0.0006         | 0              | 0.0002 | 0.0001 | 0              | 0      |                |
| 4  | SDUST  | 0.001           | 0.001           | 0               | 0.006  | 0.044  | 0.095  | 0               | 0.018          | 0.0003         | 0.053  | 0.0092 | 0.0016         | 0.0001 |                |
| 5  | BURN   | 0.0239          | 0.0024          | 0.0165          | 0.1575 | 0.6441 | 0.0011 | 0.0008          | 0.004          | 0              | 0.0007 | 0.0573 | 0              | 0      |                |
| 6  | CFPP   | 0.2874          | 0.0069          | 0.0179          | 0.0138 | 0.2718 | 0.053  | 0.0003          | 0.1655         | 0.0009         | 0.0361 | 0.0052 | 0.0012         | 0.0006 | 0.009          |
| 7  | AMSLUF | 0.727           | 0               | 0.273           | 0      | 0      | 0      | 0               | 0              | 0              | 0      | 0      | 0              | 0      | 0              |
| 8  | AMBSLF | 0.835           | 0               | 0.156           | 0      | 0      | 0      | 0               | 0              | 0              | 0      | 0      | 0              | 0      | 0              |
| 9  | AMNTR  | 0               | 0.775           | 0.225           | 0      | 0      | 0      | 0               | 0              | 0              | 0      | 0      | 0              | 0      | 0              |
| 10 | SOC    | 0               | 0               | 0               | 0      | 1      | 0      | 0               | 0              | 0              | 0      | 0      | 0              | 0      | 0              |
| 11 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 12 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 13 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 14 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 15 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 16 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 17 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 18 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 19 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 20 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 21 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 22 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 23 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 24 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 25 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 26 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |
| 27 |        |                 |                 |                 |        |        |        |                 |                |                |        |        |                |        |                |

Source profile dataset (g/g)

Sum of species in one source  
should  $\leq 1$

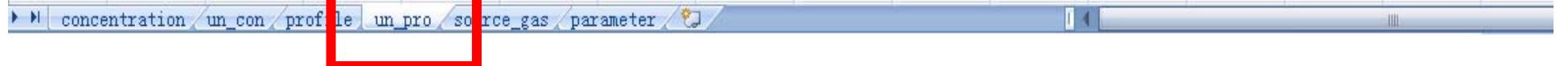
# CMBGC-Iteration 1.0

## Input file

| SID    | SO4    | NO3    | NH4    | EC     | OC     | Al     | Br     | Ca     | Cu     | Fe     | K      | Mn     | Pb     | Se     | Si   |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|------|
| LDGV   | 0.0056 | 0.0052 | 0.01   | 0.0277 | 0.0642 | 0.0024 | 0.0003 | 0.0016 | 0.0006 | 0.0016 | 0.0015 | 0.0008 | 0.0008 | 0.0003 | 0.01 |
| HDDV   | 0.0048 | 0.0014 | 0.01   | 0.1014 | 0.0774 | 0.01   | 0      | 0.0005 | 0.0001 | 0.0001 | 0.0002 | 0.0001 | 0.0001 | 0.0001 | 0.   |
| SDUST  | 0.0004 | 0.0004 | 0      | 0.004  | 0.017  | 0.001  | 0      | 0.004  | 0.0003 | 0.006  | 0.0033 | 0.0007 | 0      | 0      | 0.0  |
| BURN   | 0.0227 | 0.0018 | 0.0253 | 0.1545 | 0.1645 | 0.001  | 0.0009 | 0.005  | 0      | 0.0008 | 0.0563 | 0      | 0      | 0      | 0.00 |
| CFPP   | 0.2256 | 0.0109 | 0.0213 | 0.0222 | 0.2577 | 0.0326 | 0.0006 | 0.1053 | 0.0007 | 0.0202 | 0.0026 | 0.0011 | 0.0009 | 0.0083 | 0.06 |
| AMSLUF | 0.0360 | 0.0000 | 0.0140 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 |
| AMBSLF | 0.0420 | 0.0000 | 0.0080 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 |
| AMNITR | 0.0000 | 0.0390 | 0.0110 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.00 |
| OTHROC | 0.0000 |        |        |        |        |        |        |        |        |        | 0      | 0.0000 | 0.0000 | 0.0000 | 0.00 |

Uncertainties of source profile  
(Unit: g/g)

Pattern of “un\_pro” is the same  
to that of “profile”



# CMBGC-Iteration 1.0

## Input file

|    |         |     |        |        |        |  |  |  |  |
|----|---------|-----|--------|--------|--------|--|--|--|--|
| 1  | SID     | SO2 | CO     | NOx    |        |  |  |  |  |
| 2  | LDGV    |     | 4      | 800    | 83.7   |  |  |  |  |
| 3  | HDDV    |     | 0.71   | 13.4   | 21.9   |  |  |  |  |
| 4  | SDUST   |     | 0      | 0      | 0      |  |  |  |  |
| 5  | BURN    |     | 0.013  | 10.1   | 0.24   |  |  |  |  |
| 6  | CFPP    |     | 128    | 2.1    | 41     |  |  |  |  |
| 7  | AMSLULF |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |
| 8  | AMBSLF  |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |
| 9  | AMNITR  |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |
| 10 | OTHROC  |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |

Gas-to-PM2.5 Ratios for source emissions  
used as Constraints (Unit: g/g)



# CMBGC-Iteration 1.0

## Input file

| 1  | SID     | SO2    | CO   | NOx  |
|----|---------|--------|------|------|
| 2  | LDGV    | 4      | 800  | 83.7 |
| 3  | HDDV    | 0.71   | 13.4 | 21.9 |
| 4  | SDUST   | 0      | 0    | 0    |
| 5  | BURN    | 0.013  | 10.1 | 0.24 |
| 6  | CFPP    | 128    | 2.1  | 41   |
| 7  | AMSLULF | 0.0000 |      |      |
| 8  | AMBSLF  | 0.0000 |      |      |
| 9  | AMNITR  | 0.0000 |      |      |
| 10 | OTHROC  | 0.0000 |      |      |
| 11 |         |        |      |      |
| 12 |         |        |      |      |
| 13 |         |        |      |      |
| 14 |         |        |      |      |
| 15 |         |        |      |      |
| 16 |         |        |      |      |
| 17 |         |        |      |      |
| 18 |         |        |      |      |
| 19 |         |        |      |      |
| 20 |         |        |      |      |
| 21 |         |        |      |      |
| 22 |         |        |      |      |
| 23 |         |        |      |      |
| 24 |         |        |      |      |
| 25 |         |        |      |      |
| 26 |         |        |      |      |
| 27 |         |        |      |      |

Gases name line:

The number and sequence of gases should  
be the same to that in  
“concentration” worksheet

# CMBGC-Iteration 1.0

## Input file

|    |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|----|--------|-----|--------|--------|--------|--|--|--|--|--|--|--|--|--|--|--|--|--|
| 1  | SID    | NO2 | CO     | NOx    |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 2  | LDGV   |     | 4      | 800    | 83.7   |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 3  | HDDV   |     | 0.71   | 13.4   | 21.9   |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 4  | SDUST  |     | 0      | 0      | 0      |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 5  | BURN   |     | 0.013  | 10.1   | 0.24   |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 6  | CFPP   |     | 128    | 2.1    | 41     |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 7  | AMSULF |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 8  | AMBSLF |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 9  | AMNITR |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 10 | OTHROC |     | 0.0000 | 0.0000 | 0.0000 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 11 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 12 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 13 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 14 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 15 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 16 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 17 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 18 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 19 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 20 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 21 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 22 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 23 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 24 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 25 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 26 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 27 |        |     |        |        |        |  |  |  |  |  |  |  |  |  |  |  |  |  |

Sources name column:

The number and sequence of source should  
be the same to that in  
“profile” worksheet

# CMBGC-Iteration 1.0

## Input file

```
1   3 number of gas
2   3 range for gas constraints
3   40 coefficient of ub
4   20 step_max
5   0.02 step_constraint
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

**Key parameters for solution**



# CMBGC-Iteration 1.0

## Input file

### Key parameters for solution

```
1 3 number of gas
2 5 range for gas constraints
3 40 coefficient of ub
4 20 step_max
5 0.02 step_constraint
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

Number of gases

Should be the same to the number of  
gases in “concentration” worksheet

# CMBGC-Iteration 1.0

## Input file

### Key parameters for solution

```
1    3 number of gas
2    3 range for gas constraints
3    40 coefficient of ub
4    20 step_max
5    0.02 step_constraint
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

Range of gas constraints for global optimization solution in the model

Can be set as default value

# CMBGC-Iteration 1.0

## Input file

### Key parameters for solution

```
1      3 number of gas
2      0 range for gas constraints
3      40 coefficient of ub
4      20 step_max
5      0.02 step_constraint
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

Coefficient of up bound for global optimization solution in the model

Can be set as the average PM concentration

# CMBGC-Iteration 1.0

## Input file

Key parameters for solution

```
1      3 number of gas
2      3 range for gas constraints
3      40 coefficient of ub
4      20 step_max
5      0.02 step_constraint
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

A red arrow points from the highlighted line "20 step\_max" in the input file to a red-bordered box containing the text "Max step of Iteration".

concentration un\_con profile un\_pro source\_gas parameter

# CMBGC-Iteration 1.0

## Input file

Key parameters for solution

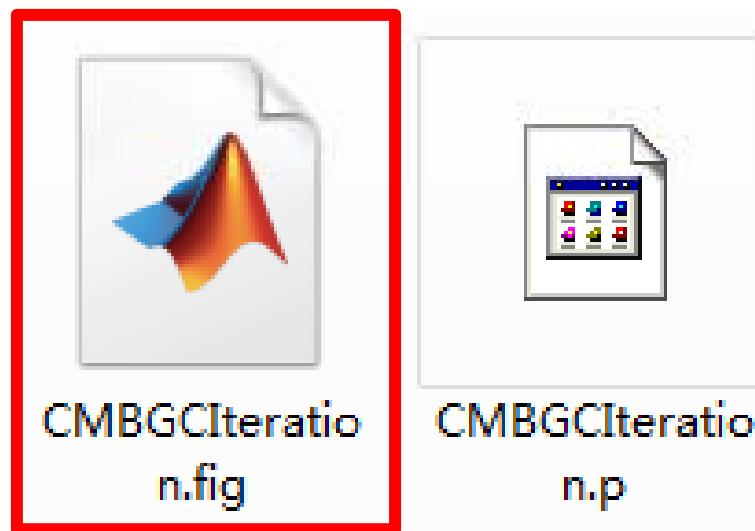
```
1      3 number of gas
2      3 range for gas constraints
3      40 coefficient of ub
4      20 step_max
5      0.02 step constrain
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
```

0.02 step constrain

Condition of Iterative convergence

# CMBGC-Iteration 1.0

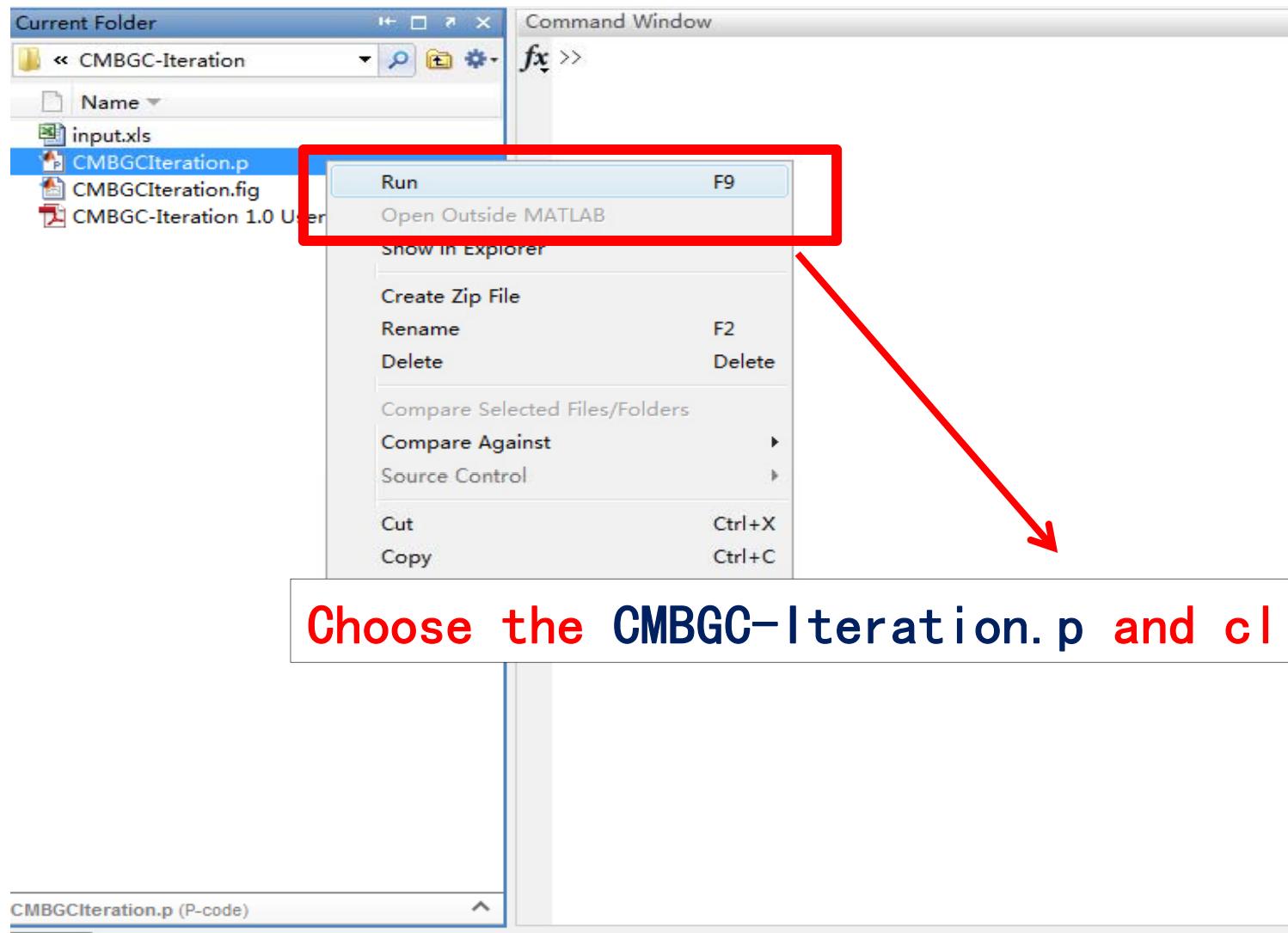
- Run the model



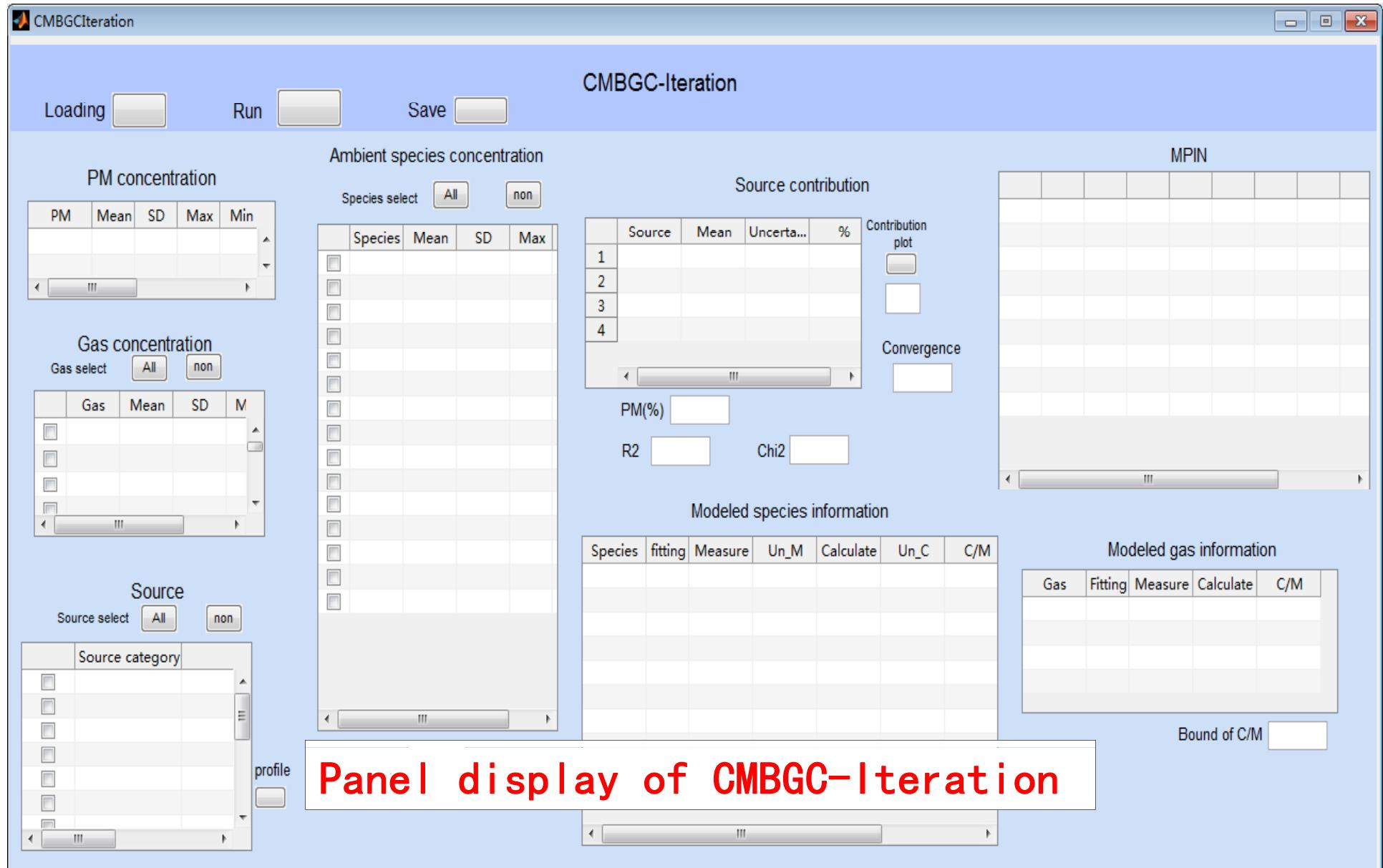
Double click the CMBGCIteration.fig file

# CMBGC-Iteration 1.0

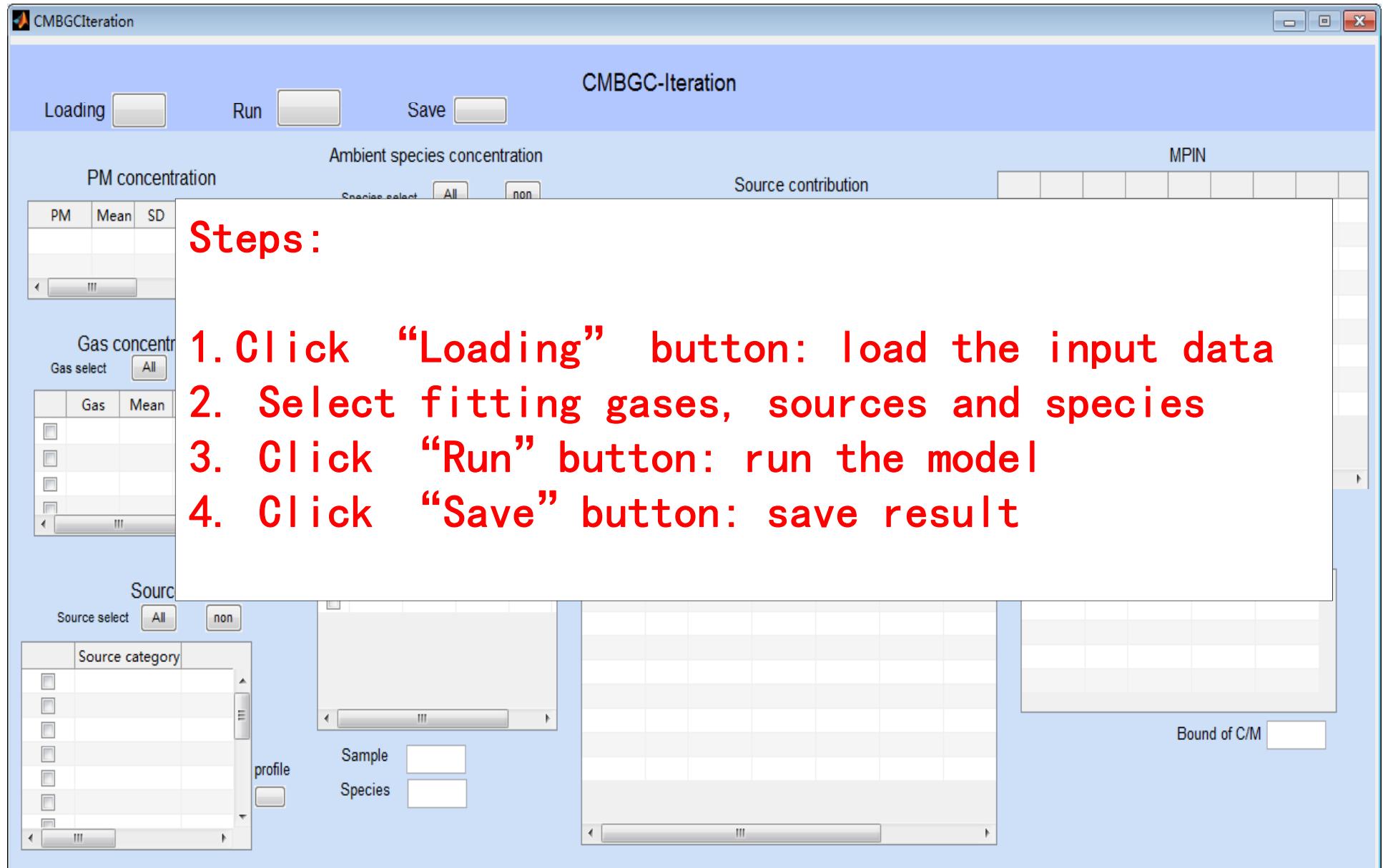
- Run the model



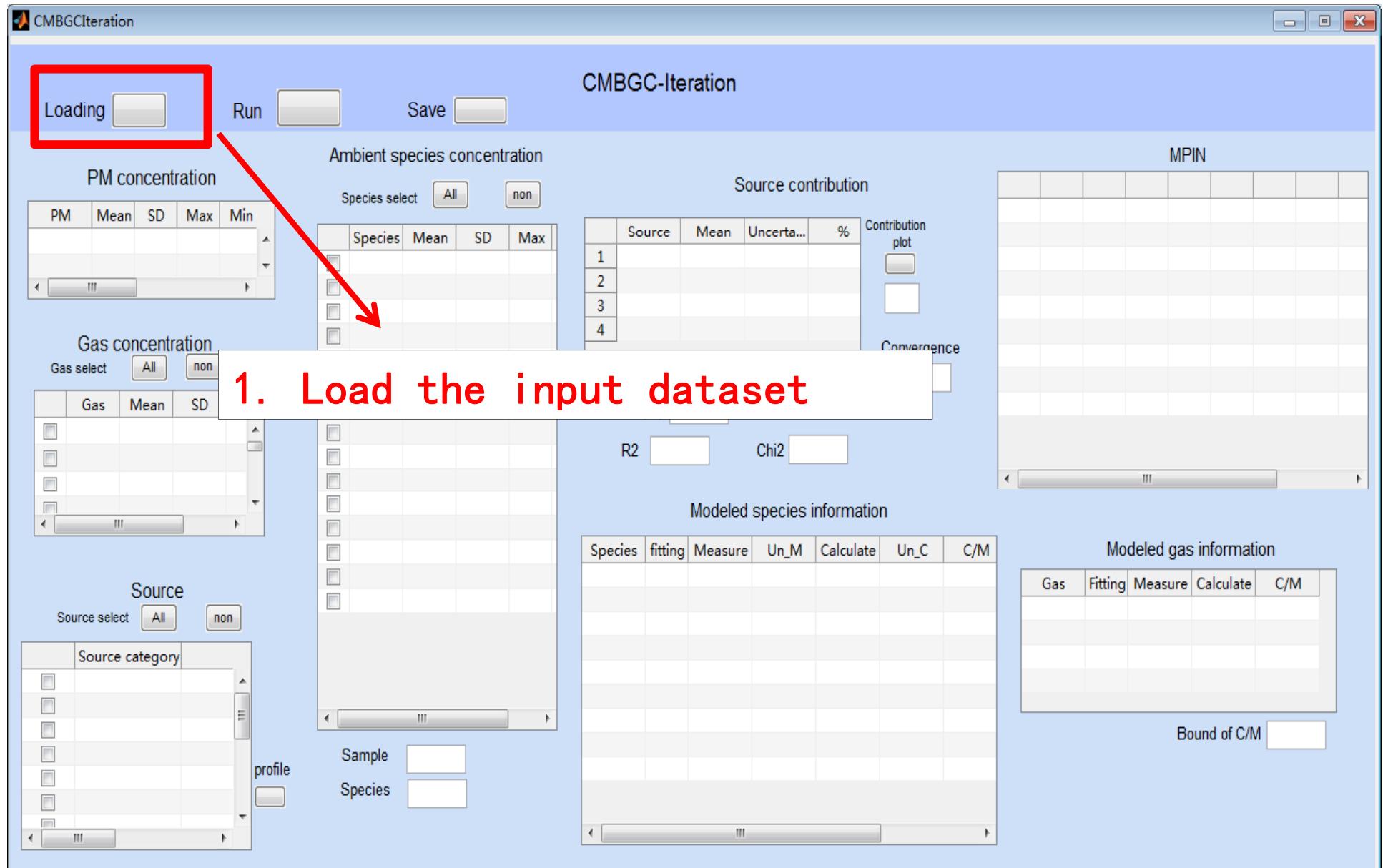
# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0

**CMBGC-Iteration**

Loading Run Save

**a** PM concentration

| PM    | Mean  | SD   | Max   | Min  |
|-------|-------|------|-------|------|
| PM2.5 | 10.28 | 4.92 | 31.00 | 0.42 |

**b** Gas concentration

Gas select

| Gas | Mean   | SD     | Max   |
|-----|--------|--------|-------|
| SO2 | 1.19   | 1.37   | 11.89 |
| CO  | 360.73 | 147.63 | 107.. |
| NOx | 37.15  | 34.91  | 298   |

**c** Source

Source select

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMSLUF          |
| AMRSUF          |

**d** Species select

Ambient species concentration

| Species | Mean | SD   | Max   |
|---------|------|------|-------|
| SO4     | 2.72 | 1.80 | 10.90 |
| NO3     | 0.87 | 0.94 | 11.10 |
| NH4     | 1.08 | 0.77 | 5.21  |
| EC      | 0.73 | 0.46 | 3.81  |
| OC      | 2.32 | 1.05 | 6.58  |
| Al      | 0.06 | 0.12 | 0.99  |
| Br      | 0.00 | 0.00 | 0.01  |
| Ca      | 0.07 | 0.08 | 0.63  |
| Cu      | 0.00 | 0.00 | 0.02  |
| Fe      | 0.08 | 0.08 | 0.62  |
| K       | 0.06 | 0.05 | 0.46  |
| Mn      | 0.00 | 0.00 | 0.01  |
| Pb      | 0.00 | 0.00 | 0.03  |
| Se      | 0.00 | 0.00 | 0.01  |
| Si      | 0.15 | 0.27 | 2.06  |
| Zn      | 0.01 | 0.00 | 0.03  |

Sample: 379  
Species: 16

Source contribution

MPIN

Display the information of input dataset

**a: concentrations of PM**

**b: concentrations of gases**

**c: categories of source**

**d: concentration of species**

Bound of C/M

# CMBGC-Iteration 1.0

**CMBGC-Iteration**

Loading Run Save

**a PM concentration**

| PM    | Mean  | SD   | Max   | Min  |
|-------|-------|------|-------|------|
| PM2.5 | 10.28 | 4.92 | 31.00 | 0.42 |

**b Gas concentration**

Gas select

| Gas | Mean   | SD     | Max   |
|-----|--------|--------|-------|
| SO2 | 1.19   | 1.37   | 11.89 |
| CO  | 360.73 | 147.63 | 107.. |
| NOx | 37.15  | 34.91  | 298   |

**c Source**

Source select

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMSLUF          |
| AMRSUF          |

**d Species select**

| Species | Mean | SD   | Max   |
|---------|------|------|-------|
| SO4     | 2.72 | 1.80 | 10.90 |
| NO3     | 0.87 | 0.94 | 11.10 |
| NH4     |      |      |       |
| EC      |      |      |       |
| OC      |      |      |       |
| Al      |      |      |       |
| Br      |      |      |       |
| Ca      |      |      |       |
| Cu      |      |      |       |
| Fe      |      |      |       |
| K       | 0.06 | 0.05 | 0.46  |
| Mn      | 0.00 | 0.00 | 0.01  |
| Pb      | 0.00 | 0.00 | 0.03  |
| Se      | 0.00 | 0.00 | 0.01  |
| Si      | 0.15 | 0.27 | 2.06  |
| Zn      | 0.01 | 0.00 | 0.03  |

**Ambient species concentration**

**Source contribution**

**MPIN**

**b: concentrations of gases**

**2.1 Select the fitting gases**

**Modeled species information**

| Species | fitting | Measure | Un_M | Calculate | Un_C | C/M |
|---------|---------|---------|------|-----------|------|-----|
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |
|         |         |         |      |           |      |     |

**Modeled gas information**

| Gas | Fitting | Measure | Calculate | C/M |
|-----|---------|---------|-----------|-----|
|     |         |         |           |     |
|     |         |         |           |     |
|     |         |         |           |     |
|     |         |         |           |     |
|     |         |         |           |     |
|     |         |         |           |     |
|     |         |         |           |     |

Bound of C/M

# CMBGC-Iteration 1.0

**CMBGC-Iteration**

Loading Run Save

**a PM concentration**

| PM    | Mean  | SD   | Max   | Min  |
|-------|-------|------|-------|------|
| PM2.5 | 10.28 | 4.92 | 31.00 | 0.42 |

**b Gas concentration**

Gas select

| Gas             | Mean   | SD     | Max   |
|-----------------|--------|--------|-------|
| SO <sub>2</sub> | 1.19   | 1.37   | 11.89 |
| CO              | 360.73 | 147.63 | 107.. |
| NO <sub>x</sub> | 37.15  | 34.91  | 298   |

**c Source**

Source select

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMSLUF          |
| AMRSUF          |

**Ambient species concentration**

Species select

| Species         | Mean | SD   | Max   |
|-----------------|------|------|-------|
| SO <sub>4</sub> | 2.72 | 1.80 | 10.90 |
| NO <sub>3</sub> | 0.87 | 0.94 | 11.10 |
| NH <sub>4</sub> | 1.08 | 0.77 | 5.21  |
| EC              | 0.73 | 0.46 | 3.81  |
| OC              | 2.32 | 1.05 | 6.58  |
| Al              | 0.06 | 0.12 | 0.99  |
| Br              | 0.00 | 0.00 | 0.01  |
| Ca              | 0.07 | 0.08 | 0.63  |
| Cu              | 0.00 | 0.00 | 0.02  |
| Fe              | 0.08 | 0.08 | 0.62  |
| K               | 0.06 | 0.05 | 0.46  |
| Mn              | 0.00 | 0.00 | 0.01  |
| Pb              | 0.00 | 0.00 | 0.03  |
| Se              | 0.00 | 0.00 | 0.01  |
| S               | 0.15 | 0.07 | 0.00  |

**Source contribution**

| Source | Mean | Uncerta... | % |
|--------|------|------------|---|
| 1      |      |            |   |
| 2      |      |            |   |
| 3      |      |            |   |
| 4      |      |            |   |

Contribution plot   
Convergence

PM(%)   
R2  Chi2

**MPIN**

**Modeled species information**

| Species | fitting | Measure | Un_M | Calculate | Un_C | C/M |
|---------|---------|---------|------|-----------|------|-----|
|         |         |         |      |           |      |     |

**Modeled gas information**

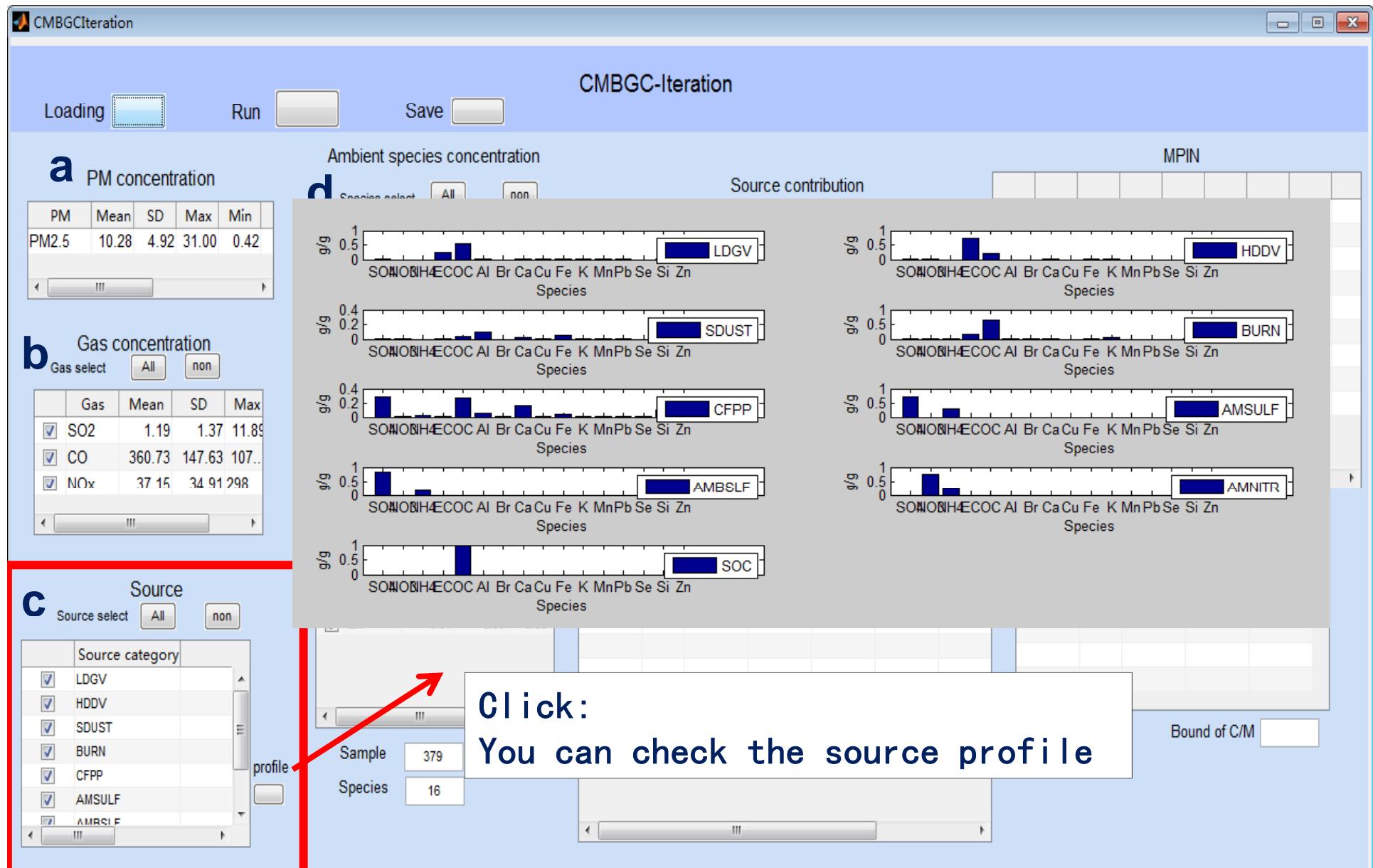
| Gas | Fitting | Measure | Calculate | C/M |
|-----|---------|---------|-----------|-----|
|     |         |         |           |     |

Bound of C/M

**c: categories of source**

**2.2 Select the fitting source categories**

# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0

**a PM concentration**

| PM    | Mean  | SD   | Max   | Min  |
|-------|-------|------|-------|------|
| PM2.5 | 10.28 | 4.92 | 31.00 | 0.42 |

**b Gas concentration**

Gas select: All, non

| Gas | Mean   | SD     | Max   |
|-----|--------|--------|-------|
| SO2 | 1.19   | 1.37   | 11.89 |
| CO  | 360.73 | 147.63 | 107.. |
| NOx | 37.15  | 34.91  | 298   |

**c Source**

Source select: All, non

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMSLUF          |
| AMRSUF          |

**d Ambient species concentration**

Species select: All, non

| Species | Mean | SD   | Max   |
|---------|------|------|-------|
| SO4     | 2.72 | 1.80 | 10.90 |
| NO3     | 0.87 | 0.94 | 11.10 |
| NH4     | 1.08 | 0.77 | 5.21  |
| EC      | 0.73 | 0.46 | 3.81  |
| OC      | 2.32 | 1.05 | 6.58  |
| Al      | 0.06 | 0.12 | 0.99  |
| Br      | 0.00 | 0.00 | 0.01  |
| Ca      | 0.07 | 0.08 | 0.63  |
| Cu      | 0.00 | 0.00 | 0.02  |
| Fe      | 0.08 | 0.08 | 0.62  |
| K       | 0.06 | 0.05 | 0.46  |
| Mn      | 0.00 | 0.00 | 0.01  |
| Pb      | 0.00 | 0.00 | 0.03  |
| Se      | 0.00 | 0.00 | 0.01  |
| Si      | 0.15 | 0.27 | 2.06  |
| Zn      | 0.01 | 0.00 | 0.03  |

**c: concentration of species**

**2. 3. Select the fitting species**

R2: [ ] Chi2: [ ]

**Modeled species information**

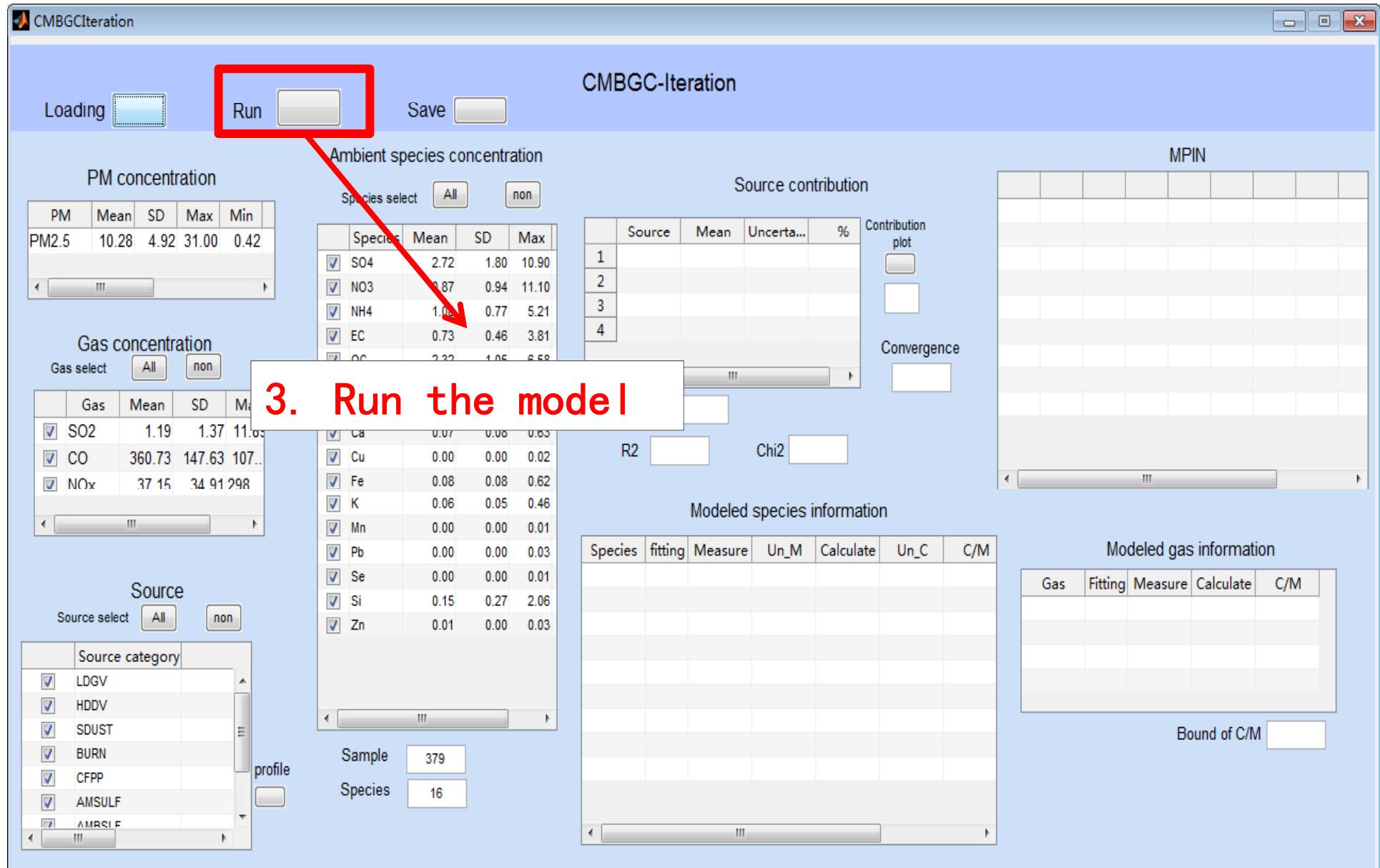
| Species | fitting | Measure | Un_M | Calculate | Un_C | C/M |
|---------|---------|---------|------|-----------|------|-----|
|         |         |         |      |           |      |     |

**Modeled gas information**

| Gas | Fitting | Measure | Calculate | C/M |
|-----|---------|---------|-----------|-----|
|     |         |         |           |     |

Bound of C/M: [ ]

# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0

**Result:**

a: Source contribution

b: Performance index

c: MPIN matrix

d: modeled species

e: modeled gases

PM concentration

Ambient species concentration

Source contribution

| Source  | Mean | Uncertainty |
|---------|------|-------------|
| 1 LDGV  | 0.47 | 0.02        |
| 2 HDDV  | 0.15 | 0.45        |
| 3 SDUST | 0.67 | 0.01        |
| 4 BURN  | 3.52 | 2.61        |
| 5 CFPP  | 0.01 | 0.01        |

Contribution plot  
1  
Convergence  
Yes

PM(%) 92.5044  
R2 0.97502  
Chi2 0.054409

MPIN

| species         | LDGV  | HDDV  | SDUST | BURN  | CFPP  | AMS... | AMB... | AI |
|-----------------|-------|-------|-------|-------|-------|--------|--------|----|
| SO <sub>4</sub> | 0.00  | -0.00 | -0.00 | 0.00  | -0.00 | -0.33  | 0.65   |    |
| NO <sub>3</sub> | -0.00 | -0.00 | 0.00  | -0.00 | -0.00 | -0.11  | 0.11   |    |
| NH <sub>4</sub> | -0.00 | 0.00  | -0.00 | -0.00 | 0.00  | 1.00   | -1.00  |    |
| EC              | -0.27 | 1.00  | 0.05  | -0.00 | 0.01  | 0.01   | -0.01  |    |
| OC              | -0.00 | 0.00  | 0.00  | -0.00 | 0.00  | 0.00   | -0.00  |    |
| Al              | -0.11 | 0.02  | 0.88  | 0.00  | 0.02  | -0.00  | -0.00  |    |
| Br              | -0.09 | -0.30 | -0.11 | 0.63  | -0.14 | -0.08  | 0.06   |    |
| Ca              | -0.13 | -0.09 | -0.65 | 0.21  | 0.87  | -0.01  | -0.02  |    |
| Cu              | 0.09  | -0.00 | -0.05 | -0.06 | 0.12  | 0.01   | -0.01  |    |
| Fe              | 0.18  | -0.02 | 0.64  | -0.06 | 0.05  | 0.01   | -0.01  |    |

Modeled species information

| Species         | fitting | Measure | Un_M | Calculate | Un_C | C/   |
|-----------------|---------|---------|------|-----------|------|------|
| SO <sub>4</sub> | *       |         | 2.72 | 0.23      | 2.68 | 0.13 |
| NO <sub>3</sub> | *       |         | 0.87 | 0.08      | 0.82 | 0.01 |
| NH <sub>4</sub> | *       |         | 1.08 | 0.09      | 1.07 | 0.09 |
| EC              | *       |         | 0.73 | 0.17      | 0.78 | 0.45 |
| OC              | *       |         | 2.32 | 0.42      | 2.86 | 0.47 |
| Al              | *       |         | 0.06 | 0.01      | 0.07 | 0.01 |
| Br              | *       |         | 0.00 | 0.00      | 0.00 | 0.00 |
| Ca              | *       |         | 0.07 | 0.02      | 0.03 | 0.01 |
| Cu              | *       |         | 0.00 | 0.00      | 0.00 | 0.00 |
| Fe              | *       |         | 0.08 | 0.02      | 0.04 | 0.00 |
| K               | *       |         | 0.06 | 0.01      | 0.21 | 0.15 |

Modeled gas information

| Gas             | Fitting | Measure | Calculate | C/M    |      |
|-----------------|---------|---------|-----------|--------|------|
| SO <sub>2</sub> | *       |         | 1.19      | 3.53   | 2.98 |
| CO              | *       |         | 360.73    | 413.92 | 1.15 |
| NO <sub>x</sub> | *       |         | 37.15     | 44.06  | 1.19 |

Bound of C/M 3

profile Sample 379 Species 16

# CMBGC-Iteration 1.0

**Result:**

**a: Source contribution**

Mean contribution ( $\mu\text{g}/\text{m}^3$ ), uncertainties of contribution, Percentage of contribution (%)

| Source | Mean | Uncertainty | PM(%)   |
|--------|------|-------------|---------|
| LDGV   | 0.47 | 0.02        | 92.5044 |
| HDDV   | 0.15 | 0.45        |         |
| SDUST  | 0.67 | 0.01        |         |
| BURN   | 3.52 | 2.61        |         |
| CFPP   | 0.01 | 0.01        |         |

R2: 0.97502      Chi2: 0.054409

**b**

**c** MPIN

| species         | LDGV  | HDDV  | SDUST | BURN  | CFPP  | AMS... | AMB... | A... |
|-----------------|-------|-------|-------|-------|-------|--------|--------|------|
| SO <sub>4</sub> | 0.00  | -0.00 | -0.00 | 0.00  | -0.00 | -0.33  | 0.65   |      |
| NO <sub>3</sub> | -0.00 | -0.00 | 0.00  | -0.00 | -0.00 | -0.11  | 0.11   |      |
| NH <sub>4</sub> | -0.00 | 0.00  | -0.00 | -0.00 | 0.00  | 1.00   | -1.00  |      |
| EC              | -0.27 | 1.00  | 0.05  | -0.00 | 0.01  | 0.01   | -0.01  |      |
| OC              | -0.00 | 0.00  | 0.00  | -0.00 | 0.00  | 0.00   | -0.00  |      |
| Al              | -0.11 | 0.02  | 0.88  | 0.00  | 0.02  | -0.00  | -0.00  |      |
| Br              | -0.09 | -0.30 | -0.11 | 0.63  | -0.14 | -0.08  | 0.06   |      |
| Ca              | -0.13 | -0.09 | -0.65 | 0.21  | 0.87  | -0.01  | -0.02  |      |
| Cu              | 0.09  | -0.00 | -0.05 | -0.06 | 0.12  | 0.01   | -0.01  |      |
| Fe              | 0.18  | -0.02 | 0.64  | -0.06 | 0.05  | 0.01   | -0.01  |      |

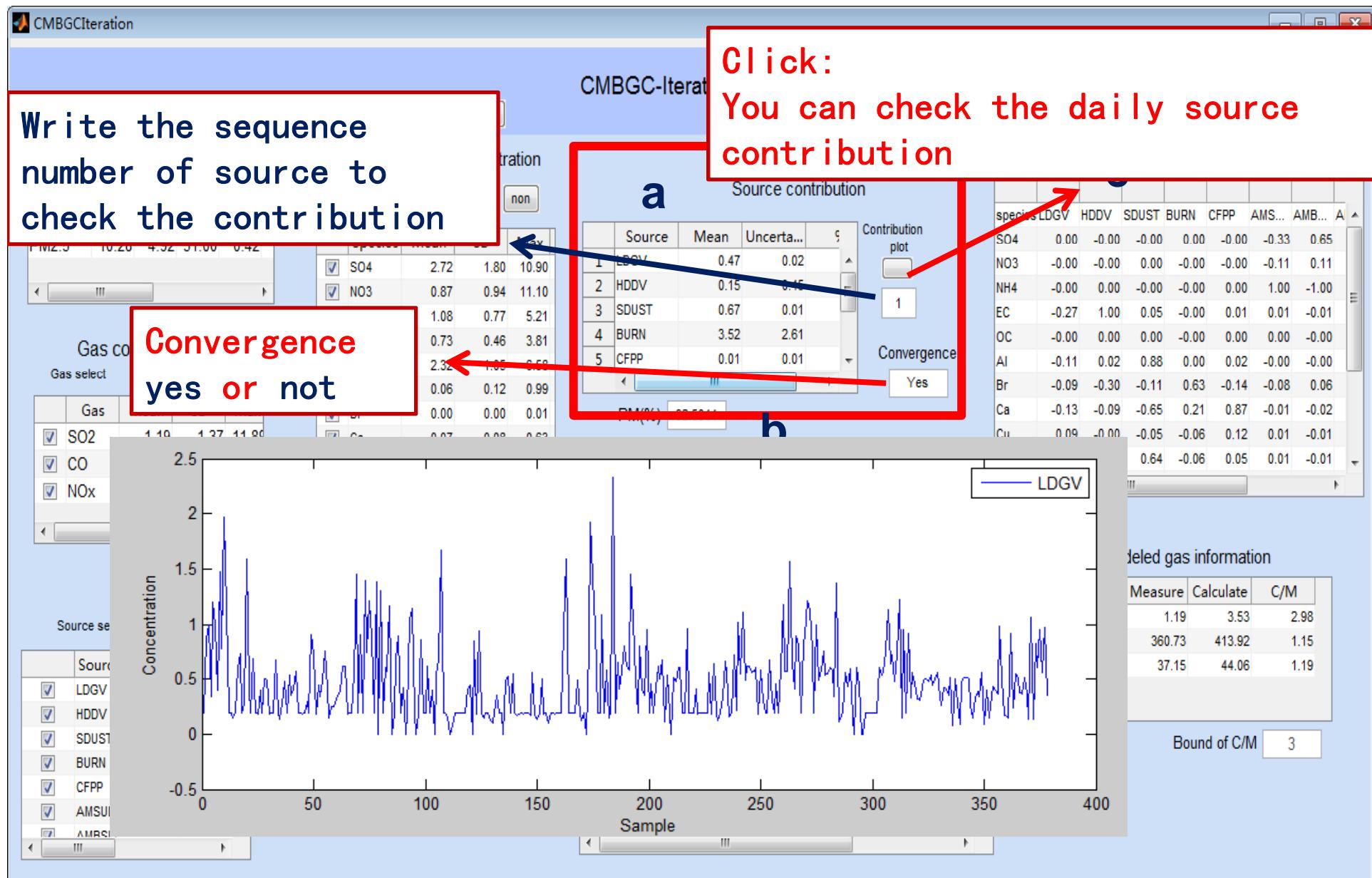
**d**

**e** Modeled gas information

| Gas             | Fitting | Measure | Calculate | C/M  |
|-----------------|---------|---------|-----------|------|
| SO <sub>2</sub> | *       | 1.19    | 3.53      | 2.98 |
| CO              | *       | 360.73  | 413.92    | 1.15 |
| NO <sub>x</sub> | *       | 37.15   | 44.06     | 1.19 |

Bound of C/M: 3

# CMBGC-Iteration 1.0



# CMBGC-Iteration 1.0

**Result:**

**b: Performance index**

PM (%) :  
(80–120%) would be satisfactory

Chi2:  
Close to 0 would be better

R2:  
Close to 1 would be better

**a Source contribution**

| Source | Mean | Uncert... |
|--------|------|-----------|
| LDGV   | 0.47 | 0.02      |
| HDDV   | 0.15 | 0.45      |
| SDUST  | 0.67 | 0.01      |
| BURN   | 3.52 | 2.61      |
| CFPP   | 0.01 | 0.01      |

Contribution plot  
Convergence  
Yes

**b**

|       |          |
|-------|----------|
| PM(%) | 92.5044  |
| R2    | 0.97502  |
| Chi2  | 0.054409 |

**c MPIN**

| species | LDGV  | HDDV  | SDUST | BURN  | CFPP  | AMS... | AMB... | A... |
|---------|-------|-------|-------|-------|-------|--------|--------|------|
| SO4     | 0.00  | -0.00 | -0.00 | 0.00  | -0.00 | -0.33  | 0.65   |      |
| NO3     | -0.00 | -0.00 | 0.00  | -0.00 | -0.00 | -0.11  | 0.11   |      |
| NH4     | -0.00 | 0.00  | -0.00 | -0.00 | 0.00  | 1.00   | -1.00  |      |
| EC      | -0.27 | 1.00  | 0.05  | -0.00 | 0.01  | 0.01   | -0.01  |      |
| OC      | -0.00 | 0.00  | 0.00  | -0.00 | 0.00  | 0.00   | -0.00  |      |
| AI      | -0.11 | 0.02  | 0.88  | 0.00  | 0.02  | -0.00  | -0.00  |      |
| Br      | -0.09 | -0.30 | -0.11 | 0.63  | -0.14 | -0.08  | 0.06   |      |
| Ca      | -0.13 | -0.09 | -0.65 | 0.21  | 0.87  | -0.01  | -0.02  |      |
| Cu      | 0.09  | -0.00 | -0.05 | -0.06 | 0.12  | 0.01   | -0.01  |      |
| Fe      | 0.18  | -0.02 | 0.64  | -0.06 | 0.05  | 0.01   | -0.01  |      |

**d Modeled species information**

| Species | fitting | Measure | Un_M | Calculate | Un_C | C/   |
|---------|---------|---------|------|-----------|------|------|
| SO4     | *       |         | 2.72 | 0.23      | 2.68 | 0.13 |
| NO3     | *       |         | 0.87 | 0.08      | 0.82 | 0.01 |
| NH4     | *       |         | 1.08 | 0.09      | 1.07 | 0.09 |
| EC      | *       |         | 0.73 | 0.17      | 0.78 | 0.45 |
| OC      | *       |         | 2.32 | 0.42      | 2.86 | 0.47 |
| AI      | *       |         | 0.06 | 0.01      | 0.07 | 0.01 |
| Br      | *       |         | 0.00 | 0.00      | 0.00 | 0.00 |
| Ca      | *       |         | 0.07 | 0.02      | 0.03 | 0.01 |
| Cu      | *       |         | 0.00 | 0.00      | 0.00 | 0.00 |
| Fe      | *       |         | 0.08 | 0.02      | 0.04 | 0.00 |
| K       | *       |         | 0.06 | 0.01      | 0.21 | 0.15 |

**e Modeled gas information**

| Gas | Fitting | Measure | Calculate | C/M    |      |
|-----|---------|---------|-----------|--------|------|
| SO2 | *       |         | 1.19      | 3.53   | 2.98 |
| CO  | *       |         | 360.73    | 413.92 | 1.15 |
| NOx | *       |         | 37.15     | 44.06  | 1.19 |

Bound of C/M 3

# CMBGC-Iteration 1.0

**a** CMBGC-Iteration

PM concentration      Ambient species concentration      Source contribution

Species select All non

Modified Pseudo-Inverse Normalized (MPIN)

Show the sensitive species for the sources

For each source, the species with 1 would be the most sensitive one for this source category

**b**

| Source category | LDGV | HDDV | SDUST | BURN | CFPP | AMSLF | AIR |
|-----------------|------|------|-------|------|------|-------|-----|
| LDGV            | *    |      |       |      |      |       |     |
| HDDV            | *    |      |       |      |      |       |     |
| SDUST           | *    |      |       |      |      |       |     |
| BURN            | *    |      |       |      |      |       |     |
| CFPP            | *    |      |       |      |      |       |     |
| AMSLF           | *    |      |       |      |      |       |     |
| AIR             |      |      |       |      |      |       |     |

Sample 379      Species 16

**c** MPIN

| species         | LDGV  | HDDV  | SDUST | BURN  | CFPP  | AMSLF | AIR   |
|-----------------|-------|-------|-------|-------|-------|-------|-------|
| SO <sub>4</sub> | 0.00  | -0.00 | -0.00 | 0.00  | -0.00 | -0.33 | 0.65  |
| NO <sub>3</sub> | -0.00 | -0.00 | 0.00  | -0.00 | -0.00 | -0.11 | 0.11  |
| NH <sub>4</sub> | -0.00 | 0.00  | -0.00 | -0.00 | 0.00  | 1.00  | -1.00 |
| EC              | -0.27 | 1.00  | 0.05  | -0.00 | 0.01  | 0.01  | -0.01 |
| OC              | -0.00 | 0.00  | 0.00  | -0.00 | 0.00  | 0.00  | -0.00 |
| Al              | -0.11 | 0.02  | 0.88  | 0.00  | 0.02  | -0.00 | -0.00 |
| Br              | -0.09 | -0.30 | -0.11 | 0.63  | -0.14 | -0.08 | 0.06  |
| Ca              | -0.13 | -0.09 | -0.65 | 0.21  | 0.87  | -0.01 | -0.02 |
| Cu              | 0.09  | -0.00 | -0.05 | -0.06 | 0.12  | 0.01  | -0.01 |
| Fe              | 0.18  | -0.02 | 0.64  | -0.06 | 0.05  | 0.01  | -0.01 |

**d**

| EC | 0.73 | 0.17 | 0.78 | 0.45 |      |
|----|------|------|------|------|------|
| OC | *    | 2.32 | 0.42 | 2.86 | 0.47 |
| Al | *    | 0.06 | 0.01 | 0.07 | 0.01 |
| Br | *    | 0.00 | 0.00 | 0.00 | 0.00 |
| Ca | *    | 0.07 | 0.02 | 0.03 | 0.01 |
| Cu | *    | 0.00 | 0.00 | 0.00 | 0.00 |
| Fe | *    | 0.08 | 0.02 | 0.04 | 0.00 |
| K  | *    | 0.06 | 0.01 | 0.21 | 0.15 |

**e** Modeled gas information

| Gas             | Fitting | Measure | Calculate | C/M  |
|-----------------|---------|---------|-----------|------|
| SO <sub>2</sub> | *       | 1.19    | 3.53      | 2.98 |
| CO              | *       | 360.73  | 413.92    | 1.15 |
| NO <sub>x</sub> | *       | 37.15   | 44.06     | 1.19 |

Bound of C/M 3

# CMBGC-Iteration 1.0

**Modeled species information**

**Species column:** shows the name of species  
**Fitting column:** shows the species selected for fitting (marked with “\*” )  
**Measure column:** shows the mean concentrations of species in PM  
**Un\_M column:** shows the mean uncertainties of species in PM  
**Calculate column:** shows the calculated mean concentrations of species  
**Un\_C:** column: shows calculated mean uncertainties of species

The screenshot shows the software interface with several windows and panels. On the left, there's a 'Source' panel with a 'Source select' dropdown set to 'All' and a 'non' button. Below it is a 'Source category' table with rows for LDGV, HDDV, SDUST, BURN, CFP, AMSULF, and AMRSULF. A 'profile' button is also present. In the center, a main window titled 'Modeled species information' displays a table with columns: Species, fitting, Measure, Un\_M, Calculate, Un\_C, and C/. The table contains data for various species like SO4, NO3, NH4, EC, OC, Al, Br, Ca, Cu, Fe, and K. A red box highlights this table, labeled 'd'. To the right, another window titled 'Modeled gas information' shows a table for gases SO2, CO, and NOx. At the bottom right, a text box says 'Bound of C/M 3'.

| Species | fitting | Measure | Un_M | Calculate | Un_C | C/ |
|---------|---------|---------|------|-----------|------|----|
| SO4     | *       | 2.72    | 0.23 | 2.68      | 0.13 |    |
| NO3     | *       | 0.87    | 0.08 | 0.82      | 0.01 |    |
| NH4     | *       | 1.08    | 0.09 | 1.07      | 0.09 |    |
| EC      | *       | 0.73    | 0.17 | 0.78      | 0.45 |    |
| OC      | *       | 2.32    | 0.42 | 2.86      | 0.47 |    |
| Al      | *       | 0.06    | 0.01 | 0.07      | 0.01 |    |
| Br      | *       | 0.00    | 0.00 | 0.00      | 0.00 |    |
| Ca      | *       | 0.07    | 0.02 | 0.03      | 0.01 |    |
| Cu      | *       | 0.00    | 0.00 | 0.00      | 0.00 |    |
| Fe      | *       | 0.08    | 0.02 | 0.04      | 0.00 |    |
| K       | *       | 0.06    | 0.01 | 0.21      | 0.15 |    |

**e Modeled gas information**

| Gas | Fitting | Measure | Calculate | C/M  |
|-----|---------|---------|-----------|------|
| SO2 | *       | 1.19    | 3.53      | 2.98 |
| CO  | *       | 360.73  | 413.92    | 1.15 |
| NOx | *       | 37.15   | 44.06     | 1.19 |

Bound of C/M 3

# CMBGC-Iteration 1.0

**CMBGCIteration**

**CMBGC-Iteration**

## Modeled species information

**C/M column:** shows the ratio of calculated and measured concentrations for species

**C/M\_un column:** shows the ratio of Un\_M of measured concentrations for species

**Residu/Un column:** shows the ratio of residual and modeled uncertainties for species

**Source**

Source select: All, non

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMSLUF          |
| AMRSUF          |

Sample: 379

Species: 16

| M    | Calculate | Un_C | C/M  | C/M_Un | Residu/Un |
|------|-----------|------|------|--------|-----------|
| 0.23 | 2.68      | 0.13 | 0.99 | 0.05   | -0.17     |
| 0.08 | 0.82      | 0.01 | 0.94 | 0.01   | -0.66     |
| 0.09 | 1.07      | 0.09 | 0.99 | 0.08   | -0.11     |
| 0.17 | 0.78      | 0.45 | 1.08 | 0.62   | 0.32      |
| 0.42 | 2.86      | 0.47 | 1.23 | 0.20   | 1.28      |
| 0.01 | 0.07      | 0.01 | 1.24 | 0.13   | 0.90      |
| 0.00 | 0.00      | 0.00 | 0.98 | 0.82   | -0.04     |
| 0.02 | 0.03      | 0.01 | 0.46 | 0.19   | -2.13     |
| 0.00 | 0.00      | 0.00 | 0.17 | 0.03   | -2.51     |
| 0.02 | 0.04      | 0.00 | 0.57 | 0.03   | -1.87     |
| 0.01 | 0.21      | 0.15 | 3.24 | 2.30   | 11.91     |

**d** Modeled species information

**e** Modeled gas information

| Gas | Fitting | Measure | Calculate | C/M  |
|-----|---------|---------|-----------|------|
| SO2 | *       | 1.19    | 3.53      | 2.98 |
| CO  | *       | 360.73  | 413.92    | 1.15 |
| NOx | *       | 37.15   | 44.06     | 1.19 |

Bound of C/M: 3

# CMBGC-Iteration 1.0

**Modeled gases information**

**Gas column:** shows the name of gases  
**Fitting column:** shows the gases selected for fitting (marked with “\*” )  
**Measure column:** shows the mean concentrations of gases  
**Calculate column:** shows the calculated mean concentrations of gases  
**C/M:** shows the ratio of calculated and measured concentrations for gases

| Gas | Fitting | Measure | Calculate | C/M  |
|-----|---------|---------|-----------|------|
| SO2 | *       | 1.19    | 3.53      | 2.98 |
| CO  | *       | 360.73  | 413.92    | 1.15 |
| NOx | *       | 37.15   | 44.06     | 1.19 |

**Source**

Source select: All, non

| Source category |
|-----------------|
| LDGV            |
| HDDV            |
| SDUST           |
| BURN            |
| CFPP            |
| AMRSULF         |

**Modeled species information**

| M    | Calculate | Un_C | C/M  | C/M_Un | Residu/Un |
|------|-----------|------|------|--------|-----------|
| 0.23 | 2.68      | 0.13 | 0.99 | 0.05   | -0.17     |
| 0.08 | 0.82      | 0.01 | 0.94 | 0.01   | -0.66     |
| 0.09 | 1.07      | 0.09 | 0.99 | 0.08   | -0.11     |
| 0.17 | 0.78      | 0.45 | 1.08 | 0.62   | 0.32      |
| 0.42 | 2.86      | 0.47 | 1.23 | 0.20   | 1.28      |
| 0.01 | 0.07      | 0.01 | 1.01 | 0.02   | 0.90      |
|      |           |      |      |        | -0.04     |
|      |           |      |      |        | -2.13     |
|      |           |      |      |        | -1.87     |

**d** Show the bound of C/M set in input file

**e** Modeled gas information

| Gas | Fitting | Measure | Calculate | C/M  |
|-----|---------|---------|-----------|------|
| SO2 | *       | 1.19    | 3.53      | 2.98 |
| CO  | *       | 360.73  | 413.92    | 1.15 |
| NOx | *       | 37.15   | 44.06     | 1.19 |

Bound of C/M: 3

# CMBGC-Iteration 1.0

**4. Save the result**

The screenshot shows the CMBGC-Iteration 1.0 software interface. The main window title is "CMBGC-Iteration". The top menu bar includes "File", "Edit", "View", "Analysis", "Help", and "About". The toolbar contains buttons for "Loading" (grey), "Run" (disabled), and "Save" (highlighted with a red box and arrow). The interface is divided into several sections:

- PM concentration:** Displays a table with columns: PM, Mean, SD, Max, Min. Data for PM2.5: Mean 10.28, SD 4.92, Max 31.00, Min 0.42.
- Ambient species concentration:** A table titled "Species select" with buttons "All" and "non". It lists ambient species: SO4, NO3, NH4, EC, OC, Al. Columns: Species, Mean, SD, Max.
- Source contribution:** A table listing sources: LDGV, HDDV, SDUST, BURN, CFPP. Columns: Source, Mean, Uncert...
- MPIN:** A table showing species concentrations across various sources (LDGV, HDDV, SDUST, BURN, CFPP, AMSULF, AMBSULF) with values ranging from -0.33 to 0.65.
- Gas concentration:** A table titled "Gas select" with buttons "All" and "non". It lists gases: SO2, CO, NOx. Columns: Gas, Mean, SD, Max.
- Source:** A table titled "Source select" with buttons "All" and "non". It lists source categories: LDGV, HDDV, SDUST, BURN, CFPP, AMSULF, AMBSULF.
- Modeled species information:** A table with columns: M, Calculate, Un\_C, C/M, C/M\_Un, Residu/Un. It lists modeled species: Fe, K, Mn, Pb, Se, Si, Zn.
- Modeled gas information:** A table with columns: Gas, Fitting, Measure, Calculate, C/M. It lists modeled gases: SO2, CO, NOx.
- Sample:** Buttons for "profile" and "Sample" (set to 379).
- Species:** Buttons for "profile" and "Species" (set to 16).

# CMBGC-Iteration 1.0

- Result

|    | A        | B        | C        | D        | E        | F        | G        | H        | I        | J        | K        |
|----|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1  | Date     | LDGV     | HDDW     | SDUST    | BURN     | CFPP     | AMSULF   | AMBSLF   | AMNITR   | SOC      |          |
| 2  | 2006/1/5 | 0.193993 |          | 0        | 0.189761 | 0.30992  | -4.3E-20 | 0        | 0.213315 | 0.200402 | 1.094407 |
| 3  | 2006/1/8 | 0.876502 |          | 0        | 0.200461 | 3.041995 | 0.118007 | 0        | 0.476396 | 0.592802 | 0.103708 |
| 4  | #####    | 1.007543 | 0.540507 | 0.183157 | 0.692743 | 0.054915 | 0.120152 | 1.214659 | 0.587993 | 0.741207 |          |
| 5  | #####    | 0.346507 | 0.23734  | 0.142343 | 0.232864 | 0.003169 | 0.124563 | 0.626495 | 0.317164 | 0.922777 |          |
| 6  | #####    | 1.238296 | 0.658799 | 0.125292 | 0.690938 | 0.016373 | 0        | 2.031739 | 3.59948  | 1.244866 |          |
| 7  | #####    | 1.018562 | 0.731049 | 0.146287 | 0.599467 | 0.148104 | 0        | 0.531261 | 0.468513 | 1.078588 |          |
| 8  | #####    | 0.396992 | 0.3593   | 1.023218 | 1.180839 | 0.000819 | 0.52876  | 0.506801 | 0.271508 | 0.49451  |          |
| 9  | 2006/2/1 | 1.476973 |          | 0        | 0.134121 | 0.699706 | 0.020236 | 2.189189 | 1.612148 | 0.661996 | 0.581551 |
| 10 | 2006/2/4 | 0.816432 | 0.874691 | 0.155177 | 0.76253  | 0.014903 | 0        | 0        | 0        | 0        |          |
| 11 | 2006/2/7 | 2.017761 | 1.06293  | 0.167117 | 0.667417 | 0        | 0        | 0        | 0        | 1.       |          |
| 12 | #####    | 1.078722 | 0        | 0.076773 | 3.723811 | 0.03493  | 1.841804 | 1.       |          |          |          |
| 13 | #####    | 0.174339 | 0        | 0.239376 | 6.357181 | 0        | 1.731074 | 2.       |          |          |          |
| 14 | #####    | 0.190209 | 0        | 0.142466 | 1.474295 | 0        | 4.690958 | 0.       |          |          |          |
| 15 | #####    | 0.147519 | 0.227849 | 0.073053 | 2.165643 | -1.4E-17 | 4.829672 |          |          |          |          |
| 16 | #####    | 0.191088 | -3.6E-21 | 0.096328 | 1.203574 | 2.91E-19 | 1.278919 | 0.       |          |          |          |
| 17 | #####    | 0.604079 | -1.6E-22 | 0.156334 | 1.060559 | 1.32E-19 | 1.796884 | 2.       |          |          |          |
| 18 | 2006/3/6 | 0.712073 | 1.42E-17 | 0.196413 | 7.423645 | 0        | 5.574883 | 3.       |          |          |          |
| 19 | 2006/3/9 | 0.19296  | -1.7E-21 | 0.523633 | 0.627631 | 1.1E-19  | 0.584028 | 1.       |          |          |          |
| 20 | #####    | 0.152698 | 7.64E-18 | 0.183394 | 7.229157 | 0.0175   | 2.009667 | 6.       |          |          |          |
| 21 | #####    | 1.650678 | 0        | 0.083071 | 4.031656 | 0.116719 | 0.545484 | 1.       |          |          |          |
| 22 | #####    | 0.423293 | 0        | 0.183426 | 1.073601 | 0        | 3.930665 | 0.       |          |          |          |
| 23 | #####    | 0.193979 | -8.7E-22 | 0.114532 | 0.314035 | 2.69E-21 | 1.613499 | 1.       |          |          |          |
| 24 | #####    | 0.707195 | 0.020388 | 0.166325 | 0.946737 | -1.8E-18 | 0.594195 | 0.       | 0.666201 | 0.205761 | 1.176282 |
| 25 | #####    | 0.18032  | 0        | 0.235105 | 4.517053 | -2.2E-19 | 5.815131 | 1.247675 | 0.370224 | 0        |          |
| 26 | 2006/4/2 | 0.168761 |          | 0        | 0.222948 | 8.07362  | 0        | 3.12256  | 3.202961 | 0.954065 | 0        |
| 27 | 2006/4/5 | 0.358642 | 7.62E-18 | 0.223367 | 5.608316 | 0.001004 | 2.614904 | 2.837898 | 1.337174 | 0        |          |
| 28 | 2006/4/8 | 0.191469 |          | 0        | 0.380178 | 1.086880 | 0.1      | 0.957576 | 1.016932 | 1.492018 | 1.110069 |

Contribution Un\_Contribution Mean\_Contribution Performance Index MPIN Modeled Species Modeled gal

**Output information:**

Daily contributions;  
 Daily contribution uncertainties;  
 Mean source contribution;  
 Performance index;  
 MPIN matrix;  
 Modeled species information;  
 Modeled gases information

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