Worst case scenario,

Model against "normal" type accident - broken line
leaky valve

Use of Computer Models for Risk Assessment and Accidental Release Under Title III, CAA Amendment

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Complying with the "MACT" provisions of Title III of the Clean Air Act Amendments of 1990 will have major impacts on facility emissions, pollution control devices and alternative chemicals and processing. Additional activities will be required under the "Residual Risk" and "Accident Prevention" subsections of Title III. The Residual Risk subsection will potentially require risk assessment modeling on populations surrounding facilities for known, probable or possible human carcinogens, and the "Accident Prevention" subsection will require a facility hazard assessment review, including plans to minimize the consequences of accidental releases. Chemicals covered by this subsection may come mainly from the EPA list of extremely toxic materials, but will specifically include ammonia, anhydrous ammonia, chlorine, hydrochloric acid, anhydrous hydrogen chloride, anhydrous sulfur dioxide and sulfur trioxide, among other chemicals.

Not all of these chemicals are on the list of Title III Hazardous Air Pollutants, and these subsections frequently go unaddressed as facilities begin planning for the CAA amendments.

This paper will review the general requirements and timetable anticipated under these two subsections, and present a summary of the currently available computer models and their capabilities relative to accidental releases, on and off site prediction of maximum concentrations, population risk assessment, identification of monitoring sites, and other potential requirements under Title III.

USE OF COMPUTER MODELS FOR RISK ASSESSMENT OF ACCIDENTAL RELEASES UNDER TITLE III, CLEAN AIR ACT AMENDMENTS OF 1990

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Much has been said about how dissatisfaction with the "risk-based" emission limitations of the national Emission Standards for Hazardous Air Pollutants (NESHAPS), programs such as the FDER "Draft Guidelines for Air Toxics" and estimates of accidental releases under SARA has resulted in adoption of the "Technology-based" emission standards of "Maximum Available Control Technology" (MACT). What has not been widely discussed has been the importance of computer emission modeling under MACT in the areas of Residual Risk and Accidental Releases (Figure 1a).

If computer modeling indicates that there is reason to believe that MACT-level emissions may represent a potential health threat (e.g. an increased cancer burden or a "residual risk"), to a surrounding population, some facilities may be required to install additional emission controls, beyond the MACT requirements, on a case-by-case and site specific basis. In addition accidental releases from each possible scenario must be analyzed, assessing the potential impacts on the surrounding population. As shown in Figure 1b, these requirements will begin to be felt as early as November of 1992. The initial list of substances to be considered includes the common industrial chemicals shown in Figure 2a. Minimum "risk management plan" components are shown in Figure 2b.

Rather than wait for these trigger dates and bemoan the negative impacts, a more practical approach is to take a proactive stance, using computer modeling and "best guess" estimates of what the regulations will be to identify "targets of opportunity" within the facility. These "targets" might be as sweeping as alternative chemicals or processing methods or as simple as reorienting of rupture disks or relocating of storage areas; these "targets" would be attacked with the goal of minimizing the impact of the new regulations when they are implemented. Careful planning now could allow a facility to avoid the "extra MACT" controls and to have a simple risk management plan requiring a minimum of personnel commitment and record keeping.

To properly select the computer model, the particular characteristics of each accidental release scenario must be determined. The common process flow sheet, such as the one in Figure 3, should be reviewed to identify possible "release points", in much the same manner as fault tree analysis. Additional characteristics to note are the physical dimensions of nearby structures and distances to property boundaries, as shown in Figure 4a. Also important is the type of release itself. As shown in Figure 4b, a liquid with a high vapor pressure leaking from a cylindrical tank into a diked area could result in an emission best characterized as a continuous release from a rectangular "area" source (as opposed to square or circular); or, depending on the liquid characteristics and peculiarities of the leak, a "point" or "line" source type model should be used.

Also important is a review of the area surrounding the facility, as in Figure 5. Distances and directions to population centers and "sensitive" receptors, such as schools, nursing homes and hospitals, and topographic features should be considered. Recall that "residual risk" modeling analyses will identify populations at risk to long-term exposure, and "risk management" modeling analyses will be concerned with sudden,higher concentration exposures and possible evacuations.

Since the information required from the two approaches is different, are the models different? Not necessarily.

There are a wide variety of models, with more being developed. In general, they can be divided into two groups, the "steady-state" and the "puff" or instantaneous type models (Figure 6 a). Steady-state models assume a continuous release over a long period of time, and are typically used in "risk assessment" type modeling. The puff type models assume a single short term release, for example a relief valve discharge, and are commonly used for modeling of accidental releases. However, if the relief valve has multiple "puffs" over short periods of time and the receptors are close, or if a liquid spill is evaporating slowly, a continuous model may prove to be easier and more accurate.

Models can also be grouped functionally into "predictive" and "response" types; the "predictive" models are more complex, require more data input and execution times, and are potentially more accurate. They are useful for "what if" determinations. The "response" models, such as those used by the Coast Guard, Fire Department and other "first responders", provide analysis of data in "real time", estimating release plume characteristics moment to moment on site after a release. They must be fast, require little data input, and generally provide graphic output.

In general they all begin with the same mathematical base (Figure 6b); the specific initial and boundary conditions, and simplifying assumptions, lead to the different results. Some models can use a full range of wind characteristics and building downwash calculations for plume prediction (Figure 7) (e.g. ISC or T-Screen), while others use a single value based on actual real time data (Cameo). some models have a physical/chemical data base associated (T-Screen and Cameo for example), which may be of benefit in particular cases.

Model output can be numeric or graphic, simple concentration vs. distance (with several wind stability classes superimposed), as in Figure 8a from T-Screen, or in isopleths as in the ISCST plot of Figure 8b. Obviously, these are better used as "predictive" models (risk assessment). Figure 9a illustrates a one-quadrant isopleth of a "puff" release with time, obviously useful to a "first responder". This particular event has a wind direction change after t = 3, moving the plume laterally. Figure 9b illustrates a release of a quickly evaporating liquid (e.g., "Spill"). If the liquid spill is small or evaporates very quickly, the similarity to the "puff" model becomes clear: conversely, if the spill is large (or deep in a diked area) and evaporates slowly, a "continuous" type area model (ISCST - area or PAL) might be more attractive than a spill model.

The ultimate selection of the model depends on an understanding of:

1. the type of information required from the analysis - don't ask the model to do what it can't do (e.g., predictive or responsive?)

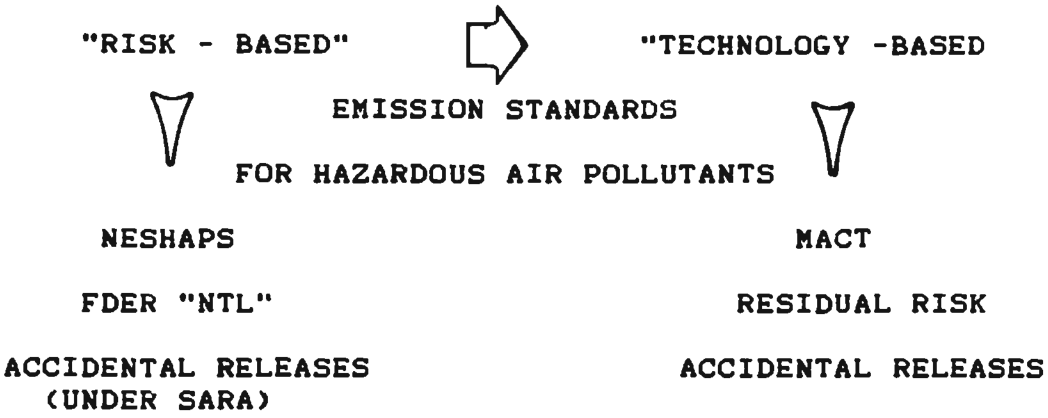
2. the initial and boundary conditions and assumptions upon which the model algorithms are based-violate them with caution.

3. the real world physical situation of the release - if it is a spill, does it evaporate quickly or slowly? Will it continue for a long time? What model types match the situation?

It is likely that several models will reasonably represent a particular situation. For example, Figure 10 might represent a "predictive" analysis of a trapezoidal area source, potentially modeled by the area source of ISCST or PAL, or by a circular pool of slowly evaporating liquid (Shell - SPILL or VAPOR). Figure 11 shows the calculated results, and it appears that for "nearby" receptors the "Spill" model, which is very easy to use, provides good agreement with the "higher accuracy" (and increased user effort) methods of ISCST.

Note that I said "appears". Actual data for both continuous and "puff" releases is very limited, and agreement of the various models is poor (unless one considers the monumental difficulties involved in obtaining an answer at all). Experimental results designed to test one model are frequently difficult to adopt to other models.

Despite careful selection of computer models, the results should be used with care, and several different models (preferably from different foundations) should be used to provide a "range" of probable values. The potential impact of these results on the facility and operations should be evaluated long before the regulations are implemented, while sufficient time remains for proactive choices.



"RISK - BASED" "TECHNOLOGY -BASED

EMISSION STANDARDS

FOR HAZARDOUS AIR POLLUTANTS

NESHAPS

FDER "NTL"

ACCIDENTAL RELEASES
(UNDER SARA)

MACT

RESIDUAL RISK

ACCIDENTAL RELEASES

Figure 1a

YEAR ONE-
LIST OF CATEGORIES AND SUBCATEGORIES OF MAJOR SOURCES - NOVEMBER 15, 1991

YEAR TWO-
MACT STANDARDS AND LIST OF SPECIES FOR ACCIDENTAL RELEASE CONSIDERATION - NOVEMBER 15, 1992

YEAR THREE-
PROMULGATION OF REGULATIONS PERTAINING TO AND REQUIRING RISK MANAGEMENT PLANS

YEAR SIX-
- *EPA REPORT TO CONGRESS ON RESIDUAL RISK FACTORS
- *FACILITY DEADLINE TO IMPLEMENT RISK MANAGEMENT PLANS

YEAR ELEVEN-
ESTABLISH REQUIREMENTS FOR RESIDUAL RISK-BASED ADDITIONAL EMISSION REDUCTIONS

Figure 1b

Initial List of Extremely Hazardous Substances Under the Clean Air Act Amendments of 1990

ammonia
anhydrous ammonia
anhydrous hydrogen chloride
anhydrous sulfur dioxide
bromine
chlorine
ethylene oxide
hydrogen cyanide
hydrogen fluoride
hydrogen sulfide
methyl chloride
methyl isocyanate
phosgene
sulfur trioxide
toluene diisocyanate
vinyl chloride

Figure 2a

Figure 2b

"REASONABLE REGULATIONS " TO PREVENT AND DETECT ACCIDENTAL RELEASES MUST INCLUDE:

*PERSONNEL TRAINING PROGRAM

*MEASURES FOR EMERGENCY RESPONSE BY FACILITY

* FACILITY RISK MANAGEMENT PLAN, INCLUDING:

HAZARD ASSESMENT OF POTENTIAL IMPACTS OF EACH RELEASE SCENARIO

FACILITY RESPONSE PROGRAM FOR EACH RELEASE SCENARIO

FACILITY RESPONDER AND EMPLOYEE TRAINING PROGRAM

T-151 TO T-156
HAZARDOUS WASTE TANK
1200 US GALLONS
11'-6" DIA x 15'-4" SS
CARBON STAINLESS STEEL
△3

T-101 TO T-110
HAZARDOUS WASTE TANKS
6000 US GALLONS
6'-0" DIA x 16'-0" SS
504 STAINLESS STEEL

H-201
THIN FILM EVAPORATOR
65 FT²
316 STAINLESS STEEL

S-101
VACUUM STILL
1600 US GALLONS
6'-0" DIA x 6'-0" S.S.
CARBON STEEL

H-101
STILL CONDENSER
SHELL & TUBE TYPE
1000000 BTU/HR, 434 FT²
CARBON STEEL SHELL/316 SS TUBES

R-1
STILL CON
150 US GALLONS
2'-6" DIA x 5'-6" SS
CARBON STEEL

R-204
VACUUM K/O POT
50 US GALLONS
2'-0" DIA x 2'-0" S.S
CARBON STEEL

T-201 TO T-210
CRUDE STORAGE TANKS
5800 US GALLONS
8'-0" DIA x 15'-6" S.S
CARBON STEEL
△2

P-302
FRACTIONATION COLUMN
48" DIA x 68'-0" SS
56 SIEVE TRAYS
304 STAINLESS STEEL

H-304
COLUMN CONDENSER
SHELL & TUBE TYPE
4500000 BTU/H, 675 FT²
CARBON ST SHELL/304 SS TUBES

H-305
BOTTOMS COOLER
SHELL & TUBE TYPE
4650000 BTU/H, 712 FT²
CARBON STEEL SHELL/
304 SS TUBES

-301 TO
RODUCT TA
5800 US GALL
10'-0" DIA x 10'-0" S
304 STAINLESS ST

R-202/203
TFE BOTTOMS TANKS
6000 US GALLONS
10'-0" DIA x 10'-0" S.S
CARBON STEEL

G-157
SOLID
GRINDER
△2

E-101
ENTRAINMENT SEPARATOR
2'-0" DIA x 5'-0" SS.
CARBON STEEL

R-101
STILL OVHD RECEIVER
200 US GALLONS
3'-0" DIA x 3'-0" S.S.
CARBON STEEL

R-103
VACUUM K/O POT
50 US GALLONS
2'-0" DIA x 2'-0" S.S.
CARBON STEEL

T-403
WATER RECEIVER
75 US GALLONS
2'-6" DIA x 2'-0" SS
CARBON STEEL

R-401
FREON WASH TANK
3000 US GALLONS
8'-0" DIA x 8'-0" S.S
CARBON STEEL

S-302/H-303
REBOILER STILL
3000 US GALLONS
10'-0" DIA x 8'-0" SS
8000000 BTU/HR
304 STAINLESS STEEL

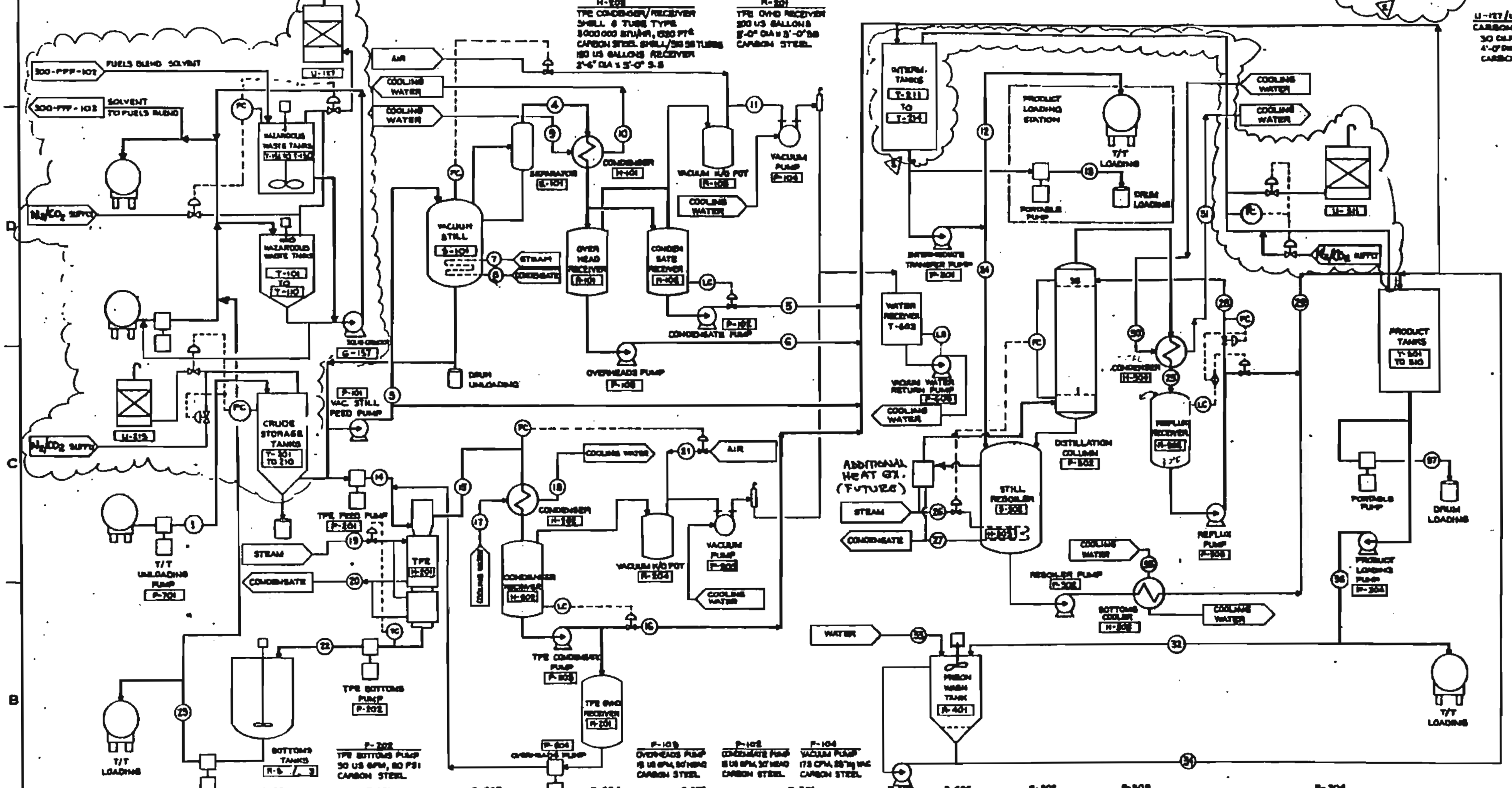
R-305
REFLUX RECEIVER
150 US GALLONS
2'-6" DIA x 5'-0" SS
304 STAINLESS STEEL

T-211 TO T-214
INTERMEDIATE STORAGE TANKS
5800 US GALLONS
8'-0" DIA x 15'-6" SS
304 STAINLESS STEEL
△2

H-202
TFE CONDENSER/RECEIVER
SHELL & TUBE TYPE
3000000 BTU/HR, 1020 FT²
CARBON STEEL SHELL/316 SS TUBES
150 US GALLONS RECEIVER
2'-6" DIA x 5'-0" S.S

R-201
TFE OVHD RECEIVER
200 US GALLONS
3'-0" DIA x 3'-0" SS
CARBON STEEL

U-127/U-215/U-311
CARBON ADSORBER
30 CU.FT ACTIVATED CARBON
4'-0" DIA x 4'-0" SS
CARBON STEEL



P-202
TFE BOTTOMS PUMP
30 US GPM, 80 PSI
CARBON STEEL

P-103
OVERHEADS PUMP
15 US GPM, 50' HEAD
CARBON STEEL

P-102
CONDENSATE PUMP
5 US GPM, 50' HEAD
CARBON STEEL

P-104
VACUUM PUMP
173 CFM, 28" Hg VAC
CARBON STEEL

P-701
T/T UNLOADING PUMP
100 US GPM, 80 PSI
CARBON STEEL

P-201
TFE FEED PUMP
30 US GPM 80 PSI
CARBON STEEL

P-101
VACUUM STILL FEED PUMP
100 US GPM, 80' HEAD
CARBON STEEL

P-203
TFE CONDENSATE PUMP
20 US GPM, 35' HEAD
CARBON STEEL

P-204
OVERHEADS PUMP
30 US GPM, 80 PSI
CARBON STEEL

P-205
VACUUM PUMP
173 CFM, 28" Hg VAC
CARBON STEEL

P-301
INTERM. TRANSFER PUMP
250 US GPM,
CARBON STEEL

P-402
WASHER PUMP
100 US GPM,
45' HEAD
CARBON STEEL

P-406
VACUUM WATER RETURN PUMP
25 US GPM, 45' HEAD
CARBON STEEL

P-302
REBOILER PUMP
100 US GPM, 30' HEAD
CARBON STEEL

P-303
REFLUX PUMP
30 US GPM, 50' HEAD
CARBON STEEL

P-304
PRODUCT LOADING PUMP
250 US GPM.
CARBON STEEL

K3

	T/T UNLOADING ①		VAC. STILL FEED ③	STILL VAPOUR ④	STILL PRODUCT ⑤	STILL OV'D ⑥	STEAM ⑦	CONDENSATE ⑧	WATER IN ⑨	WATER OUT ⑩	VENT ⑪	T/T LOADING ⑫	DRUM LOADING ⑬	TFE FEED ⑭	TFE OV'D ⑮	TFE PRODUCT ⑯	WATER IN ⑰	WATER OUT ⑱	STEAM ⑲	CONDENSATE ⑳	VENT ㉑	TFE BOTTOMS ㉒	T/T LOADING ㉓	INT TRANSF ㉔	COLUMN PRODUCT ㉕	STEAM ㉖	CONDENSATE ㉗	REFLUX ㉘	PRODUCT ㉙	WATER IN ㉚	WATER OUT ㉛	WASHER ㉜	WATER ㉝	WASHER TRANSF ㉞	COOLING WATER ㉟	T/T FEED ㊱	DRUM LOADING ㊲
DESIGN FLOW RATE CFM	—		—	320	—	—	45	—	—	—	170	—	—	—	1163	—	—	—	200	—	170	—	—	—	—	220	—	—	—	—	—	—	—	—	—	—	—
DESIGN FLOW RATE GPM	100		100	—	8.9	18	—	1.7	100	100	—	250	25	20	—	14	300	300	—	8.8	—	6	250	250	40	—	9.0	20	20	450	450	250	25	100	495	250	25
DESIGN FLOW RATE LBS/HR	42500		42500	4000	4600	6780	860	800	50000	50000	88	112500	11250	8800	4300	6500	150000	150000	4100	4100	88	3000	125000	112500	18000	4500	4500	9000	9000	225000	225000	112500	12500	45000	247500	112500	11250
TEMPERATURE °F	AMBIENT		AMBIENT	200	90	90	360	360	85	105	90	AMBIENT	AMBIENT	AMBIENT	200	90	85	105	360	360	90	200	AMBIENT	AMBIENT	90	360	360	90	90	85	105	AMBIENT	90	AMBIENT	85		
PRESS. PSIG (IN. HG VAC.)	15		10	(18)	10	10	140	140	30	40	(28)	10	10	10	(18)	10	30	40	140	140	(28)	20	10	15	5	140	140	40	40	80	40	80	50	20	60		
S.G.	0.86		0.85	0.90	0.90	0.90	—	1.0	1.0	1.0	—	0.90	0.90	0.85	0.90	0.90	1.0	1.0	—	—	—	1.0	1.0	0.90	0.90	—	—	0.90	0.90	1.0	1.0	0.90	1.0	0.90	1.0		

SOLVENT RECOVERY PLANT
PROCESS FLOWSHEET

CLIENT TRICIL RECOVERY SERVICES INC. (TRSI)

TRICIL

Figure 3

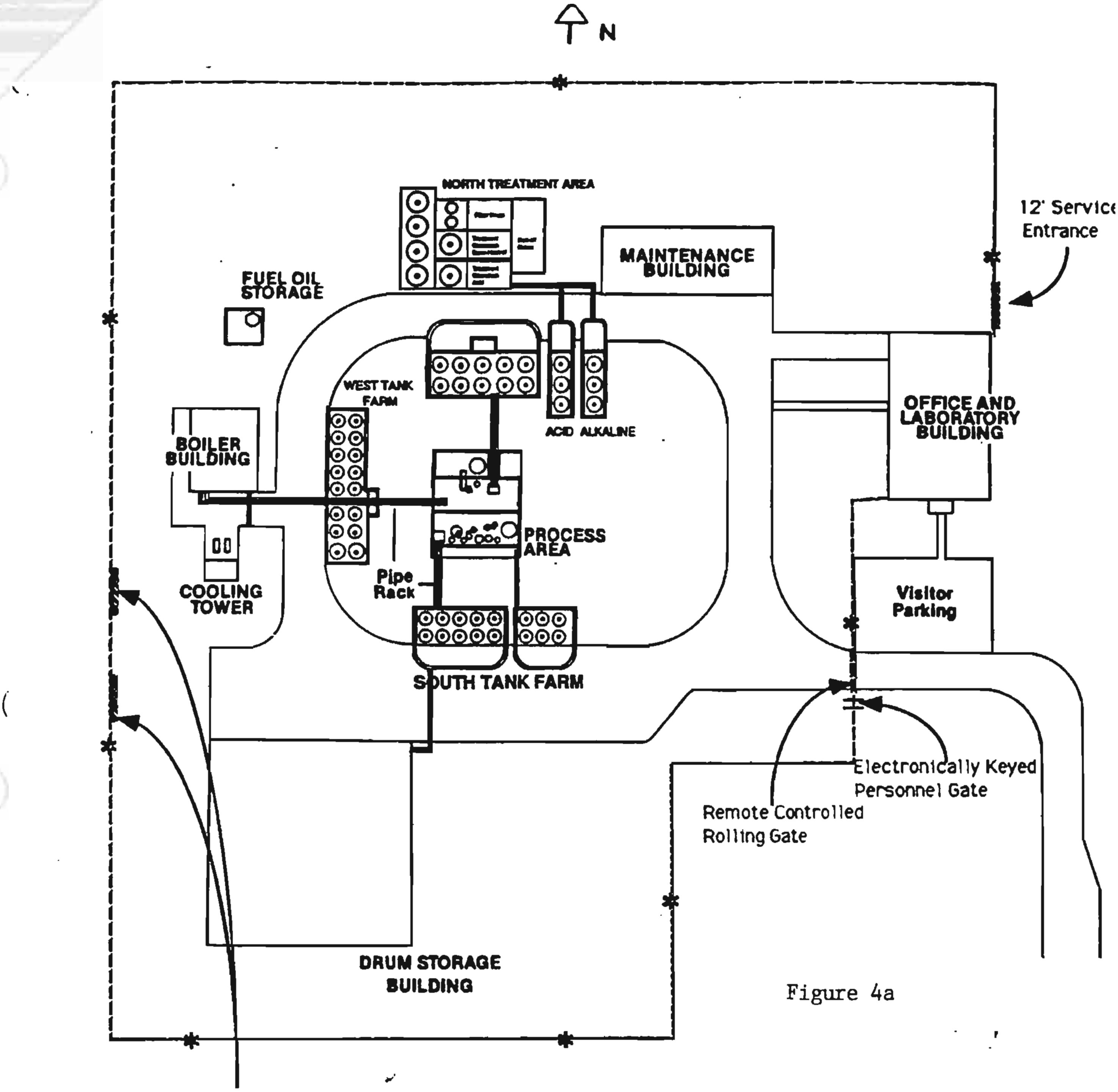
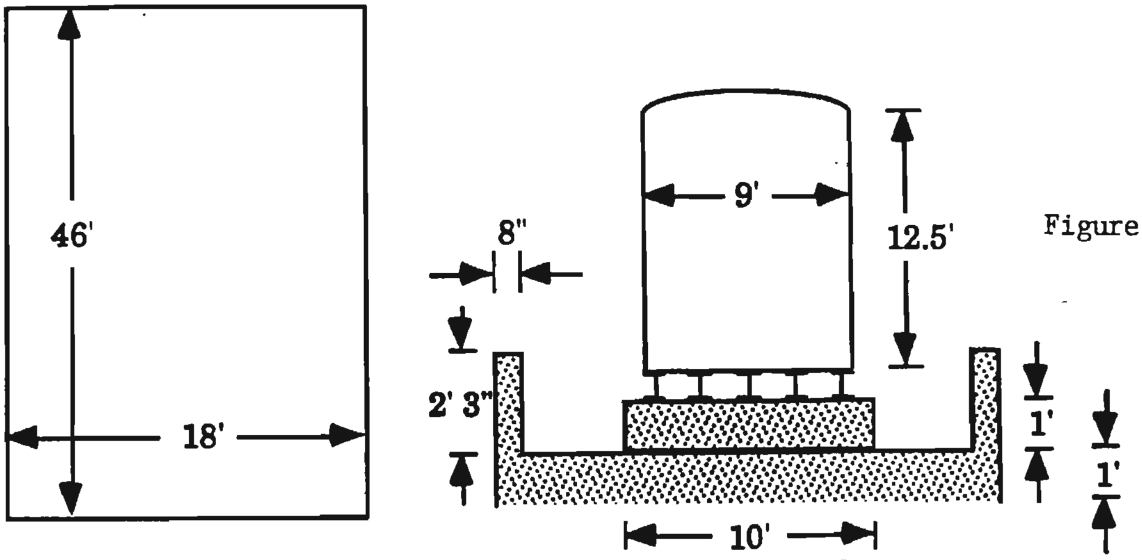


Figure 4a



6,000-gallon tanks

Figure 4b

Figure 5

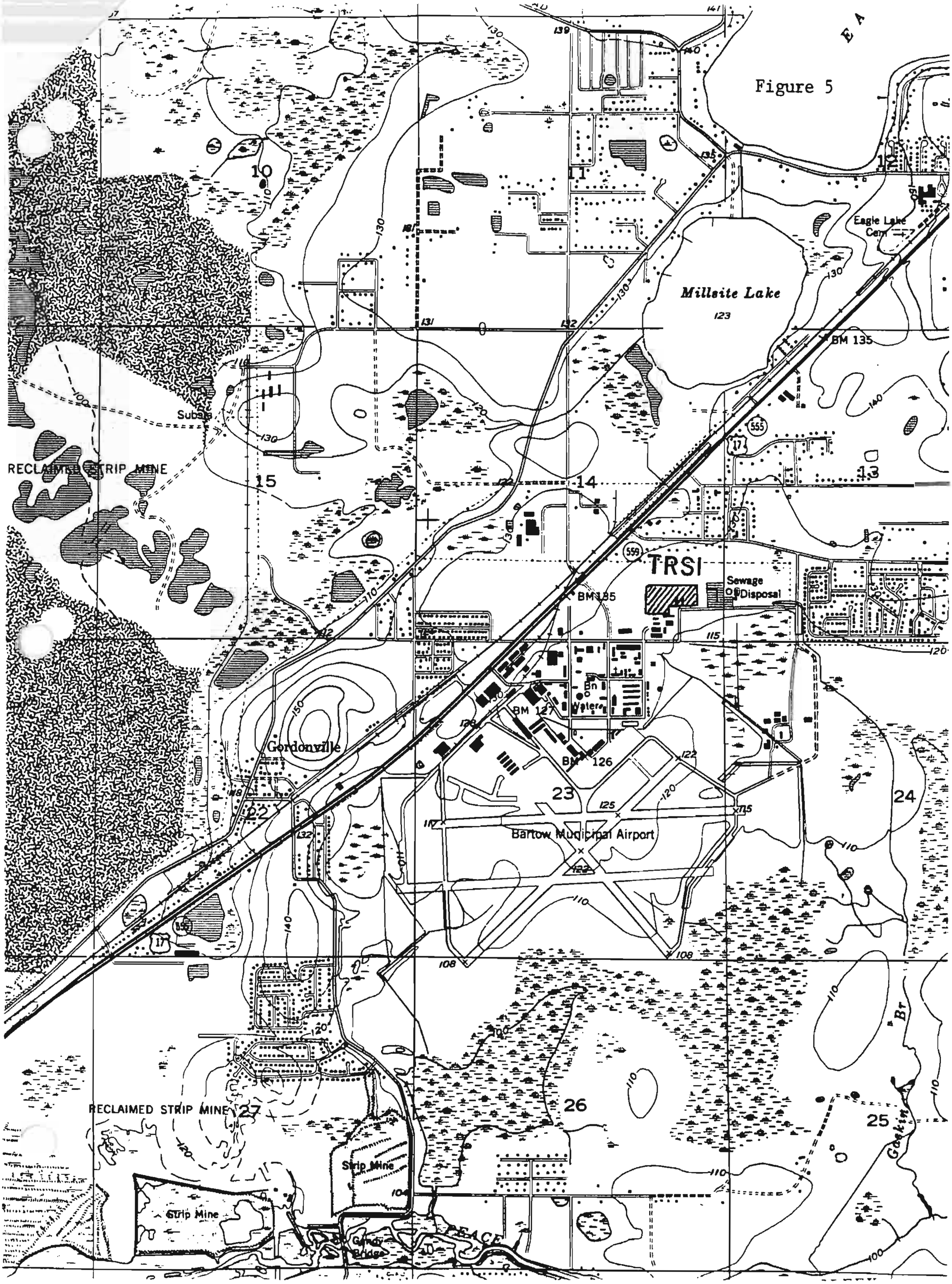

Millsite Lake
123
Eagle Lake Cem
BM 135
TRSI
Sewage Disposal
BM 135
BM 127
BM 126
Bn
Water
Bartow Municipal Airport
Gordonville
Substa
RECLAIMED STRIP MINE
RECLAIMED STRIP MINE
Strip Mine
Strip Mine
Gandy Bridge
PEACE
Goskin
Br
555
17
559
17
555
10
11
13
14
15
22
23
24
25
26
27
130
140
120
110
100

Figure 6a

STEADY STATE

SCREEN (T-SCREEN)
ISCST
COMPLEX
ISCDEP

"PUFF-TYPE"

SPILLS (SHELL)
INPUFF
TOXIC GAS
RVD

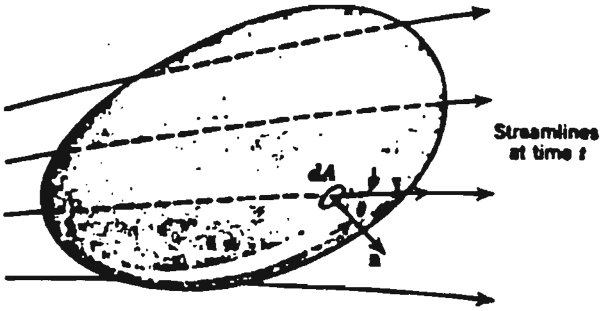
"PREDICTIVE"

ISCST

"RESPONSE"

CAMEO

Figure 6b



Fluid Flow Through a Control Volume.

$$\iint_{cs} \rho \, (\vec{u} \cdot \vec{n}) \, d\vec{A} + \frac{\delta}{\delta t} \iiint_{cv} \rho \, dV = 0$$

$$-\nabla \cdot (\rho D_{ab} \nabla w_a) + \nabla \cdot \rho_a \vec{u} + \frac{\delta}{\delta t} \rho_a - r_a = 0$$

$$\frac{\delta C}{\delta t} = -\frac{\delta}{\delta x}(Cu) + \frac{\delta}{\delta x}\left(\frac{\delta}{\delta x} D_x C\right) + \frac{\delta}{\delta y}\left(\frac{\delta}{\delta y} D_y C\right) + \frac{\delta}{\delta z}\left(\frac{\delta}{\delta z} D_z C\right) - r_a$$

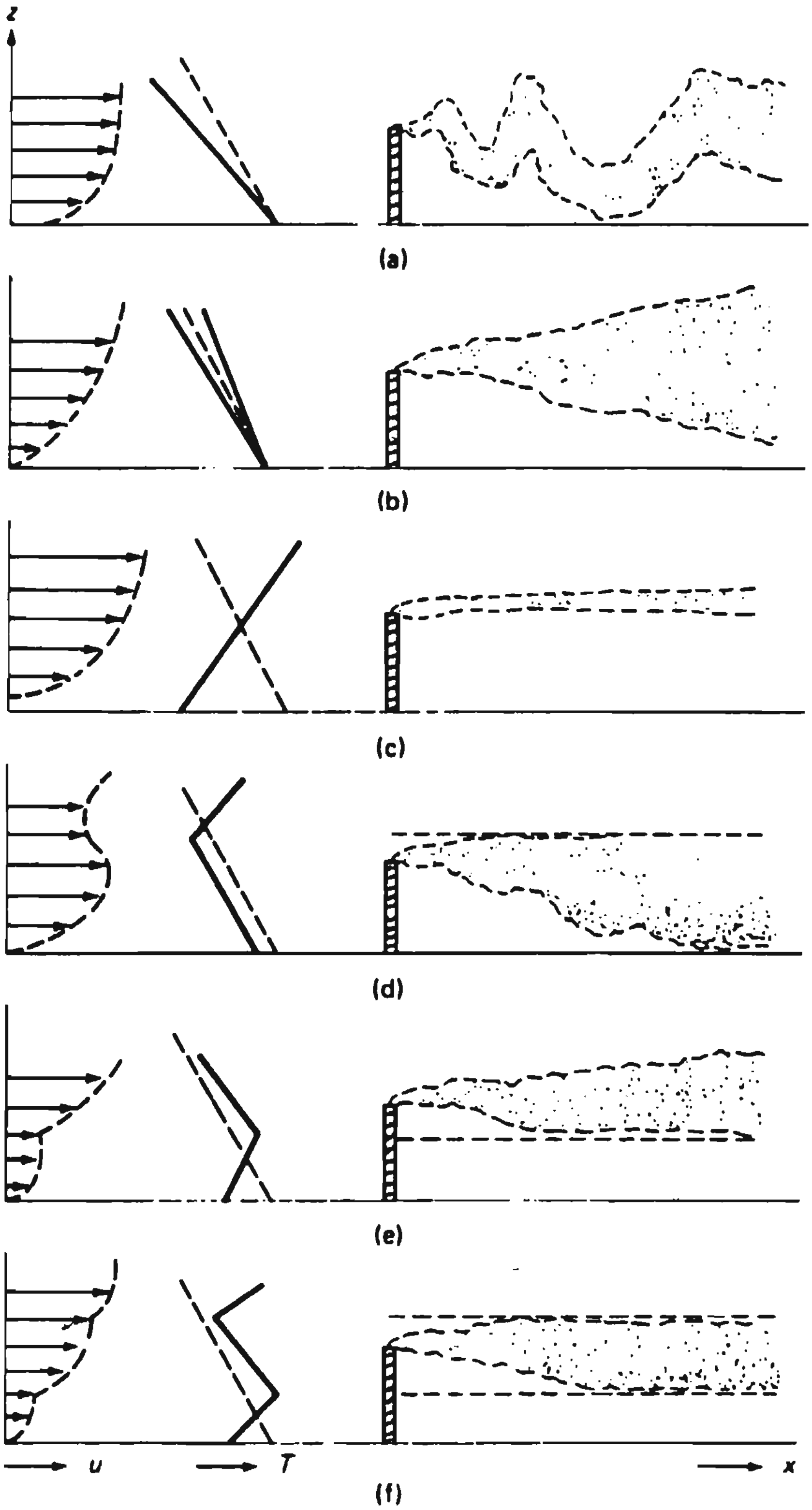


Figure 7 **Typical velocity profile, temperature profile, and plume shape in the x-z coordinate system for various atmospheric conditions. (Dry adiabatic lapse rate, - - -; ambient lapse rate, —.) (a) Looping, strong instability; (b) coning, near neutral stability; (c) fanning, surface inversion; (d) fumigation, aloft inversion; (e) lofting, inversion below stack; (f) trapping, inversion below and above stack height.**

Figure 8a

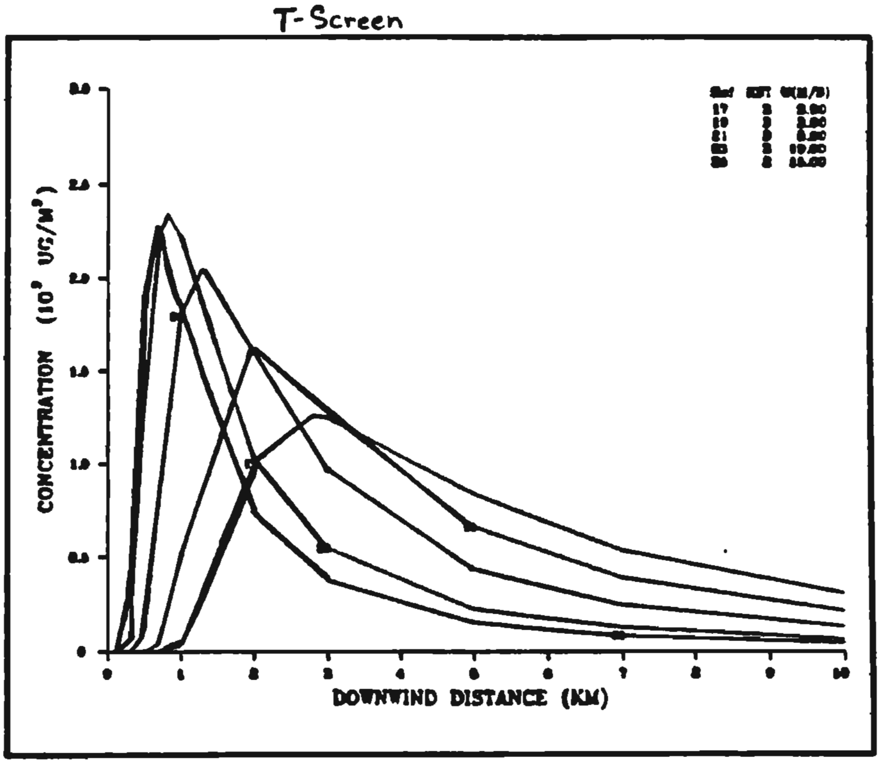
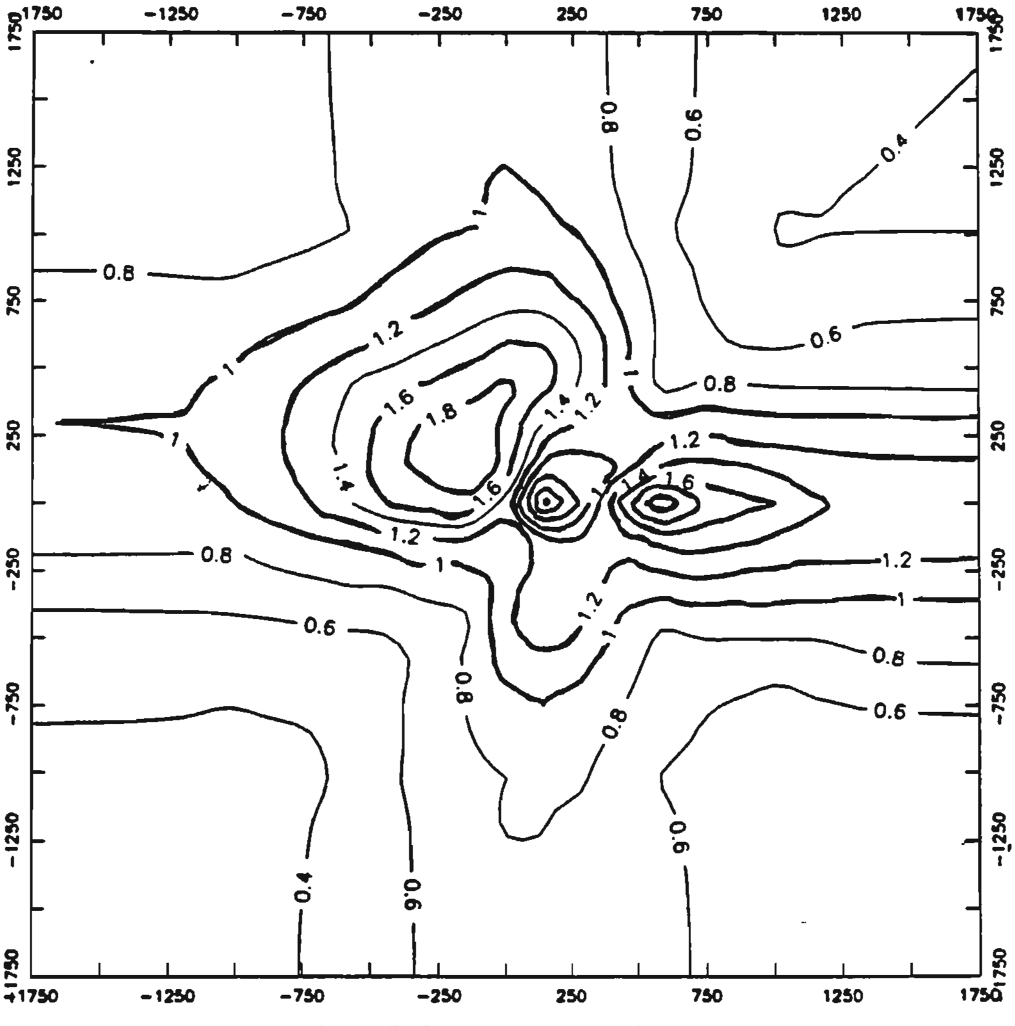


Figure 8b



HYPOTHETICAL POTASH PLANT

SCALE: 1 INCH = 500 Meters

(ISOPLETH VALUES IN MICROGRAMS PER CUBIC METER)

ISCST

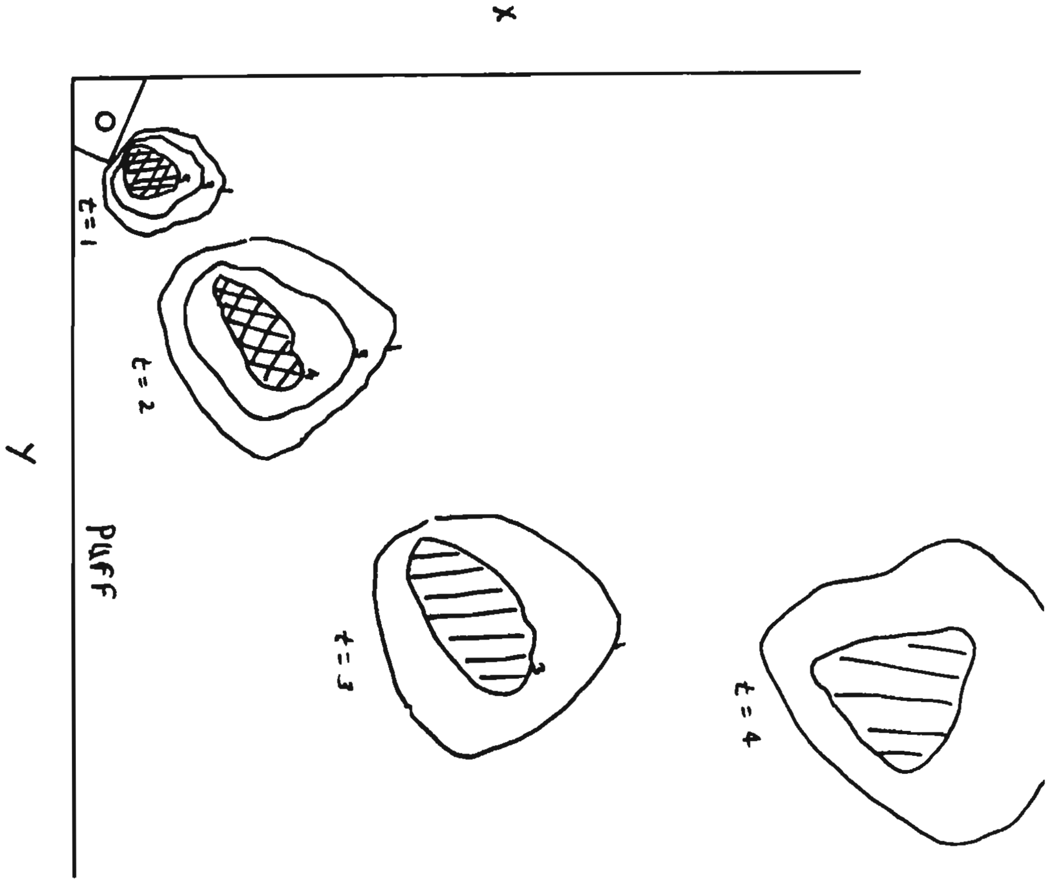


Figure 9a

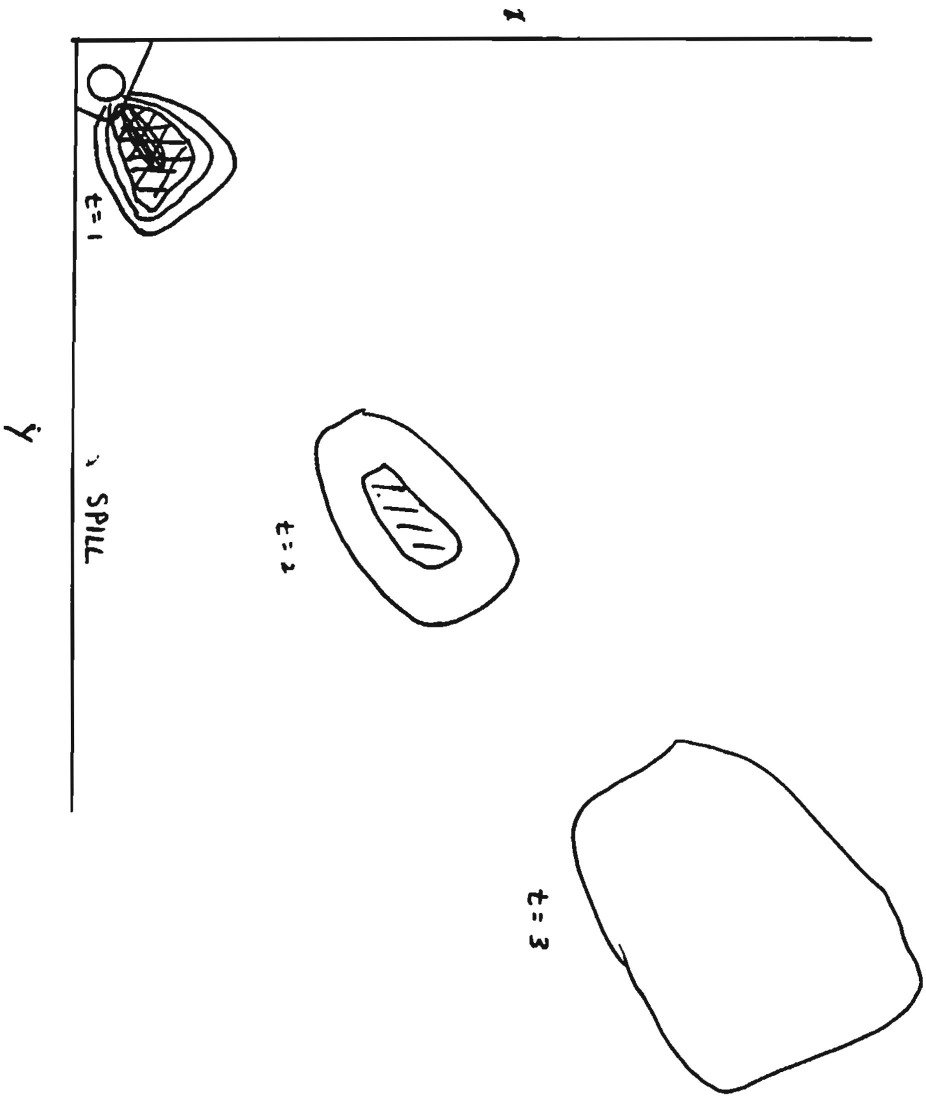


Figure 9b

Figure 10

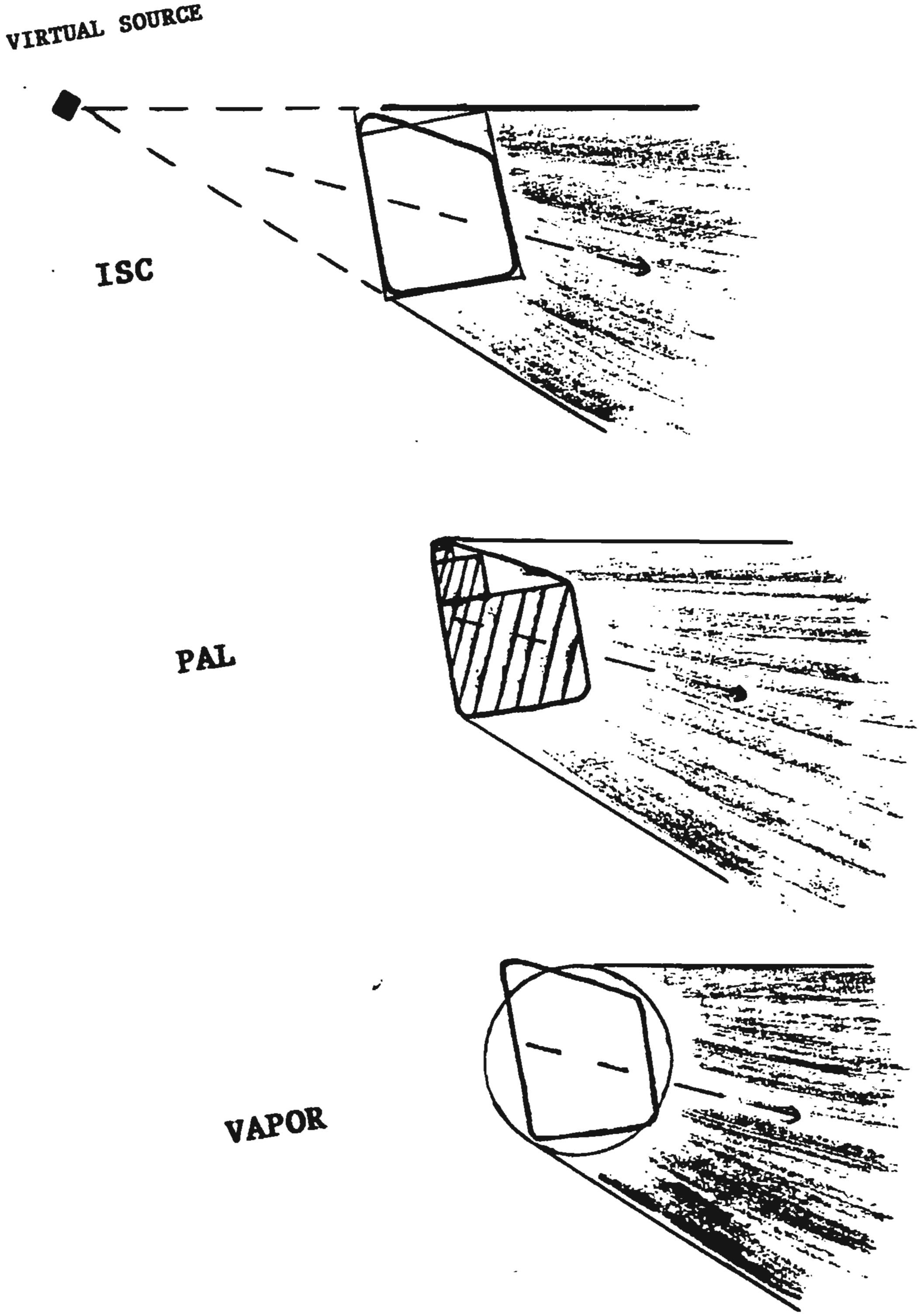


Figure 11
RECEPTOR CONCENTRATION ESTIMATES

Distance from Edge of Area Source, m	Model Results, gm/m^3				
	Vapor	ISC 1 Square	PAL	ISC 4 Square	ISC 16 Square
100	43	20	32	47	45
200	35	17	24	36	32
300	30	15	20	29	25
400	26	14	17	24	20
500	23	13	15	20	18
600	21	12	14	18	16
700	19	11	12	16	14
800	18	10	11	15	13
900	17	10	10.5	13	12
1000	16	9	10	12	11