Toxic Gas Dispersion Simulations with the CFD Code FLACS

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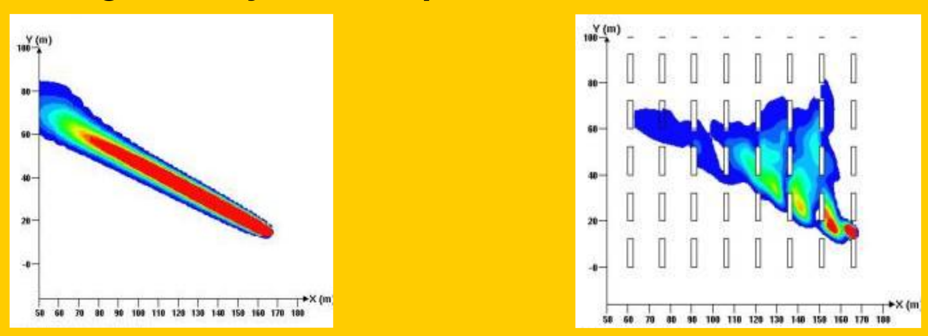
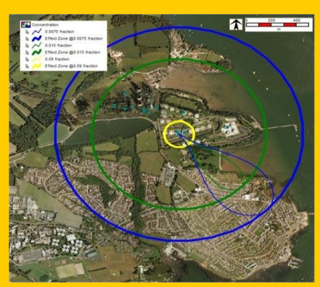
WHY USED CFD FOR DISPERSION SIMULATIONS?

- **Large influence of geometry on flow phenomena and hazards resulting from releases**

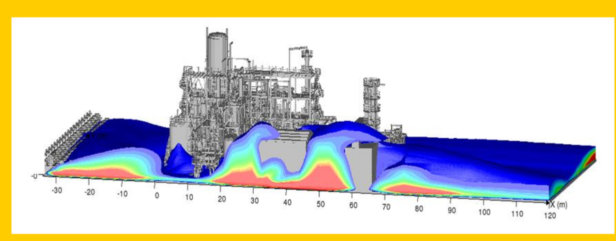


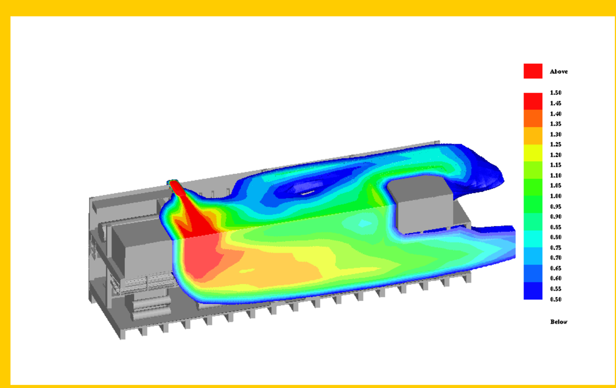
Gas dispersion (same release rate, gas type, wind direction, etc)

- **Analytical models generally neglect geometry and have other potentially unphysical assumptions such as radial symmetry of gas dispersion around release location**
- **Computational Fluid Dynamics (CFD) simulations can account for details such as obstacles and terrain features and effect of wind direction (gas may travel upwind)**



FLACS – CFD MODEL BASICS

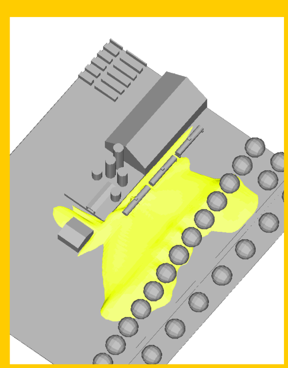




- **Specifically developed for process safety studies**
- **Full 3D Cartesian Navier-Stokes flow solver**
- **Distributed porosity concept for small, sub-grid scale obstacles**
- **Intelligent sub-grid models**
- **Possible to model atmospheric boundary layers**
- **Possible to define atmospheric stability classes**
- **Thoroughly validated against e.g. large-scale Phase3B dispersion experiments and full LNG MEP database**
- **Widely accepted by authorities worldwide**

It is possible within FLACS to add/define:

- **Geometry and buildings**
- **Vegetation and terrain contours**
- **Wind profiles, fluctuating wind**
- **Gas or liquids, single components or mixtures**



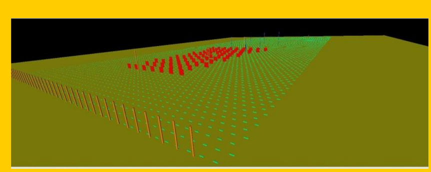
Guidelines have been developed (e.g. grid refinement near leak) based on validation

VALIDATION EXERCISE

Brief description (Details in Hanna et al., 2004)

Kit Fox 52 tests (Hanna and Chang 2001)

- **1.1-4.3 kg/s CO_2 from a pool 1.5m x 1.5m**
- **0.8-4.5 m/s wind; D, E, F neutral to stable classes**

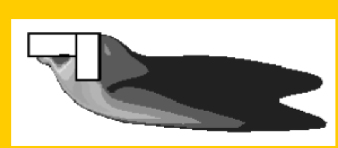


Prairie Grass 37 tests (Barad 1958)

- **40-100 g/s SO_2; 1.5-9 m/s wind; A,B,C,D,E,F stability classes**

MUST 43 tests (Biltoft 2001)

- **6 g/s propylene**
- **1.0-6.8 m/s wind; generally stable/neutral conditions**



EMU L-shaped building (Hall 1997)

- **Wind tunnel test**

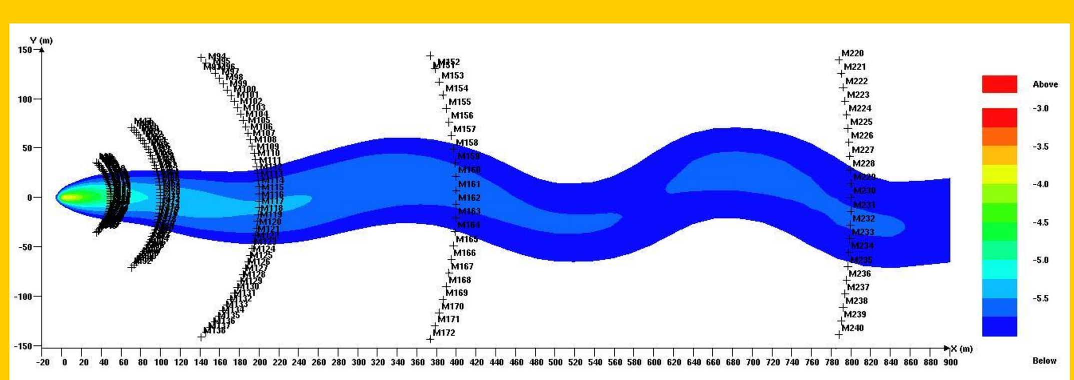
Simulation challenges

- **Concentrations to be predicted 100 to 800m downstream of leak**
- **Relatively small leaks, interesting concentrations in ppm range; Duration > 1000 s**
- **Using normal FLACS guidelines (with finer grid near leak) would require months of simulation time**
- **To be of practical interest, calculations should take less than a night (or 1-2 days)**

$\Rightarrow$ **Revised guidelines:**

- **Only a moderate or no grid refinement near the leak**
- **Coarse grid applied horizontally, somewhat finer vertically**
- **Stretching of grid outside core area, short distance to external boundaries**

Example of results and evaluation

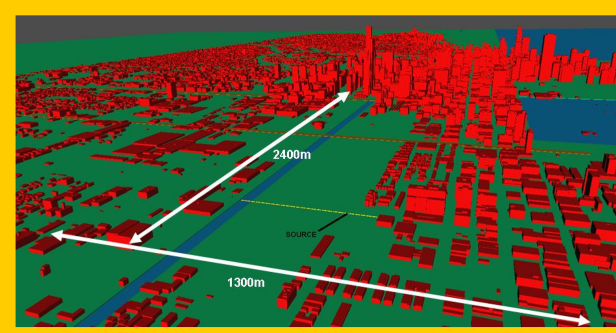


Prariie Grass Simulations, sensors in arcs at 50, 200, 200, 400 and 800 m

- **Results evaluated statistically using fractional bias, geometric mean bias, geometric variances and fraction of observations within a factor of two.**
- **General underprediction tendency of about 20 %**
- **About 86 % of the predictions are within a factor of two of the observations**
- **These results are all well within the range of acceptable model performance**

CHICAGO SIMULATIONS

- **Hypothetical chlorine release, D=10 cm hole: 225 kg/s for 300s (total release 67.5 ton) 2.4 km from downtown Chicago; 3 m/s wind (F stability). Details in Hanna et al. (2009).**
- **Geometry model prepared based on imported .shp files from Argonne NL**

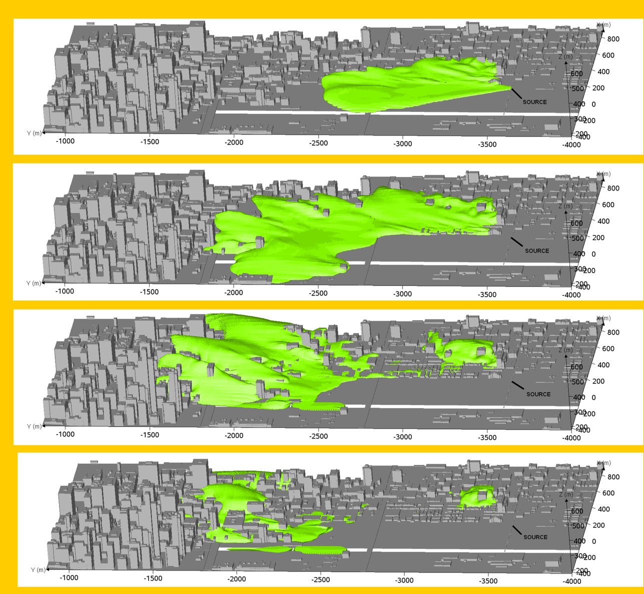


- **Two different scenarios: Wind from South (towards downtown) and Wind from East**
- **Grid used: 6m x 6m x 2m in near field, gradual stretching further away**

Results

Scenario 1: Wind from S (main observations)	***Scenario 2: Wind from E***
Dense gas behaviour clearly seen laterally	**Dense chlorine plume spreads when reaching river**
Dispersion on flat terrain similar to integral model predictions	**Plume can move upwind**
Tall buildings downtown lead to vertical mixing and quick dilution	**Lower buildings than scenario 1 (less dramatic effects e.g. vertical mixing)**
Gas pushed in between the buildings near source may remain for a long time	

100 ppmv contour plotted

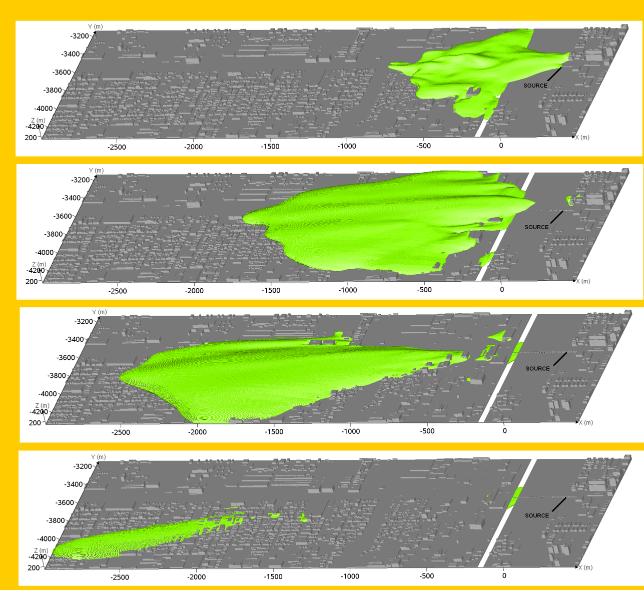


End of release (300 s)

400 s after end of release

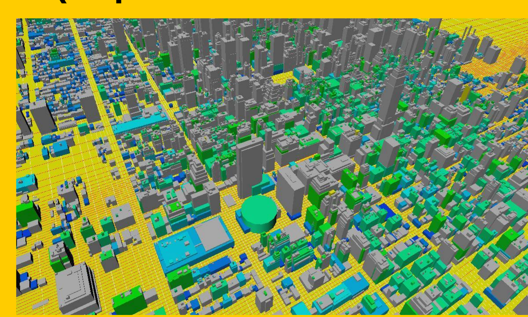
1000 s after end of release

1500 s after end of release

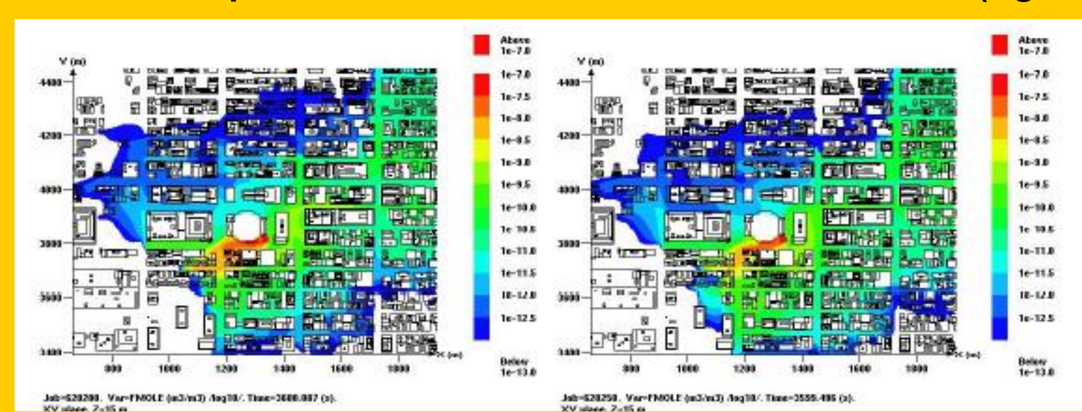


MANHATTAN (NEW YORK CITY) SIMULATIONS

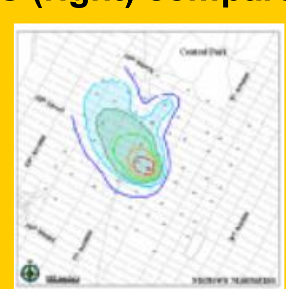
- **Wind and tracer gas release simulations in downtown Manhattan (Departmenf of Homeland security, USA); GexCon among 6 CFD modellers**
- **Geometry database imported using Vexcel, 45000+ building features covering 11.5 km^2**

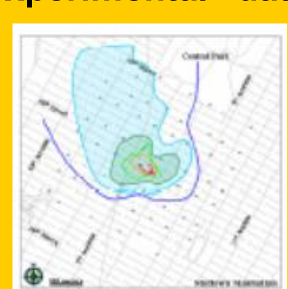


- **Details in Hanna et al (2006).**
- **Full lower Manhattan area simulated (10 km x 7.5 km x 1 km)**
- **Grid resolution in central areas 10m x 10m x 5m, stretched towards boundaries (total 2.7 M)**
- **FLACS porosity concept significant advantage compared to other tools**
- **Simulation details:**
  - **Step 1: Initialize global wind field on coarse grid**
  - **Step 2: Develop local field around buildings and street canyons by transferring to finer grid, solution “stored in library”, starting point for different calculations**
  - **Flow field is frozen, only dispersion of gas is solved – tracer gas calculations assuming constant wind field. Speed of calculations “faster than real time” (right figure below)**



- **Tracer gas calculations (right) compared with “experimental” data (left) from real releases**





OTHER EXAMPLES

- **Simulations done to “investigate” the chlorine release accident from a railcar at Festus, Missouri, USA. Pictures shown above left (Hanna et al 2009)**
- **Several studies with releases from stacks in factories or H_2S releases from “sour” gas**

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4. **Hanna, S.R., Brown, M.J., Camelli, F.E., et al., *Bull. Am. Met. Soc., 87:1713-1726 (2006).***
5. **Hanna, S.R., Chang, J.C., *Atm. Env.*, 35:2231-2242 (2001)**
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