TWENTY-FIVE YEARS OF HARMONISATION CONFERENCES – LOOKING BACK AND AHEAD

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Abstract: Throughout the series of Harmonisation conferences it has been a key issue that in the modelling community we should build upon the experiences of each other. How can we establish mechanisms which work, when it comes to pooling experiences and obtain a better utilisation of the work done in the modelling community? The paper takes a historic perspective on our efforts to do so. It recapitulates important lessons to be learnt, and also points to our current opportunities.

Key words: atmospheric dispersion modelling, model evaluation, tools for modellers, COST 732, FAIRMODE

INTRODUCTION

The series of conferences on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes has been ongoing for around 25 years. Since their beginning these conferences have been an excellent platform for disseminating information to the modelling community on common tools, procedures and guidelines, and to inspire further developments. At the harmonisation conferences it has been an issue of permanent attention that in the modelling community we should build upon the experiences of each other. So, a key question has been: How can we establish mechanisms which work, when it comes to pooling experiences and to obtain a better utilisation of the work done in the modelling community?

You may compare our dispersion modelling community to a colony of ants who are constructing a huge anthill. In our case each of us – the individual scientists – bring in some small contributions to the hill. But we should try to put some mechanisms in place to ensure that the anthill grows efficiently to a firm, durable structure of scientific knowledge.

That is where I see the role of the Harmonisation initiative: to introduce some elements of order into the construction process.

In some respects we have progressed enormously since the beginning twenty-five years ago. The Harmonisation initiative started in the era before the Internet, but it has evolved in parallel to the rise of the web. Therefore, we have been able to gain from the tremendous improvements in possibilities for information sharing that have emerged.

As a glimpse into the past I will mention that at the first workshop in Denmark in 1992 I gave a presentation entitled "Electronic information exchange in the field of atmospheric dispersion modelling". It dealt with such matters as electronic bulletin board systems (BBS) that could be accessed by dialling a phone number – something that probably sounds absurd for today's young generation of scientists.

That time was an era of communication by physical letters and data exchange by sending magnetic tapes. E-mail was just sporadically beginning to be used, and there was no World Wide Web.

The present paper will take a historic perspective on our efforts to establish mechanisms for pooling experiences within the modelling community.

When looking back I have picked a few examples of successes and failures, where there are lessons to be learnt. Some of the examples concern a specific topic that has received much attention at all our conferences: *Model evaluation*.

LESSONS FROM THE HISTORY OF THE HARMONISATION CONFERENCES
The fate of classic data sets
Around 1991 I corresponded with John Irwin of the US EPA to learn about the availability of databases with data from field experiments. He had made efforts within his organisation to preserve and digitize data archives from past experiments. He had succeeded in getting some pilot projects started, but there were not resources to follow up on them.

John became involved in the Harmonisation initiative from the beginning; he was very supportive and participated in a large number of harmonisation conferences, also after his retirement in 2004. Around 2010 John constructed a web site with access to many classic data sets, such as Prairie Grass, Kincaid, Bull Run, Hanford 67, Hanford 64 etc.

Sadly, John passed away in 2016. The website he created – *Atmospheric Transport and Diffusion Data Archive* – has now been transferred to the harmonisation web site (URL 1 and 2). The fact that such archiving of data and their publication took place as a private initiative exposes some of the missing links in the construction of our "anthill" within the scientific community. Nowadays, distribution of data sets is much easier than before. However, the task of preparing data sets for the use of others still requires many resources – more than it usually gets.

The Model Validation Kit
One example where the Harmonisation initiative has provided a widely used common tool for model evaluation was the establishment of the co-called Model Validation Kit. The kit addresses the classic problem where a single stack emits a non-reactive gas, and it includes 4 tracer data sets.

A preliminary version of the "Model Validation Kit" appeared for the workshop in Manno, Switzerland, in 1993. The subsequent year, for the workshop in Mol, the kit was streamlined, and that version was used essentially unchanged until 2005. At that time new software computing environments had made it necessary to update the package. Until 2005 the kit was distributed on CD to those research groups who requested it. This amounted to more than 250 research groups during the period 1994-2005. Since 2005, the package has been available for free download from the Internet (URL 3; Olesen 2010).

The Model Validation Kit has been a useful point of reference for a large number of studies at the Harmonsation conferences, although it does have recognised limitations. One weakness of the methodology used in the Model Validation Kit is that its results should be interpreted with great care, because it does not explicitly address the question of stochastic nature of observed concentrations. It is essential to keep in mind that in general our dispersion models describe ensemble means of an event, whereas what happens in the atmosphere can be regarded as individual realisations of an event. Our models cannot be expected to predict such fluctuations. This issue was of much concern to John Irwin and is addressed at his web site (URL 2).

FAIRMODE and other networks
In 2007, the idea of a modellers' network in support of the European Air Quality Directive was launched in a presentation by Moussiopoulos et al. at the 11th Harmonisation conference in Cambridge (Moussiopoulos et. al., 2007). During the subsequent years the network materialized in the form of FAIRMODE network (Forum for AIR quality MODElling in Europe). FAIRMODE has evolved and it is now very central in the context of the Harmonisation conferences. FAIRMODE successfully has produced many tools of common interest, such as the Delta Tool for model evaluation and the composite mapping exercise that produces a map of concentrations over Europe, as calculated by a large number of groups (URL 4).

Over the years, many other networks – e.g. COST actions and EU-funded research projects – have produced common tools of interest to the modelling community. Many of the networks have used the Harmonsation conferences as a platform for disseminating information about their tools and as a means of creating interaction with the air pollution community.

Much of the work produced by these networks has been published in the form of papers for the Harmonisation conferences. A repository of nearly all extended abstracts and a large number of presentations for the Harmonisation conferences is available on the Harmonisation web site (URL 5) (the collection of papers is not complete, because not all authors have given permission to have their papers published on the web).

Lessons from COST 732

As one example with many lessons to be learnt I will recapitulate some experiences from the COST 732 action "Quality assurance and improvement of micro-scale meteorological models" (2005-2009), which was linked to the Harmonisation initiative in many ways.

The action focused on producing guidance and protocols for quality assurance of models that are applied for describing meteorology and dispersion in an environment with many obstacles, such as a city. The action worked with several case studies, but particularly intensively with the MUST dispersion experiment that took place in the real world, but was also simulated in a wind tunnel. More that a dozen research groups worked on modelling certain scenarios from the data set. A tool (a set of Excel workbooks) was developed where the result of all research groups could be visualized and explored. During this process many problems were encountered and resolved.

Several important lessons can be learnt from the exercise – many so important and general that they deserve to be recapitulated here. Interested readers can find further information in the report with description of case studies (Schatzmann et al., 2010) and in the guidance documents produced by the action (URL 6).

Within the COST action, a "Model Evaluation Guidance and Protocol Document" was produced. One of its recommendations was to use 'exploratory data analysis' as one of the elements in model validation. Throughout the work with the data sets in the COST 732 action it was confirmed repeatedly that such exploratory analysis is crucial to reveal shortcomings of data sets, model setups and models. It was the experience that even experienced modellers sometimes do perform errors, and that these can be overlooked unless one inspects data, presented in graphical form. Conditions are best for detecting anomalies if you have a situation where several models are put into a common framework. Such a framework also makes it possible to identify features common to several models, and thereby derive an indication of the state of art. The tools developed for the MUST wind tunnel exercise provided one such excellent framework (URL 7).

As a further recommendation, when attempting to evaluate model performance it is important to consider the representativeness of the underlying data. Thus, in the case of MUST wind flow simulations, studies were performed to illustrate the effect of considering different subsets of data. The examples made it clear that a value of a certain statistical performance metric tells nothing unless it appears in a context. It was recommended that when comparing metrics for several models, metrics should not be computed by each modeller with his own methods, but with a common tool. In the case of COST 732, use of the common Excel workbooks made it transparent which data were used to compute the metrics and served to ensure consistency.

Occasionally, modellers deliver results without checking the plausibility of the complete model output. The more complex models deliver huge amounts of information. In the MUST exercise it was demonstrated that it is not sufficient to look only at the (usually small) subset of properties for which measurements are available. Much can be gained by looking at the complete model output, and a plausibility check of results is always appropriate.

In general it must be recommended to use graphical tools to get an overview of the results. Lots of things can go wrong and, in practice, they actually often do...

When making data sets available for the scientific community it is inevitable that the data sets contain errors. The way to deal with this problem deserves some attention. During the course of the COST action several versions of the MUST wind tunnel data set were used for the exercise. This led to confusion about which data a modeller should use, and to confusion about which basis was used when one considered a particular set of results. There were compelling reasons to change from one version of the data set to a new: Errors in coordinates were detected; incorrect information on source conditions appeared in one version; some data points were omitted from the data set for while, before it was decided that they were okay for use. Doublets occurred in some wind tunnel data.

All such matters led to recommendations of some simple steps that can be taken to minimize confusion in future when conducting similar model validation exercises. This can also serve as best practice when providing validation data sets for the use of others:

- Indicate clearly in files when they were created or modified, and include a log of changes.
- To the extent practicable communicate to interested parties when there is a change in files.
- To the extent practicable perform tests of data sets and tools before they are distributed widely.

The Atmospheric Dispersion Wiki

For many years we have been looking for a method to minimize the problem that researchers sometimes repeat others' mistakes, and that sometimes misconceptions can propagate. One idea took form in 2005 and was materialized in the form of a wiki.

The Atmospheric Dispersion Wiki (URL 8) was launched at the 10th Harmonisation conference in order to facilitate pooling of experiences within the modelling community. One idea behind the wiki was to put focus on warning against pitfalls and common mistakes, relevant for researchers in the modelling community. Researchers were encouraged to report on pitfalls they encountered, and which they would like to warn others against.

Furthermore, the wiki seemed well suited to communicate experiences on experimental validation data sets. Thus, the wiki contains pages concerning the Prairie Grass data set, the MUST set, and the Thompson Wind Tunnel data set. The fact that the web site is structured as a wiki allows anyone to contribute with experiences.

However, it must now be recognized that the wiki has not been a success. There have been too few contributors for it to grow, so it has not become any real focal point for exchange of experiences.

The wiki still exists, and it may continue to live its quiet life. It can still act as a resource for those seeking certain kinds of information, but in its present form it will hardly become the focal point it was intended to.

FUTURE PERSPECTIVES

There are many successful services on the Internet that may have the potential to assist the modelling community with mechanisms for pooling experiences and obtain a better utilisation of the work we do.

In a paper for the 16th Harmonisation conference (Olesen, 2014) I pointed to some web-based tools of this kind, such as Wikipedia, Google Scholar and other Google products, platforms for open source code, social/professional networks as LinkedIn, Researchgate, FigShare. I will encourage you to be inventive as to where our community can fit in and benefit from such services in future.

Regarding the future of the Atmospheric Dispersion Wiki it can be considered whether Wikipedia may serve some of the purposes that the Atmospheric Dispersion Wiki was designed for. However, Wikipedia is stiffer, less suited for communication between researchers than the Atmospheric Dispersion Wiki, so Wikipedia alone can probably not fulfil all the original aims. It is my hope that members of the audience will be able to suggest ways to revive the wiki in some form, or to suggest other structures which are capable to take over and serve the intentions of the wiki.

The future brings new challenges and new opportunities. One area where the initiative will undoubtedly be active in the near future is the question of how to make proper use of low cost sensors in our modelling activity.

CONCLUSIONS

A number of experiences on model evaluation and work with datasets for model evaluation have been recapitulated in this paper. Focus has been on a variety of issues, notably the following.

- Keep in mind that concentration measurements are results of stochastic processes, while models predict ensemble means.
- Provide and use tools that define a common framework for evaluating models and comparing their behaviour.
- For in-depth quality assurance of models /model validation exploratory analysis is indispensable. It should provide graphical output, and preferably use common tools so the behaviour of several models can be compared.
- The Harmonisation web site is a useful resource for the modelling community. Thus, it acts as a repository for extended abstracts from all the conferences. Also, John Irwin's *Atmospheric Transport and Diffusion Data Archive* as well as the *Model Validation Kit* can be found through the Harmonisation web site.
- Consider resources for best practice, such a COST documents.
- Statistical model performance metrics should appear in a context – numbers tell nothing unless there is information on the underlying data sets and on the challenges they represent.
- An open-ended question concerns the question of how to best carry on the intentions of the Atmospheric Dispersion Wiki: Can we find methods to minimize the problem that researchers sometimes repeat the mistakes of others?

As I see it, in future the Harmonisation conferences should continue to have the role as a focal point for disseminating information on common tools. The conferences should provide a platform for discussing and launching new initiatives. The activities of FAIRMODE are very relevant for the Harmonisation conferences, and also in future close links to FAIRMODE should be kept.

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