APPLICATION OF METEOROLOGICAL MODELS IN AIR QUALITY MODELLING

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1. Introduction

The history of mathematical models describing transport, spreading and transformation of atmospheric pollutants, extends back for more than a half of a century. During this time, these models have evolved considerably, in terms of their destination, structure, complexity and applicability. The problem of wintertime smog, resulting typically from coal combustion, either in industrial facilities or residential heating, has been frequenting some areas (e.g. London, Mosa Valley, Pennsylvania) for a much longer time, but the remedies were still to evolve. The Clean Air Act of 1956 introduced smokeless zones in London, however, the demand for industrial emissions limitation was present worldwide. In the early regulation attempts, the air pollution problem has been mostly perceived as spreading of plumes from industrial or power plan stacks, affecting the immediate vicinity. The first batch of calculational tools, referred here as to *dispersion models*, was introduced in 1950's to support local air pollution control policies based on so-called emission permits. The idea was to determine the allowable amount of pollutants that could be released from a planned installation without exposing the population living in the vicinity to harmful pollution levels. Models serving this purpose were called *regulatory*. Althought this procedure relied on *prevention* rather than on *remediation*, it brought gradual improvement of air quality in some regions as the newer facilities, complying with the regulations, replaced the old ones. These early dispersion models treated the process of spreading the pollutants with drastic simplifications, that limited their applicability. A typical use was to predict annual mean concentrations of a passive (non-reacting) substances within short distance (say, 20 km) from a stack. A typical model was based on an analytical solution of a simplified mass conservation equation (also termed the transport equation or, perhaps, not quite correctly, *'the turbulent diffusion equation'* (turbulence is not a diffusive phenomenon)), which yielded Gaussian distribution of pollutant concentrations across the plume, hence the term *Gaussian models*.

The next type of air pollution problems in cities begun with the increase of car use, causing emission of nitrous oxides, dust and hydrocarbons. These substances reacted in the atmosphere under the presence of solar radiation, causing *secondary pollutants*, such as ozone, to form a *photochemical smog*. Obviously, the analysis of the photochemical smog formation, or its prediction, could not be done with a Gausian model; this process was far too complex to be handled in such simplistic manner. Yet, it needed a few tens of years, to be addressed by *Eulerian numerical photochemical models* that rest on *approximate* (numerical) solutions of the full set of 'almost' *unsimplified* equations, describing transport, chemical and photochemical transformations of individual species in the atmosphere, taking into account the spatial and temporal variation of meteorological conditions over a given area.

Still another problem arose with the discovery of acidification of rivers and lakes in Scandinavia, which was attributed to long-range (transboundary) transport of air pollutants. Evidence of such transport was also supported by samples taken from remote sites, such as Arctic or Himalayan glaciers, revealing the presence of industrial pollutants and radionuclides from nuclear weapon tests. A special type of models, *Lagrangian trajectory models* was then designed. These models were based on synoptic-scale meteorological analyses of air parcel pathways (or, trajectories), and a mass balance equations describing concentration changes within a parcel moving down the trajectory.

Development of nuclear power plants, fuel processing plants, chemical factories and other facilities posing hazards to its vicinity, has caused another branch of dispersion models to emerge. These models had to take into account the flow patterns forming around the obstacles (buildings), or adopting to the terrain topography. Usually, such models could benefit from additional wind measurements taken by a local monitoring network; on the other hand, they had to be able to deliver fast, almost instantaneous prediction of the exposure of personnel, or vicinity population, to the radionuclides or toxins released during accidents. Some of these models, supplied with a proper meteorological information, were applied even in a global scale, e.g., after the Chernobyl accident in 1986. Currently, they support national emergency-response centers, such as the CANERM model in Canada.

Finally, to address global air pollution problems such as stratospheric ozone layer depletion ('the ozone hole'), worldwide increases of carbon dioxide concentrations, regional and global aerosol pollution ('brown smog'), possible climate changes ('global warning'), new, sophisticated and complex Eulerian numerical models emerges. Some of them are similar, in terms of their underlying conservation laws, to the chemical / photochemical models used in urban air basins to deal with photochemical smog; some have even greater complexity. This leading-edge branch of models is under continuos development, as the knowledge of atmospheric chemistry, and the information and computational infrastructure advances.

2. Problem definition; scale and phenomena

Problems depicted in the previous section can be characterised in terms of their *spatial* and *temporal scales*, and processes and factors that play primary role. Although it can be generally stated that basic principles of physics are universal, and stipulated that a certain set of equations could form an universal model, applicable to any problem, such approach remains impractical. The physical scales, determined by the spatial extent of a phenomenon, the period of time during which it occurs, or just the spatial and temporal variability, dictate the relative importance of individual forcings, actions or processes that occur in the course of this phenomenon. Hence, many models are built towards specific problems, taking into account only these factors and processes which are deemed to be relevant or important to a given phenomenon, or just dominant in it. However, with the growing knowledge and computational capacities, development trends are also directed towards broadening applicability of certain models. One could think of three broadly defined categories:

– single-purpose models designed towards a single particular goal, strictly related to a particular phenomenon, and a particular spatial and temporal scale. These models are the most simple ones within all the models that can be used in a given purpose, the most economic in terms of their computational and data demands, and the easiest to operate and analyse;
– more general, multi-scale and multi-purpose models that take into account many processes, and are valid for a much broader range of scales. These are typically far more complex and demanding that the former cathegory, their development cost can be several orders of magnitude higher than of the former cathegory. However, their generality makes them a feasible choice in many situations, e.g. when the particular problem is related to many phenomena, or when the problem has not been addressed by a single-purpose model;
– modular modeling systems, where a certain model can be set by the user from a collection of modules which are adequate for a particular process, phenomenon, and scales.

The above classification is somewhat simplistic, as many models can be classified as belonging to more than one cathegory with respect to their different features. Nevertheless, it illustrates the basic directions of the contemporary model design.

Meteorological phenomena can be associated with one or more of the following spatial scales. The term *global scale* usually is applied to the largest features of the atmospheric flow such as the elements of the general atmospheric circulation. *Synoptic scale* contains pressure systems – lows and highs, and their associated structures of motion – cyclones and anticyclones, with characteristic sizes of several thousand of kilometers. On the other end, *microscale* refers to the features smaller than a few kilometers, driven by local factors acting on a larger-scale background. Between the microscale and synoptic scale, the *mesoscale* contains phenomena driven by both the local and large-scale influences, that develop under interaction of processes belonging to many scales. The interaction of scales acts in both directions (top-down or bottom-up), hence the mesoscale meteorology poses many challenges to modellers.

3. Climatological approach

One of the earliest ideas utilized in applied air pollution models was to classify meteorological conditions, and to conduct computations for the resulting meteorological scenarios rather than for real situations, thereby reducing the complexity. This approach was particularly convenient for calculating long-term statistics, such as annual mean concentrations of pollutants in the ambient air. Such mean values could easily be obtained as a weighted average of the results obtained for individual cathegories, where the frequency of occurance of these cathegories served as a weighting function. Small data demand was another advantage of this method. This approach has been extremely popular in combination with a local Gaussian plume model. Other applications included local emergency-response systems, where the pre-calculated distributions could be instantaneously superimposed with the actual emission estimates, yielding the estimated exposure maps, and in wind resource estimations, where such economic computational method turned out feasible. As the computational power and data availability increased, the advantages of the climatological approach begun to fade, and the model development became controlled by the rapidly expanding knowledge of pollutant dispersion processes. Nowadays, the climatological approach is mostly regarded as obsolete.

4. Boundary-layer parameterisation

The developments of 70's and 80's of the 20-th century – most remarkably, the wide application of turbulence measurements in field experiments and the Large Eddy Simulation (LES) technique of numerical experimentation (Deardorff, 1974), resulted in a new paradigm in understanding the structure of turbulent mixing in lower atmosphere. The existing Monin-Obukhov similarity theory of the statistical structure of turbulence in the atmospheric surface layer was complemented by the inclusion of the description of the convective mixed-layer growth, the surface energy budget calculations, and combined into an applicable parameterisation of the atmospheric boundary layer. This approach employs three principal physical quantities:

- vertical turbulent momentum flux over the ground surface;
- vertical turbulent heat flux over the ground surface;
- boundary layer / mixed layer height.

The dispersion model utilizes these three parameters (calculated by so-called *meteorological pre-processor*) along with other measured quantities (wind speed & direction, vertical temperature gradient above the mixed layer), to calculate *plume dispersion parameters*, thereby replacing the climatological classification where these parameters (or, stricly speaking, their calculation) were assigned to classes. This new generation of Gaussian plume models was proposed in 80's (Weil, 1985) and eventually replaced climatological Gaussian models in the U.S. regulatory application (*Federal Register*, 2005).

5. Meteorological pre-processors

A *meteorological pre-processor* is a program, which calculates *parameters* used by a dispersion model, using available meteorological information. Usually, this “available information” means data collected from a surface weather station, belonging to the routine observation program, plus an aerological sounding from the nearest / representative location. Examples of such pre-processors are AERMET (Cimorelli *et al.*, 2004), which provides boundary layer parameters to the AERMOD dispersion model, or CALMET (Scire *et al.*, 2000), which is used with CALPUFF. A meteorological pre-processor can include some other features, such as a mass-consistent interpolation scheme which allows using data from multiple weather stations (e.g. CALMET), or including effects of flow distortion around the terrain features under various atmospheric stability conditions (e.g., AERMET). Alternately, boundary layer parameters can be computed using gridded products of meteorological centers (either analyses or forecasts) and fed into a dispersion model (e.g., CALMM5).

Computation of boundary layer parameters using routine meteorological data only involves some complexity and inacurracy. Although the the profile method (e.g., Berkowicz and Prahm, 1982), based on the well-established Monin-Obukhov surface layer similarity theory in most cases lets calculation of surface fluxes with sufficient accuracy, it requires knowledge of wind speed and temperature at two distinct levels within the surface layer, which is not the observing standard; both these measurements are available at a single heights only. Hence, additional closure is required, and the surface energy budget equation is the usual way (e.g. Holtslag and van Ulden, 1983; van Ulden and Holtslag, 1985). Unfortunately, this solution invites many inaccuracies introduced by rough methods of parameterisation and estimation of the individual budget components. Similarly, mixing heights can be derived from radiosondings, however these have low resolution and insufficient spatial and temporal coverage. Slab boundary layer models (e.g. Tennekes, 1973) are used to supplement observations under convective conditions, and diagnostic formulae (e.g. Zilitinkevich, 1972) are applied for neutral and stable cases. Particularly the latter method lacks generality and accuracy, hence the quality of the results is questionable. Nevertheless, the overall accuracy of the final results of the dispersion model is clearly better than in the climatological approach.

6. Terrain effects and diagnostic wind field models

Topography, as well as inhomogeneity of thermal and dynamic properties of the surface, causes distortion of atmospheric flow; under certain conditions, local circulations caused by differential heating can also develop. For a long time, numerical solution of the Navier-Stokes equation remained too complex and troublesome for most of practical problems. Several simplified methods were then developed for practical applications. For a more detailed discussion, readers can be referred to Lalas and Ratto (1996), Finardi *et.al*., (1997) and Homicz (2002). Here, we shall briefly discuss the basic modelling ideas and principles.

Mass-consistent diagnostic wind field models, e.g. MASCON (Dickerson, 1978), MATHEW (Sherman, 1978), NOABL (Traci *et al*., 1977) represent a method of interpolation of wind measurements taken at multiple locations, with inclusion of a requirement of impermeability of a part of the boundary, representing the terrain surface. In a simple fashion, the underlying idea can be explained as finding a correction $\vec{v}'$, applied to a first-guess field $\vec{v}_0$ (obtained by a simple interpolation), that would eliminate the divergent component of the wind field and preserve the rotational one. Let us assume that the wind data are interpolated to a regular grid, yielding the first-guess wind field $\vec{v}_0$. The resulting field will usually have non-zero divergence,

$$\sigma_0 = \mathrm{div}\bar{v}_0 \neq 0 \tag{6.1}$$

which would cause mass-consistency problems when a mass transport model is used to calculate dispersion with such field. Hence, we stipulate that

$$\sigma_0 = \mathrm{div}\bar{v}_0 \neq 0 \tag{6.2}$$

$$\mathrm{rot}v = \mathrm{rot}v_0 \tag{6.3}$$

Hence,

$$\mathrm{div}\bar{v}' = \mathrm{div}(\bar{v} - \bar{v}_0) = -\mathrm{div}\bar{v}_0 = -\sigma_0 \tag{6.4}$$

$$\mathrm{rot}v' = \mathrm{rot}(v - v_0) = 0 \tag{6.5}$$

Introduction of a flow potential function for the correction field,

$$v' = \mathrm{grad}\lambda \tag{6.6}$$

lets us rewrite (6.4)-(6.6) as an elliptic equation

$$\mathrm{div}v' = \mathrm{divgrad}\lambda = \nabla^2\lambda = -\sigma_0 \tag{6.7}$$

that could be solved yielding the correction and the final field

$$v = v_0 + \mathrm{grad}\lambda \tag{6.8}$$

A similar result can be obtained by formulation the following optimization problem: having a given first-guess vector field, find another vector field that would satisfy the minimum of the mean-square difference between the first-guess and the final solution, providing that the final solution would be non-divergent and the velocity component perpendicular to the boundary would be zero at the impermeable part of the boundary. This problem is solved by a variational technique, using Lagrange multipliers method (e.g.).

Linearized flow models, e.g. LINCOM (Troen and De Baas, 1986), FLOWSTAR (Carruthers et al., 1988) utilize simplified and linearized momentum conservation equations. To illustrate the method, let us consider the Euler equations (6.9)

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x}$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y}$$

$$u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} - g$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

describing the flow of incompressible and inviscid fluid under adiabatic conditions. Let us split the velocity field into two parts – the basic (background) flow, , and the departure (deformation) caused by the terrain:

$$u = U_0 + \hat{u} \qquad v = V_0 + \hat{v} \qquad W_0 = 0 \qquad w = \hat{w} \qquad p = P_0 + \hat{p} \tag{6.10}$$

Let us further assume that the basic flow fulfills the original equations,

$$
\begin{aligned}
U_0 \frac{\partial U_0}{\partial x} + V_0 \frac{\partial U_0}{\partial y} &= -\frac{1}{\rho}\frac{\partial P_0}{\partial x} \\
U_0 \frac{\partial V_0}{\partial x} + V_0 \frac{\partial V_0}{\partial y} &= -\frac{1}{\rho}\frac{\partial P_0}{\partial y} \\
\frac{1}{\rho}\frac{\partial P_0}{\partial z} - g &= 0 \\
\frac{\partial U_0}{\partial x} + \frac{\partial V_0}{\partial y} &= 0
\end{aligned} \tag{6.11}
$$

and that this departure is much smaller that the background velocity. Putting the basic and the departure components into the Euler equations, subtracting the equations for the basic components, and neglecting higher-order terms (products of the departures) yields a linear, homogeneous partial difference equation set

$$
\begin{aligned}
U_0 \frac{\partial \hat{u}}{\partial x} + V_0 \frac{\partial \hat{u}}{\partial y} + \hat{w}\frac{\partial U_0}{\partial z} &= -\frac{\partial \tilde{p}}{\partial x} \\
U_0 \frac{\partial \hat{v}}{\partial x} + V_0 \frac{\partial \hat{v}}{\partial y} + \hat{w}\frac{\partial V_0}{\partial z} &= -\frac{\partial \tilde{p}}{\partial y} \\
U_0 \frac{\partial \hat{w}}{\partial x} + V_0 \frac{\partial \hat{w}}{\partial y} &= -\frac{\partial \tilde{p}}{\partial z} \\
\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} &= 0
\end{aligned} \tag{6.12}
$$

where $\tilde{p} = \frac{\hat{p}}{\rho}$

Supposing that the boundary conditions can be represented by periodic functions, solutions of this equation system can be represented as Fourier series, where the individual modes can be written as

$$
\begin{aligned}
\hat{u}(x,y,z) &= Ue^{i(kx+ly+mz)}; \qquad \tilde{p}(x,y,z) = Pe^{i(kx+ly+mz)} \\
\hat{v}(x,y,z) &= Ve^{i(kx+ly+mz)}; \qquad \hat{w}(x,y,z) = We^{i(kx+ly+mz)}
\end{aligned} \tag{6.13}
$$

where *k, l, m* are the wave vector components (complex). Putting (6.13) into (6.12) yields the characteristic equation,

$$
\begin{aligned}
\Omega^2\left(k^2 + l^2 + m^2\right) &= 0 \\
\Omega &= kU_0 + lV_0
\end{aligned} \tag{6.14}
$$

which provides relationships between amplitudes of individual mode parameters (amplitude and phase). Introducing the surface impermeability stipulation as the boundary condition

$$
\begin{aligned}
\hat{w}(x, z = 0) &= U_0 \cdot \nabla h(x,y) \\
h(x,y) &= He^{ikx+ily}
\end{aligned} \tag{6.15}
$$

yields the final solution

$$
\begin{aligned}
\tilde{p} &= -\Omega^2 He^{-m_i z} e^{i(kx+ly)} m_i^{-1} \\
\hat{u} &= \Omega He^{-m_i z} e^{-i(kx+ly)} km_i^{-1} \\
\hat{v} &= \Omega He^{-m_i z} e^{-i(kx+ly)} lm_i^{-1} \\
\hat{w} &= \Omega He^{-m_i z} e^{i(kx+ly-\pi/2)}
\end{aligned} \tag{6.16}
$$

Present linearized models include some other physical effects such as momentum transport (friction) and differential heating, nevertheless the general method is similar to the above described. Compared to the mass-consistent models, they offer richer solutions, as they include at least dynamical effects, in additional to mass-consistency provided by the use by the continuity equation.

Models based on the *critical dividing streamline* concept (Ludwig *et al.*, 1991) were devised to handle the static stability issue in flows around terrain features. Under neutral stratification, the air flows both over and sideways the obstacle, while in stable conditions the part of the flow passing over the obstacle is damped by buoyancy forces. The work against these forces during the uplift of an air parcel is done at a cost of the kinetic energy of the inflow, which is limited; hence the uplift has a limited extent. Combination of this principle with the divergence minimization procedure yields the model solution.

7. Meteorological models

Present-day meteorological models consist of many modules representing individual processes. The kernel of such model is a *hydrodynamic solver*, which delivers solution of the basic equation of fluid motion, and allows to include effects of the Earth's surface curvature, rotation, topography and differential heating. Customarily, this part of the model is referred as to 'dynamics'. The other part of the model, nicknamed the 'physics' contains a rich set of modules devised to calculate radiative transfer, turbulent mixing, surface energy budget, surface-atmosphere interchange of momentum, heat and moisture, water vapour phase changes, cloud formation and precipitation, and many other processes. Meteorological models find their application in the numerical weather forecasting, climate studies, research in meteorology and geophysics, and many other fields.

Complexity of meteorological models sets high demands for their developers and users. Team development is necessary to combine knowledge in many branches of physics, mathematics and chemistry, Typically, it takes more than a hundred man-years to develop an operational weather forecast model. Community development over a network started to emerge in mid-90's as a natural trend. Running a meteorological model can be challenging, too: one must supply a rich variation of meteorological observations, from surface stations to satellite imagery, develop a data-processing system, perform quality control, objective analysis and data assimilation, supply a rich set of geophysical parameters (e.g. topography, land use, albedo, soil moisture, vegetation, oceanic ice etc.) just to launch the model. For this reason, full model execution suite is almost exclusively feasible at regional or national meteorological centers. Research groups usually cannot afford maintaining such a system, and use products of meteorological centers such as objective analysis.

8. Conservation laws & their solving; limitations

The 'dynamics' of a contemporary meteorological model is based upon the laws of conservation of mass (*the continuity equation*), momentum (*equations of motion, or the Navier-Stokes equations*) and energy (*heat transfer equation*), supplemented by some thermodynamic equations, describing relationships between the thermodynamical state parameters and water phase changes. To discuss the main problem with model dynamics, we shall restrict the discussion to a dry adiabatic system in a Cartesian coordinate framework (so-called *β-plane approximation*).

The initial value/boundary problem for this set of equations with an arbitrary initial and boundary conditions is much too complex to be solved analytically. Instead, approximate (numerical) methods are used, with some principal classes including: *finite difference methods*, *spectral methods*, *finite element methods*. In the first group, a Taylor-series expansion is used to approximate partial derivatives present in the equation system with some finite-difference expressions defined on a finite-spaced *model grid*. The simplest method of this group may be seen as replacing partial derivatives with difference quotients; this reduces the equation system to a set of algebraic equations that can be solved with a computer.

A consequence of this approach is that a certain volume of computer memory must be used to store values of the relevant physical quantities' values at all the gridpoints. Hence, computer capabilities limit the possible grid resolution. Another limitation is the computational power. But, these technical limitations are not the only ones: first, our measurement network is not dense enough to directly fill the model grid, second, the measurement are burdened with errors, third, the atmospheric dynamics exhibits tendencies to a *chaotic behaviour* – small changes in its initial state cause large differences after a few days. These problems cannot be easily circumvented, and they restrict the predictability.

An attempt to solve a set of equations, similar to (9), with a simple finite-difference method was first made during 1910-1920, by Lewis F. Richardson (1922), long before the advent of an electronic computer. He derived a suitable set of equations, designed a numerical algorithm to solve it, and attempted to obtain a solution by 6-week long hand calculations. This tedious work proved unsuccessful: Richardson obtained a clearly false pressure change of 145 hPa over a 6-hour forecast period in his two calculation points, and there was no explanation of possible causes of such failure available at that time. Much later, Courant, Friedrichs and Lewy (1928) formulated the criterion which must be met by approximate methods used for solving differential equations, to avoid rapid error growth, but it was not until 1950' s when the numerical stability issues in atmospheric models were recognized sufficiently well to develop the first weather forecast model.
The numerical stability limitations may be intuitively understood by considering an example illustrated in Fig. 8.1. Let us imagine a process, where a certain state variable oscillates, and further suppose that a continuous record of these oscillations is drawn in Fig. 8.1. as a solid line. The process is described by a physical law, which lets us calculate the temporal tendency given the current value of the state variable (a differential equation). Now let us try to obtain this variation by an approximate method, utilizing a ***current estimation*** of the state variable to ***make a forecast over a finite time step***, multiplying the tendency obtained from the differential equation by the time step lenght. This corresponds to putting a tangent to the line in Fig. 8.1. in a point, corresponding to the current time, and finding the next solution along the tangent. We see that when the time step is ***sufficiently small***, the points representing the approximate solutions fall quite close to the line representing the exact one. However, when a certain critical value, apparently related to the oscillation period of the exact solution, is exceeded, the approximate solutions rapidly start to diverge.

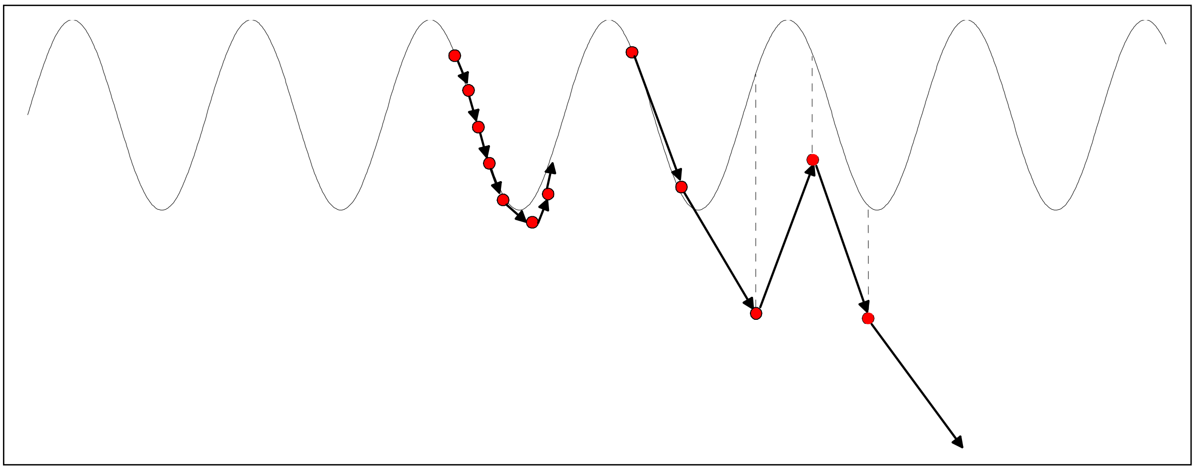

Figure 8.1. A simple idealization of the idea of stability of numerical integration methods.

An important question for now is to recognize characteristic periods of variation that can be attributed to the atmosphere, and then how to formulate the stability criteria and the integration method to ensure stability. One may expect these periods related to the external forcings the atmosphere is subject to (e.g. the surface heating/cooling in the course of diurnal cycle), to characteristic times of individual atmospheric processes, and to the internal oscillation modes related to inertial properties. Unfortunately, these periods fall into a rather wide range of temporal scales rather than to a narrow one. To ensure numerical stability, the time step must be small enough to properly reflect the *fastest component of the solution of the model equation system*, or, the phase speed *c* of the fastest wave plus the advection velocity *u*. This criterion, called the *Courant-Friedrichs-Lewy* (CFL) conditions, states that

$$C = \frac{u\Delta t}{\Delta x} \leq C_{crit} \tag{8.1}$$

where C is the *Courant number*, and C_{crit} is a certain 'critical' value (in most cases, 1) specific to the scheme under consideration.

It turns out, however, that stability properties depend on design of the approximation scheme. A scheme can be constructed as *explicit*, when values of all the quantities at a given gridpoint and a given timestep, can be computed by an explicit formula, using previous time-step values. In contrast, *implicit* schemes utilize also information from other gridpoints at the same time step; they lead to equation systems that must be solved to obtain the solution. An explicit scheme can be either *unstable* (the norm of the solutions grows every time step), *conditionally stable* (the norm of the solutions diminishes every time step when a certain CFL condition is met) or *neutrally stable* (the norm of the solutions is constant). Implicit schemes, as a rule, are *unconditionally stable*: they react to fast signals (exceeding critical Courant number) by slowing them down rather than causing the model to break. Hence, they are a viable alternative to explicit schemes; unfortunately, there is no recipe for derivation of a fully implicit scheme for nonlinear equation sets. For this reason, *semi-implicit* schemes are used. A properly designed semi-implicit scheme can circumvent some stability problems, related to the fast modes; hence, this approach appears particularly attractive for multiscale models. We shall examine this feature in more detail in the following sections.

9. Numerical weather forecasting

The first successful numerical weather forecast was made in 1950 by a group of scientists taking part in the Meteorological Project at the Princeton Institute for Advanced Studies. This project started in 1946 under leadership of John von Neumann and was directed by Jule Charney since 1948. Three elements turned out crucial to this success: the possibility of using an electronic computer, the ENIAC, the von Neumann's expertise in numerical methods and computer science, and the theoretical recognition of atmosphere's dynamics thanks to the works of Carl Rossby and his group in Norway in 30's, brought to the project by Charney. The principal idea of this project was to focus on some main features of the atmospheric flow, falling into a narrow range of scales, and to reduce the equation system, stemming from basic physical conservation laws, to a simplified approximate set, capable to describe these features, *and essentially no more*. This approach, called later *filtering*, allowed to circumvent the stringent stability restrictions, related to fast, but meteorologically unimportant internal modes such as acoustic waves, and to get some freedom in adjusting computational parameters (spatial resolution, time step), to minimize distortions in reflecting the principal features such as the large-scale vorticity advection and propagation of long (Rossby) waves.

The 'equivalent barotropic model' of the Charney - von Neumann's team, although successful in depicting the movement of a mid-latitude pressure systems, was not general enough to handle their development, mainly due to the neglection of vertical motions and their role in the cyclogenesis process, in particular the baroclinic instability. This limitation, soon recognized, needed another two years, and a next generation computer, the IAS, to overcome by a two-level baroclinic model. The Meteorology Project activities peaked around 1954, and gradually started to cease in 1955. However, the Project has laid a solid basis for the future developments and has marked the path which was followed by researchers for the next half of a century.

The 'pioneering era' of 1950's filtered models were restricted to a narrow ranges of spatial and temporal scales. It was then highly desirable to develop models applicable to a wider class of atmospheric motions, either to enable research on smaller-scale phenomena or to account for interactions between motions of different scales. The emerging approach was to return to the primitive equation system, consideration of possible filtering approximations based on an extended analysis of the atmospheric dynamics, and the introduction of the 'timestep splitting' techniques, based on splitting the general equation system into parts related to individual internal modes. This method proved successful but required, in principle, individual model design for a given range of scales and phenomena. The newest generation of models, employing semi-implicit integeration schemes has effectively overcame this problem.

Weather forecasting involves some typical scales and time ranges. For a short-range weather forecast, up to three days, it is sufficient to consider phenomena occurring in a synoptic scale, that is, over a continent. In the early 90's, models employed for this purpose covered the continent area with a grid resolution of roughly 100 km, and were called *regional*. Nowadays, their resolution exceeds 10 km, which allows to depict mesoscale features, hence the term *mesoscale* is more appropriate. Longer forecast periods, such as five days or more (medium-range weather forecast) require information from all over the globe, and *global circulation models* are uses. Long-term forecasts are attempted, but their skill is still unsatisfactory.

10. Filtering approximations

The problem mentioned in the former sections, separation of the fast and slow modes of the model is usually addressed by introducing *filtering approximations*. To illustrate this idea, it is sufficient to consider acoustic waves as an example. Under Earth's atmospheric conditions, these waves have the largest phase speeds of all the waves of dynamical origin, and have virtually no meaning in meteorological phenomena, except, perhaps, the tornadoes. The nature of an acoustic wave involves compression and expansion of the medium, that is, local density fluctuation. Scale analysis of typical meteorological phenomena shows that the local derivative of a density field in the continuity equation is much smaller than other terms and can be neglected. This simplification eliminates local density fluctuations from the model solutions, thereby filters out acoustic waves; hence it is called the *anelastic approximation*.

Further approximations can be considered when the meteorological fields are split into two parts, the reference (basic) state, and the departure from this state. This procedure involves partial linearization, and yields a better focus on meteorological phenomena occurring on a larger-scale background that may include some intense spatial variability such as pressure decrease with height. The *Boussinesq approximation* lets isolate buoyancy forces and associates them with temperature fluctuations; it is applicable to shallow motions (motions having the vertical extent much smaller than the atmospheric density scale, 8,4 km) when combined with a further simplification of the continuity equation, the *incompressibility approximation*. On the other hand, anelastic approximation should be chosen for *deep motions*. *Hydrostatic approximation* which relies on neglecting accelerations in the equation of the vertical motion component, is another important simplification. It filters out internal acoustic waves having vertical propagation component, and, when used together with selectively applied *quasi-geostrophic approximation* (approximate equilibrium of the Coriolis and pressure gradient forces in a horizontal plane), also eliminates other fast modes such as surface gravity (shallow water) waves. Hydrostatic and quasi-geostrophic approximations played a major role in theoretical investigation of atmospheric dynamics, allowing for the development of the *quasi-geostrophic theory*, the foundation of the current understanding of synoptic systems. The hydrostatic approximation can be used when the horizontal scale of the investigated phenomenon is equal to or larger than the atmospheric density scale. At the end of the 20-th century, numerical weather prediction models, were closing with their horizontal grid resolution to this 'magic' barrier of 10 kilometers, beyond which the ubiquitous hydrostatic approximation must have been abandonded. A milestone in the NWP development, reached at the end of the century, was the introduction of non-hydrostatic models into the operational service.

11. Semi-implicit schemes

In Section 8, we introduced a simple concept of stability of the numerical solution of an ordinary differential equation. Now it is time to take a closer look at this problem, with regard to a partial differential equation. Let us consider one-dimensional problem of advectional transport of a passive substance:

$$\frac{\partial \varphi}{\partial t} = -u\frac{\partial \varphi}{\partial x} \tag{11.1}$$

and its finite-difference approximation with a first-order explicit 'upstream' scheme

$$\frac{\varphi_i^{\tau+1} - \varphi_i^{\tau}}{\Delta t} = -u\frac{\varphi_i^{\tau} - \varphi_{i-1}^{\tau}}{\Delta x} \tag{11.2}$$

which yields

$$\varphi_i^{\tau+1} = \varphi_i^{\tau} - \frac{u\Delta t}{\Delta x}\left(\varphi_i^{\tau} - \varphi_{i-1}^{\tau}\right) = C\varphi_{i-1}^{\tau} + (1-C)\varphi_i^{\tau} \tag{11.3}$$

From (11.3) it follows that the solution $\varphi_i^{\tau+1}$ (at the *i*-th gridpoint and the τ+1) timestep can be calculated as a weighted average of values of φ at *i* and *i*-1 gridpoints and the timestep τ, where the Courant number *C* plays a role of a weighting factor. This corresponds to a linear interpolation of the φ function between these two gridpoints (Fig. 8.1.), and determines a point, where the section between these gridpoints (BC) is crossed by a *characteristic* of eq. (11.1), passing through the *i*-th gridpoint at the τ+1 timestep (A). In this case, a characteristic is a line along which φ value is constant, or, rather, is propagated from the τ timestep to the τ+1.

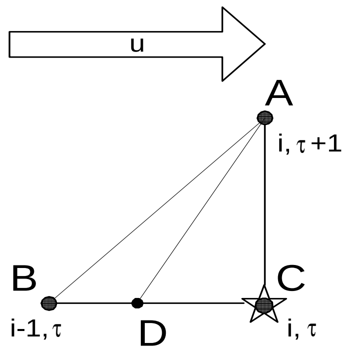

Figure 11.1. A schematic representation of the first order, explicit, uncentered approximation scheme 'upstream', (11.2).

Now let us consider the stability of the approximate solution. Using the Schwartz inequality, one can arrive to an estimation

$$\max_i \left|\varphi_i^{\tau+1}\right| = \max_i \left[C\left|\varphi_{i-1}^{\tau}\right| + (1-C)\left|\varphi_i^{\tau}\right|\right] \leq (1-C)\max_i \left|\varphi_i^{\tau}\right| + C\max_i \left|\varphi_{i-1}^{\tau}\right| \leq \max_i \left|\varphi_i^{\tau}\right| \qquad (11.4)$$

which is true when $0 \leq C \leq 1$. Otherwise, the norm of the vector representing the solution at the gridpoints will be growing every time step, and the scheme will be *unstable*. Hence, we have obtained the stability condition for the approximation (11.2) of the advection equation (11.1). One can easily see that this stability criterion is violated when the characteristic passes outside the section BC between the *i* and *i*-1 gridpoints at the timestep τ, that is, when an *extrapolation* takes place rather then *interpolation*.

Now let us consider an *implicit approximation,*

$$\frac{\varphi_i^{\tau+1} - \varphi_i^{\tau}}{\Delta t} = -u\,\frac{\varphi_i^{\tau+1} - \varphi_{i-1}^{\tau+1}}{\Delta x} \qquad (11.5)$$

or,

$$\varphi_i^{\tau+1} = \varphi_i^{\tau} - \frac{u\Delta t}{\Delta x}\left(\varphi_i^{\tau+1} - \varphi_{i-1}^{\tau+1}\right) = \frac{\varphi_i^{\tau} + C\varphi_{i-1}^{\tau+1}}{1+C} \qquad (11.6)$$

The scheme is implicit, as solving for involves, thus a set of equations must be concurrently solved. This case is illustrated in Fig. 11.2. Stability analysis shows that the condition $C \leq 1$ is no longer necessary to ensure stability, which can be easily understood from this graph.

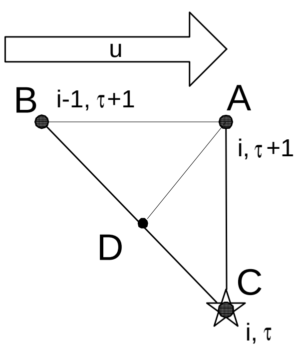

Figure 11.2. A schematic representation of the first order, implicit, uncentered approximation scheme, (11.5).

Unconditional stability is a very attractive feature of implicit schemes, however, there are some costs, drawbacks and limitations. When compared to a simple explicit scheme, with the same spatial and time steps, implicit scheme will demand more operations to be performed. Next, implicit schemes are usually more prone to numerical diffusion. Perhaps the main problem is the difficulty in treating non-linear problems with implicit schemes, as there is frequently no clue how to define an approximation that could be solved. For this reason, *semi-implicit* schemes are used. A semi-implicit scheme consists of implicit approximations used for some terms in the equation system, while other terms are treated explicitly.

For an equation system containing wave solutions, an implicit scheme will damp or slow down waves, for which the Courant number would exceed 1, hence, a distortion results rather than a breakup of instability. This feature is not necessarily a drawback and may be conscientiously used to filter out spurious oscillations.

12. Boundary conditions

Formulation of boundary conditions poses various problems and difficulties for modellers. The earth surface usually is the bottom of model domain, and its topography must be properly represented, as well as the spatially and temporally varying thermal and dynamical properties. Typically, the bottom boundary condition is derived from the non-permeability constraint (local velocity component perpendicular to the surface must be zero), however this involves use of a curvilinear, non-orthogonal coordinate system (e.g. Gal-Chen and Sommerville, 1975). This introduces complexity and awkwardness. The upper boundary condition is artificial, as the atmosphere gradually turns into void with height and has no finite limit. When the model adopts a free surface upper boundary concept, fast external, or surface modes appear and must be handled; on the other hand, using the stiff ceiling-type boundary conditions cripples the model dynamics. Models whose domain is defined over some determined extent of the globe (so-called *Limited Area Models, LAM*), must use lateral boundary conditions, which are artificial and sometimes ill-defined. This is a serious deficiency of nested-grid models, where the model operating on the inner grid receives its lateral boundary conditions from a regional, or a global model. The simplest boundary condition, representing stiff-wall type reaction, causes the waves excited within the model domain to reflect from the boundary and interphere with the 'legitimate' waves propagating out. Various types of remedies are applied, including radiative boundary conditions, sponge layers, etc.; none of these works perfecly well without any side effects. An alternative to nesting is to use variable grid resolution, which is more difficult in coding and introduces another side effect, wave diffraction. However, this solution is perhaps the least stringent and limitating, and may be seen as the best development direction in multiscale models. The variable grid resolution may be combined with non-unique time step over various part of the domain, which brings better computational economy but requires extra complexity. To summarize, there is a wealth of alternate formulations of boundary conditions for atmospheric models, none of which is perfect and absolute free of undesirable distorsions or artefacts.

13. Multiscale models

In a quest for an universal, yet practical, computer code that could be applied to a wide range of meteorological phenomena, Robert (1980) proposed a revolutionary approach to the design of a numerical model of atmospheric dynamics. In the set of equations of fluid dynamics, applied to the atmosphere, he identified terms related to the fast modes and applied *implicit* approximations for these terms. This was drastically different from the *filtering* paradigm in model design, based on *neglection* of some of these terms. The advantage was clear: the model was able to be used *just like a filtered* one when a relatively large time step was chosen, or as a full (unsimplified) model with a short time step when handling fast modes was important. This was also crucial for the model applicability to a wide range of scales, since the filtering approximations were justified by the scale analysis, valid for particular scales. Robert's hydrodynamical solver was soon adopted as a core of a meteorological model, MC2 (or MCC - *Mesoscale Compressible Community Model*), which was developed as a 'community' model by a Canadian consortium of universities, research institutes and meteorological service units (Tanguay *et al.*, 1990). Nowadays, after a quarter-of-century development, it is openly available to the researchers worldwide as a mature code.

Unfortunately, this multiscale feature applies only to the model dynamics. Small-scale processes, such as turbulence, condensation, interactions with surface become *resolvable* (directly treatable by laws of physics) only when the model resolution is sufficient. Otherwise, their effects can be only taken into account in some aggregated, *parameterized* form. The parameterizations, often based on some statistical relationships, are not universal – they are *scale-dependent*. Hence, multiscale models like MC2 are associated with extensive procedure libraries, containing parameterizations appropriate for individual scales.

Versatility of the MC2 model has been recently demonstrated in the LACES (*Large Atmospheric Computation on the Earth Simulator*) experiment. This experiment, initiated in 2003 on thence-lagerst world's computer, the

Japanese NEC's Earth Simulator, was an attempt to simulate development and further life of the hurricane *Earl* (a total of 165 hours), using a grid containing 11000 by 8460 by 67 nodes, with 1-km horizontal resolution, covering the entire North America, North Atlantic, and Arctic.

After the succesful implementation in the MC2, we see an expansion of the multiscale modeling based on the Robert's semi-implicit schemes paradigm. A good example is another Canadian weather prediction model, the GEM (*Global Environment Model*, Côté *et al*., 1998a,b). This model was initially designed as a hydrostatic, global meteorological utilizing variable grid resolution. This feature allowed to focus on some part of the global domain (such as a continent or a country), with a resolution of an order of some tens of kilometers (typical to regional models), while encompassing the whole globe, and avoiding classical nesting problems such as lateral boundary conditions. Later on, this model was extended to a nonhydrostatic formulation (Yeh *et al*., 2002), thereby turning into a *global non-hydrostatic model*, having the potential of running with 1-km resolution on some part of the domain, and, at the same time, encompassing the entire globe.

Both the MC2 and the GEM models may handle transport and dispersion of several other physical quantities such as chemical species, aerosol fractions, etc. Additional modules are attached to simulate chemical and photochemical phenomena, thereby turning these models into combined meteorological and air quality models (MC2-AQ and GEMAQ; see e.g. Kaminski *et al.*, 2002). This method of utilizing meteorological fields, calculated by the model, is called *on-line*. There are at least two advantages of this approach: (1) meteorological data are fed directly into the air quality modules, without storage limitations involved otherwise. Hence, it is possible to use more detailed meteorological information in the air pollution model, and to achieve better results. (2) coding economy, as the air quality utilizes the same subroutines, as the meteorological model, for calculating the airborne transport. For complex air quality models, the cost of calculating the meteorological models becomes an affordable fraction of the total computational cost, therefore this approach is feasible. However, running a meteorological model requires some additional skills and data, so the decision must be balanced.

14. Data processing, analysis and assimilation; reanalysis

Meteorological models exhibit a pronounced sensitivity to initial conditions, resulting from numerous instabilities occuring in the atmosphere. Modelers recognized quite early the potential for improving forecast skill, associated with refining the initial conditions. Hence, enormous effort has been spent on data analysis and processing associated with setting the initial conditions. This effort includes:
- Quality control.
- Objective analysis.
- Data assimilation methods such as 4D-VAR.

The purpose of the quality control (QC) is to eliminate data contaminated by significant errors. Most QC methods involve checking the consistency of a weather report, in terms of agreement between various related physical quantities. Other QC method involve examination of continuity of time series, spatial correlations, etc.

The transformation of irregularly spaced weather data onto a regular model grid is handled by objective analysis techniques, that is, by a computer algorithm. The most popular method is the multivariate optimum interpolation method, as formulated by Gandin (see Daley, 1991). It takes into account statistical properties of meteorological fields, such as spatial autocorrelation function and cross-correlation of individual variables. This method is theoretically optimal in a sense of minimization interpolation errors provided that statistical properties of meteorological fields are known.

Optimization criteria can be formulated in both the space and time domain, including some physical constrains as represented by the meteorological model. A sophisticated error minimization procedure, accomplished in the time and space domain, with the model used to provide specific interpolation function, is called the 4D-VAR, or FDDA (four dimensional variational data analysis). This method proved to be the most succesful, despite its complexity and large computational cost.

A typical data assimilation procedure, carried out at a meteorological center, involves short (one to a few hours) model forecasts interspersed with objective analyses. In the latter, the forecast is used as a 'background' or 'initial approximation', and combined with newly incoming data. This procedure is repeated continously. At certain selected times, such as 00Z and 12Z, principal forecast runs (e.g. 2 or 3-day forecasts) are branching from this assimilation cycle. A very important point is that the assimilation cycle is likely the best source of processed meteorological information: it is quality controlled, it includes data from many types of measurements, synchronized and combined, it is interpolated to a regular grid with the physical constraints imposed by the meteorological model. It can also be available in relatively short (1 hour) archiving time period.

Recognition of usefulness of the data assimilation cycle product has led to establishing *reanalysis projects* (e.g. Kalnay et al., 1996). These projects, executed in world-leading meteorological centers, constituted long-time (40 years or so) runs of the data assimilation suites, providing uniformly processed meteorological data suitable for short-time climate variability studies. With their spatial resolution increasing in subsequent runs, the reanalysis results are likely the best available climatology for air pollution and other engineering studies. At present, reanalyses are now attempted with the inclusion of atmospheric chemistry, primarily to recognize the changes in atmospheric composition and its effects on the radiational equilibrium and the climate. Results of these projects can be also useful in air pollution studies, for example, to produce initial conditions for high-resolution models.

15. Ensemble forecasting

Recognition of the chaotic properties of the atmosphere has made us to acknowledge the predictability limitations of deterministic forecasts. In early 90's, ensemble forecasting was initiated to break this barrier. Ensemble forecasting involves multiple model runs, initiated with properly perturbed initial conditions; different models are also tried. In contrast to the deterministic approach, the final forecast is based on the entire ensemble of results rather than on a single one. Statistics based on the ensemble provide the most-likely scenario, as well as a measure of its likelyhood, extreme results can be also individually considered. As this concept proved successful, it is also tried in other problems such as an air quality forecasting. A good discussion of the ensemble forecasting can be found in Kalnay (2003).

16. Summary

In this paper, we have discussed several ways of using the meteorological information in air quality studies and forecasting. The basic situations and choices can be classified as follows:

1. climatological approach;
2. sequential processing of the raw meteorological measurements from a single station;
3. processing of meteorological data from a limited area network of observations;
4. using products of meteorological centers (forecasts, data assimilation cycle analyses, reanalysis results);
5. using dedicated meteorological models, or meteorological models combined on-line with the air quality models.

The particular choice depends on the particular problem and its spatial scale. Local problems may be treated with simpler approaches (preferably #2) while the large-domain tasks such as transboundary transport or real-time air quality forecasting or emergency response system will, as a rule, demand more complex treatment (#3-5). The choice of a proper meteorological input is undoubtedly one of the keys to the succesful air quality forecasting.

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