Chapter 9

Applications in atmospheric sciences

9.1 ▪ Numerical weather prediction

9.1.1 ▪ Presentation of the domain

Obviously, weather forecasts have always been of paramount importance. They have often been the epitome of risk assessment in agriculture; ship navigation and sailing; air navigation; battlefield tactics; extreme events such as storms, tornadoes, and floods; and more recently for renewable energy, such as wind energy and solar energy.

At the end of the nineteenth century the Norwegian school of meteorology, led by Wilhelm Bjerknes, built the foundations of modern meteorology. Modern communications, e.g., telegrams, allowed meteorologists to almost instantaneously transfer observation results to draw charts of pressure, temperature, humidity, and wind speed. Weather forecasting emerged from the art of the forecaster to interpreting these charts and their extrapolation in space and time.

After the Second World War, scientific computation and new measurement devices, such as radar, fostered the ambition of weather forecasting. Solving at least approximately the fundamental equations that govern the atmospheric motions became possible, thus enabling comparison between observation charts and the numerical output of mathematical models. NWP was born.

With the increase in the number of observations and in the accuracy of the numerical models, enabled by the increase in computational power, the quality of meteorological forecasts has steadily increased over the years.

9.1.2 ▪ Examples of DA problems in this context

NWP is extremely challenging. Solving the primitive equations at very high resolution and incorporating finer physics, such as cloud microphysics and constituent chemistry and physics, is a first major hardship. The second hardship is fundamental and is due to the chaotic atmosphere dynamics, as first explained by the famous meteorologist Edward Lorenz. The main consequence is that any small perturbation in one of the meteorological fields increases exponentially with time. Hence, a fine estimation of the meteorological fields, whose deviations from the true ones can be seen as an error, is bound to diverge exponentially with time from the truth. NWP at the mid-latitudes has a finite horizon of predictability of about 10 days [Lorenz, 1965, 1982; Dalcher and Kalnay, 1987].

A solution to overcome this second hardship is to correct the estimation of the fields by correcting the initial condition of a forecast using information coming from measurements. That is why DA is critical in NWP. It was first introduced in the form of computationally cheap interpolation methods, Cressman interpolation, and later statistical interpolation. Using background climatological information and a variational analysis, this led to the introduction of 3D-Var in the 1990s. At the beginning of the 2000s, optimal control over a time window was used to obtain a model-consistent trajectory and led to the introduction of 4D-Var in the field [Rabier et al., 2000]. A few years later, the EnKF was also experimented with and put into operation [Houtekamer and Mitchell, 2005]. Nowadays, operational centers implement hybrid and 4DEnVar methods (see Chapter 7) to combine some of the benefits of the filtering and variational methods while trying to avoid their drawbacks.

As opposed to many components of the earth system, the atmosphere is a very well observed part. The improvements in NWP skills have come from the increase in the model resolution and from the ability of DA to make good use of observations, but also from the fast-increasing flux of observations, most of them stemming today from space platforms.

The exponential increase in the number of observations, mostly due to satellite measurements, has benefited NWP in the southern hemisphere, where the synoptic observation system (i.e., the global-scale traditional observation network) is much sparser than in the northern hemisphere due to the oceans. These observations, after thinning, are fed into the DA systems.

The increase in the model resolution and the improvement in the parameterizations have decreased representativeness errors and more generally model error to a point that errors have become of the same magnitude as the initial condition error growth induced by the dynamics, at least for the standard way of measuring NWP performance. In turn, this implies that the determination of the initial condition remains of paramount importance, as well as the role played by DA. DA is also meant to play a significant role in model error mitigation by, for instance, state parameter estimation.

9.1.3 ▪ Focus: Evaluating the skill of NWP

The improvement in NWP is objectively measured by standard skill tests routinely issued by the operational centers. The increase in performance has recently been qualified as “The quiet revolution of numerical weather prediction” in Bauer et al. [2015]. This is first justified by the achievements of the NWP community, which have not been publicized as much as others in other sciences, such as fundamental physics. Second, the progress has been due to many factors from both the scientific and technical sides, some of them already mentioned. Third, this progress has been steady over three decades, with no clearly publicized breakthrough. Figure 9.1 shows this steady improvement over the years using a standard skill score of NWP applied to an observable: the geopotential height at 500 hPa, from the ECMWF. As hinted at in the previous section, the gap between predictability over the northern and southern hemispheres has reduced considerably because of the uniform coverage of satellite observations.

An empirical model for the error growth in NWP is [Lorenz, 1982; Dalcher and Kalnay, 1987]

$$\frac{\mathrm{d}E}{\mathrm{d}t} = (\alpha E + \beta)\left(1 - \frac{E}{E_\infty}\right), \tag{9.1}$$

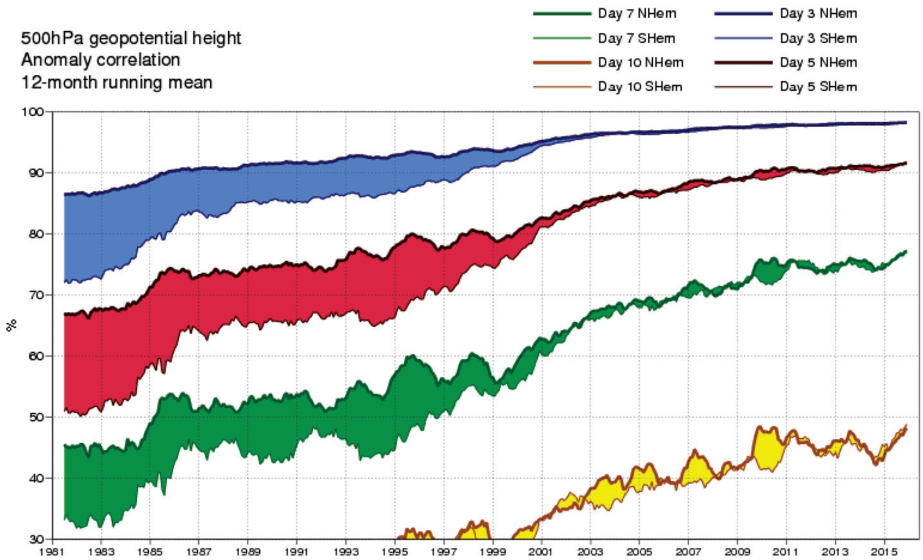

Figure 9.1. *Anomaly (difference between the actual value and the climatological value) correlation coefficient of the* 500 *hPa height forecasts for the extratropical northern hemisphere (upper curves) and southern hemisphere (lower curves), and for a forecast horizon of* 3, 5, 7, *and* 10 *days.* *©2016 ECMWF, reprinted with permission.*

where α is the dynamical error growth due the chaotic nature of the model, β is the model error source term, and E_∞ is the asymptotic error level at which error saturates because of the finite volume of phase space. A typical error growth curve that follows this model is plotted in Figure 9.2. In the short term, error growth is dominated by model error, which exceeds the uncertainty on the initial condition. The exponential

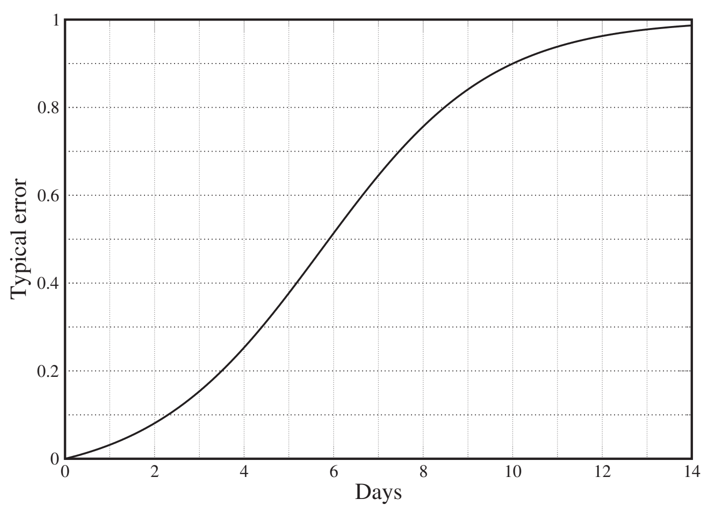

Figure 9.2. *Typical error growth following the empirical model* (9.1)*. The asymptotic error is* $E_\infty = 1$, $\alpha = 0.5$, *and* $\beta = 0.025$.

growth due to the uncertainty on the initial condition finally takes over but will ultimately saturate.

This empirical model allows us to roughly attribute the improvement in the forecast to either the estimation of the initial condition or the mitigation of model error, using a simple fit to the skill scores [Simmons and Hollingsworth, 2002; Magnusson and Källén, 2013]. Such an analysis confirms that the improvement mostly comes from both the reduction of the error in the initial condition (thanks to DA) and the reduction in model error. Both turn out to be equally important. The initial condition can be addressed by DA, whereas model error can only be partly mitigated by DA. The increase in the number of observations has been a less important factor in the most recent trend analysis [Magnusson and Källén, 2013], typically since the 2000s.

9.2 ▪ Atmospheric constituents

The primary goal of DA in meteorology or oceanography can be identified with the inverse problem that consists of estimating the initial condition of the state vector. This is justified by the strong sensitivity of the errors to the initial condition due to the chaotic dynamics of the primitive equations. In addition to the fluid itself, the primitive equations account for the transport and evolution of the water content of the atmosphere but do not describe all the other trace constituents of the atmosphere.

9.2.1 ▪ Presentation of the domain

These trace constituents are critical [Seinfeld and Pandis, 2016]. They can form air pollution with huge sanitary impacts, such as ozone or fine particulate matter in the boundary layer. They strongly affect the radiative budget and climate: the ozone in the stratospheric ozone layer to protect us from ultraviolet radiation and carbon dioxide as the main global contributor to global warming of the atmosphere. The atmosphere can hold harmful pollutants such as radionuclides in the wake of a nuclear accident, or ashes after a volcano eruption, with radiative forcing impact and with annoyance for airplanes.

To simulate these additional species, one should add to the primitive equations the transport equations of the species, the reactions among them, and the emission and loss processes in the atmosphere. There are hundreds of species of interest in various forms: gaseous, aqueous, particulate matter, and aerosols, to name a few. Their chemical and physical dynamics can be strongly nonlinear. However, their dynamics are barely chaotic.

9.2.2 ▪ Examples of DA problems in this context

As a consequence, the main issue in controlling and tracking these species may not be in determining the initial content of the species in the atmosphere. An accurate quantitative estimation of the concentrations usually requires the estimation of all the influential factors, such as the emissions or the sinks, the chemical kinetic rates, and the microphysical thermodynamical coefficients of the many parameterizations required to simulate the species. Moreover, the estimation of these forcings is often interesting per se, not only for nowcasting or predicting the species concentrations.

In particular, the estimation of the emissions is highly relevant. It is critical in the definition of abating policies for air quality or for the earth system's response, leading to global warming. When estimating these factors rather than the concentrations, DA is actually used to solve an inverse problem. There is indeed a very strong connection between the methods of DA and the mathematical techniques developed long ago in inverse problems, as already heavily emphasized in this book [see also Bocquet, 2012b, and references therein]. For instance, the concept of background in DA is tantamount to the concept of regularization in mathematical inverse problems, which is pivotal in the understanding of emission inverse problems.

The application of DA to the estimation of the fluxes of pollutants began in the 1990s with the goal of estimating greenhouse gas fluxes, such as carbon dioxide and methane [Chevallier, 2012, and references therein], but also to estimate primary pollutants or precursors of secondary pollutants, such as nitrogen oxides, carbon monoxide, sulfate dioxide, or other trace but harmful species, such as heavy metals [Elbern et al., 2012, and references therein].

With this objective in mind, filtering approaches are not the most efficient techniques. Indeed, to estimate an emission flux, one would like to later use concentration observations that are causal consequences of these emissions. Hence, smoothing techniques are usually preferred, such as 4D-Var, BLUE equations but applied over a time-window, or an EnKS. That said, the EnKF has also been successfully used for forecasting and parameter estimation in this context.

9.2.3 ▪ Focus: Inverse modeling of the radionuclide emission from the Fukushima-Daiichi nuclear power plant accident

In the case of an accidental release of pollutant in the atmosphere, it is crucial to forecast the plume and the contaminated zones, for instance to implement safety protocols to protect the population. Numerical transport models are used to simulate the dispersion of the pollutant. Figure 9.3 shows the large-scale dispersion of cesium-137 that came from the nuclear accident of the Fukushima-Daiichi nuclear power plant (FDNPP). Cesium-137 is a harmful radionuclide with a 30-year half-life that is carried over large distances in the form of particulate matter.

These models requires several input fields. In an accident context with a pointwise source, the critical inputs are the meteorological fields obtained from meteorological models, wind and precipitation, and, above all, the pollutant source term. An incomplete and erroneous knowledge of these inputs has dramatic consequences on the reliability of the plume forecast. Given that accidental releases are, fortunately, exceptional, and because it is dangerous to perform in situ measurements, the source term is very difficult to estimate.

The inverse modeling problem consists of locating the source or, more often, when the location is known, estimating the time rates of the release. This is called source term estimation.

Since in this context the model can often be assumed linear in the source term, several inference methods can be used to estimate the source term, such as 4D-Var, BLUE over the accident time window, an ensemble smoother, stochastic optimization, the simplex method, or Monte Carlo Markov chains. However, the main difficulty often comes from the paucity of the observations. Moreover, the knowledge of the prior statistics of the errors is rather poor. Hence, it is tempting to use the observations to infer part of these statistics, in a fashion similar to the estimation of the regularization parameters in inverse problems [Michalak et al., 2005; Davoine and Bocquet, 2007].

In the wake of earlier estimation of the Chernobyl source term, several estimations of the FDNPP source term using DA techniques have been published [Winiarek et al., 2012; Stohl et al., 2012; Saunier et al., 2013; Winiarek et al., 2014]. Figure 9.4 shows

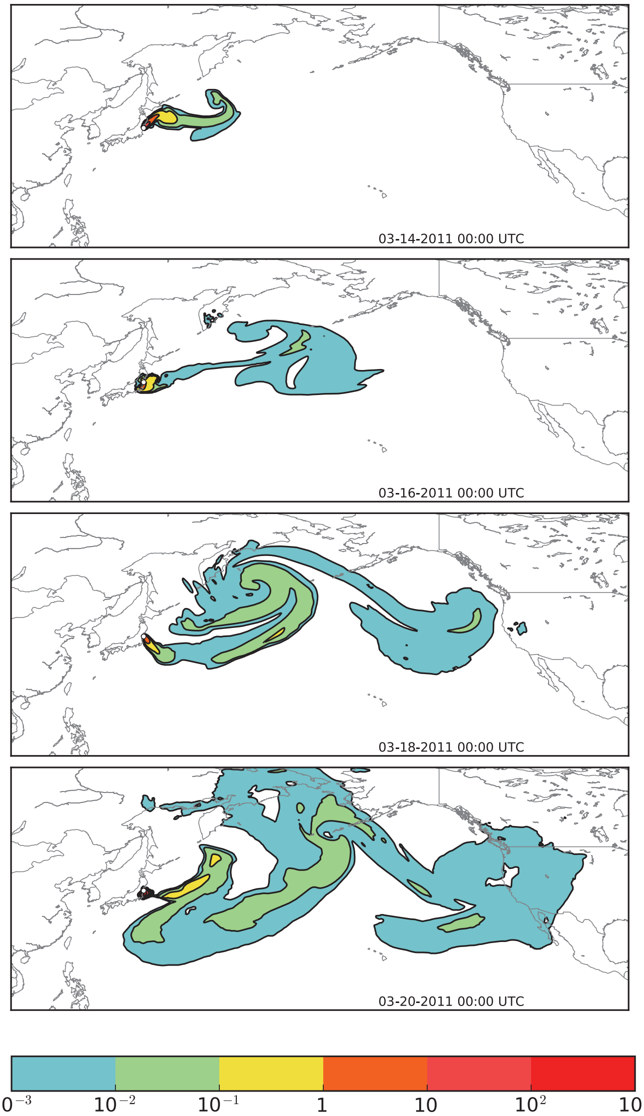

Figure 9.3. *Cesium-137 radioactive plume at ground level (activity concentrations in becquerel per cubic meter) emitted from the FDNPP in March 2011, as simulated by the* POLYPHEMUS/POLAIR3D *chemical transport numerical model [using the setup from Winiarek et al., 2014].*

an estimation of the cesium-137 source term from the FDNPP. It has been obtained using DA methods, where the error statistics are estimated while accounting for the non-Gaussianity of the errors induced by the positiveness of the emission rates. Once the source term is estimated, the numerical model can be used to simulate the contaminated zones, in the air on short notice and in the soil in the longer term. Figure 9.5 compares the observations of cesium-137 deposited near the FDNPP to the simulation deposition field obtained using the estimated source term.

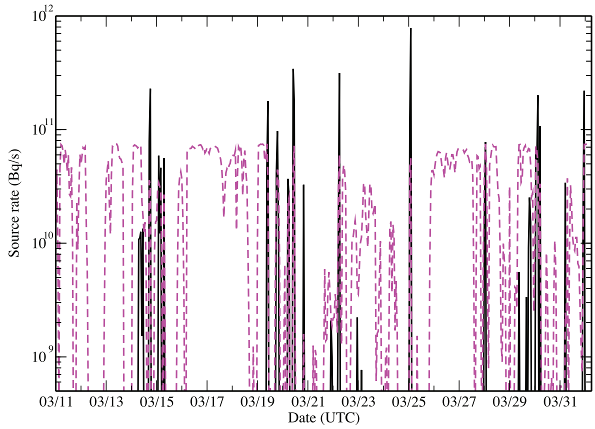

Figure 9.4. *Cesium-137 source term as inferred by inverse modeling (from Winiarek et al. [2014]). Estimated total:* 12×10^{15} *becquerel (Chernobyl was about* 85×10^{15} *becquerel). The pink curve represents the diagnosed uncertainty related to the inversion. Reprinted with permission from Elsevier [Winiarek et al., 2014].*

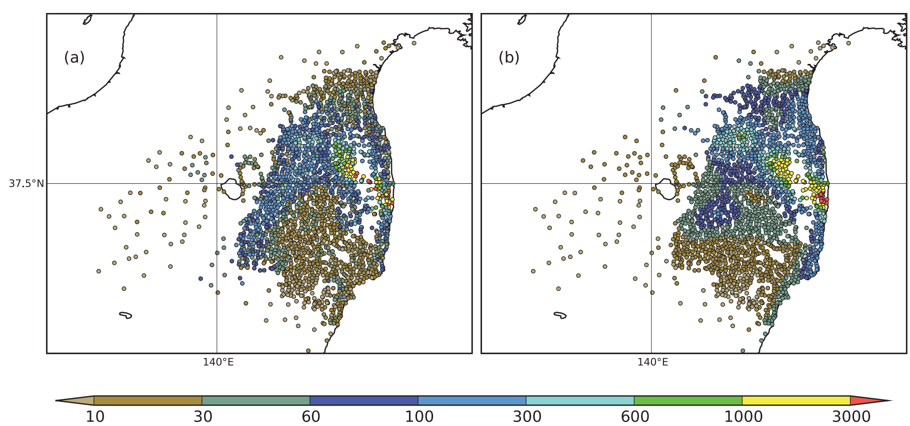

Figure 9.5. *Deposited cesium-137 (in kilobecquerel per square meter) measured* (a) *and hindcast* (b) *near the FDNPP. Reprinted with permission from Elsevier [Winiarek et al., 2014].*