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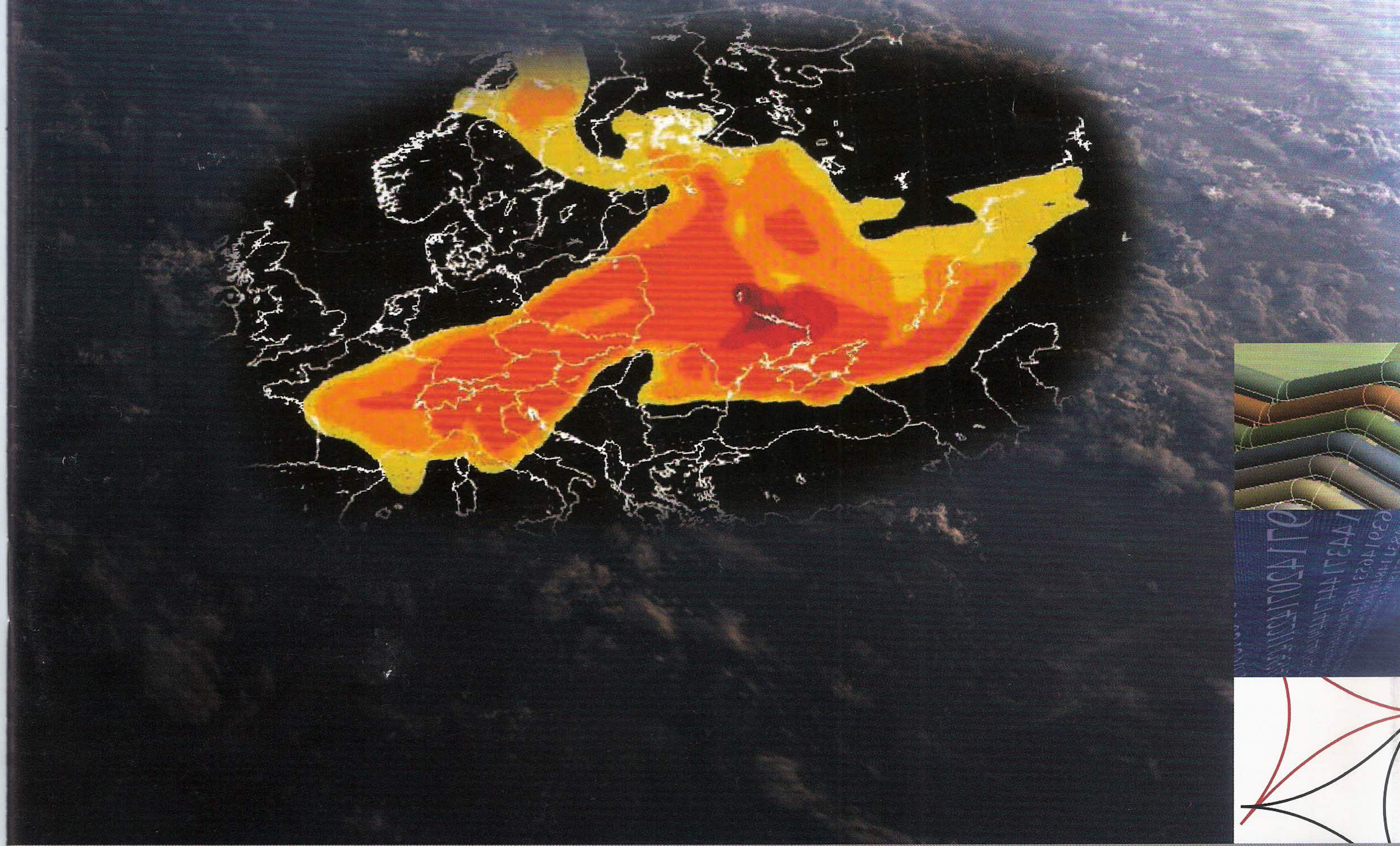
analysing the atmosphere

using CFD to model our surroundings



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INTRODUCTION TO ATMOSPHERIC MODELLING

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It is obvious, even trivial, to every living being on the surface of the earth that the medium we are living in has an activity on its own (called weather) with which we deal on a daily basis and which impacts widely many of our activities, including the economy.

Atmospheric motions are seemingly random on various scales. Though different in nature, randomness appears on the planetary scale and time scales of the order of days, months (climate and global weather) in chaotic, but to some extent, predictable structures. It appears also for flows at the microscale in the meteorological terminology (i.e. flow scales of the order of tens of metres and seconds to minutes on domains of the order of several kilometres). The attempt to predict the seemingly random flow of the air in our atmosphere dates back to early in the last century when Lewis Fry Richardson worked on numerical methods for weather prediction at the Meteorological Office in the UK [1]. The first numerical solutions provided for atmospheric flows are obtained from simplified and projected formulations of the fluids equations on a sphere in the rotating frame. The simplification retains the largest equilibrium terms producing the so-called barotropic and baroclinic balanced equations for planetary scales motions. Similarly, given the large horizontal to vertical aspect ratios of the geometry and flow motions on such scale, a shallow water version was used. Since then, the basics for meteorology analysis and forecast have relied on a common set of equations known as primitive equations applied for geostrophic stratified flows.

Much more detailed phenomena are included in the mesoscale modelling tools (on much shorter scales than planetary scales) with e.g. non-hydrostatic motions, cloud micro physics, local flows patterns related to either terrain features, heat sources or small scale active weather systems (storms, squall lines..etc). Both large scale and mesoscale models exploit closure schemes to represent sub-grid scale turbulence with semi-empirical laws for turbulent diffusivity. However, neither of these application types employs fine enough resolution for the modelling of atmospheric flow patterns induced by local/microscale features in the surface layer: such as buildings, obstacles, strong localised momentum and mass sources, as required for flow and dispersion simulation of impact or risk studies for industrial activities. Indeed, for atmospheric dispersion modelling, in 1955, the US military also worked to simulate the weather through the simplified Navier-Stokes equations in order to predict contaminant spread over time and space in the context of nuclear and chemical warfare under the Joint Numerical Weather Prediction Unit (JNWPU), a joint project between the U.S. Air Force, Navy and Weather Bureau. The complete history of weather prediction models can be found at the Atmospheric General Circulation Modelling website [2].

With the advent of faster digital computing, new ideas were advanced on how to solve the challenging Navier-Stokes equations governing the atmospheric flows on the largest scale that could possibly be experienced on Earth for fluids. Soon, weather predictions became an important aspect of our everyday lives. Technologically, adding the solution of a transport equation on these weather models, to represent the evolution of concentration of a pollutant in the air was only a very small additional step.

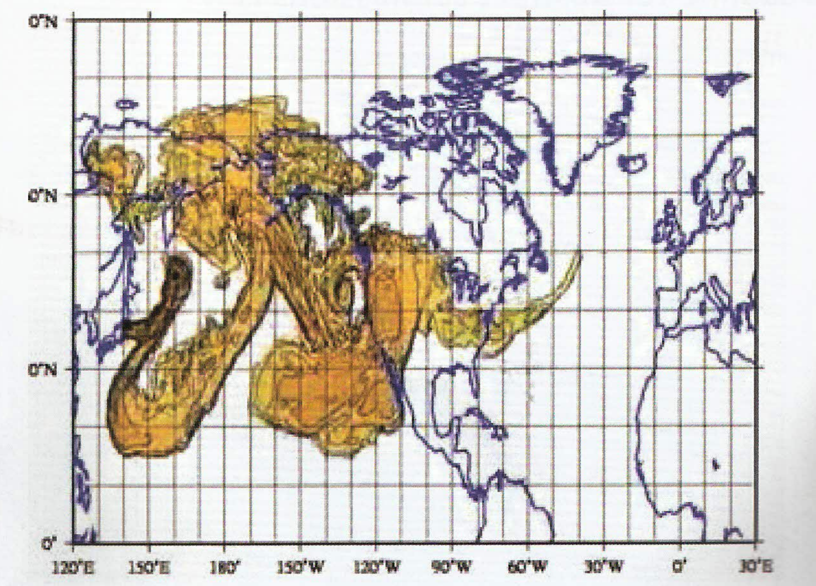

Figure 1: Example of simulated radioactive component dispersion contours following Fukushima accident [3]

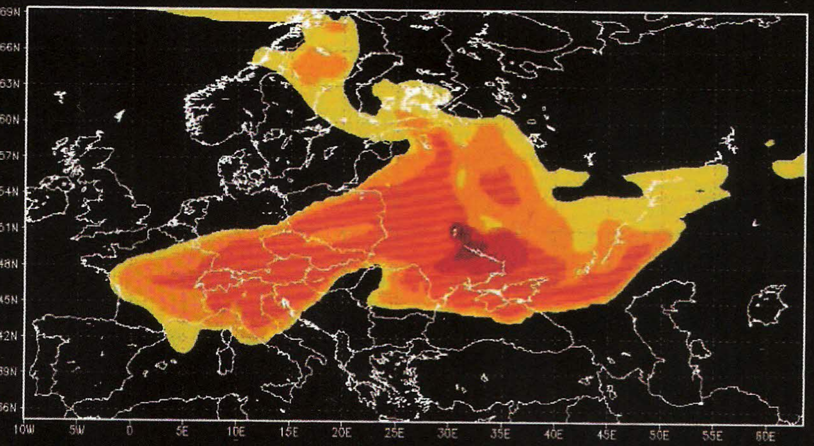

Figure 2: Example of Recent Simulated Radioactive Component Dispersion Contours Following Chernobyl accident [4]

Over the years – and usually in response to major natural events or industrial accidents - the general public at large has become quite accustomed to comprehending dispersion through modelling. Recent - and unfortunate - examples of this are the Fukushima accident or the Eyjafjallajökull volcano eruption, in which prediction of contaminant plumes were available within days or even hours of the event with severe consequences on the local population including evacuation and grounding of flights.

This rapid response capability compares this with the situation in 1986 with Chernobyl accident, when the French government could affirm - with no real scientific challenge at that time - that the cloud did not cross the French borders.

On a less dramatic note and away for the public eye, the economic and social development of developed countries is now greatly influenced by the regular use of atmospheric modelling, through the current awareness of environmental impact and health issues related to pollution. Indeed, besides weather forecast and exceptionally large events/accidents, atmospheric modelling is used by regulatory bodies to assess the compliance of existing or proposed industrial facilities with respect to environment norms and public safety. The technology can also be used for emergency response planning in anticipation of potential accidental chemical releases.

The software tools used to predict atmospheric flow and the spread of pollutants were restricted for quite some time to analytical and 2D tools based on Gaussian models. With improved computer capabilities and the development of advanced numerical models and schemes, atmospheric modelling has finally come of age with the use of Computational Fluid Dynamics (CFD).

The current use of CFD for any kind of flows still requires a fair amount of assumptions to be made in order to break down the problem into manageable pieces solved in a reasonable period of time. In much the same way, atmospheric modelling can be categorised according the level of accuracy required and the type of assumptions to be made. Depending, for example on the length scale (local, regional or continental), the simulation would require a different set of models and assumptions. In the remainder of this article, the main focus will be on solving atmospheric CFD Reynolds-Averaged Navier-Stokes (RANS) modelling on a local scale (also called micrometeorological scale).

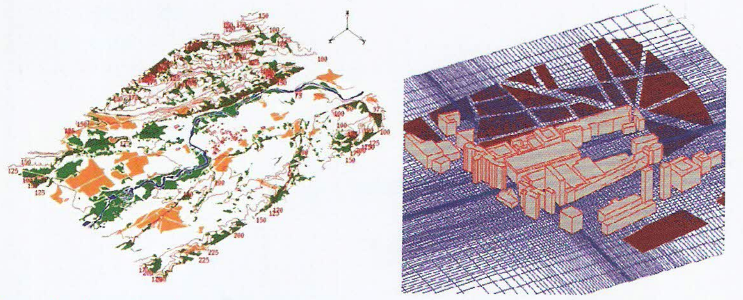

Figure 3: Example of a Numerical Model of Terrain Including Land Usage (left) and Buildings (right)

The steps required to successfully complete an atmospheric dispersion simulation will be very familiar to any person working with CFD on a regular basis. They are:

1. Collection and analysis of data
2. Set up of assumptions
3. Creation of model geometry
4. Grid generation
5. Definition of Source terms
6. Imposition of Boundary conditions
7. Specification of Initial conditions
8. Execution of the numerical solution
9. Analysis of the results

In the interests of brevity, each of these items will not be discussed in detail here. However, for further information on the subject the reader is expected to revert to the excellent Best Practice Guidelines issued by the COST732 action [5] as well as to the extensive internet link list on the NAFEMS website [6].

A person undertaking simulations in this area will, of course, be aware that the numerical accuracy expected in the simulation of atmospheric flows is, of course, less important than the one expected for, say, aeronautical studies, due to the lack of control one has over input data accuracy. Depending on the type of study to be carried out, the importance of the above data will change. An impact analysis in which the annual average concentration of a pullutant is to be assessed, will require the input data to be as realistic as possible but will adhere to average values and situations. An industrial hazard assessment on the other hand will generally seek to take into account the worst-case scenario by setting all variables towards the most adverse effect. The minimum data required for an atmospheric dispersion modeling:

- Terrain elevation and altitude often obtained from Land Geographic Surveys, either in digital or hard copy format. Satellite data, now freely available, can also be of help.
- Site map with obstacles, heat sources etc.
- Weather data: wind velocity, temperature and atmospheric stability from meteorological services often represented by a windrose.
- Source emission : from the industrial unit or from some general data (e.g. vehicles/day for road emission).

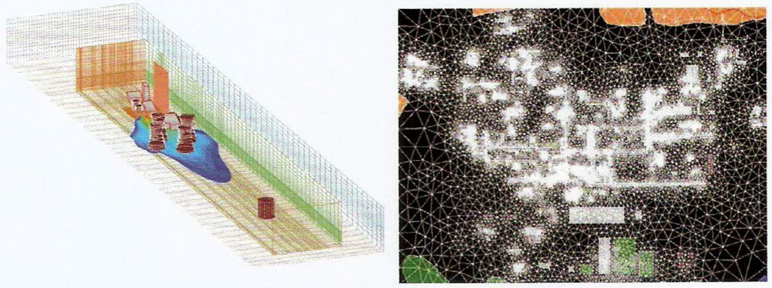

Figure 4: Example of Embedded Structured Mesh (left) and of a Unstructured Mesh (right)

Among the data listed above; atmospheric stability might be a new concept to analysts coming from a more conventional CFD background and is therefore worthy of further discussion. Atmospheric stability is the resistance of the atmosphere to vertical motion and is a function of vertical variation of temperature. A large decrease of temperature with height corresponds to an "unstable" condition which promotes vertical currents and mixing. A reduction in termperature with height corresponds to a "stable" condition which inhibits vertical motions. Many local factors influence atmospheric stability, such as wind speed, local heat sources/sinks and surface characteristics. Atmospheric stability also varies during the day and according to the season and can therefore not be an output of the simulation and yet the behavior of a pollutant plume will depend on it.

The atmospheric stability will therefore take the form of a set boundary condition which will be designated by a stability class, as developed by Pasquill in 1961. The air flow simulation will start in the numerical domain according to the chosen Pasquill stability class and the flow solution will then be influenced locally by the presence of buildings and other obstacles like large equipment or terrain elevations as well as heat sources/sinks. The wind coming from various directions will develop along preferred paths through and around obstacles. Thus it is important to not only have an accurate representation of plant layout under consideration but also the neighbouring buildings with their heights. This numerical model of terrain should also include a representation of the vegetation in order to capture the effect of its drag on air flow and water bodies like lakes, rivers etc, for their influence on air flow by temperature variation. The solution domain boundaries have to be far enough from the emission point, so that the assumed boundary conditions have a minimal impact the local wind patterns, including in those in the vertical direction.

Indeed, in the specific case of atmospheric flow modelling with CFD, one has to take into account both an accurate description of the atmospheric boundary layer with background profiles for winds, temperature and turbulence (all varying with altitude), and simultaneously, solving the local (internally produced) turbulence from mechanical processes (shear layers, wakes, momentum sources) and thermal sources related e.g. to industrial processes or urban heating.

The former are prescribed with appropriated formulations based on modified Monin-Obukhov profiles that relies on key micrometeorological parameters (Energy budget at ground, roughness length, friction velocity, M-O length, mixing length.....etc). Several formulations based on similarity theory and prognostic 1D closure model for the turbulence profiles and on the aggregate of atmospheric boundary layer (ABL) measurements for various experimental sets spanning as much as possible the diverse atmospheric stability regimes.

The locally produced turbulence must be calculated in the RANS CFD approaches with closure equations - the most frequently used being the k-ε model for turbulent kinetic energy k and its dissipation rate ε. Again in the various versions of the k-ε formulations (standard, RNG, low Reynolds...etc). One has to take care regarding the specific conditions of the flow in the ABL and thermal stratification on the sink and sources terms in the turbulence equations. All these specific properties and processes influence the atmospheric turbulence and may have an impact on the RANS mean flow solution through the turbulent diffusivity which in turn has a direct and significant influence on contaminant dispersions.

Atmospheric flow applications can also be quite a challenge to mesh. The pollutant release can be quite small and, in the case of accidental releases, the speed and momentum associated with it can be quite large, which in turn requires a fine mesh with cells that can be a few centimetres wide. On the other hand, if the plume is expected to reach a height of a few kilometres the scale of the affected region will be very much larger. Despite the rapid advances in computational hardware, simulations incorporatring fine cells of the order of centimetres cannot be carried out over such a a large extent. Solutions include working on the mesh (structured, unstructured, non-uniform or even embedded) or on the source term by taking a step away from the emission and considering a large area or volume as emission source.

The choice of the wind direction and magnitude to impose as a boundary condition is once again dependent on the type of study to be carried out. If an annual impact on air quality is sought for, a large number of wind conditions reflecting the windrose need to be considered. This could include up to 3 to 5 different velocities for each wind sector amounting to 30-100 weather conditions. If an industrial risk assessment is to be performed, then the critical wind conditions need to be investigated, keeping in mind that criticality will be a function of the

Pasquill class	Definition
A	very unstable
B	unstable
C	slightly unstable
D	neutral
E	slightly stable
F	stable

Table 1: Definition of Pasquill Atmospheric Stability Classes

Surface windspeed		Daytime incoming solar radiation			Nighttime cloud cover	
m/s	mi/h	Strong	Moderate	Slight	> 50%	< 50%
< 2	< 5	A	A – B	B	E	F
2 – 3	5 – 7	A – B	B	C	E	F
3 – 5	7 – 11	B	B – C	C	D	E
5 – 6	11 – 13	C	C – D	D	D	D
> 6	> 13	C	D	D	D	D

Table 2: Occurrence of Atmospheric Stability Classes

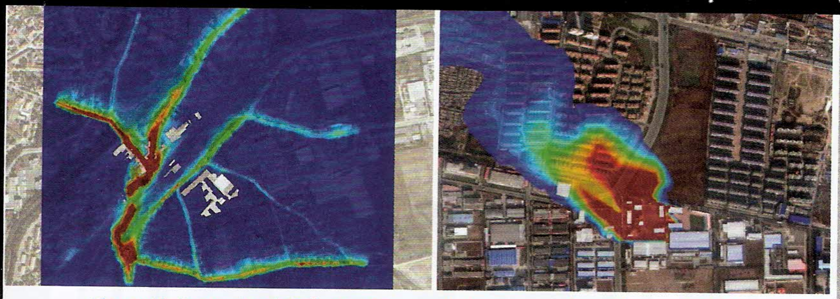

Figure 5: Example of Pollutant Concentrations on a Road Network (left) and from an Industrial Source (right) at 1.5 m high

source characteristics (cold/hot, violent/mild) and of the target (far/close, below/above the release point).

The source terms used in the simulation also require an extensive discussion, if only to correlate them to the mesh used, although it is only possible to provide an overview here. It could be a point source (stack or pipe rupture), a line source (road), an area source (pool evaporation or dust fly-off), a volume source (complete collapse of a tank) or jet-like (pressurized emission). The choice of solver will be based to a large extent on the type of source that needs to be accounted for: a transient compressible solver for a high-jet accident emission, a steady-state incompressible solver for traffic pollutant, for example.

As obvious as it may sound; the results have to be analysed keeping in mind the ultimate objective of the simulation. The concentrations of each pollutant need to be compared to thresholds in air quality if the aim is to look for environmental impact and in toxicological effects if accidental releases are being considered. The thresholds for these two major types of studies are not defined in the same way. For environmental impact studies, the thresholds will usually be annual average (requiring that all results specific to one wind condition are weighted with the occurrence frequency of that wind and summed up) or percentiles (the percentage of measures below a certain level which requires a cell-by-cell analysis).
For risk assessment studies, one common way to analyse the results are doses, which are the integration of pollutant concentration over the time for which an individual would be exposed to it. This integration is not linear, however, as the degrading response of the body over time is taken into account.

Other possible applications of CFD in atmospheric modelling include its use as an operational decision-making tool. Examples are given below among many others.

Sensor Location Optimization

A major immediate economic benefit of 3D modelling is in the optimisation of detector/ sensor positioning, so that they don't need to be positioned intuitively in large numbers on a complex site. For a classical sensor network, conventional strategy relies upon prior identification of the potential leaks (from processes, storage, pumps and manifolds). Then, a usually dense and close range set of sensors is located with as many patches as necessary to cover all possible locations of leakage. Such empirical methods result in an expensive sensor network without any guarantee of its efficiency. Furthermore for equipment such as long pipelines or storage tank parks, with the potential for multiple source leakages, there are never enough sensors. One has to distribute a limited number of detectors over a large area with no way of knowing which way the pollutant will go in the event of release.

CFD could be put into use by simulating the release of pollutants from all likely leak sources and in all likely wind conditions. Such simulations are done with generic unitary emissions such as puffs of pollutants. Streamlines for pollutant dispersion over the site are established in 3 dimensions and the optimal sensor mapping is done using a composite turbulence map and the pollutant stream line map. Locations where turbulence is minimal and stream lines from most likely sources or most severe leaks pass, represent the most appropriate detection sites. Alternatively, using the adjoint solution of the advection-diffusion equations from all positions of the sensors on a predefined network and for relevant 3D flow patterns, one can construct a visibility function depicting the spatial coverage of the network and the time lags/delay for detection.

Source Retrieval by Retro-Tracing from Sensor Network to Leak Source and Real-Time Management

Techniques used for identifying the source from the sensor, such as retro-trajectories or adjoint methods, are based on inverse CFD modelling of flow and dispersion. For any given network of sensors, these methods provide a measure of "visibility" ensuring a proper mapping of the area - both for process locii (i.e. known possible locations) and for diffuse/distributed emission zones. With such an optimised network, any gas detection by one or more sensors can be quickly traced back to the likely leak source automatically in a matter of minutes after the leakage initiation. Coupled with in situ weather measurements and/or external data from weather services for forecasting in the following hours, the evolving dispersion of the toxic gas could be simulated and used for evacuation and emergency actions undertaken on the identified source.

This article is only intended to provide a flavour of atmospheric modelling and is not intended to address all of the issues facing the analyst in an exhaustive manner. All interested readers are encouraged to gain further insight into this fascinating subject through the links listed in NAFEMS website [4]. This article owes much to the authors in this list.

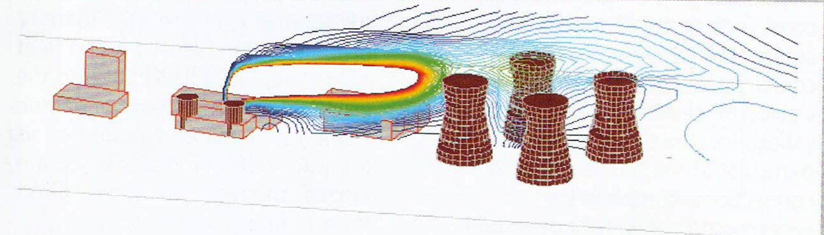

Figure 6 : Example of a Plume Dispersion on a Vertical Plane

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