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Supplement of

Retrieving CH_4-emission rates from coal mine ventilation shafts using UAV-based AirCore observations and the genetic algorithm–interior point penalty function (GA-IPPF) model

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S1. Introduction for GA-IPPF

The main advantage of GA-IPPF is that it can retrieving methane emission sources without diffusion parameters. When supplied with concentration data, meteorological data, and location information, the emission characteristics can be precisely determined by GA-IPFF. The function of the genetic algorithm (GA) is to define the range of each unknown parameters, and the IPPF would calculate final solutions of each unknown parameters based on the domain determined by GA. The specific explanation of the two algorithms is presented as follows:

S 1.1 Genetic algorithm

GA is a kind of bionic algorithms that draw on natural selection in biology. By simulating the evolution of an artificial population, the GA retains a set of suitable individuals in each iteration after selection, crossover, and mutation, and the population evolves over several generations, i.e., many iterations, and the final retained individuals will result in an approximately optimal fitness function. Detailed steps are as follows:

Step 1:In this study, we selected real number encoding method for GA. That is encoding the floating point number itself, including dispersion parameters, wind and other unknow parameters in formula 1.

Step 2: Initializing populations. Maximum number of evolutionary generations in this section is set as 1000, the number of initial populations is set as 900. The individuals are randomly generated within the selected range, that is the lower boundary and upper boundary in this article.

Step 3: Calculate fitness function. The fitness function is the criterion for judging the strengths and weaknesses of individuals, F is regarded as fitness function in this step, obviously, we want to find the individual with the smallest value of fitness in the genetic iteration.

$$F = \sum_{i=1}^{n} (C_m^i - C_s^i)^2 \qquad \text{ES1}$$

Step 4 :Selection. The purpose of selection is to select multiple pairs of superior individuals from the current population, each pair of superior individuals is called a pair of parents, and let the parents generate new offspring by crossover and mutation until the number of individuals in the next generation reaches the population limit. There are many ways of selection, in this article, we choose the roulette wheel method, in which the probability of an individual being selected is inversely proportional to the size of its fitness function.

Step 5 :Crossover. It simulates chromosome crossover in the biological system, and the certain codes of the parents, like genes, are crossed over according to the crossover probability, and a new offspring is created after the crossover. The crossover method we adopted is to randomly generate genetic vectors to determine the crossover position.

Step 6 : Mutation. That is the mutation in biological community model. Coding genes are altered according to a given mutation probability.

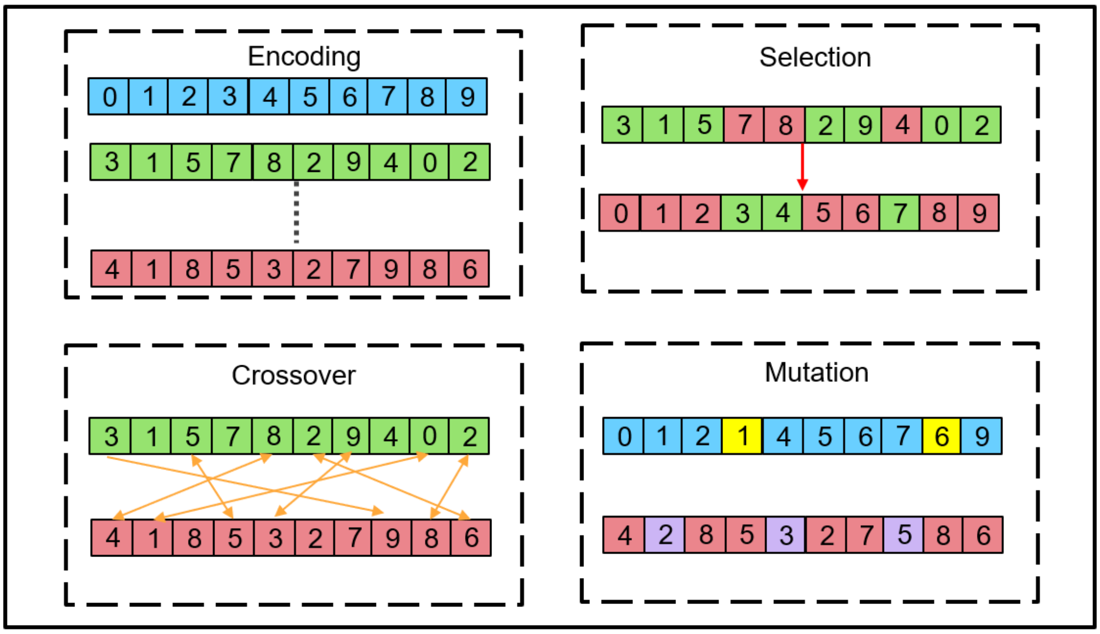

Figure S1. Steps in GA, including Coding, Selection, Crossover and Mutation

Step 7: Termination discriminations. Whether to terminate the iteration depends on the fitness of the offspring generated by crossover meets the requirements and reaching the maximum evolutionary algebra T. if terminated, the iteration with the smallest fitness is regarded as the output. Conversely, the process would be returned to Step 3.

After the calculation of GA algorithm, we can derive the points with smaller fitness functions in the initial definition domain. However, the GA algorithm is stochastic and has the possibility of falling into local optimal solutions. We repeat the GA algorithm 10 ,000 times and get 10,000 potential solutions. Furthermore, the boundary of the 10,000 potential solutions are considered as the more precise domain, and then, the optimal solution would be found by using IPPF algorithm:

S 1.2 IPPF

Interior point penalty function (IPFF) is appropriate to solve the problem of inequality constraints, and the calculated solution is within the feasible region. Hence, it would promise the final results in parameters domain calculated by GA, especially for Q. This method could adjust values of the input meteorological parameters to promote the optimal solution, including wind speed and wind direction.

Step 1 : Determine initial points , $x^{(0)} \in D_0$ （D_0 is parameters domain）; Penalty parameter sequence

$\{\mu_k\}, \varepsilon > 0, k = 1$.

Step 2 : Constructing auxiliary functions

$$F_{\mu_k}(x) = F(x) - \mu_k^{-1} \sum_{i \in I} \log g_i(x) \qquad \text{ES2}$$

$$F = \sum_{i=1}^{n} (C_m^i - C_s^i)^2 \qquad \text{ES3}$$

g_i is inequality constraint.

$$lb < x_i < ub, i = 1,2,3......10 \qquad \text{ES4}$$

Step 3 : $x^{(k-1)}$ is regarded as initial points, it was used to solving the unconstrained formula $\min F_{\mu_k}(x), x \in R^n$

Step 4 : Termination discriminations, if

$$\mu_k^{-1} \sum_{i \in I} \log g_i(x) \leqslant \varepsilon \qquad \text{ES5}$$

Then, the solution of $x^{(k)}$ can be regarded as the output. Otherwise, return to step 2.

Finally, $x^{(k)}$ is treated as the optimal solution of the unknow parameters, including emission rate, diffusion parameters and effectively emission height of CH_4 source.

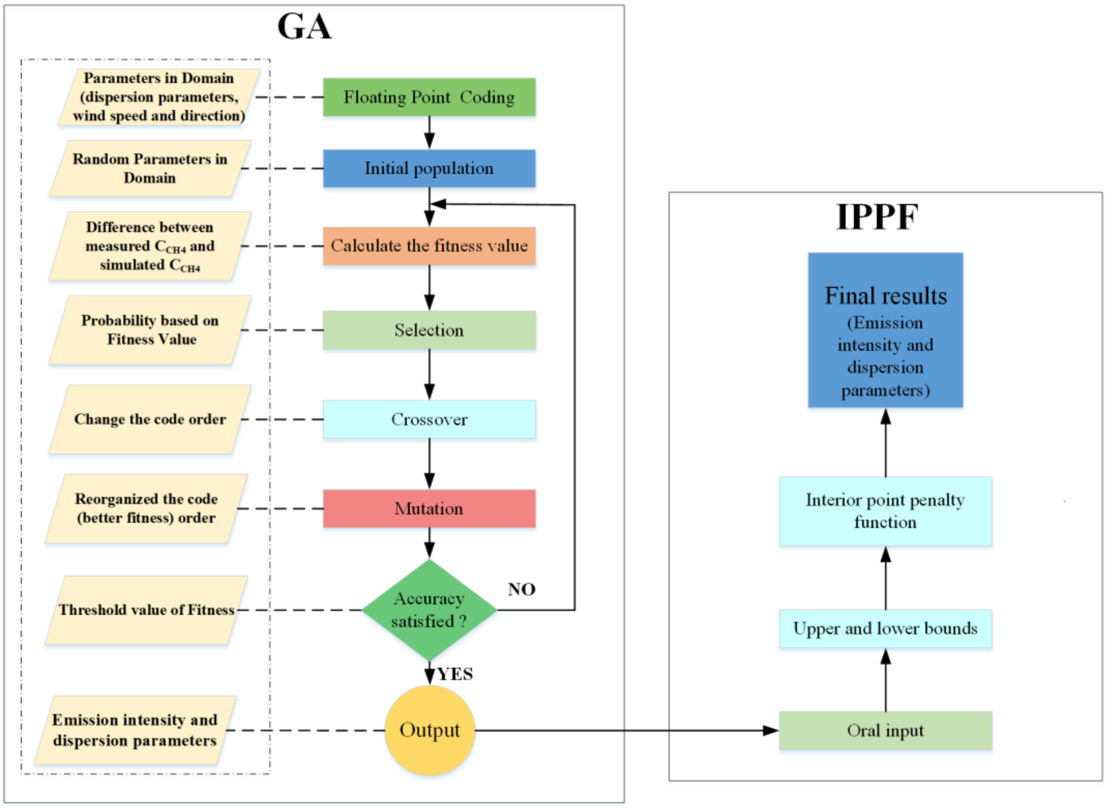

Figure S2. Detail processes of GA-IPPF

S2. Retrieved results by GA-IPPF in each Flight

The retrieved parameters based on the collected data in the other Flights in 2017 8/18 and 8/21 are shown in this section. Table S1 presented the detailed methane diffusion parameters by GA-IPPF. And Figure.S3 showed the simulated methane concentration in each collected position through the parameters in Table S1.

Table S1. Retrieved parameters by GA-IPPF in each Aircore Flight around Pniówek coal

Parameters	Flight 4	Flight 8	Flight 12	Flight 14	Flight 17	Flight 18
Initial wind speed (m/s)	3.4	2.3	2.4	3.5	2.7	3.4
Initial wind direction (°)	36.1	10	117.4	107.6	207.8	154
Emission intensity (kt/hour)	639.3±17.3	1415.5±57.3	1449.8±57.3	730.6±22.3	342.5±13.3	742.0±22.3
Wind speed (m/s)	3.7±0.3	2.2±0.2	3.2±0.2	4.8±0.3	4.0±0.2	3.1±0.3
Wind direction (°)	9.0±1.3	59.0±1.2	123.2±1.2	111.2±1.7	169.6±1.8	180±2.1
a	0.03±0.01	1.50±0.02	0.19±0.01	0.21±0.02	0.3±0.01	0.5±0.01
b	1.2±0.02	0.62±0.01	1.18±0.02	1.02±0.01	1.2±0.03	0.97±0.01
c	0.49±0.01	0.33±0.02	0.41±0.02	0.06±0.01	0.05±0.01	0.08±0.02
d	0.5±0.01	1.1±0.01	0.56±0.02	0.89±0.01	0.98±0.02	0.78±0.02
B (mg/m^3)	1.54±0.01	1.42±0.01	1.51±0.01	1.41±0.01	1.41±0.01	1.47±0.01
Emission height (m)	17.2±1.5	20.4±2.1	57.4±2.2	43.3±1.6	30.5±1.1	33.6±1.3
Reflection index	0.98±0.02	0.99±0.01	1±0.01	0.98±0.01	0.97±0.01	1±0.01

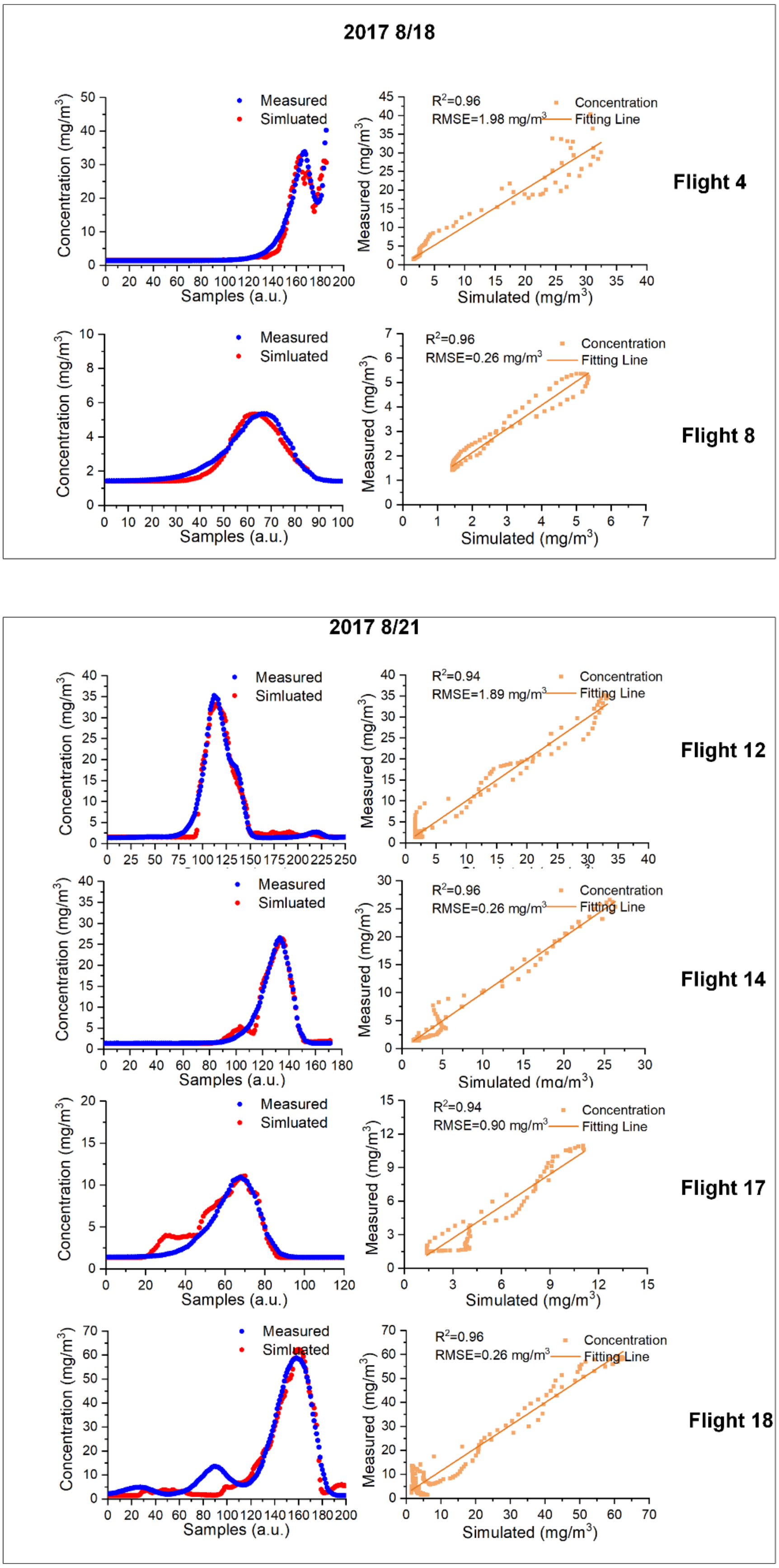

Figure.S3. The rebuilt the methane diffusion based on retrieved parameters in each Aircore Flight around ventilation shaft of Pniówek coal.

S3. Instruction for the peaks in Flight 15

In this section, we simulate the spatial distributions of atmospheric CH_4 enhancements due to the emission of a strong point source. parameters are shown in Table S2. The diffusion of CH4 is simulated according to formula 1.

Table S2. Parameters setting in CH_4 diffusion simulation

Parameters	Values
Wind speed (m/s)	2.5
Wind direction (°)	90
Emission rate (kg/s)	300
a	0.11
b	0.93
c	0.1
d	0.93
H (m)	20
B (ppb)	2000

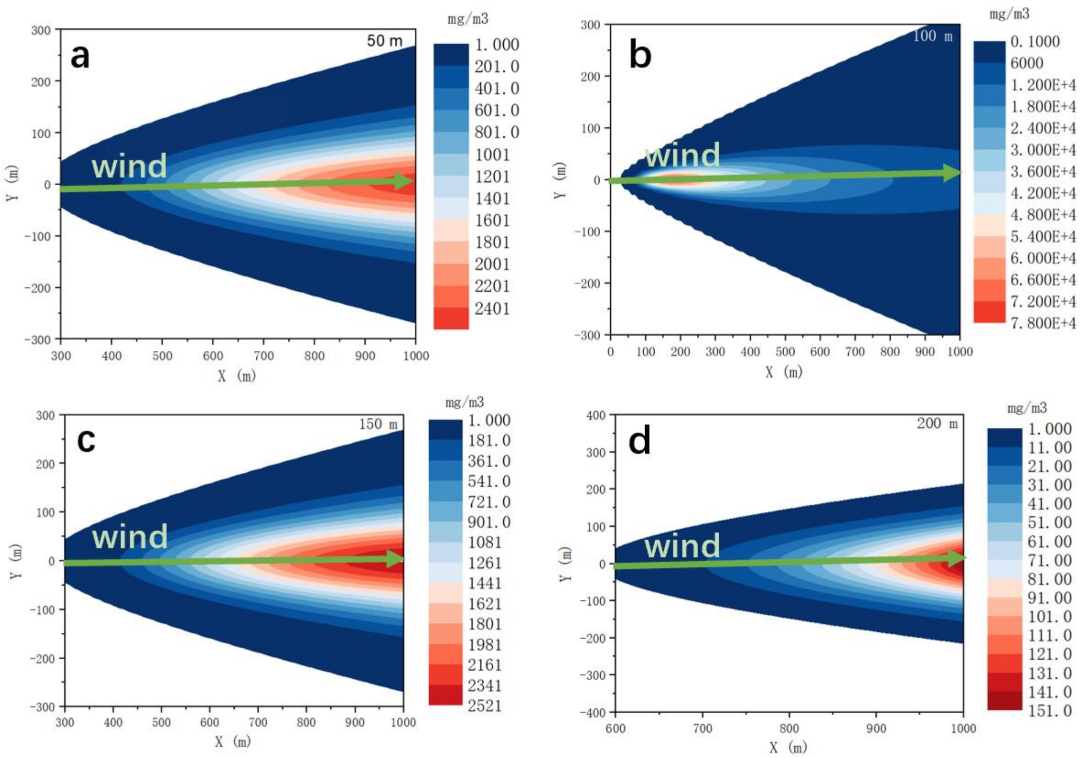

Fig.S4 Simulated diffusions of CH_4 at different heights, a.50 m; b.100 m; c.150 m and d. 200 m.

According to Gaussian diffusion, at a certain height, the closer the spatial position to the downwind direction is, the greater the diffusion value is. Fig.S4 showed that there are different hot spots in different heights, which could explain the hots in collection Flight.

S4. Rebuild methane diffusion in 2-D by different quantification model

In this section, we rebuild the 2-D plume of CH_4 dispersion in Flight 6 and Flight 15 based on the different methods, including NLSF, GA-IPPF, inventory, Mass balance and Gaussian inversion. It worth nothing that 2-D plume rebuild by NLSF, GA-IPPF and inventory are according to formula 1. Relative diffusion parameters in inventory are as same as that retrieved by GA-IPPF in each Flight. 2-D plume rebuilt by Masa balance is according to formula 12. 2-D plume rebuilt by Gaussian inversion is according to formula 13.

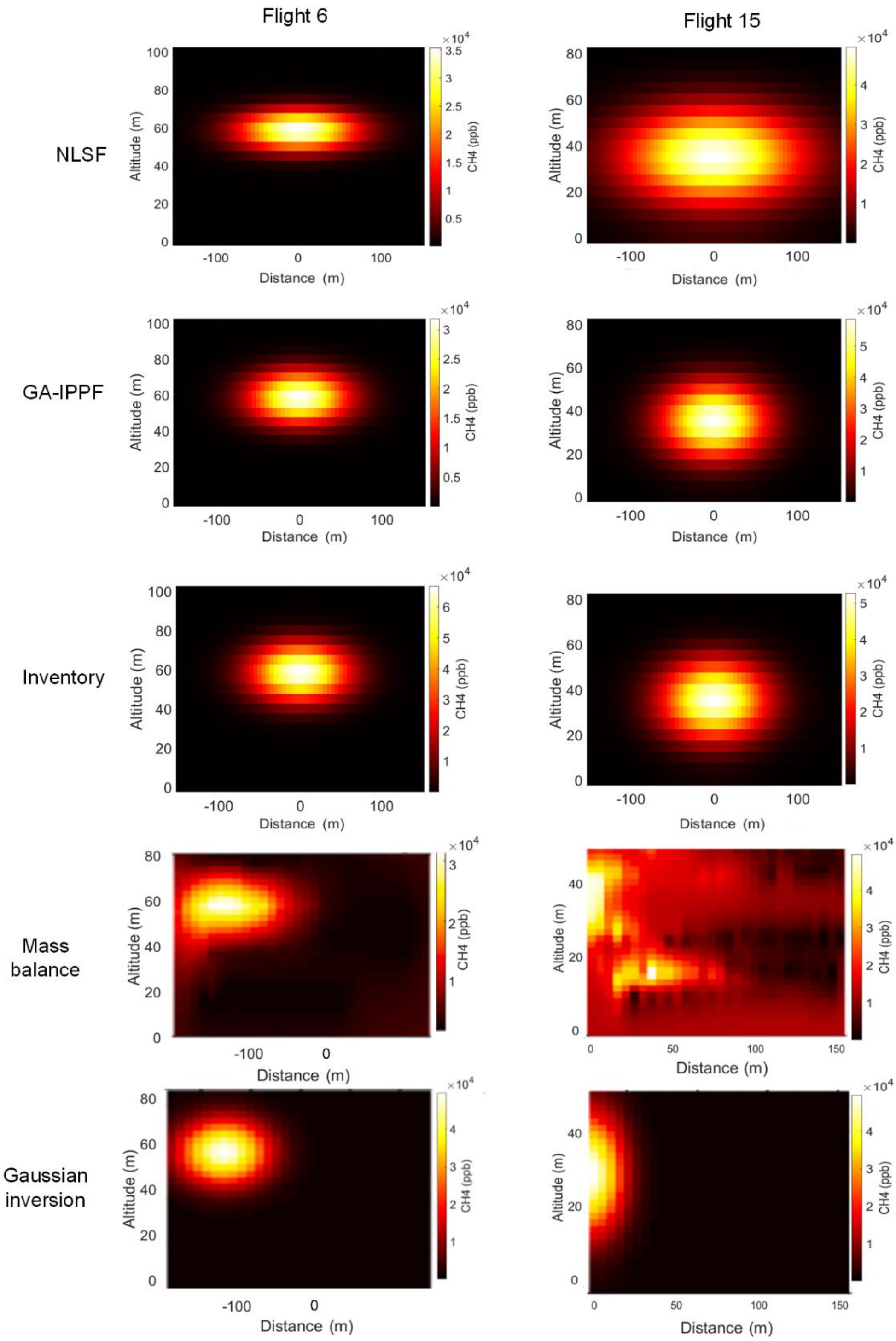

Fig.S5 2-D plume rebuilt by different methods in Flight 6 and Flight 15