

VARIATION IN THE CONCENTRATIONS OF CONSTITUANTS IN A PLUME WITH *fluidyn*-PANACHE

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ABSTRACT

Contrary to the usual belief, various constituents of a pollutant emission may have very different dispersion behaviour in the atmosphere. This is due to the specific heats and molecular weights of these gases. Their proportional concentrations may change very rapidly if the terrain and meteorology have a varying temperature or altitude profile.

Fluidyn-PANACHE software is used in this case for simulating the PANACHE of CO and SO₂ from a stack. PANACHE solves Navier Stokes equations in a curvilinear mesh espousing the terrain and obstacles. The solver and the numerical scheme have been adopted for atmospheric flows with or without chemical reactions.

METHODOLOGY

PANACHE is a self contained software package designed for environmental studies and also for simulating various gaseous emissions into the atmosphere.

PANACHE has been designed specifically for non technical people. The users are architects, city planners, geologists, environmental designers, pollution and fire brigade personnel, etc. and a host of other professionals who are involved in the task of improving the fragile and increasingly threatened environment.

In relation to the gaseous emissions due to industrial mishaps on a large or small scale, PANACHE provides a full fledged application to follow the evolution of a gas cloud and to calculate its real consequences.

In addition to the above it is also capable of predicting wind velocity and temperature distribution over a three dimensional complex terrain topography.

The equations solved by PANACHE to describe the convection and diffusion are those of mass conservation, species conservation, Navier-Stokes equations of momentum and the energy conservation equation.

The gravity effect can be taken into account by the Boussinesq hypothesis or considering full gravity.

The turbulence modelling for the atmospheric boundary layer was done using the Nieuwstadt and Van Ulden (1978) K model for the steady, horizontal, homogeneous, stable boundary layer (Businger and al, 1971; Deardorff and al, 78,79; Hanna, 68) .

The resulting system of equations were solved for the CO & SO₂ plumes using the PANACHE code.

The above system of equations was solved for the SO₂ and CO plumes using the alternate Lagrangian Eulerian method, developed by the Los Alamos Group (Hirt and al, 74; Pratch, 75; Van Leer, 77)

PRESENT TEST CASE

The physical model considered refers to the plume of a thermal power station consuming 3000 tons of coal per day.

The coal is assumed to have a sulphur contains that leads to a sulfur dioxide emission of about 750 g/s. Carbon monoxide is the other component computed, one can assumed that its flow rate is 150 g/s.

The stack height is 50 m, the diameter 10 m. The temperature and the mass flux are assumed to be 400 K and 75 kg/s respectively.

The wind velocity, supposed uniform, is assumed to be 4 m/s at the domain entrance, that means 100 m upstreams of the stack.

The atmospheric temperature is taken to be initially 300K.

BOUNDARY CONDITIONS AND COMPUTATIONAL DETAILS

The whole integration domain extends to a maximum of 700 m in the axial z direction, 600 meters in the crosswind or y direction and 300 meters in the direction perpendicular to the ground (x axis) (fig.1 and 2).

The automatic grid computed by PANACHE is curvilinear (Body Fitted Coordinates) structured and non uniform (fig.3). The grid used was $(x,y,z) = 12 \times 25 \times 25$.

The boundary conditions used were as follows :

- a) At the "inlet" of the computational domain, specified wind velocity, temperature and pressure were used.
- b) The chimney stack was located typically 100 m away from the inlet. At this location, specified mass flux for sulfur dioxide and carbone monoxide, the temperature of gases, assumed to consist only of SO₂, CO and air with the following composition :

SO ₂ :	10 000 ppm mass
CO :	2 000 ppm mass
Air :	988 000 ppm mass.

Pressure and exit velocity were described.

- c) At all the other "free" boundaries, atmospheric pressure was assumed to prevail a condition, that would allow the calculation of a correct inflow/outflow at these boundaries, from overall continuity consideration.

RESULTS AND CONCLUSIONS

Fig. 4 and 5 show the wind profile at 1 meter from the ground. On fig. 4 a large domain view allows influence of obstacles (buildings, hills). Fig. 4 shows the 3 dimensional effect generated by the 2 hills (venturi effect).

In fig. 6 isosurface of 1 ppm concentration is drawn and the concentration at ground level for both pollutants considered.

The results show very different behaviour of pollutant. Carbon monoxide is "stopped" by the 200 meter high hills, instead of So₂ plume can go over it.

This is due to the differences in molecular weight

$$(M_{wCO} = 28,01 \text{ g/mole} \quad M_{wSO_2} = 64,06 \text{ g/mole})$$

and heat capacity :

$$(H_{cCO} = 0,249 \text{ kcal/kg/K} \quad H_{cSO_2} = 0,149 \text{ kcal/kg/K})$$

of both pollutants. SO_2 heavier than air ($M_{wair} = 29 \text{ g/mole}$) will be more affected by the gravity effect than the carbon monoxide.

A complete three dimensional Navier-Stokes model available in PANACHE for the proper characterization of chimney plumes has been developed and applied to a realistic case of a coal burning power station chimney.

The results produced by fluidyn-PANACHE seems to be quite impressive in giving a correct picture of transient pollutant dispersion on uneven terrain with obstacles. It is thus an economical tool for prediction of the spread of hazardous gases, either accidental or deliberate, and a helpful package for city planners environmental engineers and a host of other professionals involved in the task of maintaining our fragile and increasingly threatened environment.

PANACHE DESCRIPTION

- 3D Fluid Mechanics, high precision finite volume scheme
- Deterministic solution with accurate representation of topography/ meteorology/ emission source
- Correct sensitivity to changes of parameters
- Designed for field engineers-non specialists

SIMULATION by PANACHE

- Topography : automatic curvilinear mesh generation for the terrain and around obstacles
- Atmosphere : calculated thermal inversion, wind profile
- Turbulence : due to obstacles and surface roughness

- Far Field and near Field (close to obstacles-2nd order)
 - Thermal Exchange - with ground and Chemical Units
 - Water Bodies, Forests, Fields : temperature, roughness, condensation
 - Sources and Pollutants data base
 - Calculation in a window drawn on a map by the user
 - On site measurements : used for inverse calculation to correct initial data and improve the model
- PANACHE APPLICATIONS: ACCIDENTS - INDUSTRIAL or VEHICULAR
- Exact simulation of buildings/chemical units
by curvilinear mesh and a 2nd order solver
 - Heavy Gas Dispersion : exact modelling of low lying areas and the heat exchange with the ground
 - Pollutant sources : multiple kind and coupling with FLUIDYN-CONTAINER(explosion of reservoirs)
 - Fire and Chemical Reaction
 - Effect of changes in wind, sun/shadows with time
- PANACHE APPLICATIONS: CHRONIC IMPACT
- Multiple Sources: stacks, routes, Stagnant/Waste water
 - Particles : Sulfur, Charcoal
 - Chemical Reaction with air, humidity or between gases.
 - Scavenging, Acid Rain: Pollution absorption by droplets
 - Odor Propagation : even in still air

- Pollution Control Devices efficiency evaluation
- Site choice for Pollution measuring Instrumentation
- Effect of Topographical changes
- Wind Field around buildings or in accidented topography

DATA REQUIRED, ANALYSIS and RESULTS

- Only topographical and meteorological information required
- Pre- & post- processors integrated with numerical solver
- Inverse Analysis approximation for lacking data
- Model accuracy improved by previous calculations
- Data base, prepared in advance for various atmospheric conditions for a site, used for quick accidental situations
- Interactive Data entry and Results Analysis
- Iso-curves pollution concentration, temperature, etc.
- Surface representation of pollutants level in 3D space
- Wind profile charts in 3D space
- Multi-window, video animation, interactive presentation

REFERENCES

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- 2) Deadorff Jw (1978), Journal Geophysical Resources, 83,1889
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- 7) Pracht WE (1975), Journal Computational Physicals 17, 135
- 8) Van Leer B (1977), Journal Computational Physicals 23,263.

FIGURES

- 1 Bird's eye view of terrain
- 2 Isometric view of the considered site
- 3 Automatic mesh generation of site (plane $x=1$: soil surface)
- 4 Wind field at 1 m height. Effect of hills and obstacles
- 5 3D effect of the two hills presence
- 6 Isoconcentration plume equal to 1 ppm of SO_2 & CO with map of corresponding concentrations on ground