

## J14.1 SOURCE EMISSIONS AND TRANSPORT AND DISPERSION MODELS FOR TOXIC INDUSTRIAL CHEMICALS (TICs) RELEASED IN CITIES

Steven Hanna<sup>1</sup>, Rex Britter<sup>2</sup>, Joseph Leung<sup>3</sup>, Olav Hansen<sup>4</sup>, Ian Sykes<sup>5</sup>, Peter Drivas<sup>6</sup>, Jeffrey Weil<sup>7</sup>, and David Strimaitis<sup>8</sup>

<sup>1</sup>Hanna Consultants, Kennebunkport, ME; <sup>2</sup>Cambridge University, UK; <sup>3</sup>Leung Inc., Rancho Palos Verdes, CA; <sup>4</sup>GexCon, Bergen, Norway; <sup>5</sup>L-3Com, Princeton, NJ; <sup>6</sup>Bedford, MA; <sup>7</sup>Un. Colorado, Boulder, CO; <sup>8</sup>TRC Solutions, Lowell, MA

### ABSTRACT

The major scientific issues concerning source emissions models and dispersion models for Toxic Industrial Chemicals (TICs) are discussed, with emphasis on chemicals stored and/or transported as pressurized liquefied gases (e.g., chlorine, anhydrous ammonia, and sulfur dioxide). Many tons of a gas/aerosol mixture can be released and have been released into the atmosphere in one or two minutes in railcar accidents. Some recommendations are given for specific source emissions equations, with scientific rationale provided. Field experiments on TIC source emissions are reviewed and some results of evaluations of models for droplet formation in flashing jets are presented. The characteristics of various dispersion models for TIC releases in urban areas are reviewed. A hypothetical chlorine railcar release in Chicago is simulated with a CFD model (FLACS) and with several widely-used simpler models and the results compared. The CFD model-simulated effects of the urban buildings on the dense gas transport and dispersion are discussed, such as constraints by buildings near the source, reductions in transport speed, diversion of the dense gas down drainage slopes, increases in turbulence intensities, and hold-up in building wakes after the main cloud has passed.

### 1. OBJECTIVES AND BACKGROUND

The authors have been carrying out research on Toxic Industrial Chemical (TIC) source emissions models and dispersion models for several years.

The source emissions model improvements have been under study for two years, where the main objective is to suggest improvements for the toxic industrial chemical (TIC) source emissions models in HPAC (DTRA, 2008). Currently these source emission models are included in the Industrial Facilities (IFAC) and Industrial Transportation (ITRANS) modules (DTRA, 2004) and in the SCIPUFF transport and dispersion module (Sykes et al, 2007). The study team is making use of TIC emissions models suggested by

the chemical industry (CCPS, 1996) and detailed field experiments such as those involving two-phase jets (CCPS, 1999, Witlox et al., 2007). The highest priority scenarios concern releases of many tons of pressurized liquefied gases such as chlorine, anhydrous ammonia, and sulfur dioxide. In most cases, these releases become dense due to their high molecular weight, their cold temperature, and or/their imbedded liquid droplets. For most scenarios, the worst case will be when all of the released material quickly ends up in the gas phase or as a fine aerosol as it is transported downwind.

The existing TIC source emissions equations have been reviewed (Hanna et al., 2008b), and some recommended equations are being evaluated with data from TIC field experiments, emphasizing recent experiments with pressurized liquefied gases. In addition, the source inputs required by SCIPUFF are being reviewed to ensure a smooth transition to SCIPUFF (Hanna et al., 2008c). An expert workshop on the topic was held in March, 2008, and resulted in a set of conclusions and recommendations described by Hanna and Britter (2008).

The authors have also been developing and testing transport and dispersion models for dense TIC releases, with recent focus on complex urban and industrial areas (Hanna et al., 2008d). Most TIC accidents and high-priority scenarios involve the presence of industrial buildings, tanks, and other obstacles, or urban areas with complex building shapes. The buildings obstruct the flow and cause changes in the rates of dispersion, and any ditches or slopes may enhance drainage flows. Hanna et al. (2009) applied a CFD model (FLACS) to a real chlorine accident at a chemical processing plant in Festus, Missouri, and to a hypothetical chlorine release at a railroad crossing in Chicago. The intent was to investigate the effects of the buildings and of terrain on the dense gas cloud. Also, several widely used simpler dense gas TIC models were applied to the Chicago scenario.

### 2. SOURCE EMISSIONS MODELS

The highest priority TIC release scenario involves storage of pressurized liquefied gases,

---

*Corresponding author address:* Steven R. Hanna, 7 Crescent Ave., Kennebunkport, ME 04046-7235, [hannaconsult@roadrunner.com](mailto:hannaconsult@roadrunner.com)

such as chlorine, anhydrous ammonia, and sulfur dioxide. These TICs are important because they are inhalation hazards, they are frequently stored and transported around the U.S. in large quantities (say 50 to 100 tons per container vessel), and they have low boiling points (i.e., high saturated vapor pressures). Because of their low boiling points and the fact that they are stored as pressurized liquids, when the vessel ruptures, the TIC “flashes” into a gas-aerosol mixture with high velocity. For holes of diameter 10 cm or larger in the vessel, nearly all of the 50 to 100 ton contents may be emitted to the atmosphere in a matter of minutes.

Some major TIC source emission model concerns are: thermodynamic state of the stored material, rupture size(s) and type, response of materials within the storage vessel including rapid phase change, heat transfer processes and foaming (level swell), phase of release, flashing depressurizing jet, and aerosol drop size distribution and subsequent proportions of rainout and suspended small aerosol drops. Figure 1 is a schematic diagram showing the regions of importance in a flashing jet and the symbols used, going from the storage vessel to the point where the jet pressure decreases to nearly ambient values. Figure 2 shows the temperature-entropy curve for chlorine at various pressures, illustrating how an isentropic release could involve all-liquid, all-gas, or two phase processes, depending on the storage conditions. The simpler all-gas or all-liquid cases have well-known analytical solutions. For two-phase releases, some approximations such as the Homogeneous Equilibrium Model (HEM) provide an analytical solution. Unfortunately, real scenarios always have complications such as jagged holes at unknown locations on the tank, length of the pipe extending a short distance from the tank, release rate that varies in time, and poorly-known weather conditions.

Relevant field and laboratory experiments have been reviewed and a subset chosen for source emission model evaluation, including: Modelers’ Data Archive (MDA), RELEASE (flashing jets and droplet sizes), FLADIS and URAHFREP, FLIE, DNV JIP flashing jet studies (Witlox et al, 2007), and those from Richardson (2006). Project Madison (1 ton chlorine cylinders) field data should be available within one year.

Figures 3, 4, and 5 provide examples of the comparisons of droplet size model predictions with observations. The two models are the CCPS (1999) RELEASE model and the Witlox et al. (2007) JIP model. The two data sets are the CCPS (1999) RELEASE data and the Witlox et al. (2007) JIP data package. It should be mentioned, though, that the JIP data contain direct observations of droplet diameter, while the CCPS RELEASE data use the CCPS RELEASE model to back-calculate the droplet diameters from observations of the rate of deposition of liquid on the ground surface. The vertical axis in the three figures is the ratio of

predicted to observed droplet diameter,  $D_{pred}/D_{obs}$ . In Figure 3,  $D_{pred}/D_{obs}$  is plotted versus superheat,  $\Delta T$ , which is the difference between the storage temperature and the TIC saturation temperature at ambient pressure (i.e., the TIC boiling point). Smaller droplets are expected at larger superheat because the jet will breakup due to flashing or expanding bubbles in the droplets. It is seen that the two models tend to overpredict the droplet diameter at small superheat and underpredict it at large superheat. The model error is less than a factor of two for about 60 % of the points. Figures 4 and 5 plot  $D_{pred}/D_{obs}$  versus orifice velocity for the JIP droplet model and the CCPS RELEASE droplet model, respectively. Figure 4 shows that the JIP droplet model tends to overpredict the droplet diameter at small orifice velocities and underpredict (by about a factor of two) at larger velocities. Figure 5 shows that the CCPS RELEASE model has little bias for the CCPS data, but that is expected since the model was tuned to those data. However, the CCPS model tends to underpredict the observed JIP droplet sizes by about a factor of 5, where the prediction is based on the RELEASE “mechanical” model. This model, selected by the RELEASE algorithm, gives smaller sizes than the “flashing” model, which overpredicts the JIP observations by about a factor of 2.

The research is also addressing the hand-off from the source emission model to the HPAC/SCIPUFF dispersion model. Hanna et al. (2008c) present a review of general methods for the transition (mostly based on physics-based dimensionless criteria), as well as a review of the methods in HPAC (mostly based on arbitrary criteria concerning jet velocity and excess temperature). It is concluded that, while the current methods in HPAC are adequate, they are subjective in many places, and could be improved by having the transition criteria based on the fundamental physics relations. New criteria are being recommended, but must account for the fact that SCIPUFF currently handles only the accelerations in a vertical jet and not the accelerations in jets at other angles. SCIPUFF is being modified, however, to treat accelerations of jets at any angle.

To attempt to identify topics in the area of TIC source emissions where there is a consensus, an expert workshop was held in March 2008 and a summary and set of recommendations written (Hanna and Britter, 2008). The experts used the Festus, MO, and the Project Madison videos of chlorine releases to provide a focus for discussions. In addition, the group agreed that the foaming inside the vessels was important and its parameterization considered a key element of the TIC source emission model.

### 3. DISPERSION MODELS FOR URBAN AND INDUSTRIAL SCENARIOS

Most accident or terrorist scenarios involving TIC releases include complications due to complex terrain and/or obstacles such as urban or industrial buildings and obstacles. Most of the widely-used dense gas dispersion models generally do not account for the presence of obstacles, other than perhaps through an enhanced surface roughness, and account only for simple linear slopes, at best. HPAC/SCIPIUFF is in this category (Sykes et al., 2007). However, the HPAC system does have the capability to use mesoscale meteorological models for inputs, with grid sizes down to 100 m. In this case any terrain can be resolved down to 100 m resolution, and the linear slopes required by SCIPIUFF can be also prescribed at 100 m resolution. Some users have run HPAC/SCIPIUFF to represent dense gas dispersion over terrain using 10 m resolution (in that case, a mesoscale meteorological model would not have been used, since the resolution would be too small for the model). Alternatively, a Computational Fluid Dynamics (CFD) model can be used, and it can resolve the 3-D building geometry and terrain down to resolution of 1 m. In between the simple slope models and the CFD models, there is a class of models (e.g., QUIC, see Williams et al. 2005) that can treat dense gases and can apply mass-consistent diagnostic wind approaches to 3-D urban geometries and terrain.

The CFD models and the diagnostic wind models take many minutes to run on a computer and therefore are not useful for emergency response applications. This drawback can be bypassed in specific urban areas by running the CFD model beforehand for certain meteorological conditions that have a high expectation, and saving the resulting 3-D time dependent wind fields for use during an emergency (see the CT-ANALYST model described by Moses et al. 2006).

Most dense gas dispersion models used for emergency situations are in the simpler category. Examples of these models and the ones that were compared here are SCIPIUFF (Sykes et al., 2007), SLAB (Ermak, 1990), HGSYSTEM (Witlox and MacFarlane, 1994), ALOHA (NOAA, 1992) and PHAST (Witlox and Holt, 1999). In a previous study, the above simple models were compared for the release scenarios at three railcar accidents involving chlorine releases at Festus, Missouri; Macdona, Texas; and Graniteville, South Carolina (Hanna et al., 2008a). In the current study, these simple dense gas models are compared with the FLACS CFD model (Hansen et al., 1999, 2001, 2007) for the Festus scenario and for a hypothetical Chicago railcar release scenario. FLACS is designed for simulating the transport and dispersion of industrial chemicals in the atmosphere and has previously been evaluated with the Kit Fox field observations of dense gas dispersion in obstacle

arrays (Hanna et al., 2004). We first present a qualitative evaluation of FLACS for the Festus, Missouri, chlorine railcar accident, and then compare the FLACS solutions with the simple models' solutions for a hypothetical chlorine railcar release in Chicago.

To demonstrate that the FLACS CFD model can satisfactorily simulate the dispersion of a chlorine cloud from a large railcar accident, the model was run for the Festus, Missouri accident scenario. The accident took place while a railcar was offloading chlorine at a chemical processing facility (see Hanna et al., 2008a, for more details of the release conditions). Figure 6 presents two side-by-side simulations of the observed and simulated chlorine clouds at Festus. The edge of the visible cloud in the FLACS simulations is assumed to occur at a concentration of 2000 ppm. It is seen that the model can satisfactorily simulate the complex jet flow under the railcar and the effects of nearby buildings, tanks, and trees. There were no chlorine concentrations available to allow quantitative testing of the model.

Next, FLACS and the simpler models were applied the Chicago scenario. All of the simpler models, except SCIPIUFF, were included in Hanna et al.'s (1993) comprehensive dense gas model evaluations with observations from several field sites. The conclusion of that evaluation was that these few models were in the group of better-performing models.

A hypothetical Chicago scenario was devised where a chlorine railcar suddenly had a 10 cm diameter hole in its lower side at a busy rail junction (see Figure 7 for a photograph of the site). The release rate and the initial jet behavior (including thermodynamics) were calculated using standard analytical source emissions models. This source emission information was provided to FLACS. Other model inputs were two wind direction scenarios, as well as the very large 3-D building geometry file at a resolution of about 1 m over the entire city. The terrain was assumed to be flat, with the exception that Lake Michigan was 2 m lower, and the Chicago River was 2 m lower.

Figure 8 shows the FLACS-simulated cloud boundaries (assumed to be the 100 ppm contour) for one of the Chicago scenarios. This is the south wind scenario, where south is to the right of the figure. Plots are shown for simulation times of 400 s and 1500 s. Note that the release was initiated at 100 s and stopped at 400 s.

The top panel of Figure 8, at 400 s, shows that the dense gas cloud is relatively shallow and broad while it is over the flat open area extending about 1 km to the north of the release site. However, the east (far) edge of the cloud does extend into the buildings, which cause enhanced vertical spread and also cause holdup or retention of the cloud behind buildings.

After 1500 s, as seen in the second panel of Figure 8, the cloud extends into the tall buildings in

downtown Chicago, causing more vertical mixing and retention behind buildings. It is interesting that there is part of the cloud that hangs back, remaining within the building complex closer to the source. This has important implications for emergency response planning.

An east wind scenario was also run, giving similar results to those seen in Figure 8. The most interesting new feature of the east wind run is that, when the dense cloud encounters the Chicago River "valley" (2 m deep) about 300 m west of the source release point, part of the cloud moves laterally (north and south) along the river.

The SCIPUFF, SLAB, HGSYSTEM, ALOHA, and PHAST models were also run for the Chicago scenario in Figure 8. Figure 9 contains the variation with downwind distance of the maximum 10 min average chlorine concentration for FLACS and for the five simpler models. It is seen that all models' simulations are in the same factor of ten range at all distances. The FLACS CFD model simulations are within this range most of the time, indicating rough agreement with the maximum (cloud centerline) concentrations. However, Figure 9 shows that the FLACS concentrations are a factor of two to five higher than the others at distances of 500 and 1000 m, which is when the cloud is still in the flat open area in Figure 8. Most of the simpler models are treating the entire domain as if it has an urban roughness length, without accounting for the flat area. The SCIPUFF model is able to account for variations in roughness length with distance.

## 5. FURTHER COMMENTS

The two research topics discussed here - TIC source emissions models, and TIC dispersion models in urban areas - are recognized to have several difficult scientific issues and are the subject of active research by many groups throughout the world. The bottom line, however, is to provide protection to persons who may be harmed by an accidental or intentional release of a TIC. Consequently, we are trying to focus on scientific areas that make a difference, and are trying to downplay scientific areas that may be of great academic interest but have little effect on the bottom line. The mass emission rate of the TIC to the atmosphere from the storage vessel is a major concern, as well as the removal rate in the near field due to deposition to the surface or due to chemical reactions. Also, a fundamental question in urban areas is whether the buildings cause increases or decreases in concentration when compared to the same TIC release scenario in a flat rural area. There are several competing scientific effects - for example, the buildings cause a decrease in wind speed (which will cause increases in concentration) but also cause an increase in turbulence (which will cause decreases in concentration). The buildings can also constrict the

lateral spread of the plume in the near field and can "hold-up" the TIC material in building wakes for many minutes (which will both cause increases in concentration).

Another effect of obstructions is the blocking of the initial jet momentum. For example, at Festus (see Figure 6) the jet hit the side of the railcar and was diverted under and around the railcar. At the Graniteville accident, the jet was directed 45 degrees downward and caused a crater in the ground under the railcar. The blocking effect will reduce the momentum of the jet and is thus likely to reduce the amount of ambient air entrained into the jet. As a result the concentration may remain high for a longer time. These effects have not been adequately studied and should be the subject of future laboratory and field studies, as well as model development and application studies.

The modeling and the field experiments both demonstrate that one should not assume that, within a few hundred meters of the source release location, the TIC cloud is going to be transported "downwind". Even over perfectly flat and open terrain, the dense TIC cloud will slump in all directions due to gravity effects. Thus the cloud will slump in an upwind direction also. This upwind and lateral movement will be accentuated if the terrain has a slope in those directions. And in urban areas or industrial sites with many buildings, tanks, and other obstructions, the wind flow near street level is chaotic, with vortices around buildings and with street canyon channeling. This can cause the TIC cloud to move in any random direction for a few hundred meters, even if it is not dense. Thus emergency responders and the general population are not "safe" unless they keep out of a circle of radius several hundred meters surrounding the release location. Persons who are inside that circle should shelter in place and, as the Chicago FLACS simulations showed, should assume that some of the TIC cloud is trapped in building vortices even 30 or more minutes after the main cloud has passed.

This guidance for emergency responders and for the public will be refined as the research progresses over the next few years.

## ACKNOWLEDGEMENTS

This research has been sponsored by the Defense Threat Reduction Agency (DTRA) and the Department of Homeland Security / Transportation Security Administration (DHS/TSA). The DTRA program manager is Rick Fry and the DHS/TSA program manager is Jack Aherne. The DHS/TSA funding came through a subcontract with Northrop Grumman with Curtis Schuhmacher as project manager.

## REFERENCES

- CCPS/AIChE, 1996: Guidelines for Use of Vapor Cloud Dispersion Models, 2nd Edition, ISBN No: 0-8169-0702-1, Pub No: G-40, 271 pp.
- CCPS/AIChE, 1999: RELEASE: A Model with Data to Predict Aerosol Rainout in Accidental Releases, ISBN No: 0-8169-0745-5, 184 pp.
- DTRA, 2004: HPAC 4.04 V&V Tech. Doc., Subsection 3.2 on Industrial Facilities (IFAC) Model (22 pages) and Subsection 3.3 on Industrial Transportation (ITRANS) Model, 8725 John J. Kingman Rd, Ft. Belvoir, VA 22060 (15 pages).
- DTRA, 2008: HPAC Version 5.0 SP1 (DVD Containing Model and Accompanying Data Files), DTRA, 8725 John J. Kingman Rd, Ft. Belvoir, VA 22060.
- Ermak, D.L., 1990: Users Manual for SLAB: An Atmospheric Dispersion Model for Denser-than-Air Releases. UCRL-MA-105607, Lawrence Livermore Nat Lab, Livermore, CA.
- Hanna, S.R. and R.E. Britter, 2008: Conclusions and Recommendations from Workshop on Toxic Industrial Chemical (TIC) Source Emissions Model Improvements (25-26 March 2008). Report P098-3 by Hanna Consultants, Kennebunkport, ME., prepared for DTRA, Ft. Belvoir, VA.
- Hanna, S.R., J.C. Chang and D.G. Strimaitis, 1993. Hazardous gas model evaluation with field observations. *Atmos. Environ.* **27A**, 2265-2285.
- Hanna, S.R., S. Dharmavaram, J. Zhang, I. Sykes, H. Witlox, S. Khajehnajafi and K. Koslan, 2008a: Comparison of six widely-used dense gas dispersion models for three actual chlorine railcar accidents. *Process Safety Progress.* **27**, 248-259.
- Hanna, S.R., Hansen, O.R., Dharmavaram, S., 2004. FLACS air quality CFD model performance evaluation with Kit Fox, MUST, Prairie Grass, and EMU observations. *Atmos. Environ.* **38**, 4675-4687.
- Hanna, S.R., O.R. Hansen, M. Ichard and D.G. Strimaitis, 2009: CFD model simulations of dispersion from chlorine railcar releases in industrial and urban areas. *Atmos Environ.* **43**, 262-270. online at <http://dx.doi.org/10.1016/j.atmosenv.2008.09.081>
- Hanna, S.R. G. Lee, R. Britter, O. Hansen, and P. Drivas, 2008b: Toxic Industrial Chemical (TIC) Source Emissions Improvements - Task 1: Review of HPAC Source Emissions and Alternate Algorithms, Draft Report number P098-01 to DTRA, Ft. Belvoir, VA.
- Hanna, S.R. G. Lee, R. Britter, O. Hansen, and P. Drivas, 2008c: Matching of TIC Source Emissions Model Outputs with SCIPUFF Inputs, Draft Report number P098-02 to DTRA, Ft. Belvoir, VA.
- Hanna, S.R., G. Lee, R. Britter, O. Hansen, D. Strimaitis, P. Drivas and T. Spicer, 2008d: Study of Toxic Industrial Chemical (TIC) Releases and Dispersion from Railcar Accidents or Terrorist Activities. Report P101-1 by Hanna Consultants, Kennebunkport, ME., prepared for Northrop Grumman Mission Systems and DHS.
- Hansen, O.R., O. Talberg and J.R. Bakke, 1999: CFD-based methodology for quantitative gas explosion risk assessment in congested process areas: examples and validation status. Proceedings, AIChE/CCPS Int Conf and Workshop on Modeling the Consequences of Accidental Releases of Hazardous Materials, San Francisco, ISBN 0-8169-0781-1, pp. 457-477.
- Hansen, O.R., J. Renoult and J.R. Bakke, 2001: Explosion risk assessment: how the results vary with the approach chosen. Fall Symp Proc., Mary Kay O' Connor Process Safety Center, Dept. of Chem. Eng., Texas A&M University, 3122 TAMU, College Station, TX 77843-3122, pp. 395-410.
- Hansen, O.R., J.A. Melheim and I.E. Storvik, 2007: CFD-Modeling of LNG Dispersion Experiments, Proceedings of 7<sup>th</sup> Topical Conference on Natural Gas Utilization, AIChE Spring Meeting, Houston.
- Moses, A., K. Obenschaun and J. Boris, 2006: Using CT-Analyst as an integration tool for CBR analysis, Proc. of SPIE, vol. 6201, pp62016V, doi: 10.1117/12.666122
- NOAA/HMRAD and EPA/CEPPO, 1992: ALOHA Users Manual and Theoretical Description. Reports available from NOAA/HMRAD, 7600 Sand Point Way NE, Seattle, WA 98115 and on CAMEO/ALOHA web site.
- Richardson, S.M., G. Saville, S.A. Fisher, A.J. Meredith, and M.J. Dix, 2006: Experimental determination of two-phase flow rates of hydrocarbons through restrictions, *Process Safety Environ. Prot.* **84 (B1)**, 40-53.
- SAFER Systems, 1996: Description of Modeling Algorithms, TRACE Version 8.0. Looseleaf notebook available from SAFER Systems, 4165 E. Thousand Oaks Blvd., Suite 350, Westlake Village, CA 91362.
- Sykes, R.I., S.F. Parker, D.S. Henn, and B. Chowdhury, 2007: SCIPUFF 2.3 Technical Documentation, DRAFT Technical Report for Contract No. DTRA01-03-D-0013, L-3 Titan Corporation, Princeton, NJ, 336 pp.

Williams, M., M.J. Brown and A. Gowardhan, 2005: Adaptation of the QUIC-PLUME model for heavy gas dispersion around buildings. AMS Atmos. Sci. and Air Qual. Conf., San Francisco, paper 8.6, [http://ams.confex.com/ams/ASAAQ2005/Techprogram/paper\\_90901.htm](http://ams.confex.com/ams/ASAAQ2005/Techprogram/paper_90901.htm).

Witlox, H., M. Harper, P. Brown, and V. Cleary, 2007: Flashing liquid jets and two-phase droplet dispersion - II. Comparison and validation of drop size and rainout formulations. *J. Haz. Mat.*, **142**, 797.

Witlox, H.M.W. and A. Holt, 1999: A unified model for jet, heavy and passive dispersion including droplet rainout and re-evaporation", Int Conf and Workshop on Modelling the Consequences of Accidental Releases of Hazardous Materials, CCPS/AIChE, San Francisco, 315-344.

Witlox, H.W.M. and K. McFarlane, 1994: Interfacing dispersion models in the HGSYSTEM hazard-assessment package, *Atmos. Environ.*, **28**, 2947-2962.

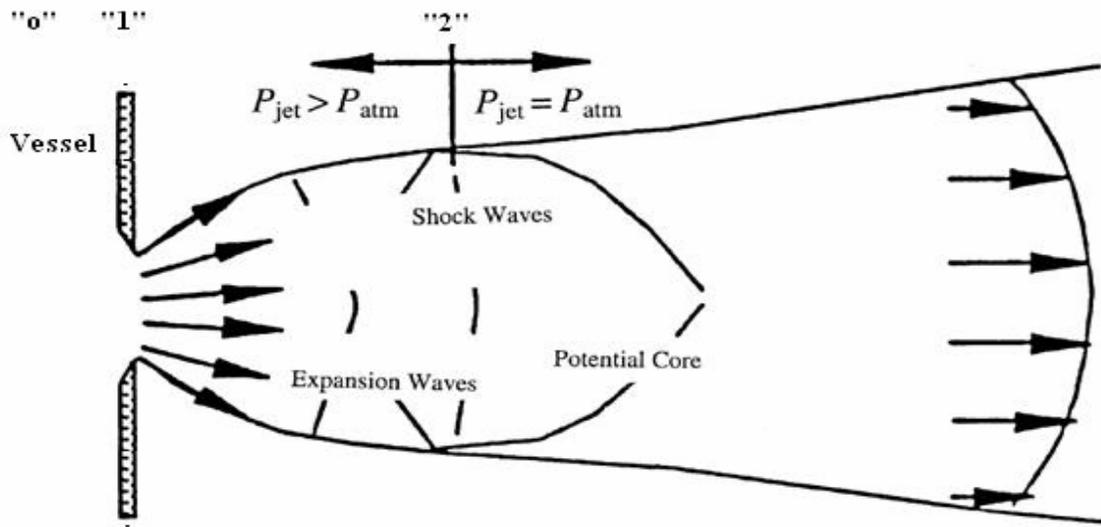


Figure 1. Diagram showing regions of concern for a release of a pressurized liquefied gas.

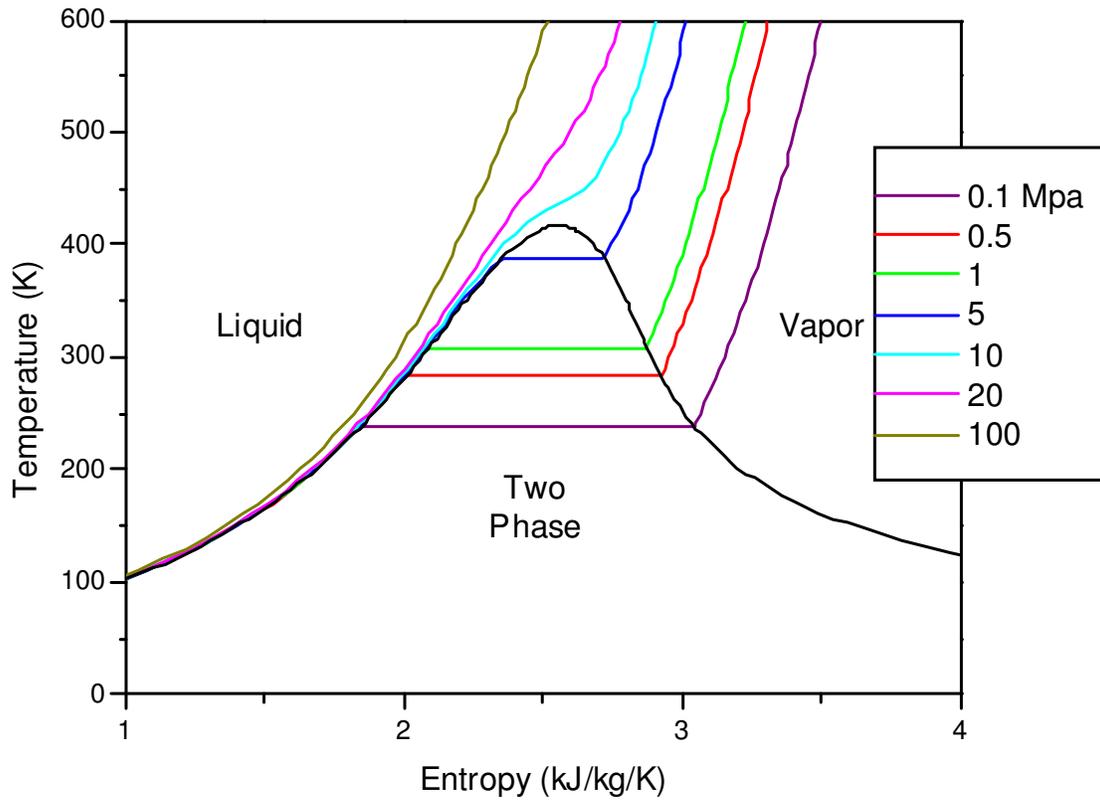


Figure 2. Temperature-entropy diagram for chlorine

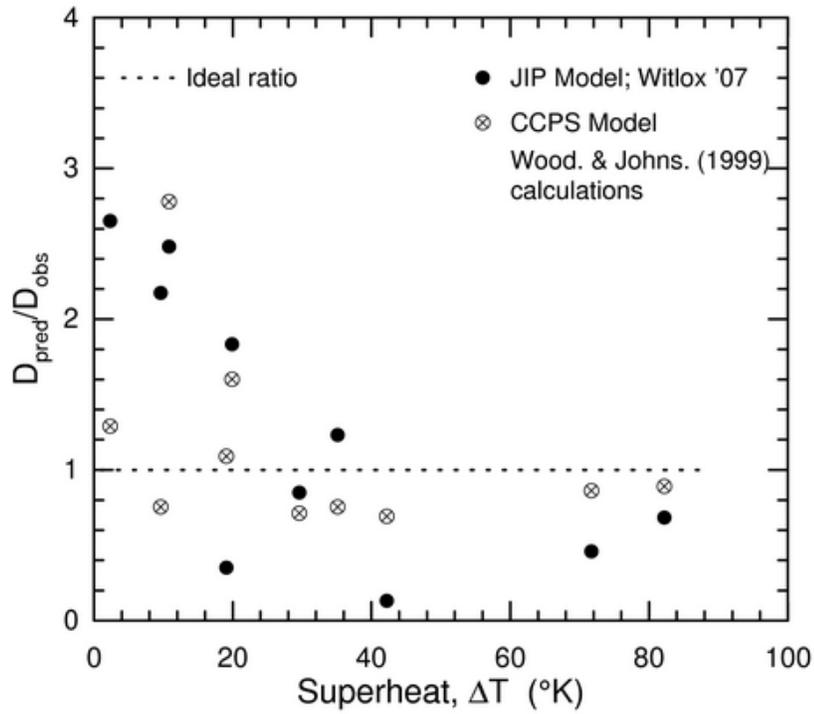


Figure 3. Droplet size ratio plotted versus superheat for the CCPS (1999) RELEASE observations for two models – the JIP model by Witlox et al. (2007) and the RELEASE model by CCPS (1999).

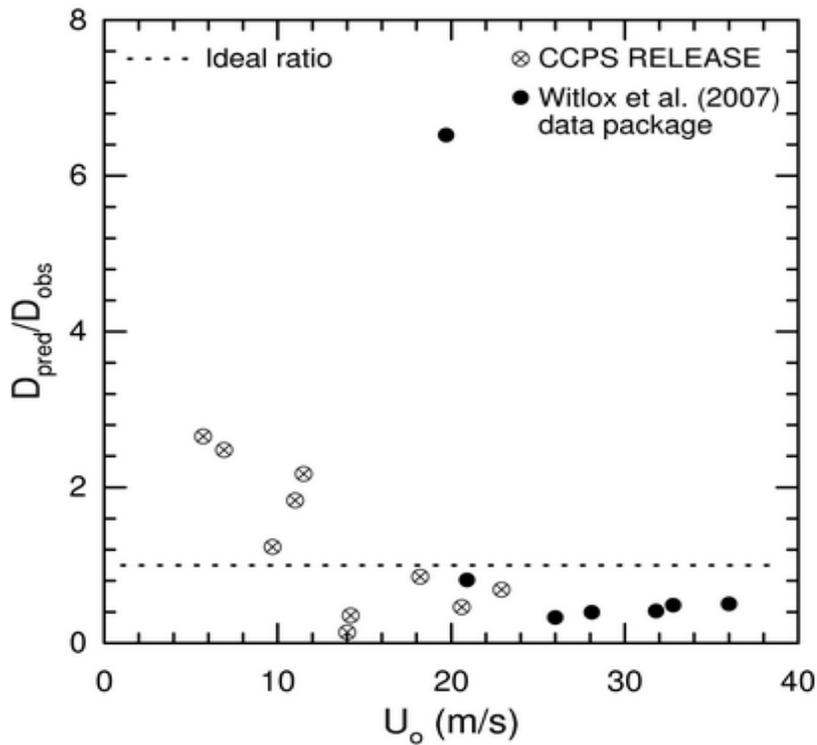


Figure 4. Droplet size ratio plotted versus orifice velocity for the CCPS (1999) RELEASE observations and the JIP observations (Witlox et al., 2007) for the JIP model by Witlox et al. (2007).

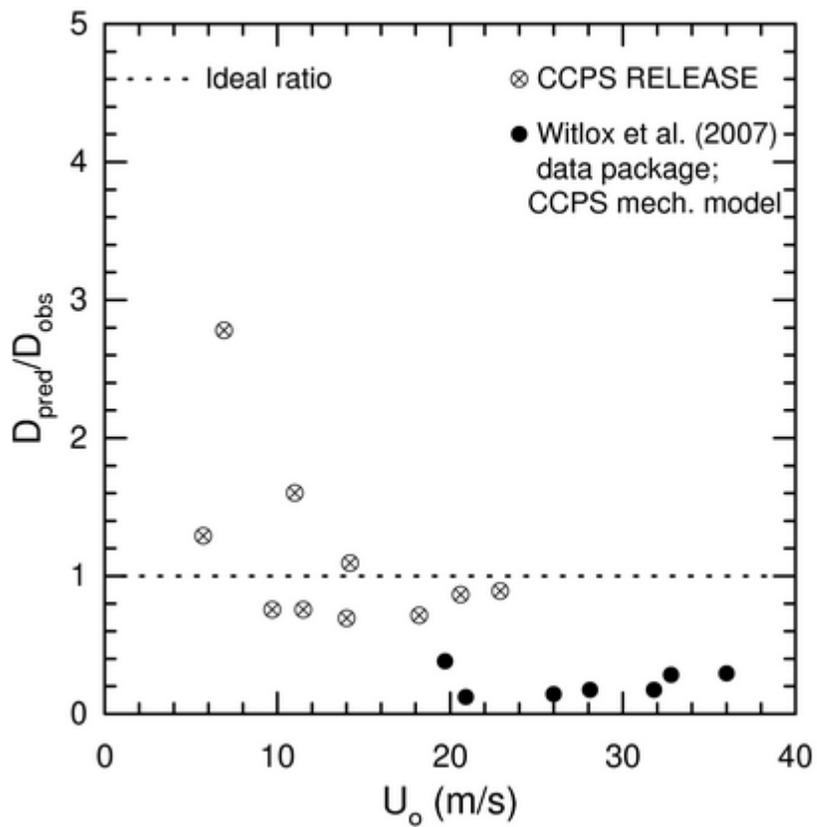


Figure 5. Droplet size ratio plotted versus orifice velocity for the CCPS (1999) RELEASE observations and the JIP observations (Witlox et al., 2007) for the CCPS(1999) RELEASE model.



Figure 6. Festus results. Comparison of frames from Fox News videos on the left and FLACS-simulations on the right (where the 2000 ppmv level is shown) for two different views. Videos are provided courtesy of Fox News.



Figure 7. Photograph of railroad junction in Chicago, looking towards the east-northeast. The hypothetical release location is the junction to the right of the small two-story station house. Jack Aherne (DHS/TSA) provided the photograph.

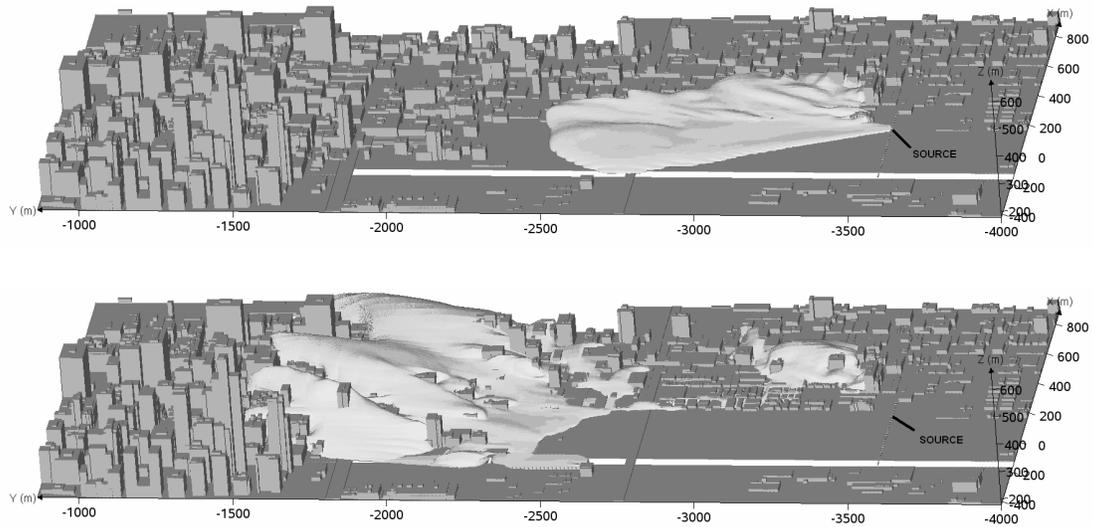


Figure 8. Examples of FLACS CFD model results from Chicago scenario 1 (south wind), where 100 ppmv contours are shown, for  $t = 400$  (top) and  $1500$  s (bottom). The view is to the east. The winds are from right to left (i.e., from the south).

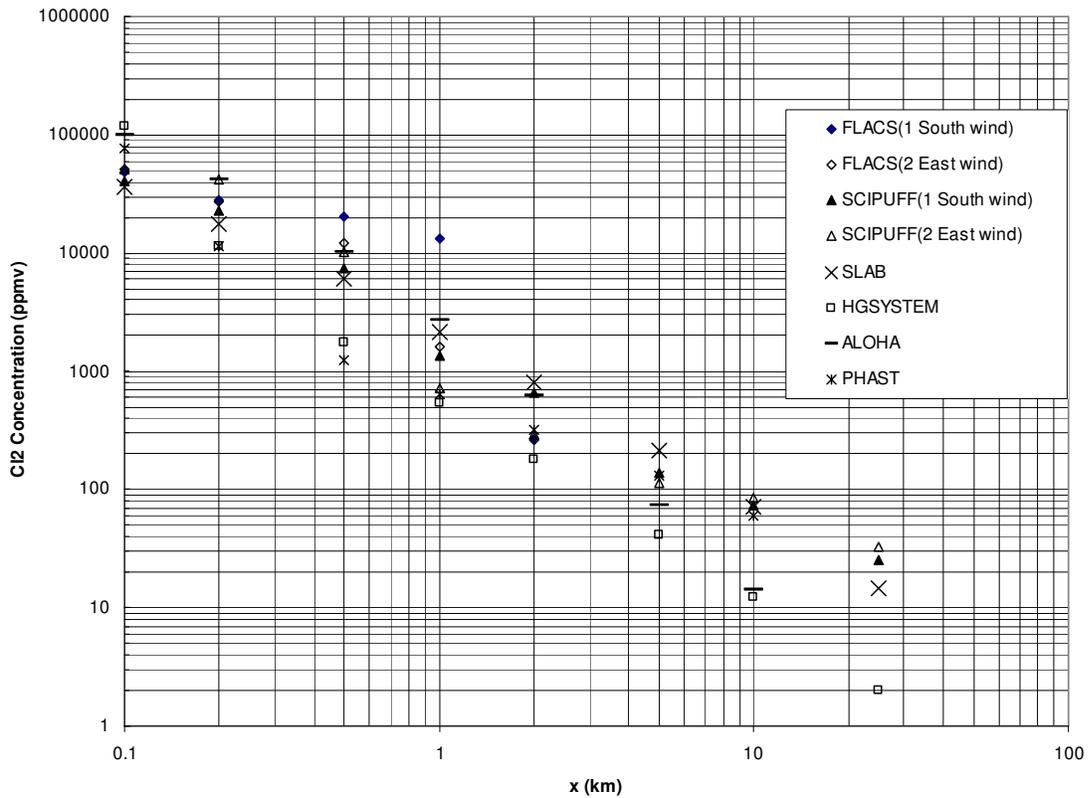


Figure 9. Plot of maximum 10 min average concentration (ppm of chlorine) versus downwind distance,  $x$ , for the models FLACS, SCIPUFF, SLAB, HGSYSTEM, ALOHA, and PHAST for the Chicago scenarios.