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UCRL- JC 109835
PREPRINT

Atmospheric Modeling of the July 1991 Metam Sodium Spill into California's Upper Sacramento River

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This paper was prepared for presentation at the
Air & Waste Management Association
85th Annual Meeting
Kansas City, Missouri June 22-26, 1992

March 5, 1992

Lawrence Livermore National Laboratory

ABSTRACT

The California Office of Emergency Services asked the Department of Energy's Atmospheric Release Advisory Capability (ARAC) at the Lawrence Livermore National Laboratory to determine the maximum credible air concentrations from a spill of metam sodium into California's Upper Sacramento River. About 19,000 gallons of metam sodium herbicide were spilled into the river approximately 3 miles north of Dunsmuir, California, due to a tank-car derailment on the night of July 14, 1991.

The herbicide moved in the river toward the northernmost finger of California's largest reservoir, Lake Shasta, 45 miles to the south. As it flowed down the deep canyon, the water-soluble metam sodium decomposed into hydrogen sulfide and methylamine gases. Residents along the river were advised to evacuate the area, and a 50-mile stretch of Interstate 5 was temporarily closed. Response officials were also concerned that sunlight would readily evaporate the enlarged slick once it arrived into the still water of Lake Shasta on July 16.

On July 15, ARAC used its three-dimensional emergency response modeling system to determine the highest instantaneous and 8-hour average air concentrations of toxic gas by-products over upper Lake Shasta. A quick response was possible using on-line topographic and geographic data bases in combination with forecasted southwestern surface winds. The worst-case calculation showed that the gases would be well below any health hazard.

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INTRODUCTION

The Atmospheric Release Advisory Capability (ARAC) is a real-time emergency response and preparedness service that was developed and has been operating at the Lawrence Livermore National Laboratory (LLNL) in Livermore, California, for the past 17 years. ARAC is a national resource with a suite of dispersion models to simulate the consequences of accidental releases of material into the atmosphere on local to global scales. Funded by the Departments of Energy (DOE) and Defense (DOD), the primary role of ARAC has been to provide calculations for radiological releases. Any U.S. federal agency can request the services of ARAC through DOE as delineated in the Federal Radiological Emergency Response Plan.

This paper provides a background on how ARAC has been drawn into responses other than radioactive material releases, summarizes its modeling system, and focuses on its response to the July 1991 spill of metam sodium from a railroad tank car into the upper Sacramento River in California.

BACKGROUND

Since the beginning of its initial operations in 1974, ARAC has been involved in over 500 responses, primarily exercises with its supported agencies. In accordance with its charter, ARAC has been used for major domestic radiological events where the U.S. government was involved. In addition, as Table I indicates, ARAC has been also used for nonradiological releases within the United States and for a variety of international incidents. In fact, requests for assistance involving nonradiological releases have equaled those involving radioactive releases.

The current ARAC system has evolved according to the demands and expectations of its supported agencies as well as its experience with responses.[1] For example, early in the history of ARAC, a 1976 North Carolina train accident revealed that real-time meteorological data automatically formated for use in the dispersion models was essential to a rapid response. In 1978, the unique request by DOE to estimate the atmospheric consequences of Russian nuclear-powered COSMOS satellites during reentry burn-up caused the ARAC team to develop a high-altitude particle fall model. As a result, ARAC was prepared for COSMOS 1402 in 1981. ARAC's largely manual response to the 1979 Three Mile Island accident indicated the need for on-line U.S. topography and geography data bases. The 1986 Chernobyl accident propelled ARAC to implement continental-to-hemispheric scale models supported by world-wide terrain and mapping data.

Each response resulted in expanded capabilities. Consequently, ARAC was ready with the necessary models and data bases to simulate the daily regional-scale soot concentrations from the Kuwaiti oil fires in the Persian Gulf region from May to October 1991.[2] Also, when the U.S. Air Force asked ARAC to determine the impact of the Mt. Pinatubo ash cloud on regional flight operations, the capabilities were in place to make that real-time assessment.

One of the most recent requests came through an Agreement In Principle between DOE and the state of California. While supporting local agencies in response to a July 14, 1991, railroad tank car spill into the upper Sacramento River, the California Office of Emergency Services (OES) contacted the DOE San Francisco Office in Oakland to request ARAC's assistance in estimating the air concentrations due to the evaporating by-products of the metam sodium when it reached the still waters of upper Lake Shasta.

TABLE I. Notable ARAC responses.

YEAR	LOCATION	SOURCE	RELEASE
1976	North Carolina	Train accident	Uranium hexafluoride*
1978	Northern Canada	COSMOS 954 reentry	Fission products
1979	Three Mile Island Harrisburg, Penn.	Nuclear power plant	Mixed fission products
1980	Damascus, Arkansas	Titan II missile	Missile fuel*
1981	Indian Ocean	COSMOS 1402 reentry	Fission products
1982	South Carolina	Savannah River Plant	Hydrogen sulfide leak*
1986	Gore, Oklahoma	Sequoyah Fuels Plant	Uranium hexafluoride*
1986	Chernobyl, USSR	Nuclear power plant	Mixed fission products
1988	Amarillo, Texas	Pantex Plant	Tritium gas release
1988	Miamisburg, Ohio	Mound Plant	Tritium gas release
1991	Persian Gulf	Nuclear facilities Kuwait oil fires	Mixed fission products Smoke*
1991	Philippines	Mt. Pinatubo	Volcanic ash*
1991	Northern Calif.	Railroad car spill	Toxic gas products*

*Release involved toxic chemicals.

ARAC SYSTEM

The original concept, prototype development, and initial operations from 1974 to 1982 were directed by DOE. From 1983 to 1986 the system was redesigned and a high level of automation was implemented to support up to 100 facilities within the DOE-DOD nuclear community. Figure 1 depicts the automated flow of information during an ARAC emergency response with the current system. This simplified diagram represents only the top-level system functions of the ARAC Emergency Response Operating System (AEROS) that contains over a million lines of computer code. AEROS automatically assembles necessary information for the model runstream once the minimum accident data have been entered with the "problem questionnaire." The questionnaire may either be completed on a computer system at one of the remote support facilities or entered at the ARAC center based on information gathered from any site by telephone.

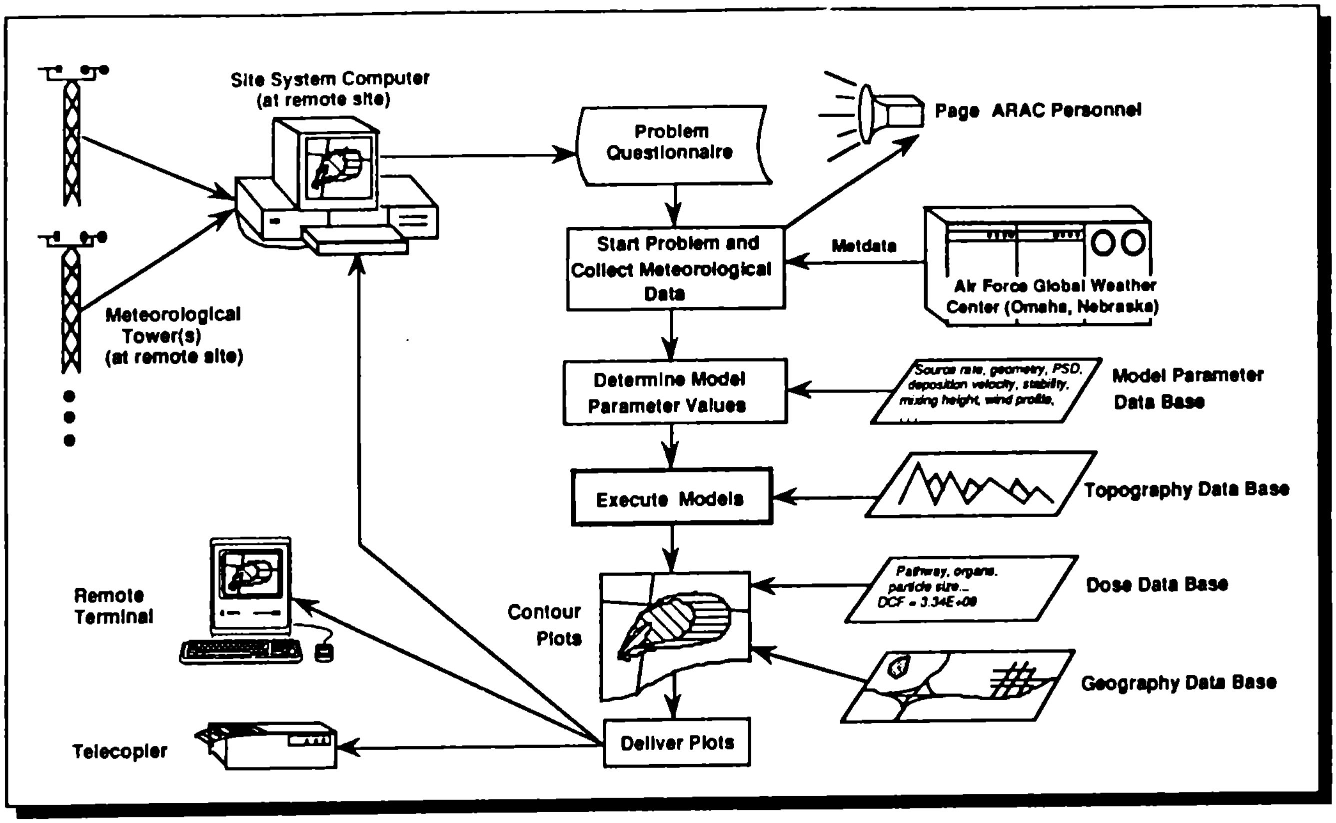

Figure 1. ARAC Emergency Response Operating System functions.

Hourly surface and twice-daily upper-air meteorological data (metdata) are automatically acquired from the ARAC dedicated link to the U.S. Air Force Global Weather Center. Within two minutes, the metdata is received, decoded, and formatted for model input. Meteorological variables (such as atmospheric stability, mixing height, and vertical wind power law profile parameters) can be determined from on-line algorithms or input by the assessment meteorologist running the models. A variety of source term inputs such as release rate, source geometry, particle size distribution, and deposition velocity are estimated from the questionnaire information. Once model inputs are prepared, the following series of six computer codes are run:

- TOPOG - Topographic grid generation
- MEDIC - Meteorological data interpolation code
- MATHEW - Mass-adjusted three-dimensional wind field
- ADPIC - Atmospheric dispersion by particle-in-cell
- DOSE - Application of radiological dose factors
- PLOT CONTOUR - Graphical contour plots generator.

These codes, which represent the primary regional-scale diagnostic three-dimensional dispersion model system, have been validated against several tracer studies.[3] An on-line continental United States topographic data base with a resolution of 0.5 km x 0.5 km is used by TOPOG to produce a 51 x 51 x 15 Eulerian grid with block-form terrain for the lower boundary of the model system. MEDIC uses an inverse-distance-squared ($1/R^2$) weighting of wind speed and direction observations and wind power profile laws to initialize the three-dimensional winds for MATHEW. MATHEW minimizes divergence in the initial wind field by adjusting horizontal wind vectors and generating vertical winds according to mass consistency. This wind field provides the transport component for ADPIC. A maximum of 20,000 Lagrangian marker particles is available to represent up to nine different sources or species. These are dispersed using either gradient (K-theory) or Monte Carlo diffusion schemes in ADPIC. Sources may be either instantaneous puffs or continuous plumes with time-varying release rates. Half-life decay, particle-size-dependent settling, dry deposition, and rainout are computed each time step for each source. For radionuclides, the DOSE code applies dose factors to the desired individual organs or the whole body through inhalation, immersion, or ground exposure pathways. PLOT CONTOUR produces a variety of plots using a geographic map overlay. For general map coverage of the United States, ARAC uses the U.S. Geological Survey (USGS) 1:2,000,000 Digital Line Graph (DLG) data base.[4]

Plot types include deposition of material on the ground, instantaneous and time-integrated doses, or air concentrations at selected levels above ground. Species or sources may be combined as required and contoured according to specified isopleth values. A legend is shown on each plot that describes the release, species involved, and type, units, and valid time for the contours.

After a quality assurance review by an assessment meteorologist, the plots may be transmitted to a supported site computer by a 1200-baud modem or faxed to the on-site emergency response manager. The time to create and deliver plots to a supported site computer can be as little as 15 to 30 minutes after receipt of accident information. For nonradiological incidents, the response time depends on the complexity of the source term, the availability of meteorological data, and the preparation of unique model input parameters.

Typically, ARAC response time is equally split between computer (or voice) communications with the site, automated (or manual) model input preparation, model execution, and human interaction with the system. ARAC currently uses 7 million instruction per second Digital Equipment Corporation (DEC) VAX 8550 computers to run the models and microVAXES to communicate with DEC PC350/380 site computers at 1200 baud. In one year, ARAC plans to upgrade the VAXes with machines that are ten time faster and begin replacing the site computers with Unix-based workstations communicating with ARAC at 9600 baud.

SACRAMENTO RIVER SPILL RESPONSE

Description of Spill

Seven cars on a 97-car train were derailed on a curve of track at about 2150 PDT on July 14, 1991. The accident occurred on a portion of track known as the Cantara Loop, about 3 miles north of Dunsmuir (a community of about 3,000 in a mountainous area of Northern California [Figure 2]). One of the derailed cars, a tank car filled with metam sodium (a soil fumigant), was on a bridge over the upper Sacramento River. The car fell into the river, was punctured, and spilled the metam sodium. The Material Safety Data Sheet indicated that the yellow-green solution readily mixes with water and decomposes to toxic gases, methylamine, methylisothiocyanate, and/or hydrogen sulfide. The California Highway Patrol closed a 50-mile stretch of Interstate 5 that parallels the north-south river valley, and citizens were evacuated along the river.

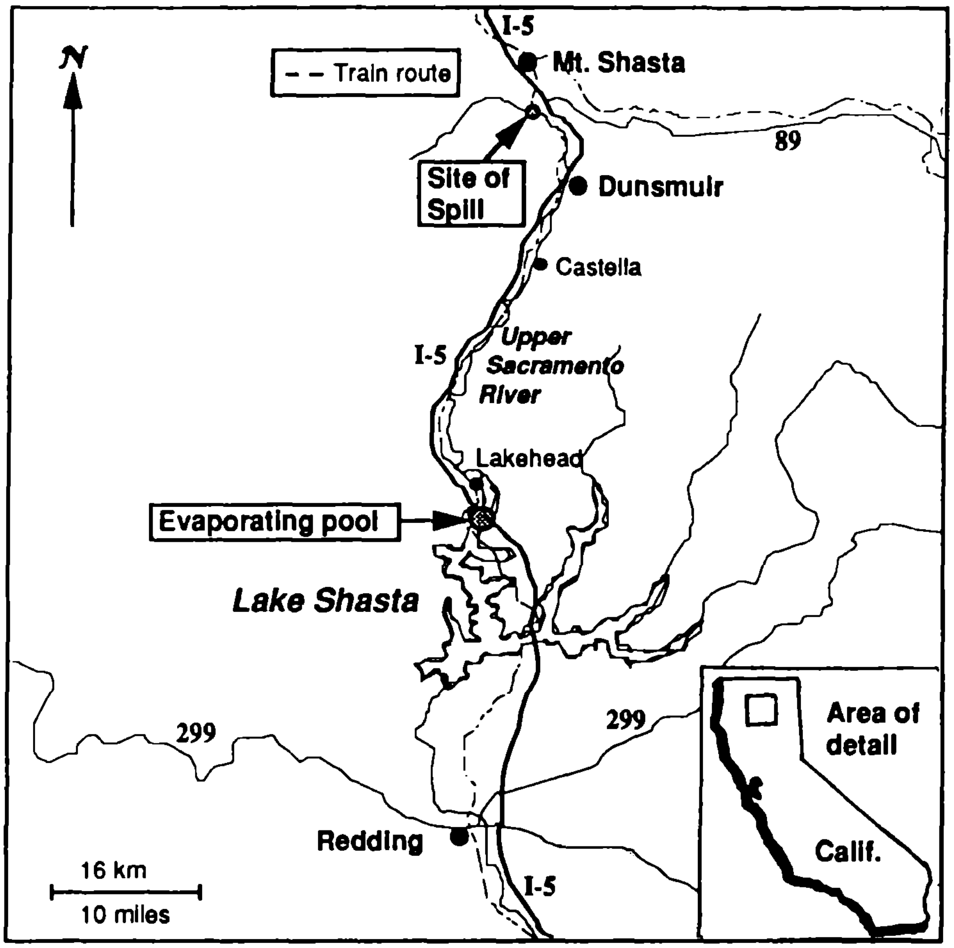

Figure 2. Map of the upper Sacramento River and Lake Shasta region.

Timeline of Events

By the afternoon of the next day (Monday, July 15), the spill had travelled about half way down its 40-mile trip toward Lake Shasta. It was estimated that the slick would arrive at the upper reaches of Lake Shasta by Tuesday morning, July 16. The multi-agency response group was concerned that the elongated slick might create a large cloud of toxic gases due to the increased amount of strong summer sunlight once it reached the more exposed still water of the lake . The question of whether or not to evacuate residents and vacationers along the Sacramento River arm of Lake Shasta led the OES to request dispersion modeling from ARAC.

Table II briefly lists the chronology of events relevant to the involvement of ARAC. The OES first obtained approval to use ARAC through the DOE San Francisco Office on the afternoon of July 15, and then provided ARAC with a source term estimate by 1700 PDT. ARAC was asked to estimate the maximum instantaneous and 8-hour average air concentrations for the pool evaporation from 0600 to 1100 PDT on Tuesday, July 16. ARAC responded in about 1-1/2 hours, and within that time all pertinent input data were collected, terrain data were extracted, a model grid was built, MATHEW/ADPIC was run, and plots were delivered to OES.

TABLE II. Timeline of ARAC involvement in the response to the July 1991 Sacramento River spill.

DATE	TIME (PDT)	EVENT
Sunday, July 14	2150	Derailment of tank car causes spill of metam sodium into upper Sacramento River
Monday, July 15	1500	OES makes initial inquiry to ARAC
	1645	DOE approves use of ARAC services by OES
	1700	OES provides ARAC with source term estimate
	1830	ARAC delivers plots to OES
Wednesday, July 17	0300	Spill begins to arrive at Lake Shasta
Saturday, July 20	1800	Aeration of spill on Lake Shasta begins

Model Grid

A 20 km x 20 km x 700 m grid was centered on the northern tip of the Sacramento arm of Lake Shasta where the pool of metam sodium was expected to slow down and evaporate. This grid uses the maximum resolution of the on-line topographic data base with each grid cell representing 0.5 km x 0.5 km. Figure 3 illustrates a view of the simulated terrain looking from the south over the model domain.

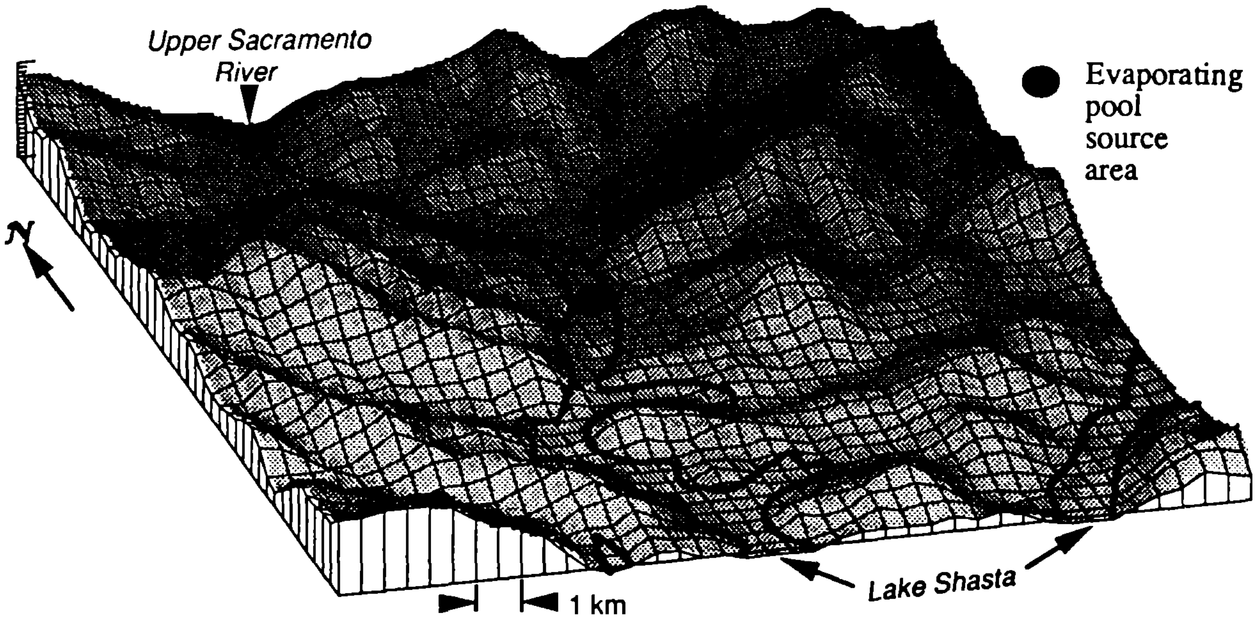

Figure 3. Perspective view of model grid terrain.

Source Term Estimate

Table III lists the Material Safety Data Sheet (MSDS) data and assumptions used by OES to determine a realistic amount of hydrogen sulfide gas that could evaporate on the northern tip of Lake Shasta. A similar calculation gave 200 lbs/hr for the methylamine release. A one-mile-diameter circular area was used for the source. When the spill did arrive in the lake early Wednesday morning, it was 1-1/2 miles long and was estimated to contain between 11,000 and 12,000 gallons of metam sodium. This compared well to the 9,500 gallons expected to reach the lake.

TABLE III. Source term assumptions.

19,000 gal	Tank car volume
x 0.327	Purity of solution as metam sodium
x 9.7 lbs/gal	Metam sodium density (using a specific gravity of 1.162 g/ml)
60,000 lbs	Approximate maximum metam sodium spilled in river
x 0.5	Assume one half of spill in river arrives at the lake
x 0.5	Assume one half of the metam sodium in the lake evaporates
x 0.33	Ratio of molecular weight of H_2S to metam sodium
5,000 lbs	H_2S evaporated from the lake surface
÷ 5 hr	Assume slick evaporates over 5 daylight hours
1,000 lbs/hr	Hydrogen sulfide release rate

Meteorological Conditions

As with many real-world events, representative meteorological data for accidents are usually in short supply. Routine observations are taken by the National Weather Service (NWS) at Mt. Shasta, 50 miles north of the northern tip of Lake Shasta and in Redding about 10 miles south of the evaporating pool area. Winds were from the south on Monday afternoon. ARAC relied on the NWS forecast of southwesterly winds at 5 m/sec over the Lake Shasta area for Tuesday morning, July 16, for model input. The forecast proved accurate, since actual winds on Tuesday morning were from 200° at 3 m/sec at 0800 PDT.

Figure 4 shows the wind field produced by MATHEW at 50 m above ground with terrain features taken into account. Wind vectors are displayed for every other grid cell or every 1 km. The map is centered on the Lake Shasta metam sodium pool source area. One of the drawbacks of the USGS 1:2,000,000 DLG data is that map feature information is internal to the data base. Labeling the map remains a device-dependent complexity. The Sacramento River arm of Lake Shasta is in the center of the map; Interstate 5 is the solid line winding from south to north across Lake Shasta. The numbers on the perimeter of the map refer to Universal Transverse Mercator coordinates in kilometers. One problem discovered during this response was that the DLG map and the terrain were shifted about 0.5 km or the maximum resolution of the terrain data. This required some editing of terrain cell heights and rerunning of the models before releasing the plots. This problem occurred because of the coarse spatial resolution of the 1:2,000,000 USGS data base.

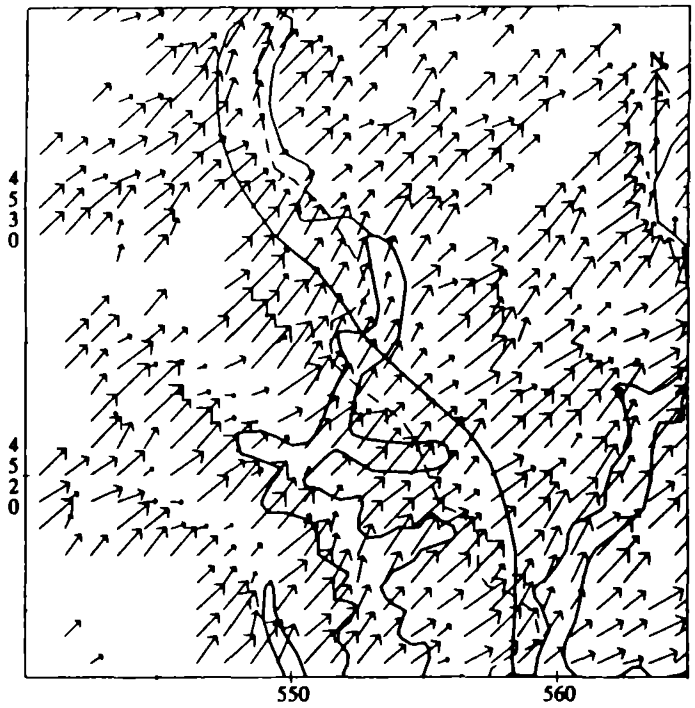

Figure 4. MATHEW wind vectors for Tuesday, July 16, 1991.

Dispersion Conditions

ARAC estimated that the atmospheric stability would be neutral all day. Figure 5 shows instantaneous cross-section and overhead views of the particle location at 1000 PDT or 4 hours after the release began. The figure shows how the gas spread across the tip of the lake and moved up the western facing slopes of the ridge north of the lake. After 5 km of travel, the gas cloud rose to 600 m above ground. This excellent upslope flow dispersion readily diluted the cloud.

Contour Plots

Contour plots were produced for instantaneous and 8-hour average methylamine and hydrogen sulfide air concentrations. The maximum modeled values are compared with the American Conference of Governmental Industrial Hygienists threshold limit values in Table IV. With its higher emission rate, the H_2S became the primary concern. Comparing instantaneous concentrations with a 15-minute average short-term exposure limit adds considerable conservatism.

TABLE IV. Modeled concentrations compared with threshold limit values.

	METHYLAMINE (ppm)	H_2S (ppm)
Short-Term Exposure Limit (STEL)	--	15
Maximum instantaneous modeled concentration	2.4	9
Time-Weighted Average (TWA)	10	10
Maximum 8-hour modeled concentration	0.12	0.6

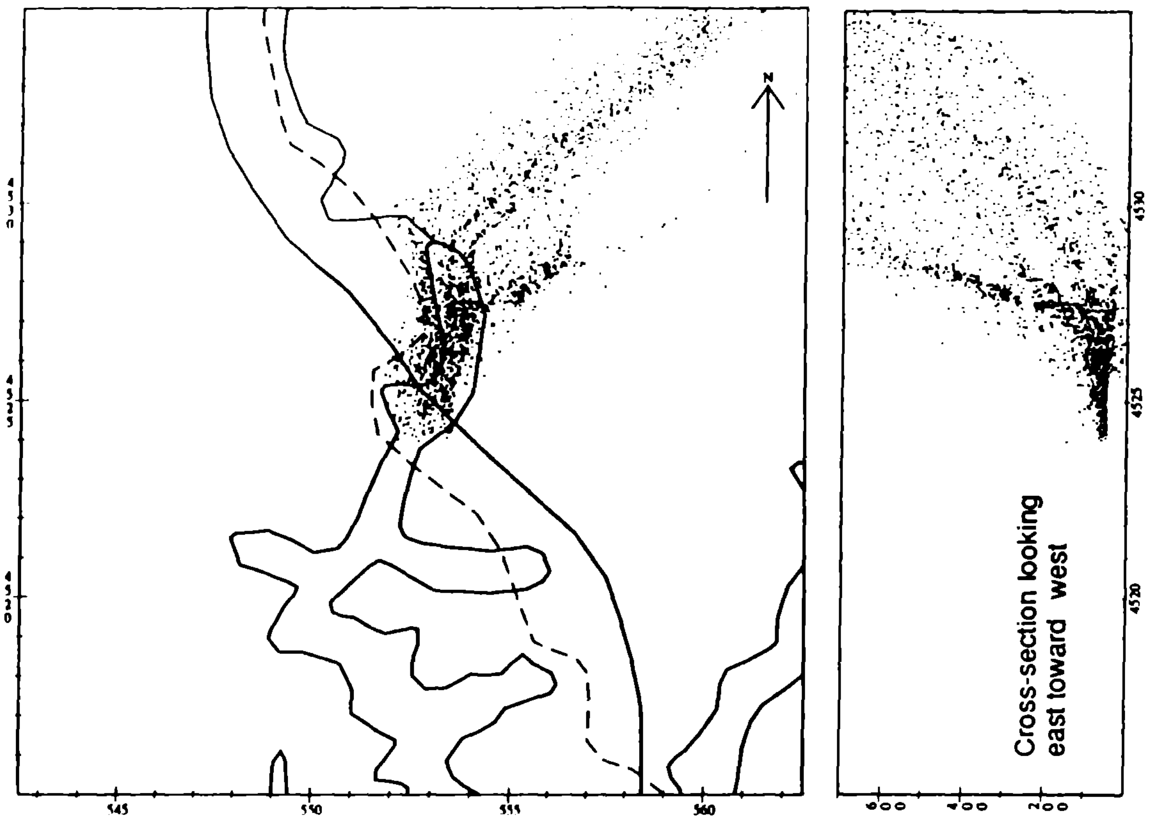

Figure 5. Instantaneous views of particles 4 hours after the beginning of the release.

Figure 6 shows a sample contour plot for the 8-hour H_2S integrated air concentration. The instantaneous H_2S and methylamine plots showed a similar pattern with contours extending northeastward. The maximum values were all located on the lake. Based on these calculations, an evacuation of the area was not considered necessary.

Southern Pacific officials began aerating the metam sodium pool early Sunday morning, July 20. Maximum air concentration measured within the water curtain surrounding the aerator was 4 to 5 ppm. Although this concentration was measured over an aerated lake surface, it compared favorably with the model's maximum instantaneous concentration of 9 ppm by quiescent evaporation.

CONCLUSIONS

A federal emergency response developed to respond to accidental radiological releases in the atmosphere was used to simulate the toxic gas clouds above an evaporating pool of metam sodium during the response to the July 1991 upper Sacramento River spill in northern California. Using an on-line terrain data base and forecasted wind conditions, the model appeared to produce a reasonable estimate of the hazard from the evaporating pool on Lake Shasta. This event, coupled with ARAC's history of responses, begs the question,

Does the United States need a national *toxic chemical* emergency response modeling capability?

With a proven modeling system in place, the framework for developing such a capability exists at ARAC. Significant new developments with default source terms, release mechanisms, toxic chemical (MSDS) data bases, and exposure indicies would have to be added to the system. In addition, new tools such as dense gas models would need to be engineered into the operational environment. Moreover, training of the ARAC operations staff would have to be extended to include toxic chemicals. Federal funding for this expansion is currently being considered for ARAC supported sites in the latter half of the 1990s. Support of the expansion by states could broaden the availability and capability of response to major industrial or transportation accidents throughout the country. Until such support is in place, ARAC will continue to respond to toxic chemical releases as best as it can on a case-by-case basis with the current system.

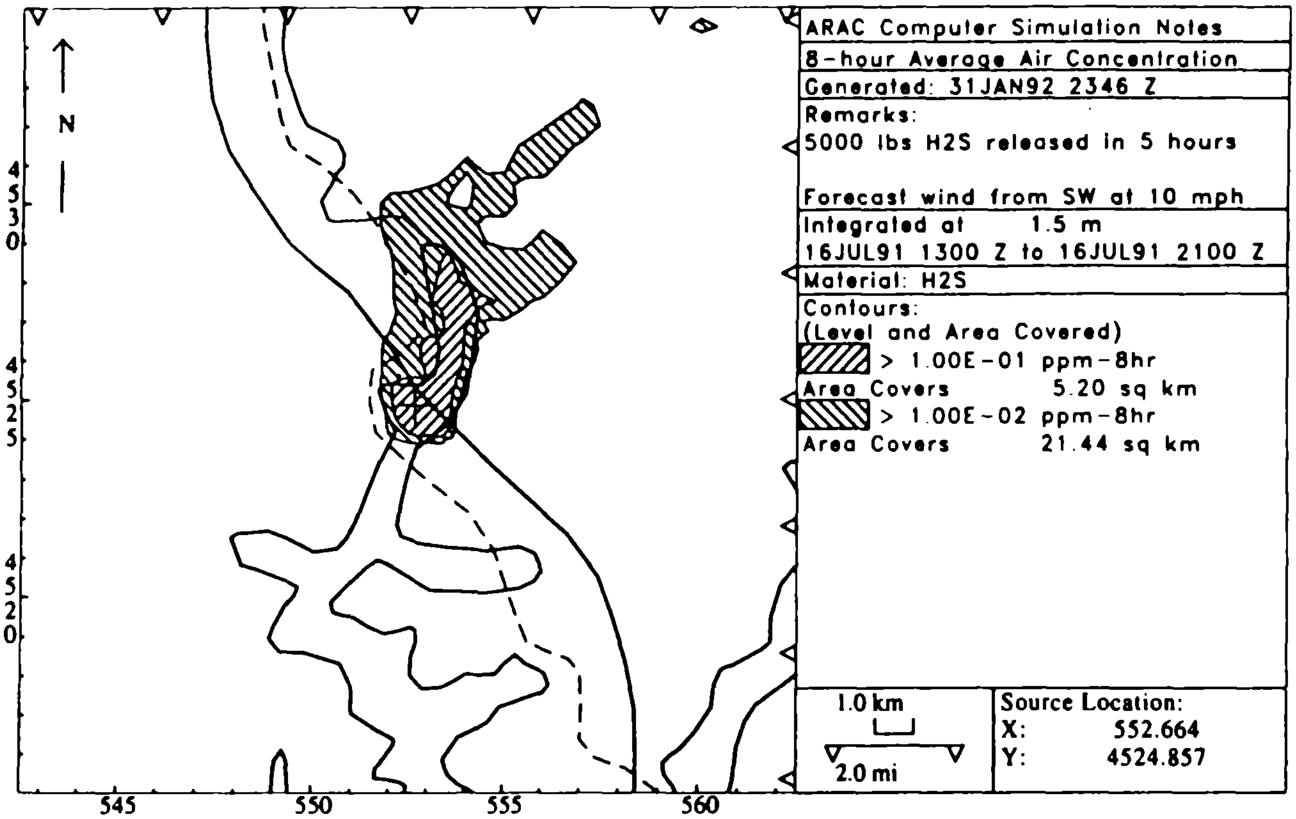

Figure 6. Plot of 8-hour H_2S integrated air concentration for 0600-1400 PDT on July 16, 1991.

Acknowledgment. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-eng-48.

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