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OVERVIEW OF GIFFORD'S 1959 PAPER THAT FIRST JUSTIFIES INVERSE MODELLING

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Abstract: There is great interest now in inverse modelling in order to estimate air pollution source emissions. This type of modelling goes by several other aliases (e.g., top-down, backwards, adjoint, sensor data fusion, receptor, source term estimation). Many groups employ a procedure where the transport and dispersion (T&D) model is run "backwards", starting at a sampler location. The scientific and mathematical justifications for this methodology were first proposed over 60 years ago in a brief (2 page) but seminal paper by Gifford (1959). He pointed out that, when run in forwards or backwards mode, the solution describes a probability distribution in space. In forwards mode, the probability distribution describes the distribution of pollutant concentrations, and, in backwards mode, it describes the distribution of probabilities that the source is at a certain location. Gifford's simple but elegant explanation was consistent with his belief in the principle of Occam's razor (the simplest explanation is probably the best).

Key words: *Inverse modeling, source term estimation**,** Gifford, probability distributions*

INTRODUCTION

Over 60 years ago, Gifford (1959) published a short paper in which he attempted to simplify calculations of contributions of mass emissions of pollutants from multiple sources, spread over an area, to pollutant concentrations at a downwind receptor. In those days before the widespread use of computers, many scientists searched for analytical "short cuts" (Gifford's words).

There is much current interest in determining mass emission rates from upwind sources using observed concentrations at several sensors, along with knowledge of local winds and stability. For example, what are the actual methane emissions from a chemical facility? Or, what is the location and magnitude of a chemical agent released upwind of a military facility? There are many disciplines studying this problem and they use multiple approaches and nomenclature (e.g., inverse, top-down, backwards, adjoint, sensor data fusion, receptor, source term estimation). Hanna and Young (2017) provide a brief review of the several alternate methods and point out that there is a need for harmonization.

The current paper relates Gifford's suggested methodology to recently developed inverse modeling methods.

SOME EXAMPLES OF CURRENT INVERSE MODELS' USE OF GIFFORD'S APPROACH

At the core of any of the many available inverse modeling systems is a transport and dispersion (T&D) model. It is important that the T&D model have minimal mean bias (otherwise the estimated mass emission rate could have an error proportional to the mean bias).

The complexity and uncertainty of the source term estimation calculation quickly grows with the number of unknowns [number of sources, source locations, emissions variation with time, elevation of source (e.g., stack height), movement of source (i.e., automobile, ship, airplane)]. In most of the many published applications, the source is assumed to be at at known level (ground level or at a specific stack elevation) and is not moving.

For the simplest problem – a single source of known location, with concentrations observed at a few sensor locations (including one or two near the middle of the plume), a ”brute-force” iterative procedure, with the T&D model run in normal forward mode, may be sufficient. An example of a simple approach is the EPA OTM33A method (Brantley et al., 2015). For complicated problems, advanced statistical optimization methods are used, including “genetic algorithms”, “Bayesian inference”, “simulated annealing”, and “evolutionary strategies”. The advanced genetic and evolutionary methods attempt to assure that the solution is the best across all possibilities.

The EPA Brantley et al. (2015) source term estimation model applications involve scenarios where the source location is known (or at least is narrowed down to one of several possible locations close to each other in a specific industrial facility). They show, using field experiments with tracers, and measuring concentrations at a plant fenceline with a moving van, that they can estimate the mass emission rate within ±30 % about 70% of the time. It is important to note, though, that this success rate is partly due to the fact that they require that the wind and the concentration observations be steady before making an STE calculation. The scenario being addressed by Brantley et al. (2015) is depicted in their photo in Figure 1, where the van and instrumentation are used in their field experiments. In this photo the van is travelling forwards and the small time series plot labelled CH_4 (methane) is intended to show what might be observed

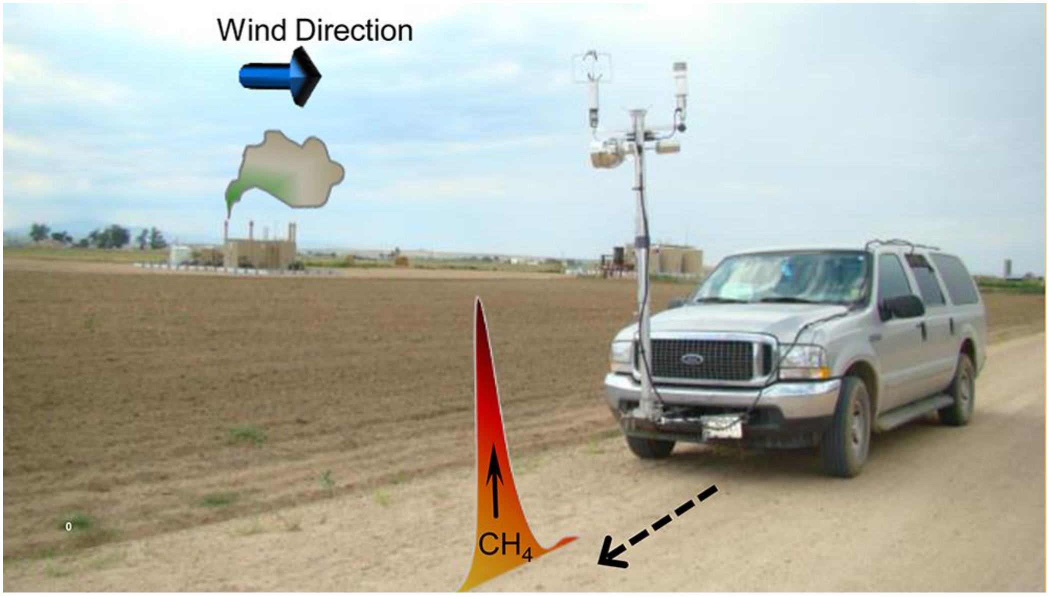

Figure 1. Photo from Brantley et el. (2015), showing van and instruments used in their OTM33A source term estimation methodology.

Bieringer et al. (2015) employed the “backwards plume” concept in developing their source term estimation method, which has the SCIPUFF adjoint model as its basis. They produced a useful diagram illustrating the methodology (see Figure 2 below). The letters CBR represent chemical, biological, and radiological. In their words: “Our inputs in this case would be the concentration observations and weather information. A T&D model is then run with the reversed winds (panel B). The logical conjunction of the inverse plumes defines the source location that would produce the measured concentration. The back-plumes from sensors within the pollution plume are combined with an ‘and’ operator (i.e., only locations in all such plumes are potential sources). In contrast, the back-plumes from sensors not within the pollution plume are combined using ‘and not’ (i.e., only locations outside those plumes are potential sources). Panels C and D show this process. Panel D shows the source location area which results. With the source location in hand, one can proceed much more successfully with source strength estimation via the forward methods.”

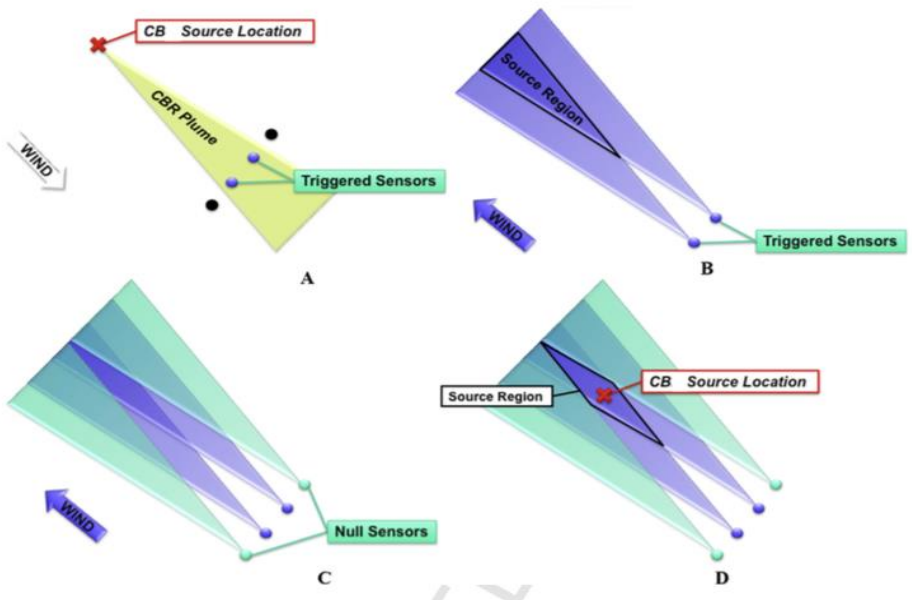

Figure 2. Depiction of a backwards transport and dispersion model STE method (Bieringer et. al. 2015). The dark diamond in part D is the best estimate of the source location. The acronym CBR refers to chemical/biological/radiological agents.

The success of STE depends on having at least 2 or 3 sensors that are reporting significant (non-zero) concentrations, preferably in the middle and near the edges of the pollutant cloud. Hopefully, if sensors are located along the plume centerline at various distances downwind, the concentrations are decreasing with distance. It is also very useful to have one or two sensors outside of the plume, recording zero. Those "null" sensors can help identify locations where the source is not. Even with wind directions that are close (say 10 or 20°) to being aligned with the source and sensor locations, the plume edge may only graze the sensor network, leading to uncertain STE estimates.

In the adjoint inverse modelling method, a forward T&D model is run in the backwards direction, adjusting parameters to fit concentration observations. This adjoint method (e.g., used in SCIPUFF, Sykes et al. 2014) adheres to Gifford's (1959) concept that the dispersion model produces a spatial field of probabilities. With this probabilistic framework, the probability fields from each sampler's back-plume are assumed to be independent. With several sampler locations to consider, the problem turns into a statistical optimization problem.

Sykes (2007) and Chowdhury and Sykes (2008) published examples of the model's applications to the ETEX field experiment, where the tracer release was from a location in NW France and there were about 200 sensors scattered around Europe. In this application, bith the source magnitude and its location were assumed to be unknown. Figure 3 shows the adjoint inverse model's probability distribution of predicted source locations for one of the ETEX tracer releases. The highest probability is the red colored area in the center of the color contours. A major focus of the two papers was to test methods for combining observations from neighboring sensors in order to speed up the solution. For example, if there is an area with a group of 10 sensors that are observing concentrations that are all within 30 % of each other, then they can be considered as one sensor in the model calculations.

Platt and Deriggi (2012) present results of an exercise where several source term estimation models were applied to the Fusion Field Trial 2007 (FFT07) data. A set of about 100 samplers were set out in a square array, and tracer gas was released upwind of the array. The models covered the range from adjoint to complex statistical optimization. It was assumed that the location and the magnitude of the source were unknown. The results were mixed, with the models predicting within a factor of two some of the time, but producing large magnitude errors in a few cases. As mentioned earlier, results are better if the samplers provide a more detailed coverage of the plume (along wind and laterally).

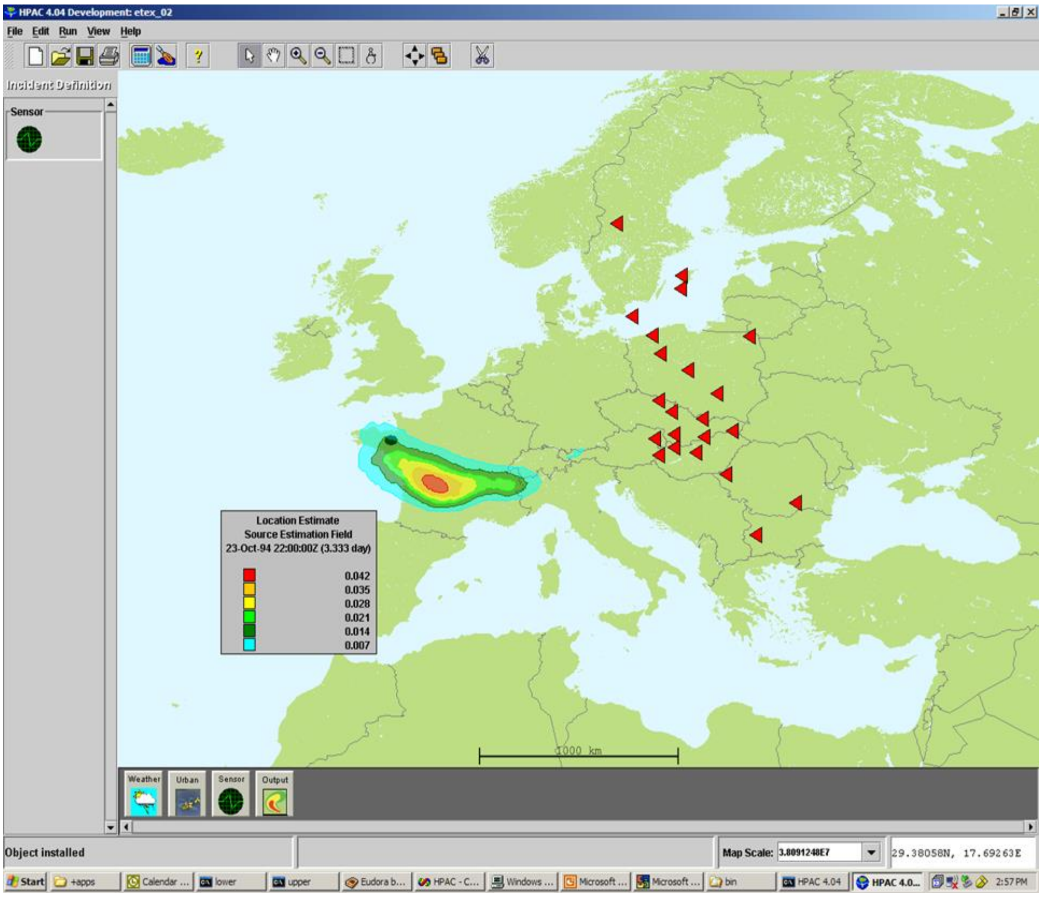

Figure 3. SCIPUFF adjoint model predictions of probabilities (color contours) of source location using observstions from sensors (triangles) during an ETEX field experiment (from Sykes, 2007). Actual source was at black dot near the NW corner of France.

FURTHER COMMENTS

I am pleased to see a recent increase in references to Gifford's 1959 paper in published papers on inverse modeling and STE. Because the paper was 60 years old and its title did not reflect its application to inverse modeling, it was neglected at first. I hope that the curren paper can further advance recognition of Gifford's contribution.

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