The Application of 3D QRA Technique to the Fire/Explosion Simulation and Hazard Mitigation within a Naphtha-Cracking Process

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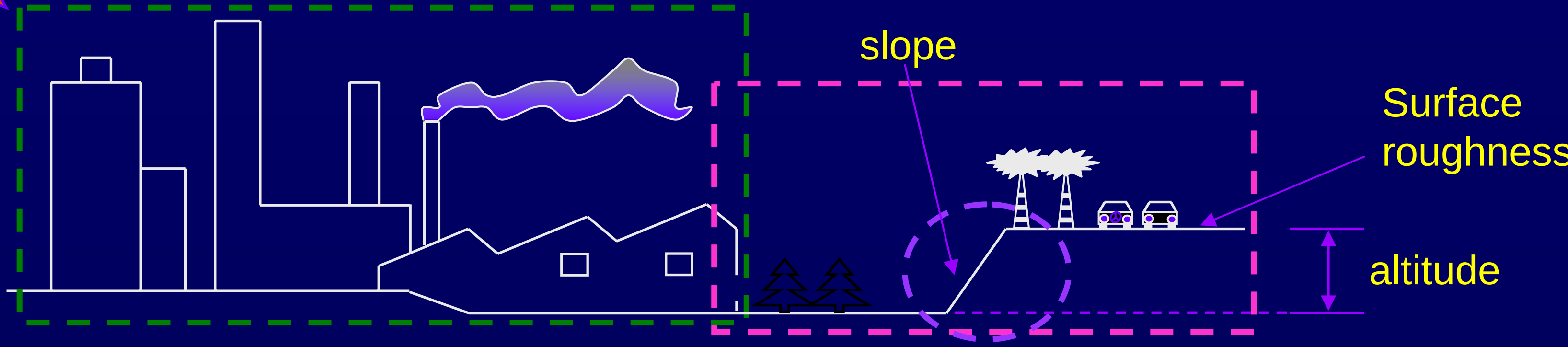
Preface

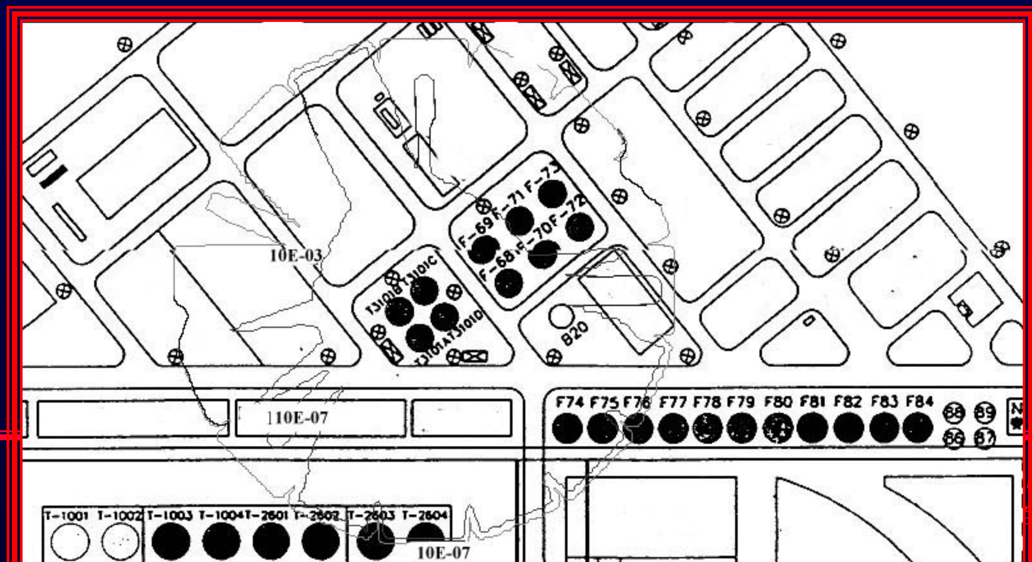
- Owing to the continuous growth of global population, the requirement of raw materials and energy has also increased during the past decades. The petrochemical industry, which supports the daily life of human beings, also becomes more prosperous and even larger at the same time. Common petrochemical plants usually have complex producing processes and store a large amount of hazardous substances.

- A very serious consequence such as flammable and explosive accident may happen once these substances are ignited accidentally; therefore, people have to pay close attention to the environment and public security problems for the industry.

Preface (cont.)

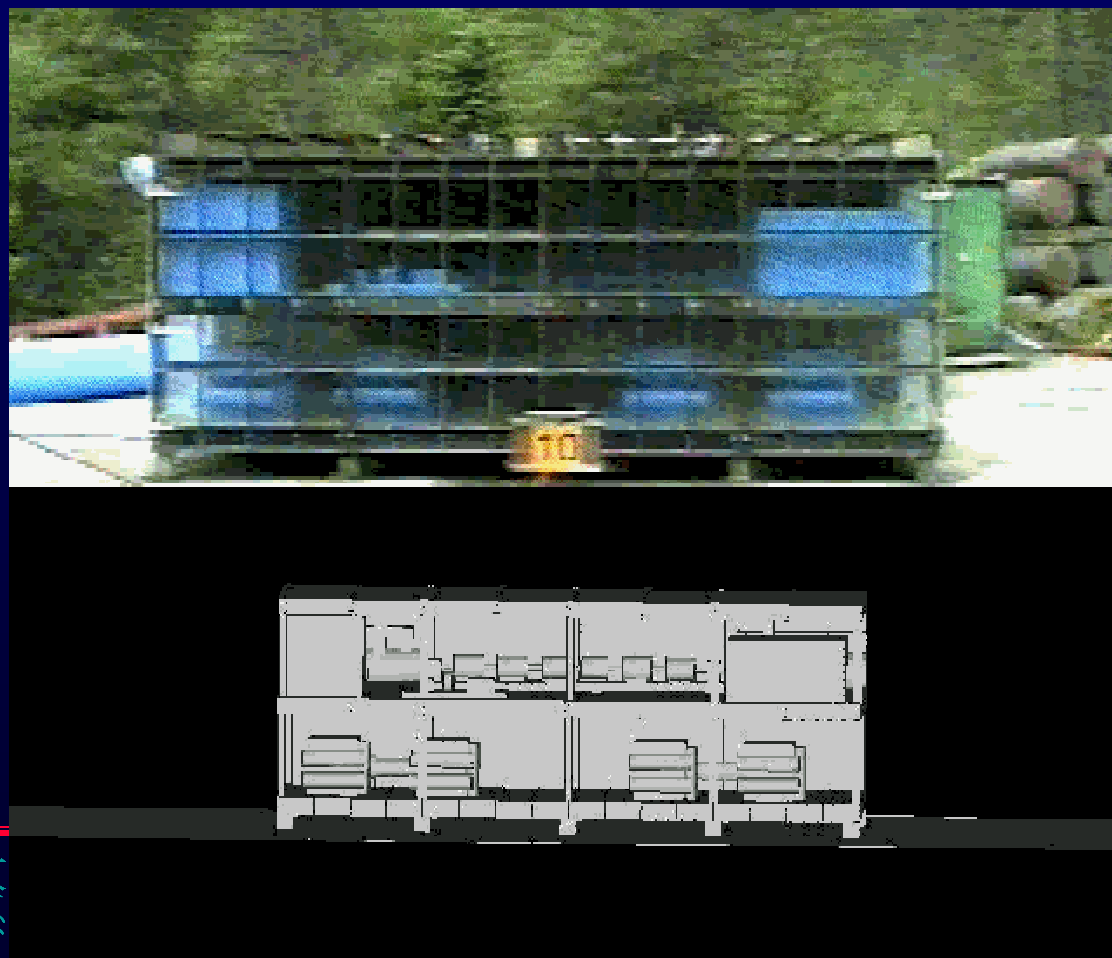


- The traditional risk analysis technique (such as SAFETI etc.) can only predict two-dimensional personnel risk within certain process area; it usually neglected the influence of building blockage and terrain effect therefore its simulation results were quite different from the real situations.



Preface (cont.)

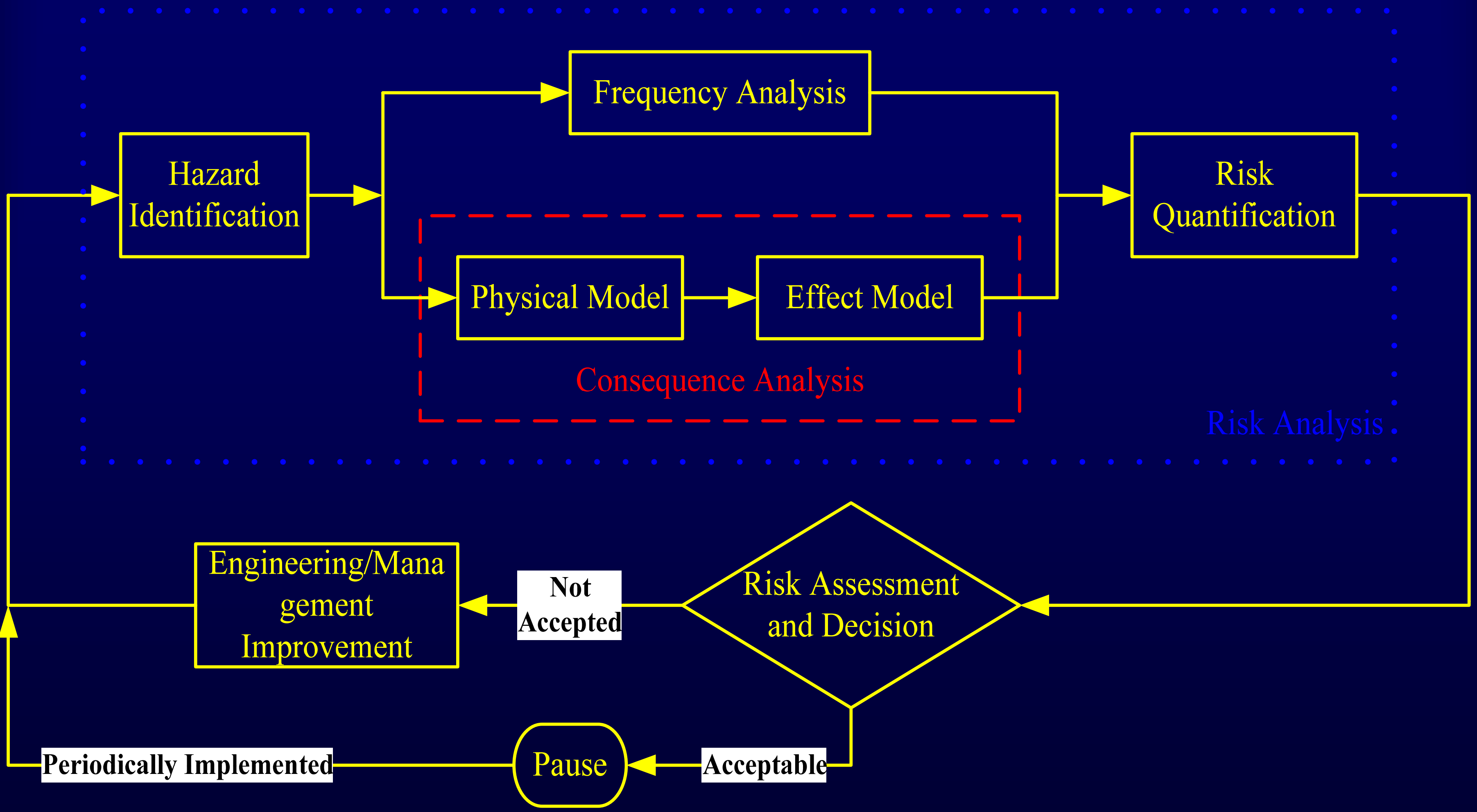
- A more rigorous model such as CFD (computational fluid dynamics) can resolve the previous limitations; however, it didn't find out a proper way to handle the complexity of risk calculation.



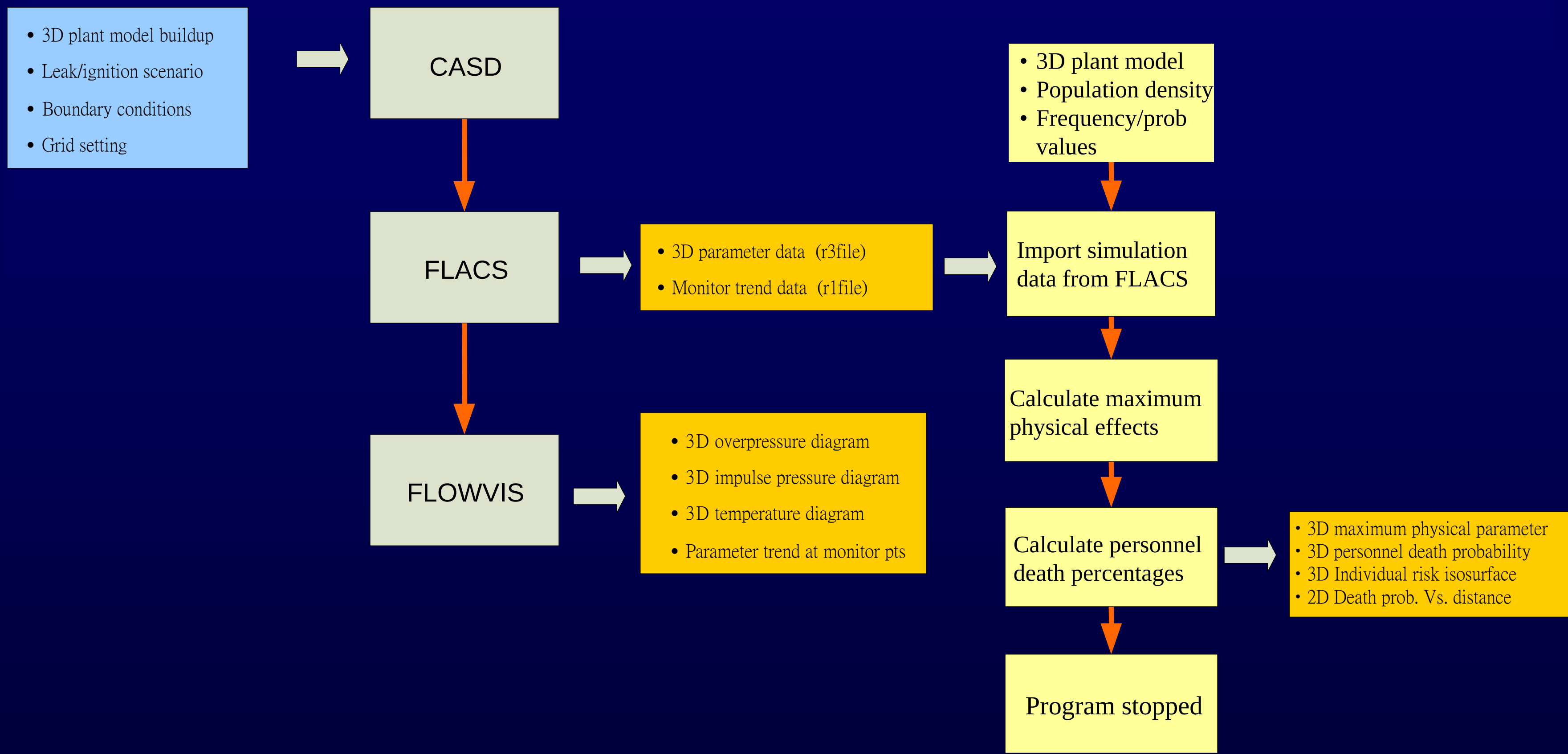
Preface (cont.)

- A 3D risk analysis technique was developed in this research via combing the results of CFD simulations with some post-processing procedures and was applied on a fire and explosion simulation within a petrochemical plant's process area.

Research method



Research method (cont.)



Physical model (FLACS)

Effect model +
risk analysis module

(1) Physical Model

- FLACS software was employed as the physical model to calculate all kinds of fire & explosion consequences (P, J, T…)
- FLACS is a kind of CFD (computational fluid dynamics) software, it includes 3 parts:
  - CASD (computer aided scenario design)
  - flacs (flame acceleration simulator)
  - FLOWVIS (flow visualization)
- The 3D, real time simulation results can be shown in the movie files

(2) Effect Model

- This research used CVF6.6 and MATFOR graphical library to develop the "effect model" and the "risk analysis module"

- In order to predict the maximum hazard impact degree within the hazard impact area, the "maximum physical effects" in each coordinate (x, y, z) within hazard elapse time were selected to convert the time dependent variables (P(x, y, z, t), J(x, y, z, t), and T(x, y, z, t)) into time independent variables via Eq(1)

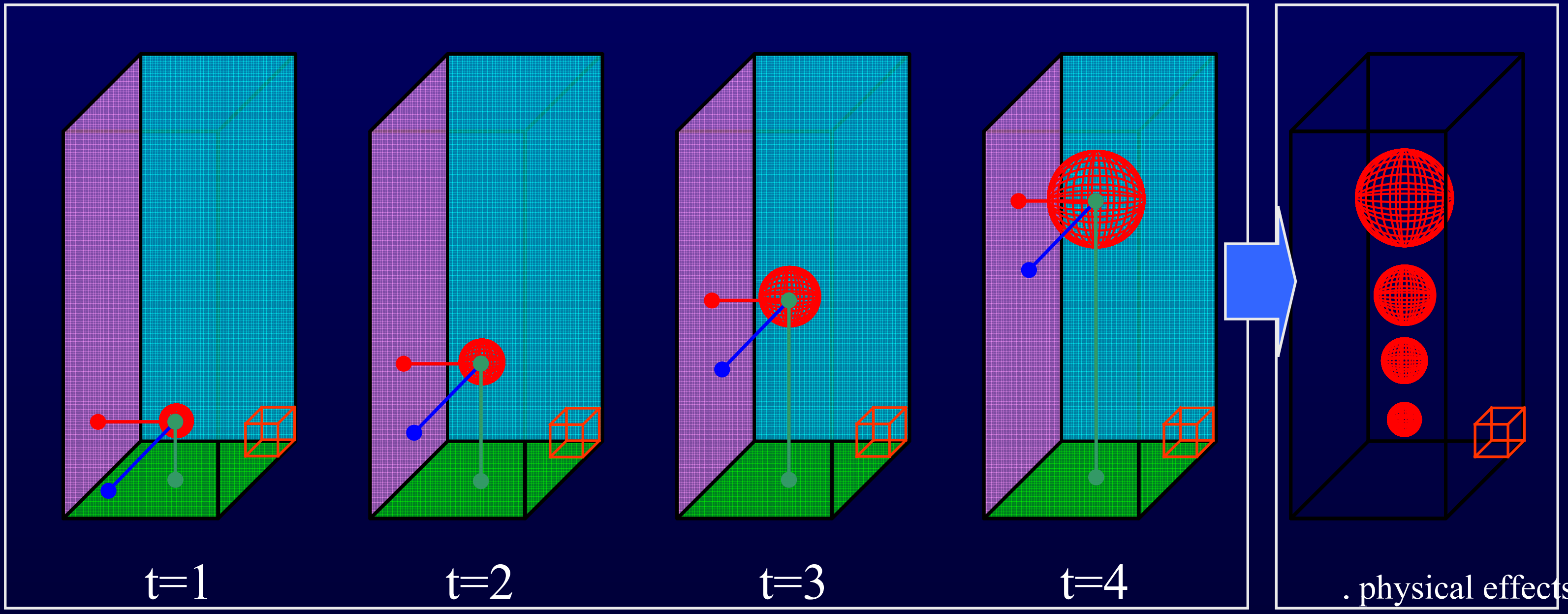
$$F_{\max}\left(x,y,z\right) = \underset{t_0 \le t \le t_f}{Max}\, F\left(x,y,z,t\right) \qquad (1)$$

- $T_{max}(x, y, z)$ will later be converted into "radiation heat" via Eq(2).

$$I_{\max}\left(x,y,z\right) = 5.67\times 10^{-8}\left(T_{\max}^{4}\left(x,y,z\right) - T_{a}^{4}\right) \qquad (2)$$

Maximum physical effects

$$V_{\max}(x,y,z) = \underset{t=1\sim n}{Max}\, V(x,y,z,t)$$



FLACS

Risk analysis module

Death probability calculation

Physical quantity $\xrightarrow{(3)}$ Probit value $\xrightarrow{(4)}$ Death probability

Hazardous physical effects	FLACS output	Conversion formula	Probit function
Thermal radiation	K	$I_{x,y,z} = 5.67 \times 10^{-8}\left(T^4 - T_a^4\right)$	$Y_{x,y,z} = -14.9 + 2.56 \ln\left(\frac{t_e I_{x,y,z}^{4/3}}{10^4}\right)$
Over-pressure	barg		$Y_{x,y,z} = -77.1 + 6.91 \ln\left(P_{x,y,z}\right)$
Impulse pressure	Pa · s		$Y_{x,y,z} = -46.1 + 4.82 \ln\left(J_{x,y,z}\right)$

$$P_{Di}\left(x,y,z\right) = \frac{1}{\left(2\pi\right)^{1/2}} \int_{-\infty}^{Y_i(x,y,z)} \exp\left(-\frac{u^2}{2}\right) du$$

Frequency Analysis

- According to the previous research [I *et al.*, 1999], the common tank rupture frequency is between $2 \times 10^{-6} \sim 1 \times 10^{-5}$/yr

- Based on the published document and the experience, this research divided the incident frequency (F_I) into 3 categories,
  - possible ($F_I = 1 \times 10^{-5}$/yr)
  - impossible ($F_I = 1 \times 10^{-6}$ /yr), and
  - extremely impossible ($F_I = 1 \times 10^{-7}$ /yr)

Quantitative Risk Analysis

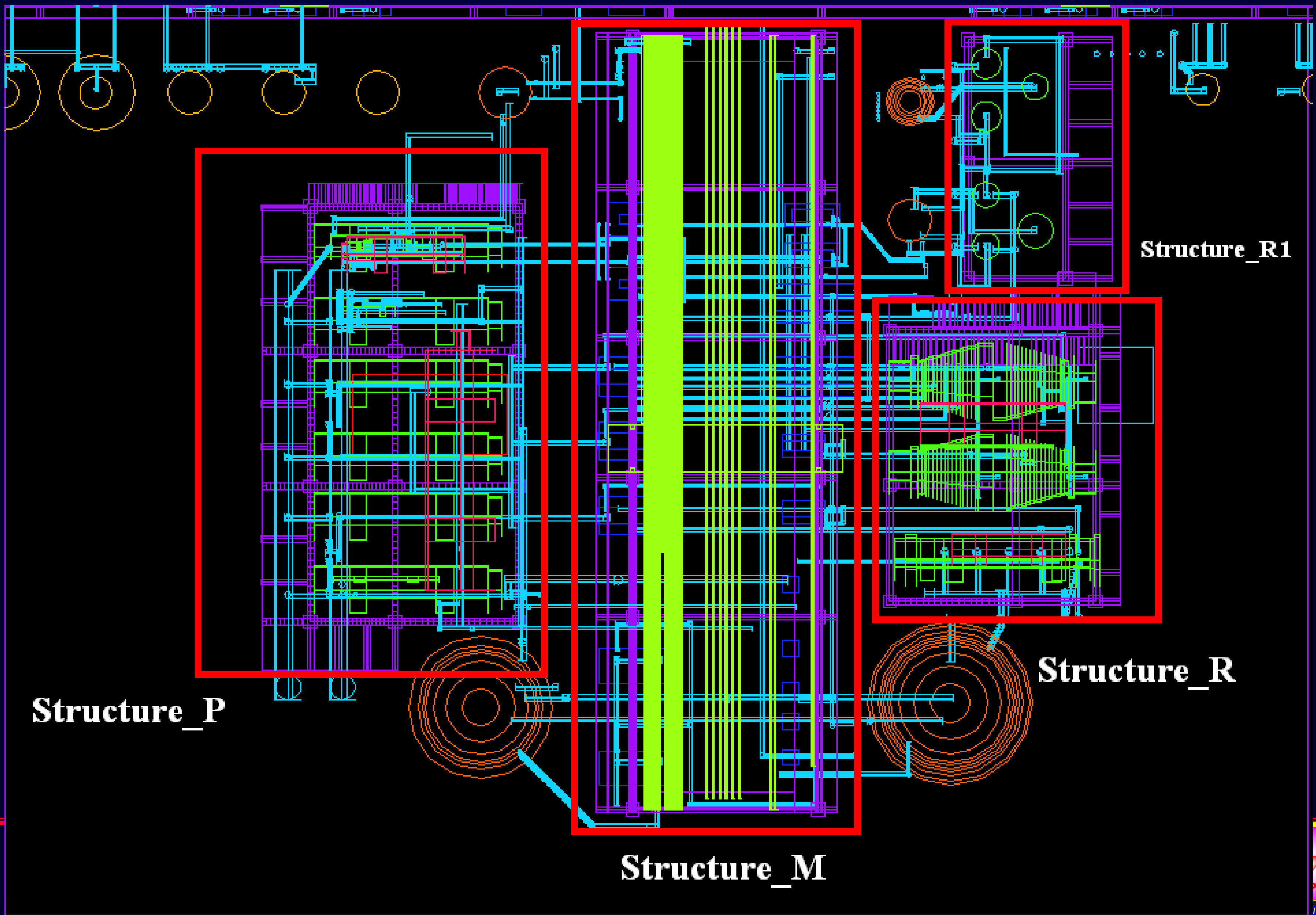
- 3D death percentage generated from effect model can be applied to predict the IR value by combining incident frequency, atmospheric conditions, and ignition probability, etc.; the total IR value is the cumulative summation of IR values under different hazardous physical effects from certain enumerated incidents as Eq(5)

$$IR(x,y,z)=\sum_{i=1}^{n} F_I P_I P_{WIND} P_{Z,i}(x,y,z) P_{D,i}(x,y,z) \qquad (5)$$

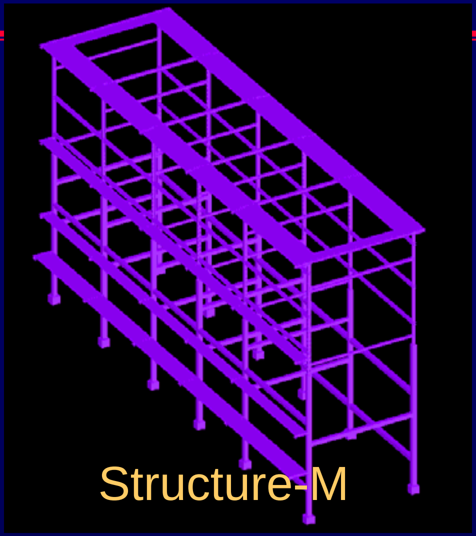
  - IR(x,y,z): the individual risk at specific location (x, y, z)
  - n: the number of the hazardous physical effect, the default effects are explosion overpressure (P), pressure impulse (J), and heat radiation (I)
  - F_I: incident frequency; P_I: ignition probability of the released cloud
  - P_{WIND}: probability of wind directions
  - $P_{Z,i}$ and $P_{D,i}$: personnel appearance probability & death percentage at coordinate (x, y, z)

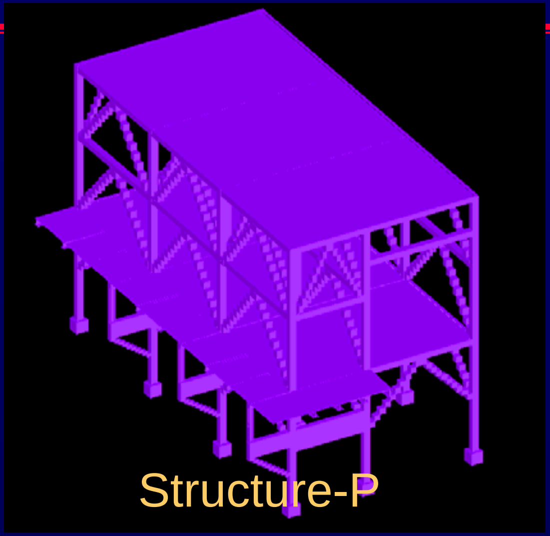
Introduction to the Simulation Site

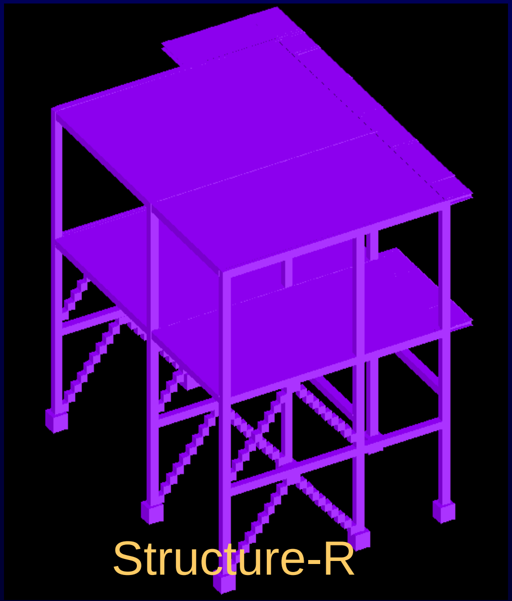
Fig. 1 Equipments layout of the simulation site

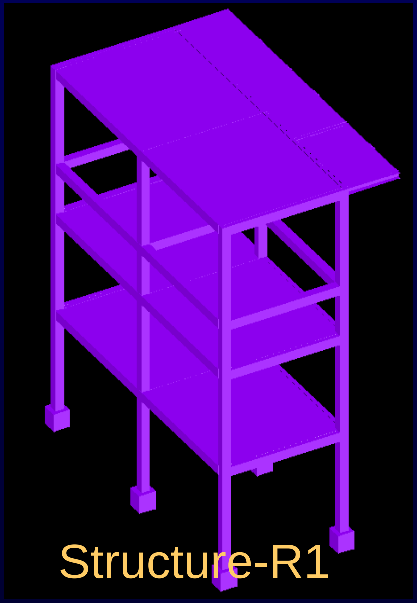


Structure

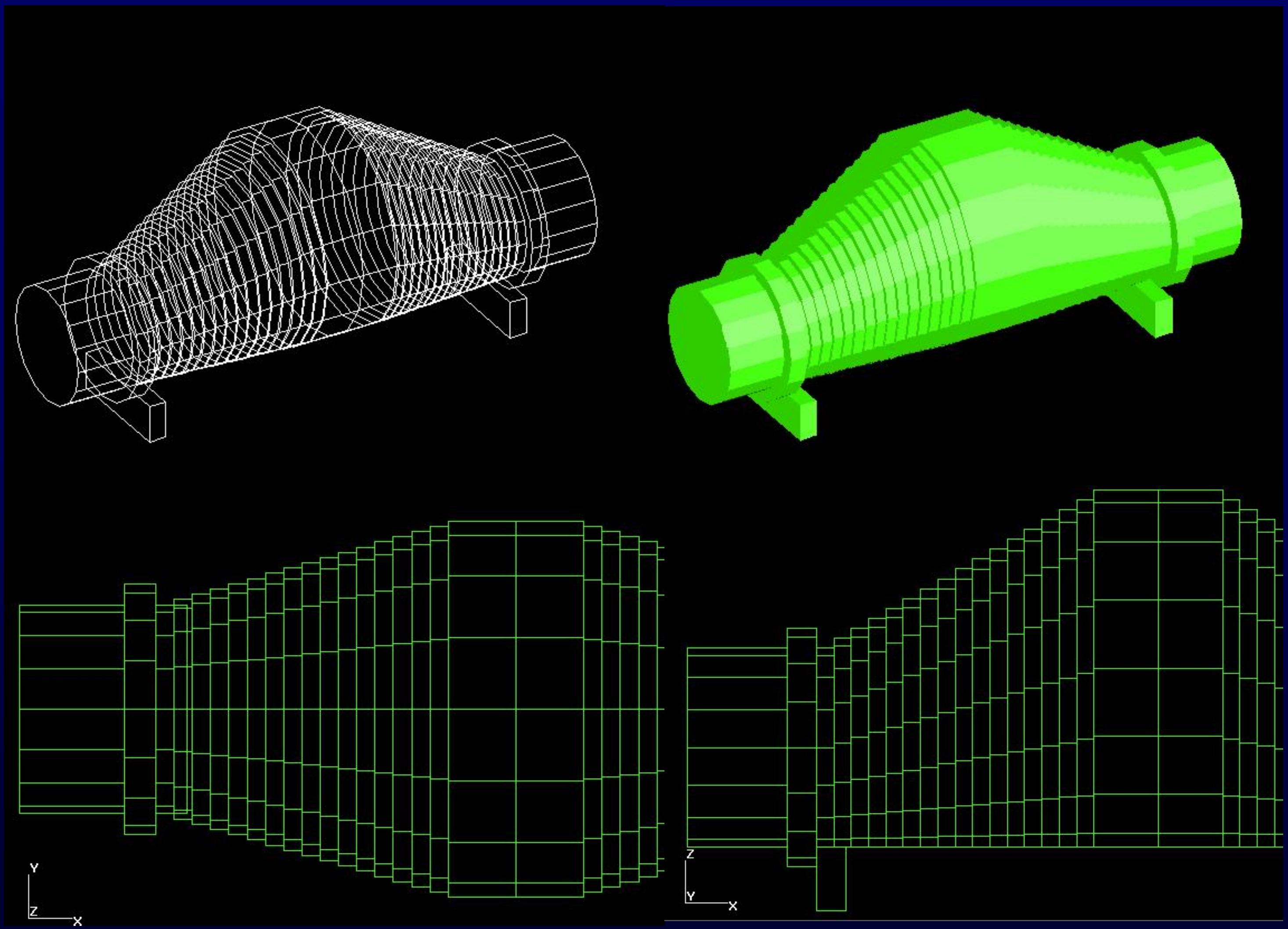




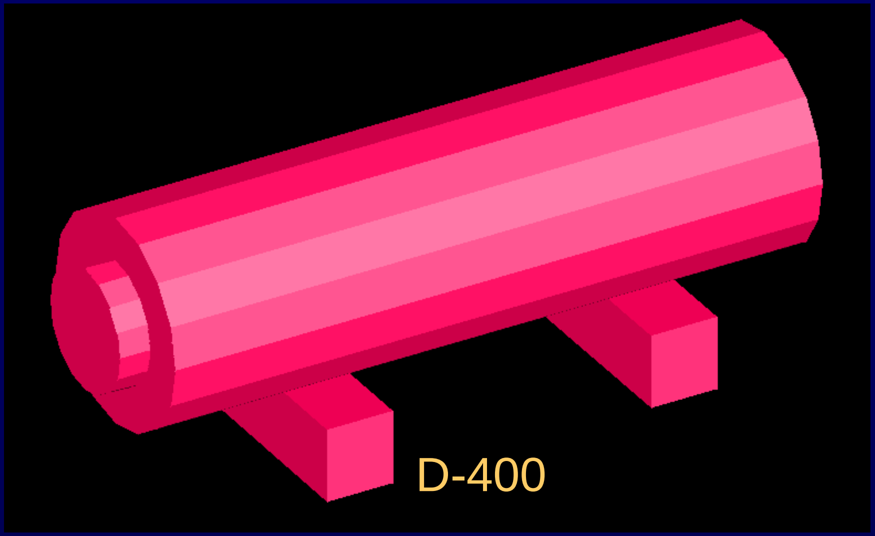


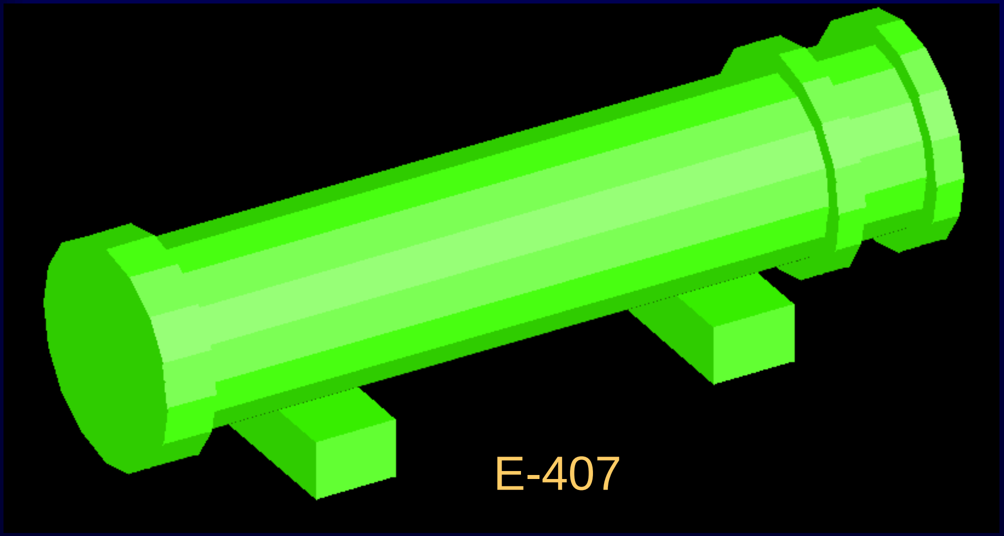


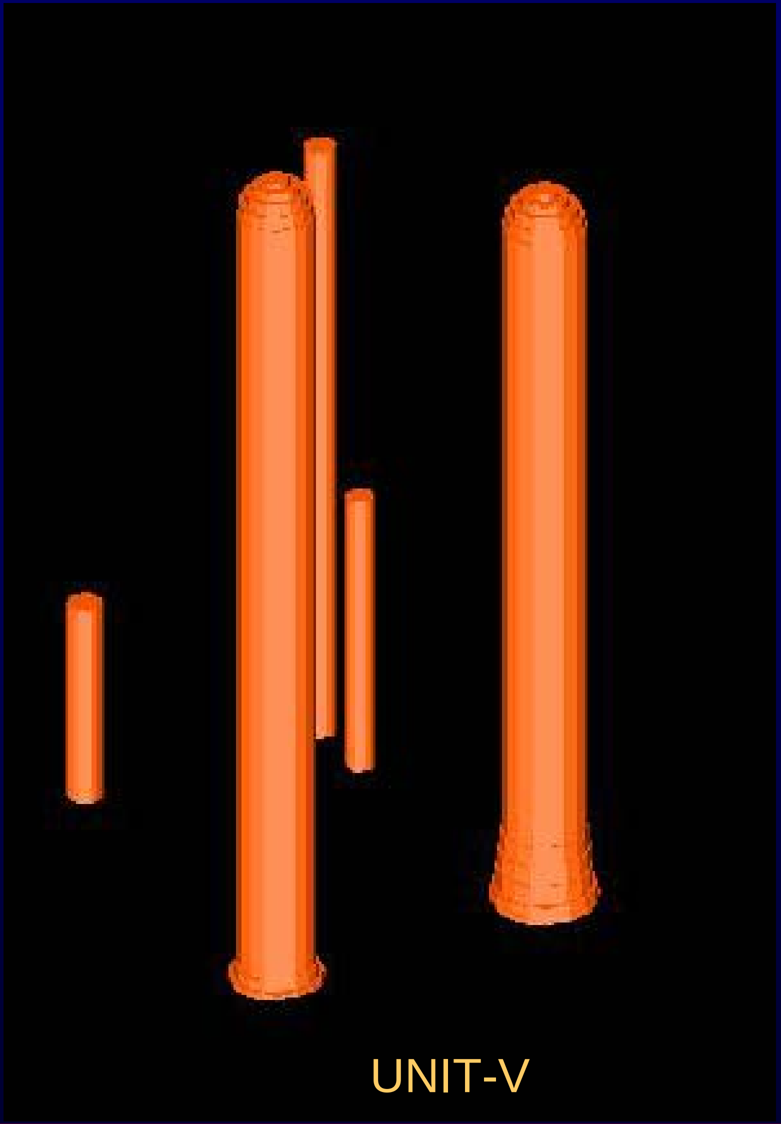
Equipments



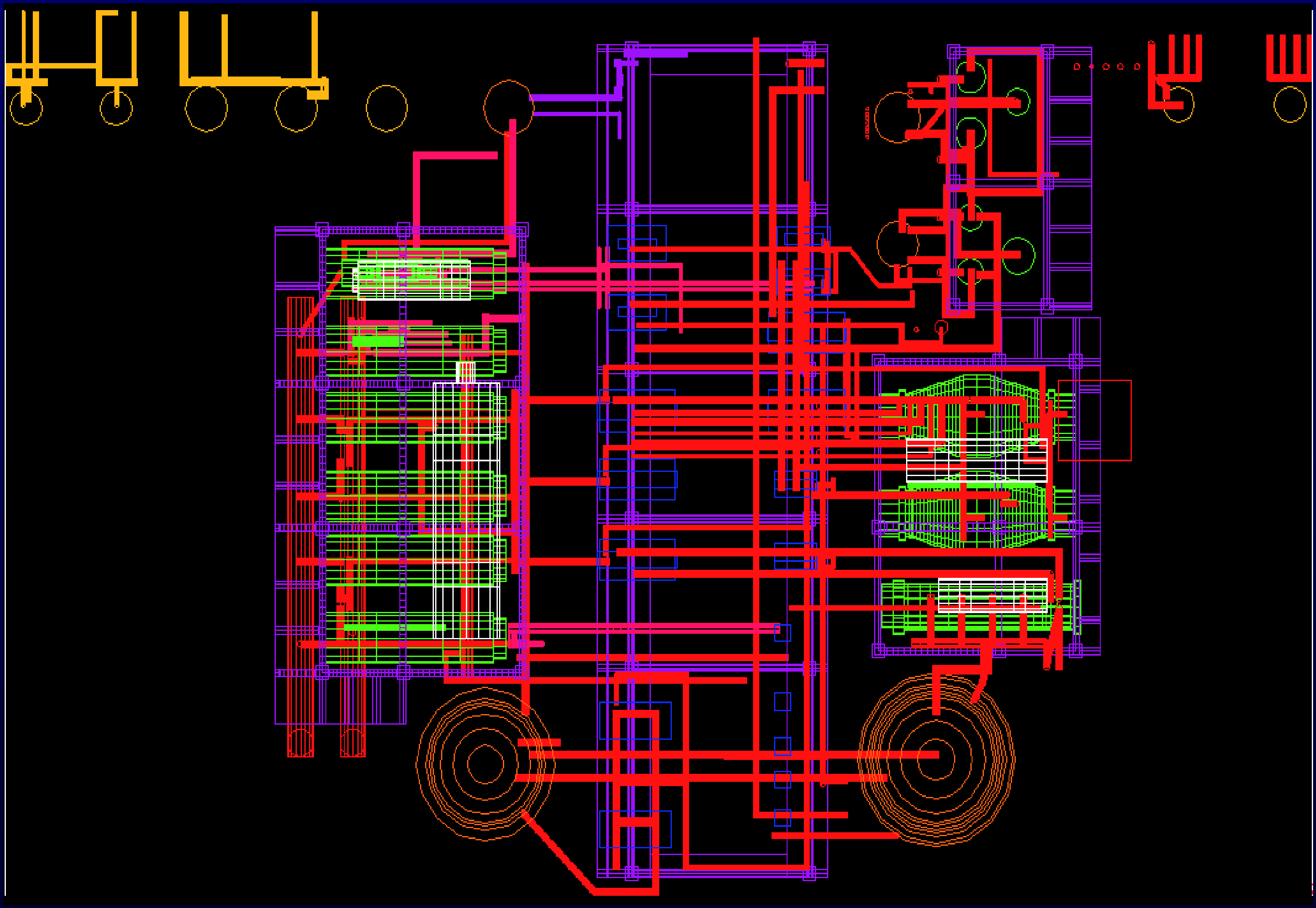
Equipments (cont.)



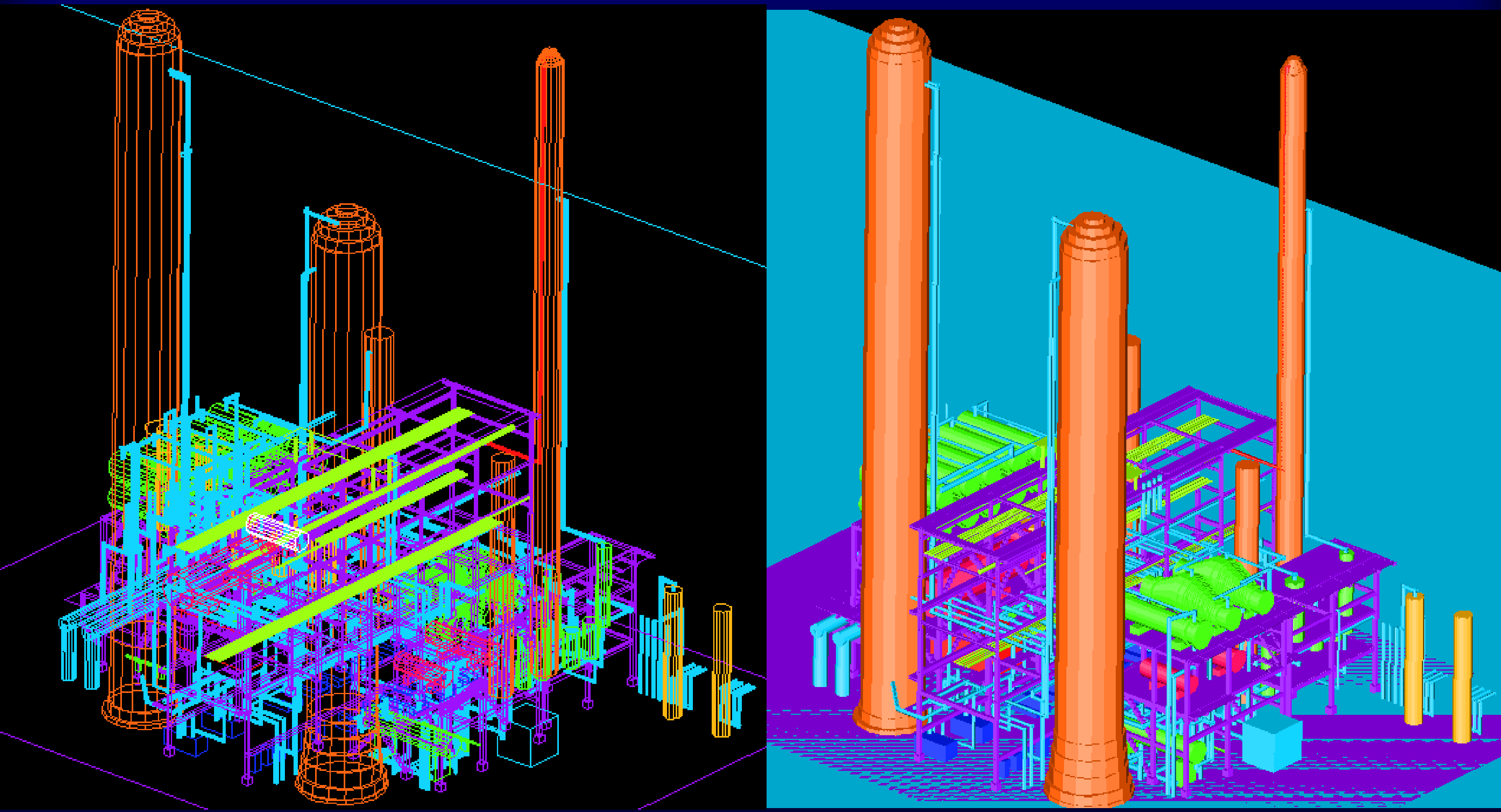




Pipeline



3D isometric diagram

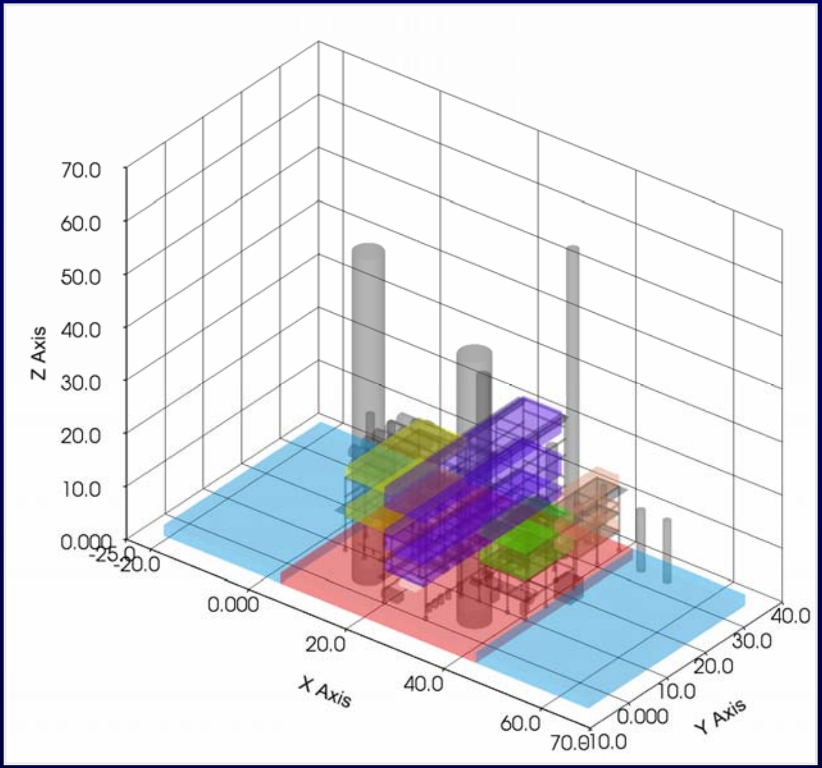


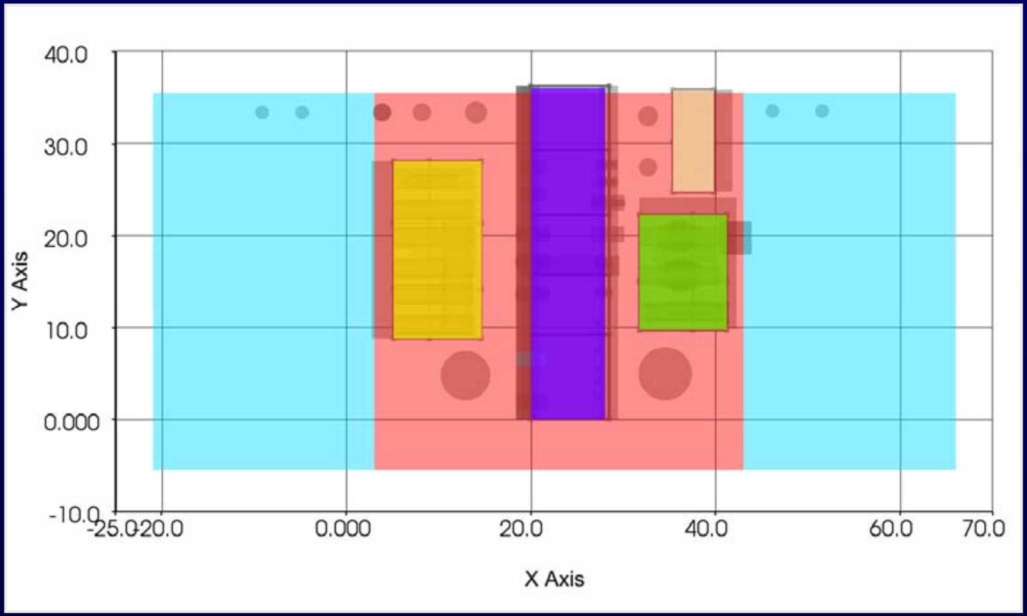
Modeling of simulation area

Population Distribution & Probability

Location	Coordinate range (grid number) ①	Number of person ②	Probability of appearance (Pz) ③	Population density (②×③/①)
Ground areas	(19:38, 15:36, 2:2)	3	0.081	6.09E-04
P-2F	(20:24, 23:31, 5:5)	3	0.081	6.57E-03
P-3F	(20:24, 23:31, 9:9)	3	0.081	6.75E-03
R-2F	(34:38, 23:29, 6:6)	3	0.081	8.10 E-03
R-3F	(34:38, 23:29, 8:8)	3	0.081	9.00 E-03
R1-2F	(36:38, 30:34, 4:4)	3	0.081	2.21E-02
R1-3F	(36:38, 30:34, 6:6)	3	0.081	1.87 E-02
R1-4F	(36:38, 30:34, 8:8)	3	0.081	1.62E-02
M-2F	(27:32, 18:34, 5:5)	2	0.038	2.24E-03
M-3F	(27:32, 18:34, 7:8)	2	0.038	1.12E-03
M-4F	(27:32, 18:34, 11:12)	2	0.038	1.12E-03
Vacant lots	(27:32, 18:34, 11:12)	1	0.008	3.03E-05

Population Distribution & Probability (cont.)



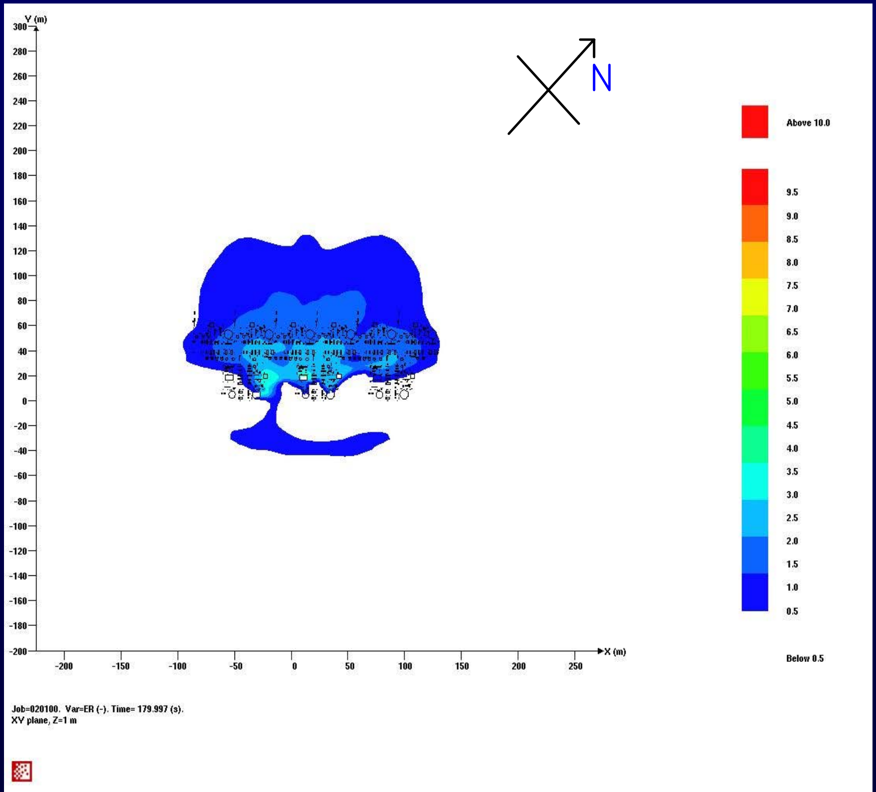


Wind probability (0.023%+0.08%)/2 =0.15%

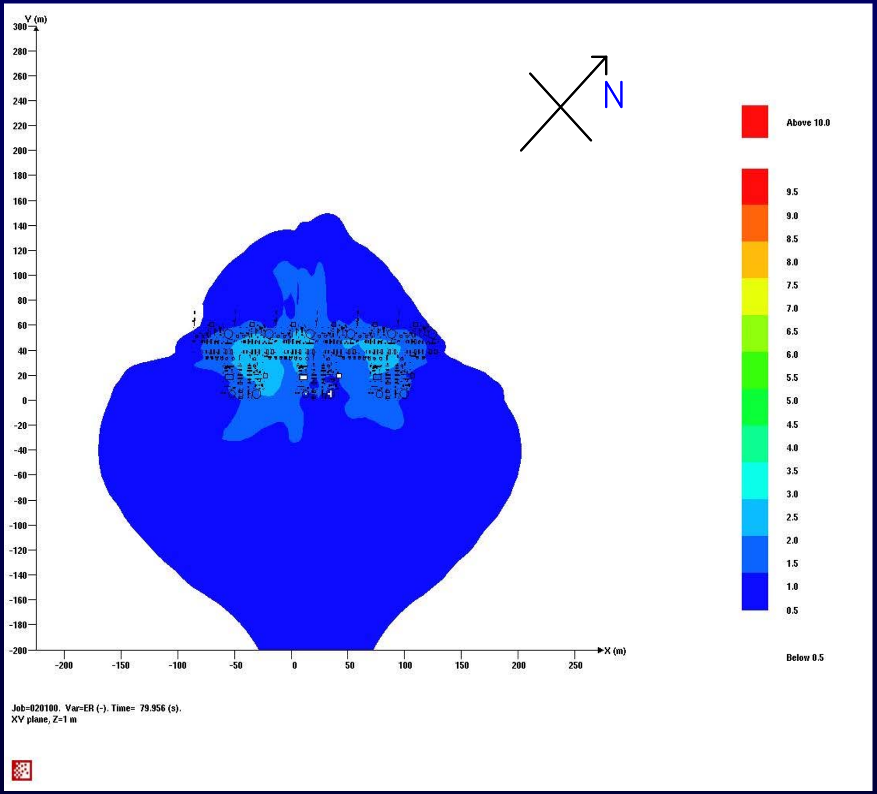
Speed (m/s) Direction	1.0 - 2.5	2.5 - 4.0	4.0 - 6.0	>6.0	Total	Calm
NNE	5.79	1.06	0.09	0.01	6.95	17.5
NE	4.43	0.42	0.05	0.01	4.91	
ENE	3.73	0.31	0.04	0	4.08	
E	2.77	0.2	0.03	0	3	
ESE	0.15	0.02	0.02	0	0.19	
SE	**0.23**	**0.08**	0.04	0.01	0.36	
SSE	1.66	2.19	1.46	0.35	5.66	
S	2.44	2.07	0.77	0.1	5.38	
SSW	1.19	0.44	0.03	0.01	1.67	
SW	0.93	0.59	0.08	0.03	1.63	
WSW	1.43	1.04	0.1	0.04	2.61	
W	3.24	3.77	0.45	0.08	7.54	
WNW	2.92	5.03	2.18	0.1	10.23	
NW	3.25	3.1	1.39	0.1	7.84	
NNW	3.41	1.91	0.47	0.11	5.9	
N	9.34	4.26	0.85	0.1	14.55	
Total	46.9	26.48	8.04	1.04	82.5	

Wind setting – SE wind (2.5m/s)

Gas cloud dispersion influenced by wind (Z=1m)



with wind

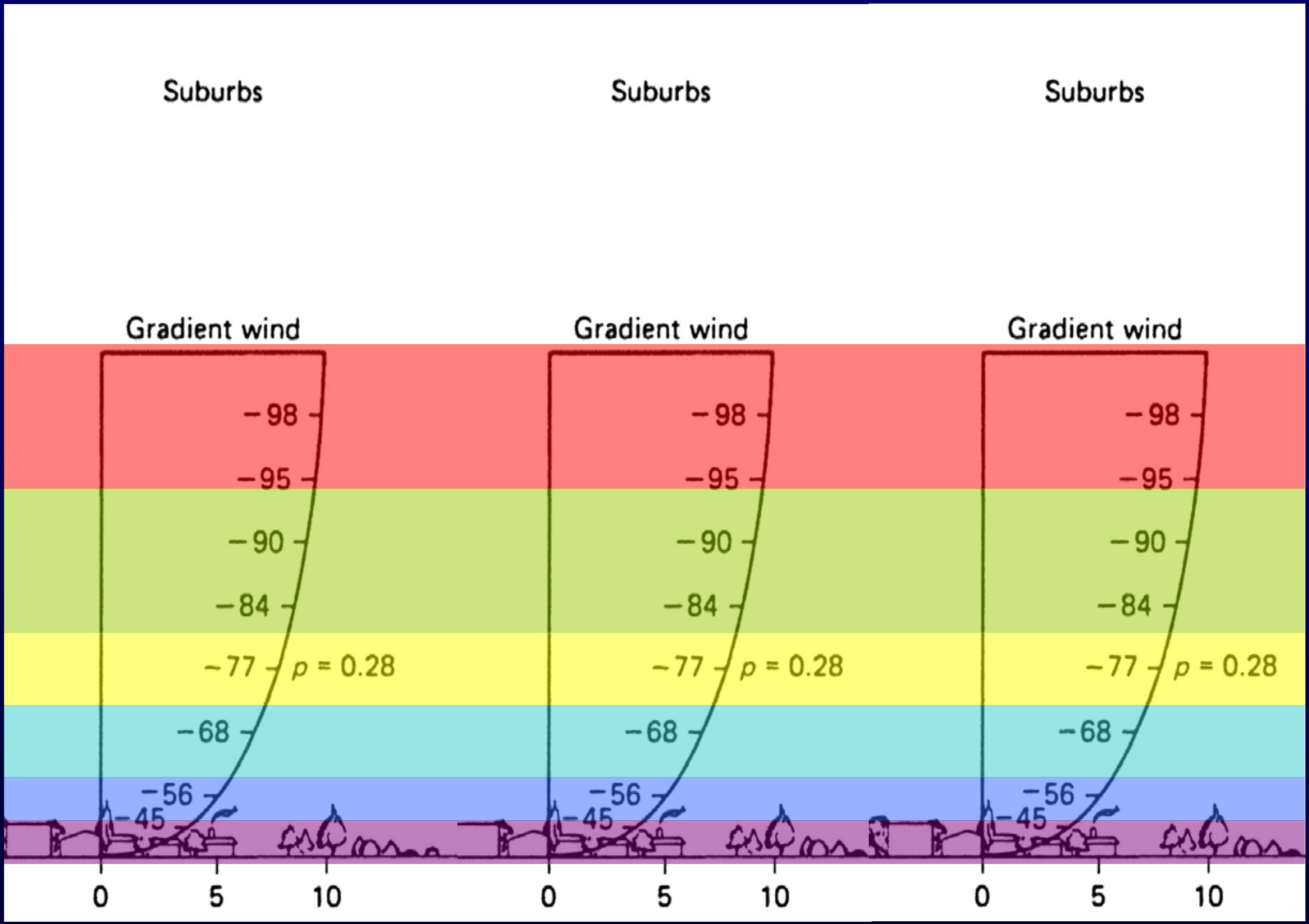


without wind

Boundary conditions

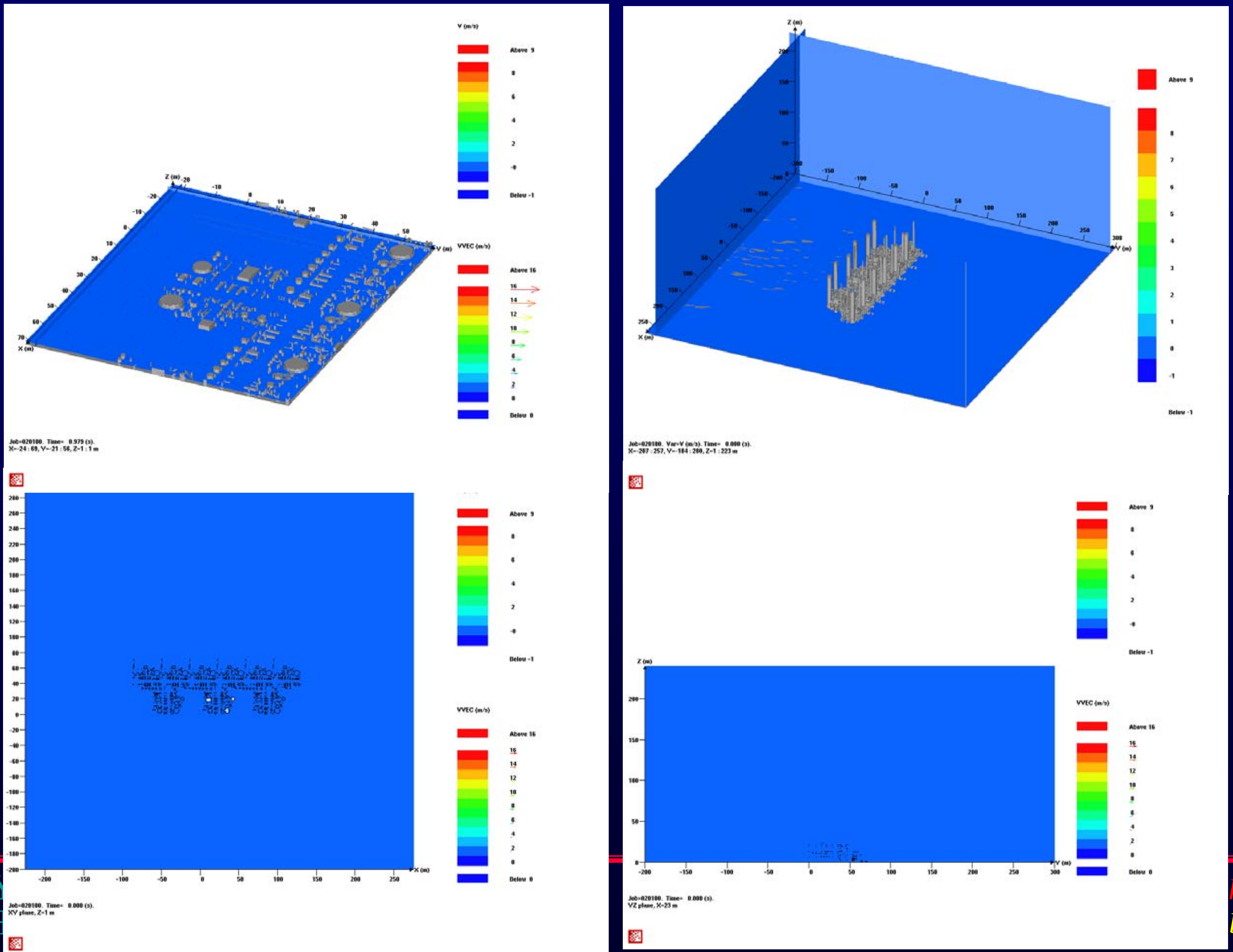
Boundary	Parameter setting	Wind speed (m/s)	Wind direction
X-LO	WIND	2.5	+Y
X-HI	WIND	2.5	+Y
Y-LO	WIND	2.5	+Y
Y-HI	NOZZLE	-	-
Z-LO	NOZZLE	-	-
Z-HI	NOZZLE	-	-

Illustration of gradient wind



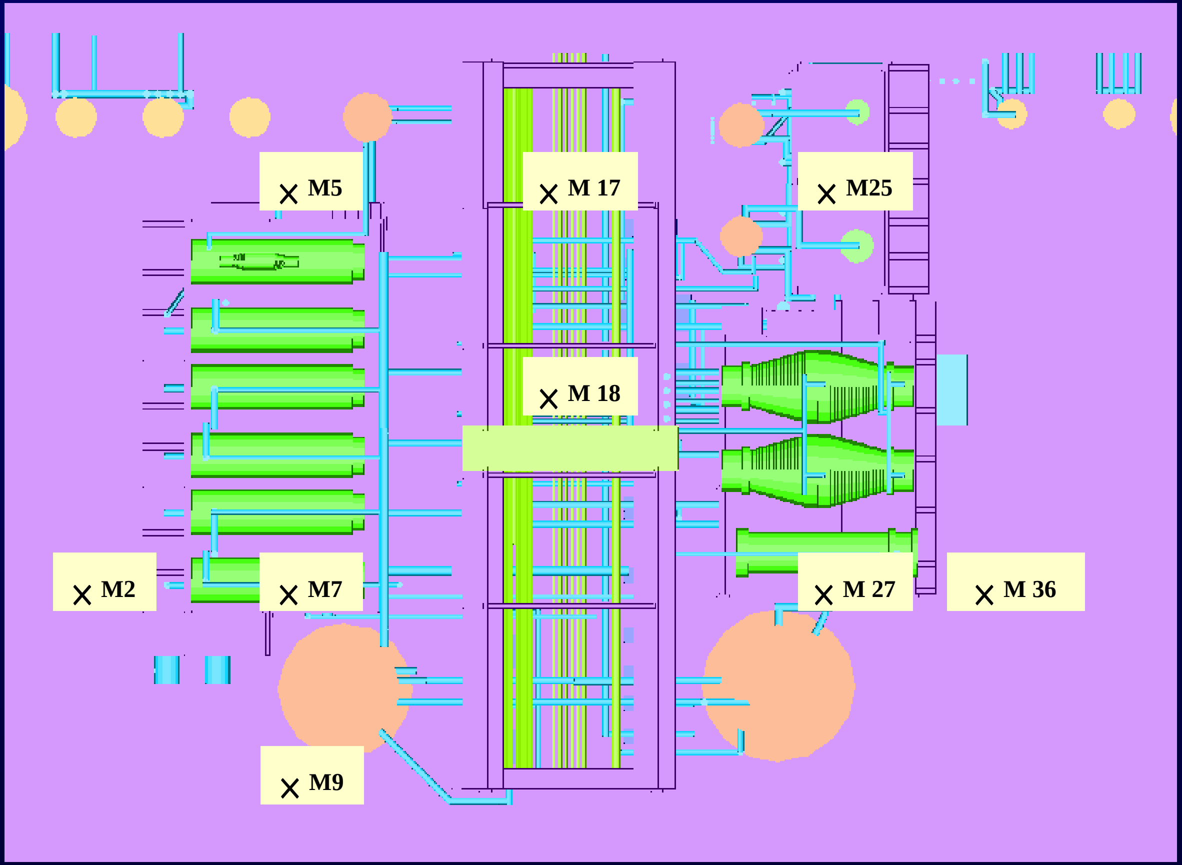
The colors stand for different wind speeds in direction of Y

Wind field simulation



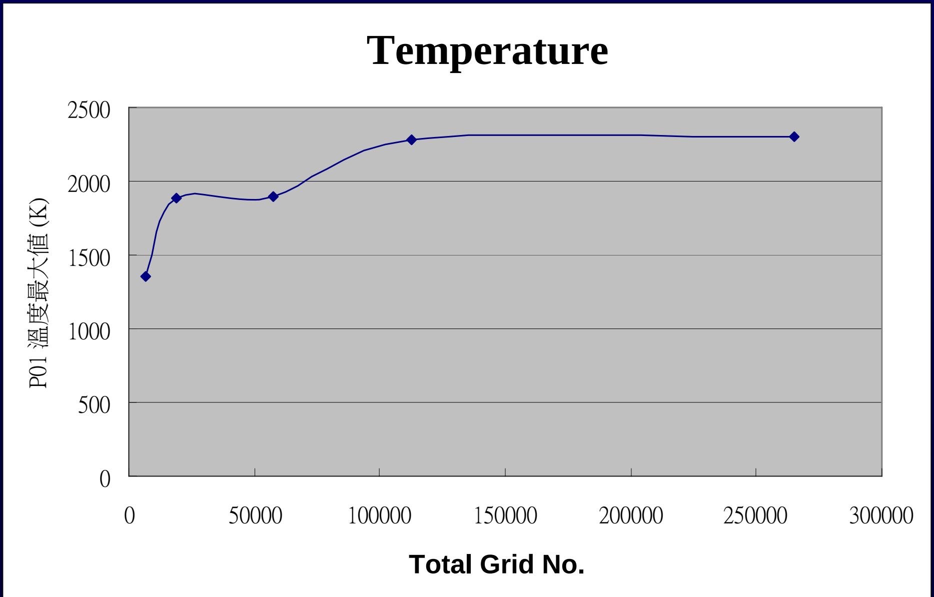
Location of monitor points

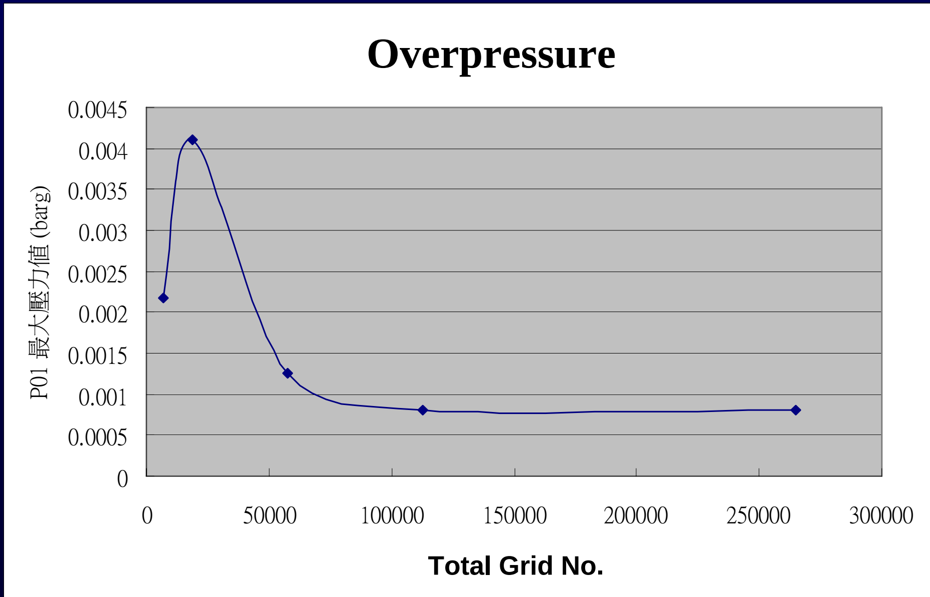
Monitor Point No	X（m）	Y（m）	Z（m）
P2	0	10	1.5
P5	10	30	1.5
P7	10	10	1.5
P9	10	0	3.0
P17	20	30	1.5
P18	23	20	1.5
P25	37	30	1.5
P27	37	10	1.5
P36	45	10	1.5



Independent tests for simulation grids

Test No	1	2	3	4	5
Grid size (m)	10*10*10	5*5*5	2.5*2.5*2.5	2*2*2	1*1*1
(x,y,z) (grid no.)	(24, 24, 12)	(34, 33, 17)	(50, 46, 25)	(61, 56, 33)	(82, 77, 42)
Total grid no.	6,912	19,074	57,500	112,728	265,188





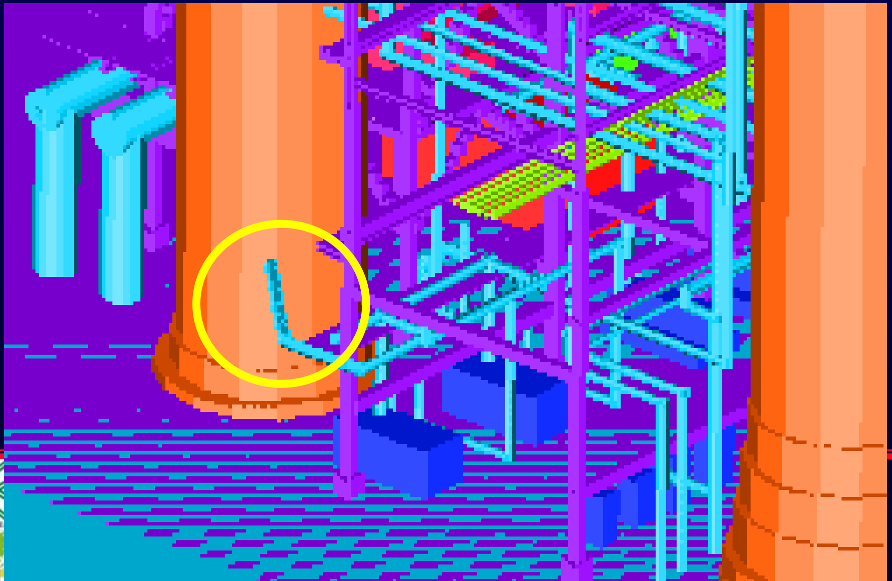
Simulation scenarios

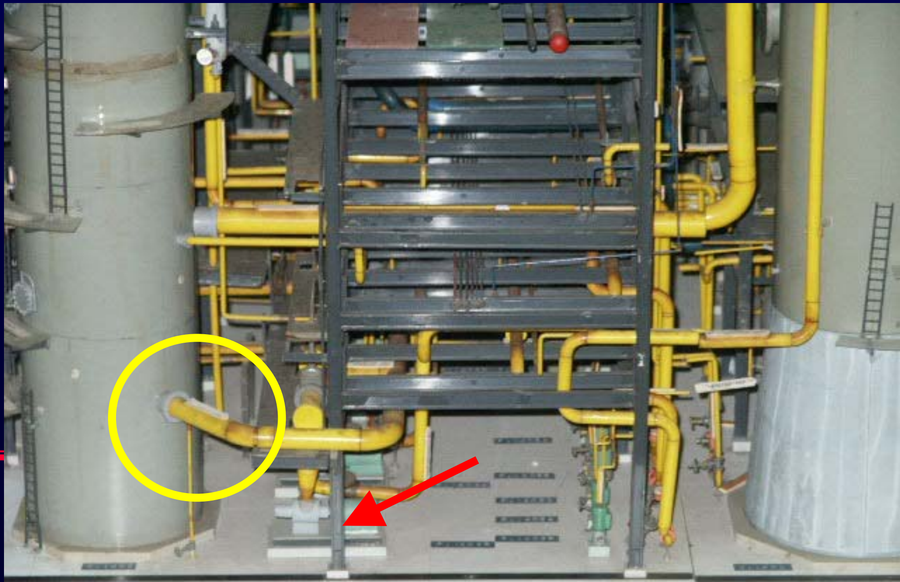
Case No.	1	2	3
Scenario	Distillation column collapse	Reflux tank rupture	Reflux tank rupture
Gas volume (m^3)	28,730	1,767	1,767
Gas conc. (%)	100	100	100
Ignition time (sec)	11	0.5	0.5
Ignition point (m)	(59, 25, 1)	(16, 12, 3)	(16, 12, 3)
Mitigation measure	No	No	Water spray

Results and Discussion

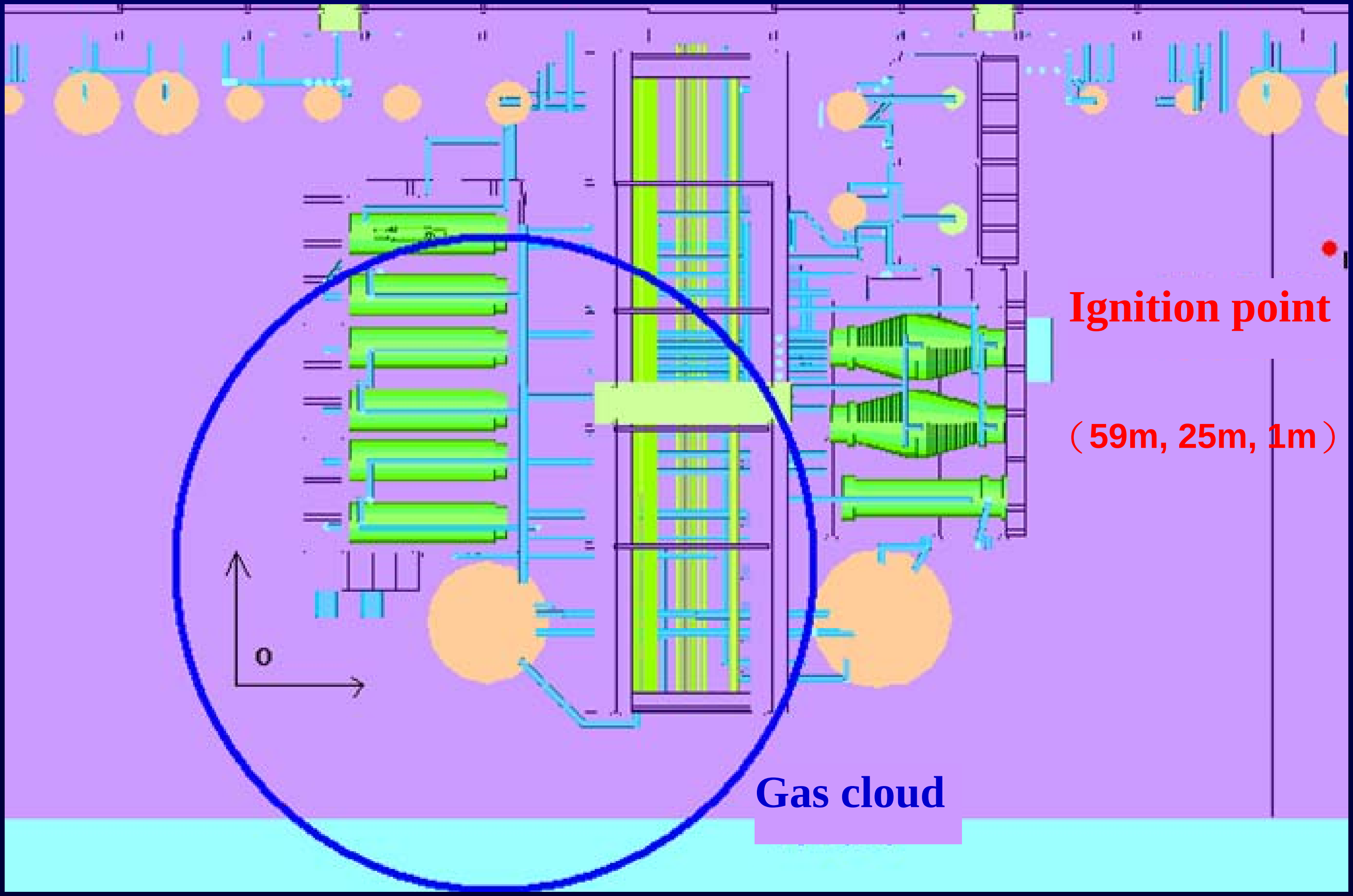
Case 1: Distillation column collapse incident

- A large scale vapor cloud ignition case that originated from a distillation tower collapse incident (support breaking due to ext. fire).
- The released chemical contains 95% propylene (with 3.5% propane, 1.5% ethane) and forms a 38 m diameter (volume expands 270 times), 100% concentrated spherical gas cloud.
- After 11 sec dispersion, the gas cloud was ignited by an ignition point.

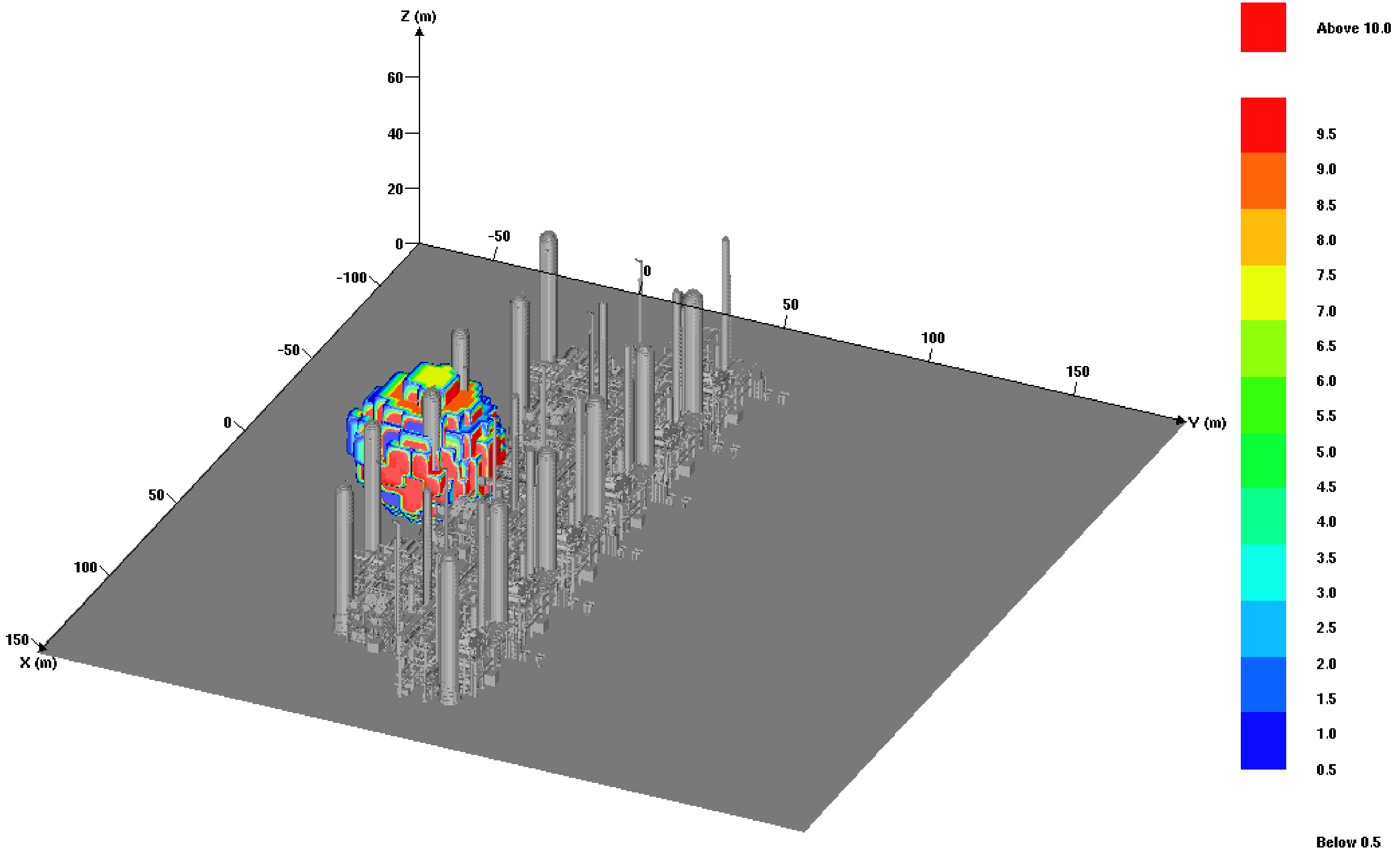




Case 1: gas cloud & ignition point

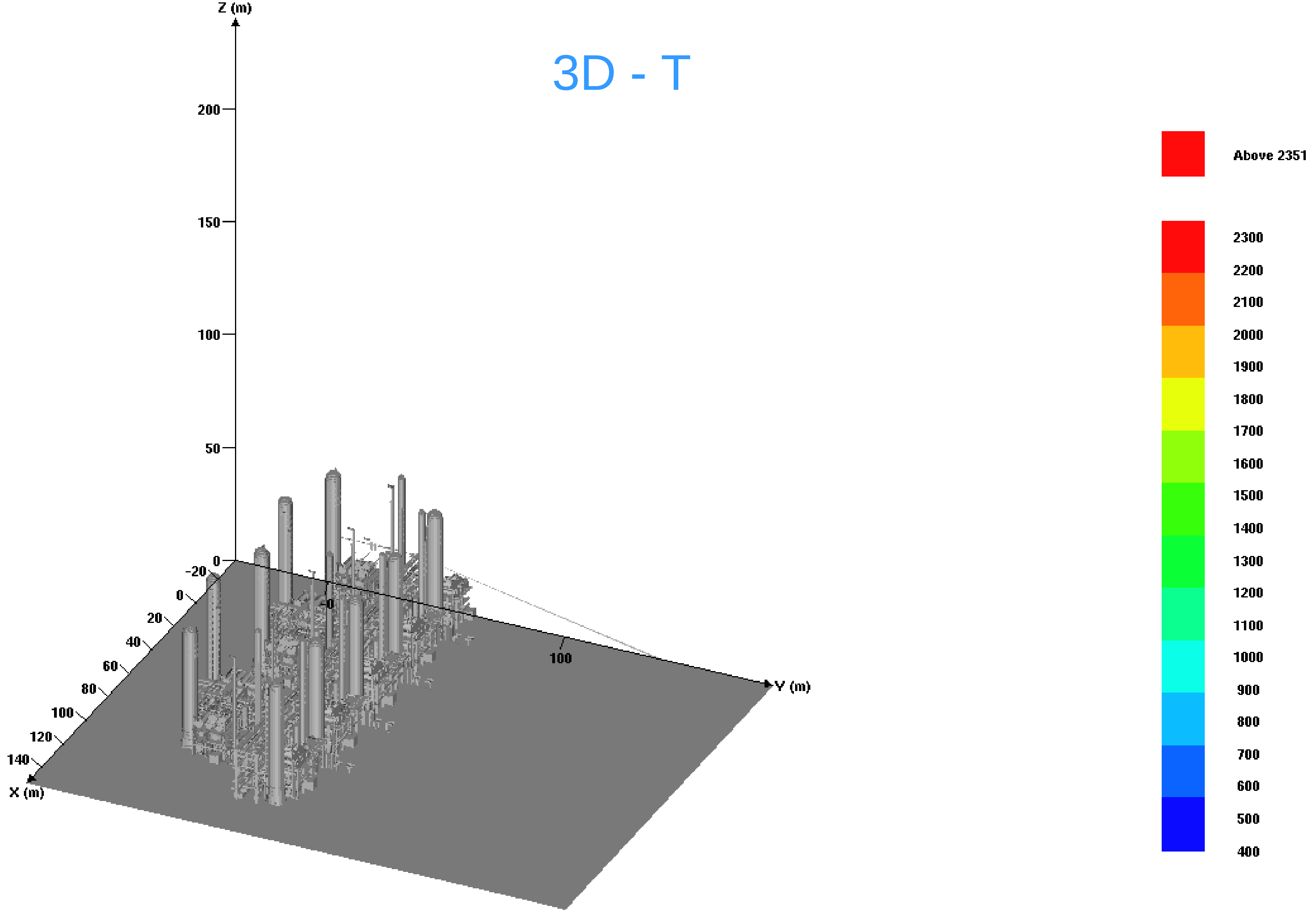


3D - ER



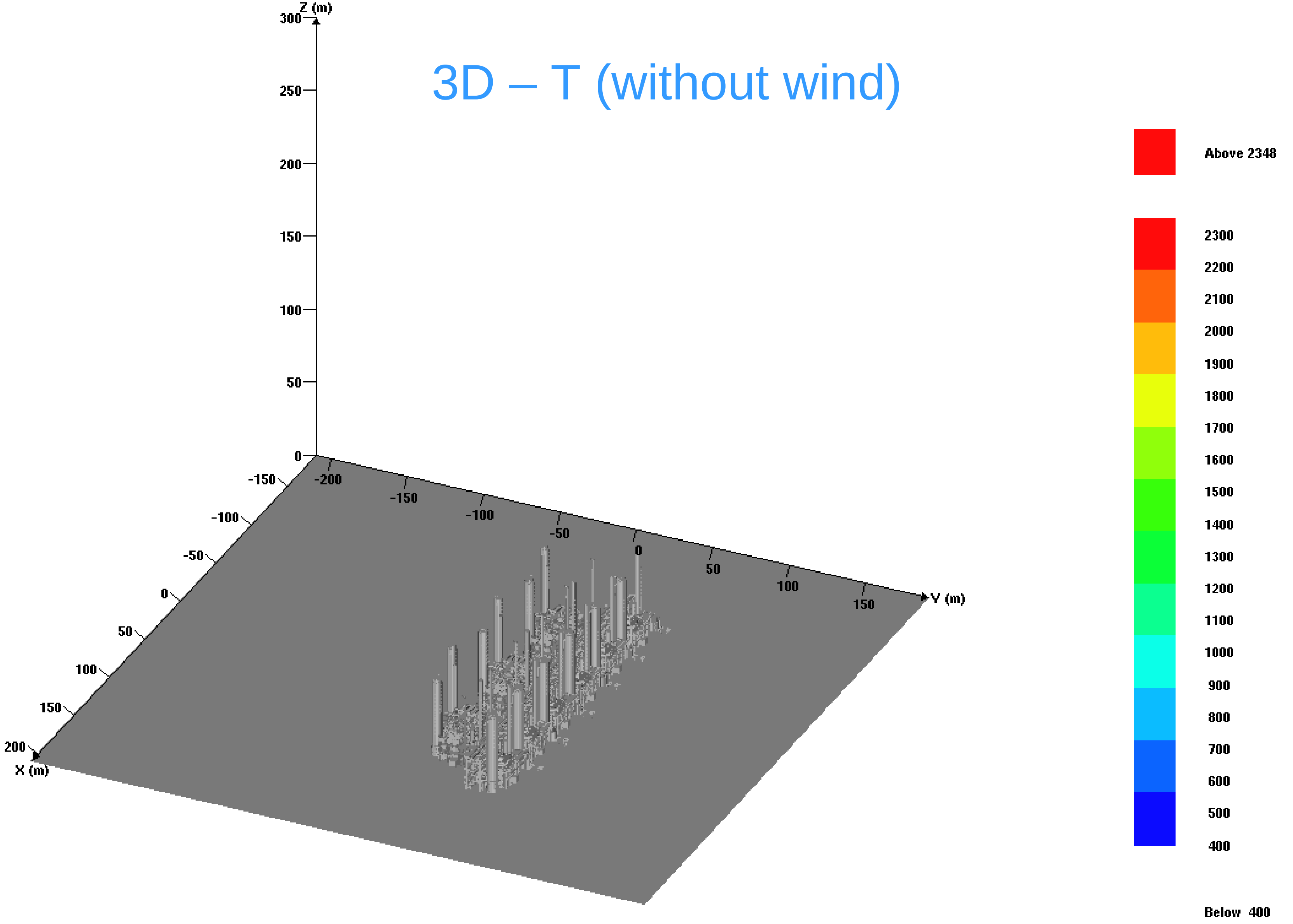
Job=020100. Var=ER (-). Time= 120.016 (s).
X=-118 : 143, Y=-68 : 175, Z=1 : 72 m

3D - T

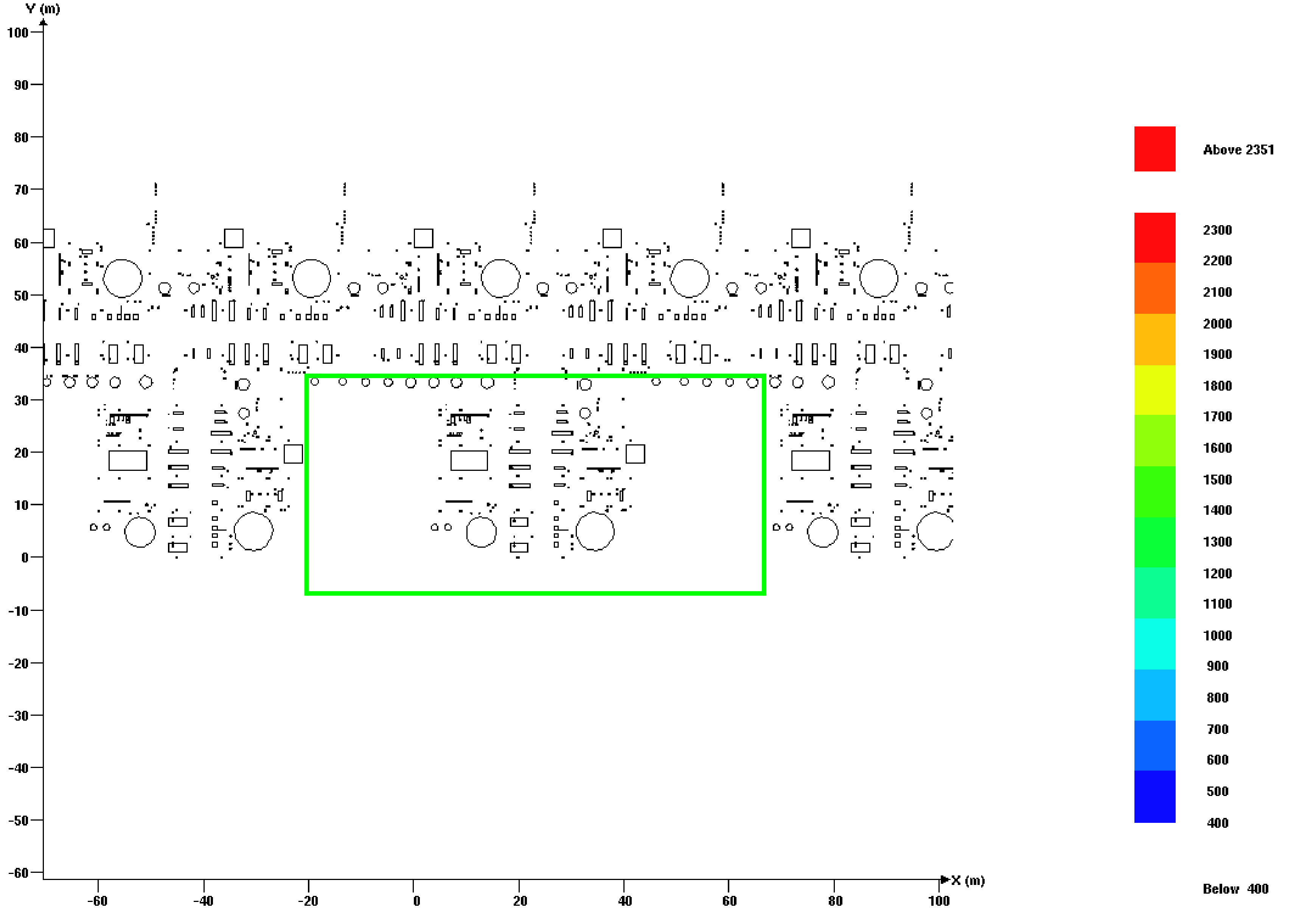


Job=020100. Var=T (K). Time= 120.016 (s).
X=-32 : 143, Y=-35 : 175, Z=1 : 223 m

3D – T (without wind)



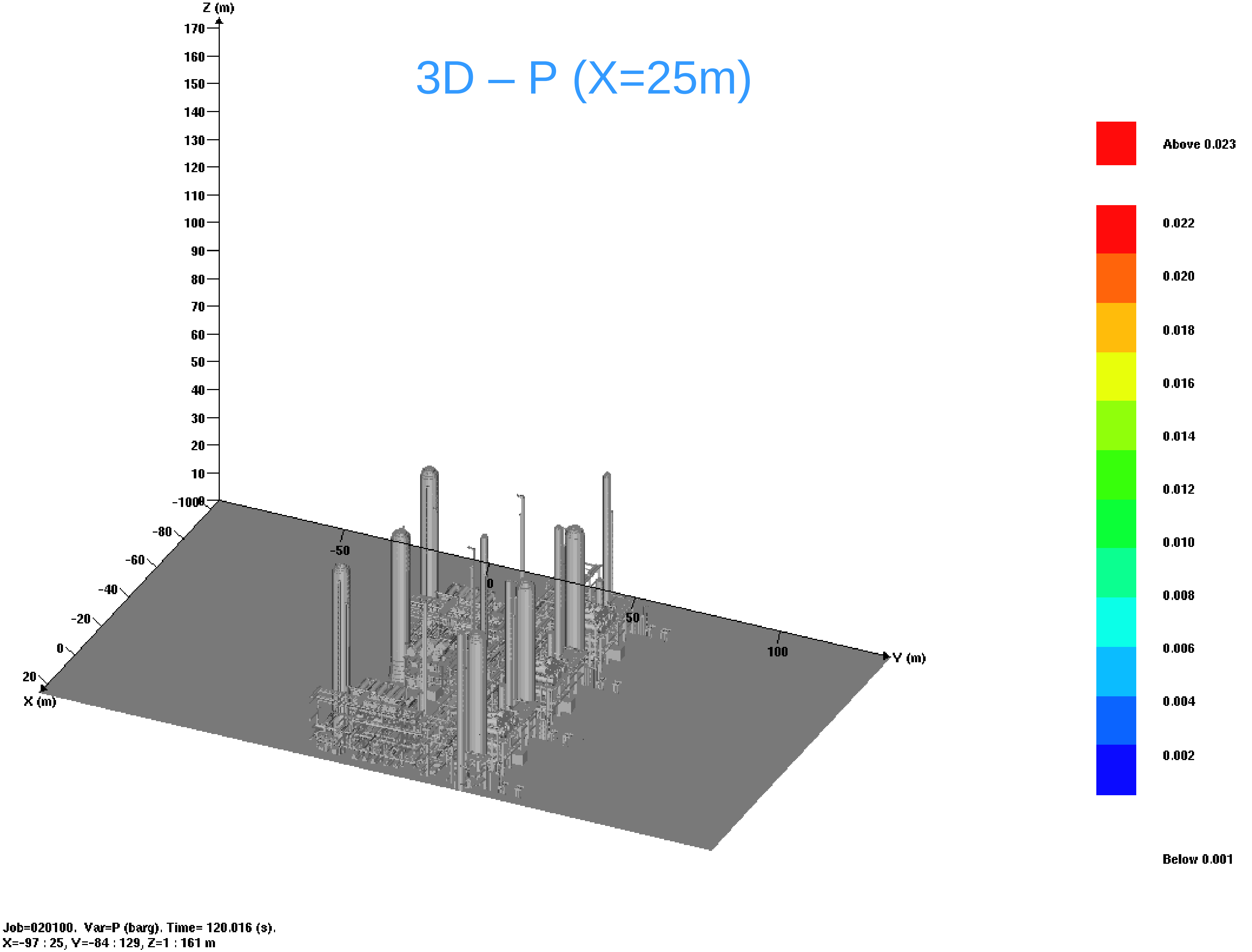
Job=020100. Var=T (K). Time= 0.000 (s).
X=-175 : 195, Y=-191 : 179, Z=1 : 280 m



Job=020100. Var=T (K). Time= 120.016 (s).
XY plane, Z=1 m

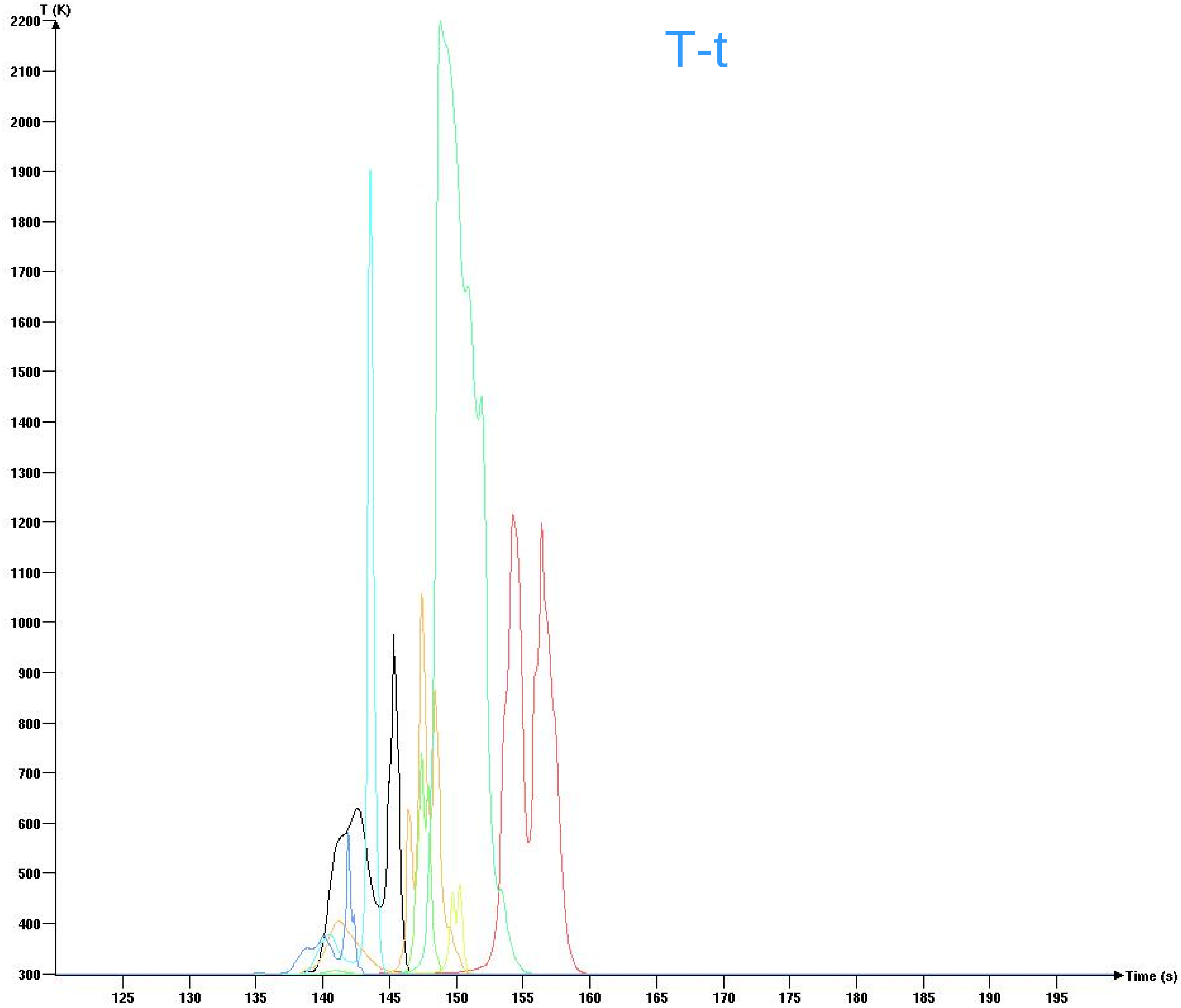
2D – T (Z＝1m)

3D – P (X=25m)



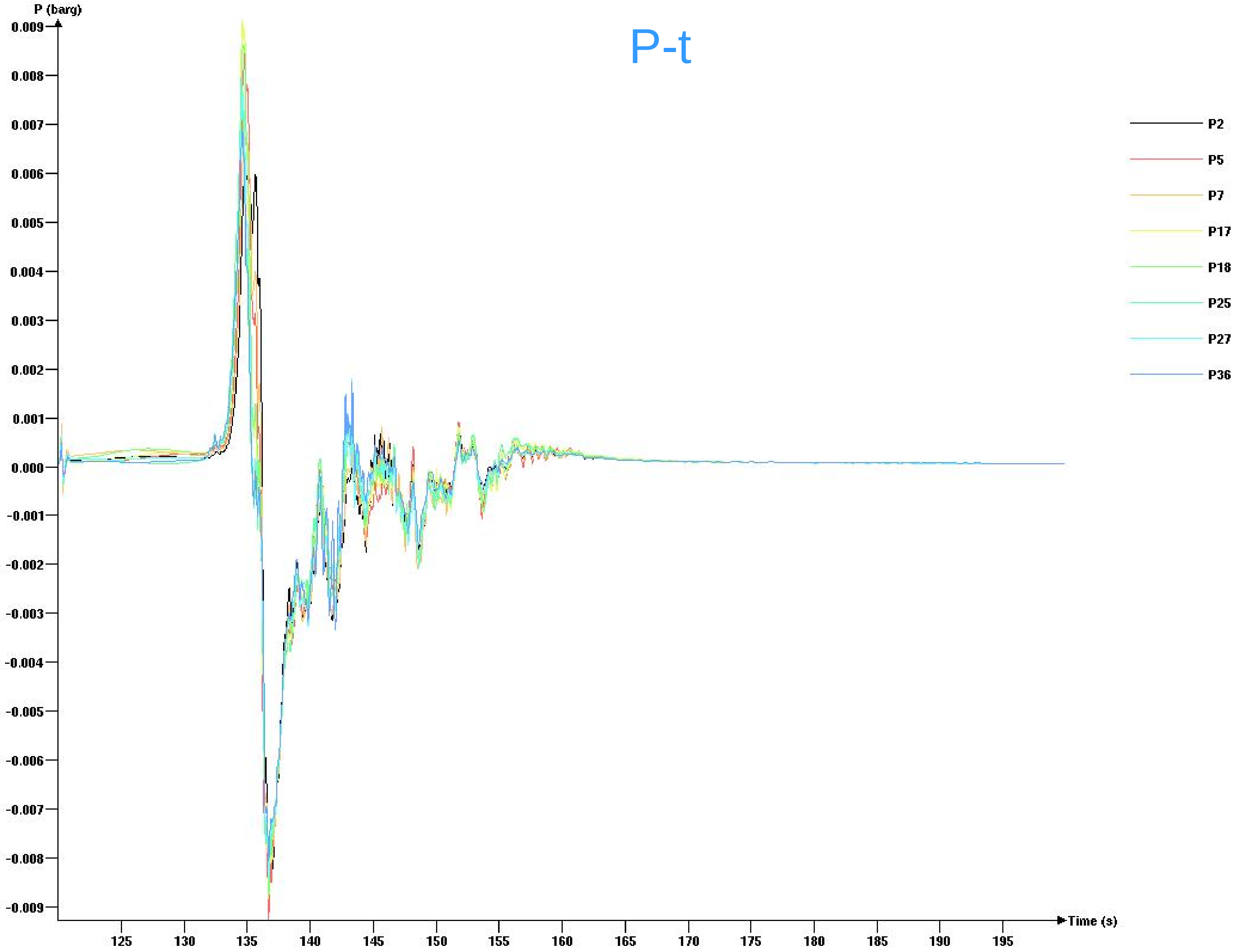
Z (m)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
-100
0
-80
-60
-40
-20
0
20
X (m)
-50
0
50
100
Y (m)
Above 0.023
0.022
0.020
0.018
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
Below 0.001
Job=020100. Var=P (barg). Time= 120.016 (s).
X=-97 : 25, Y=-84 : 129, Z=1 : 161 m

T-t



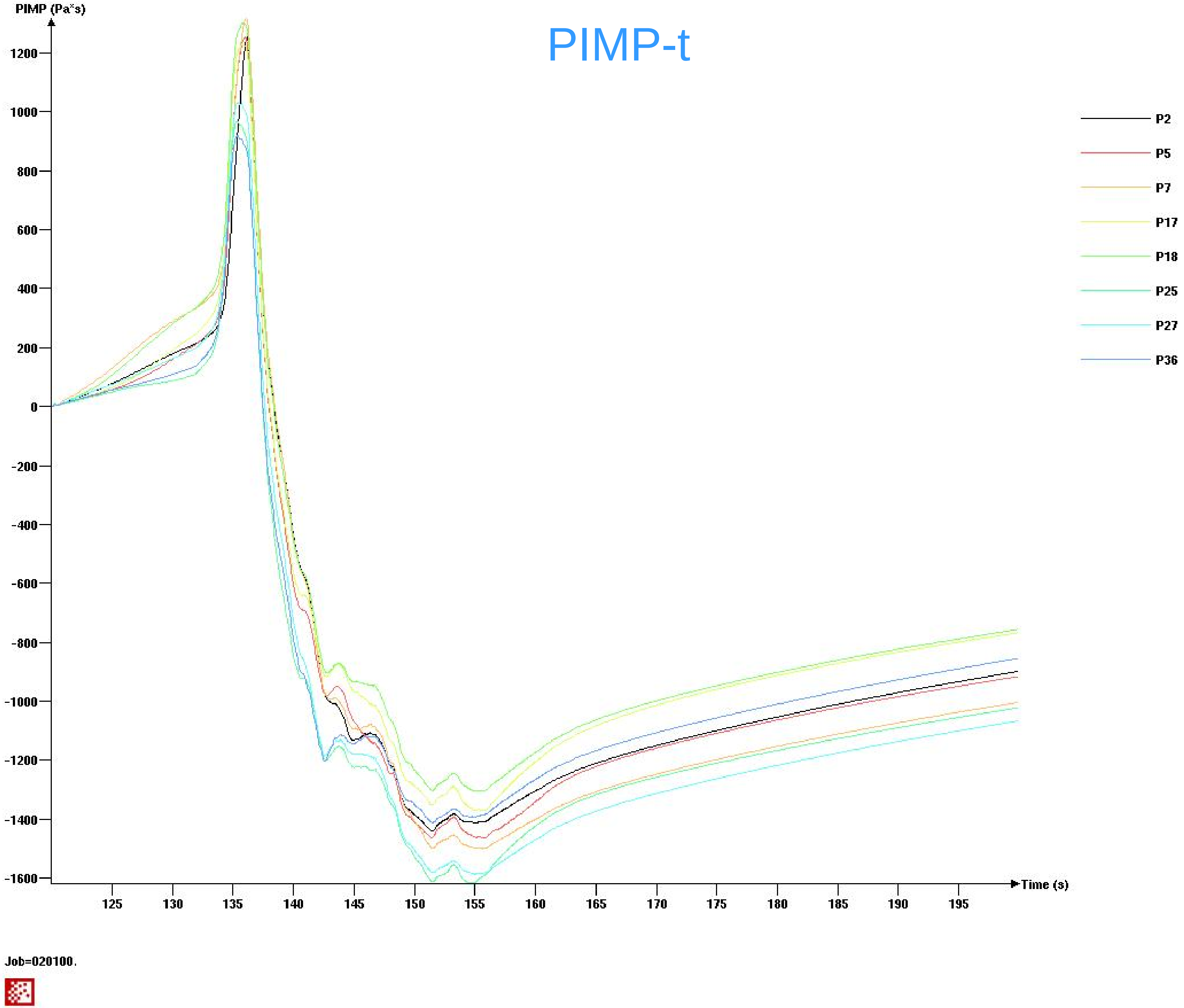
Job=020100.

P-t



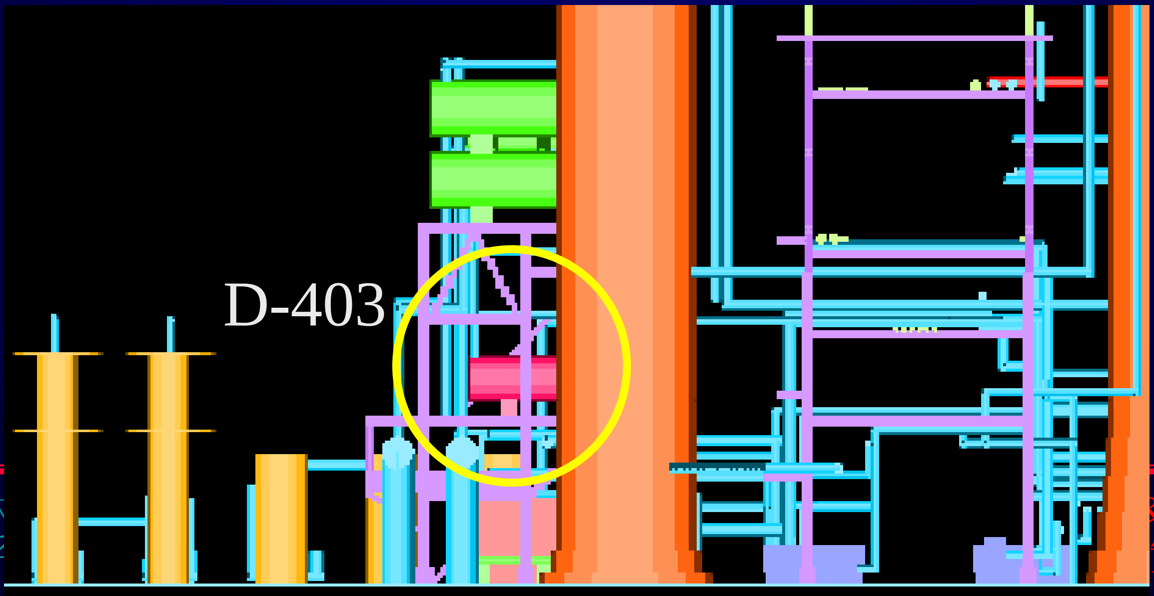
Job=020100.

PIMP-t

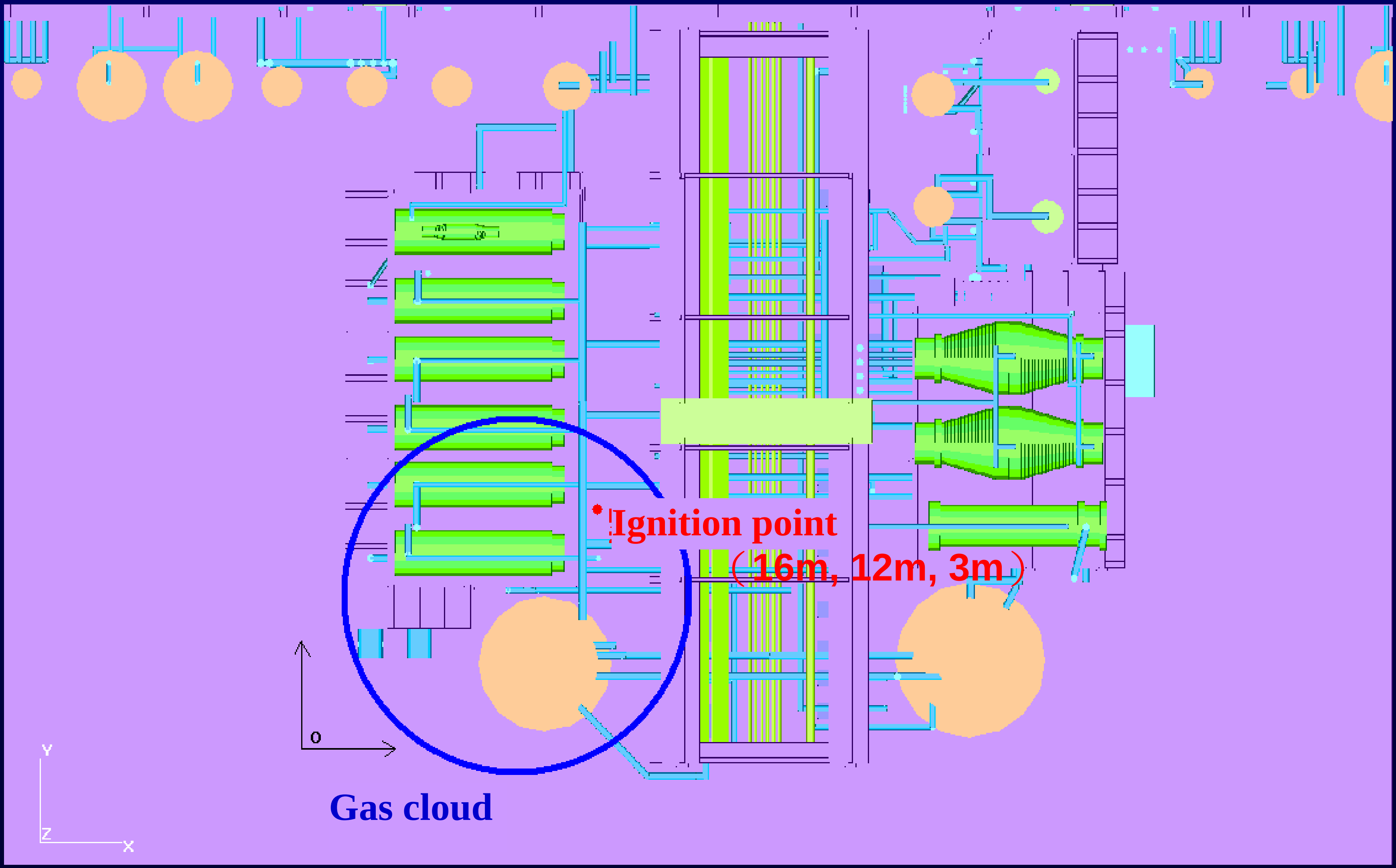

PIMP (Pa*s)
1200
1000
800
600
400
200
0
-200
-400
-600
-800
-1000
-1200
-1400
-1600
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
Time (s)
P2
P5
P7
P17
P18
P25
P27
P36
Job=020100.

Case 2: reflux tank rupture incident

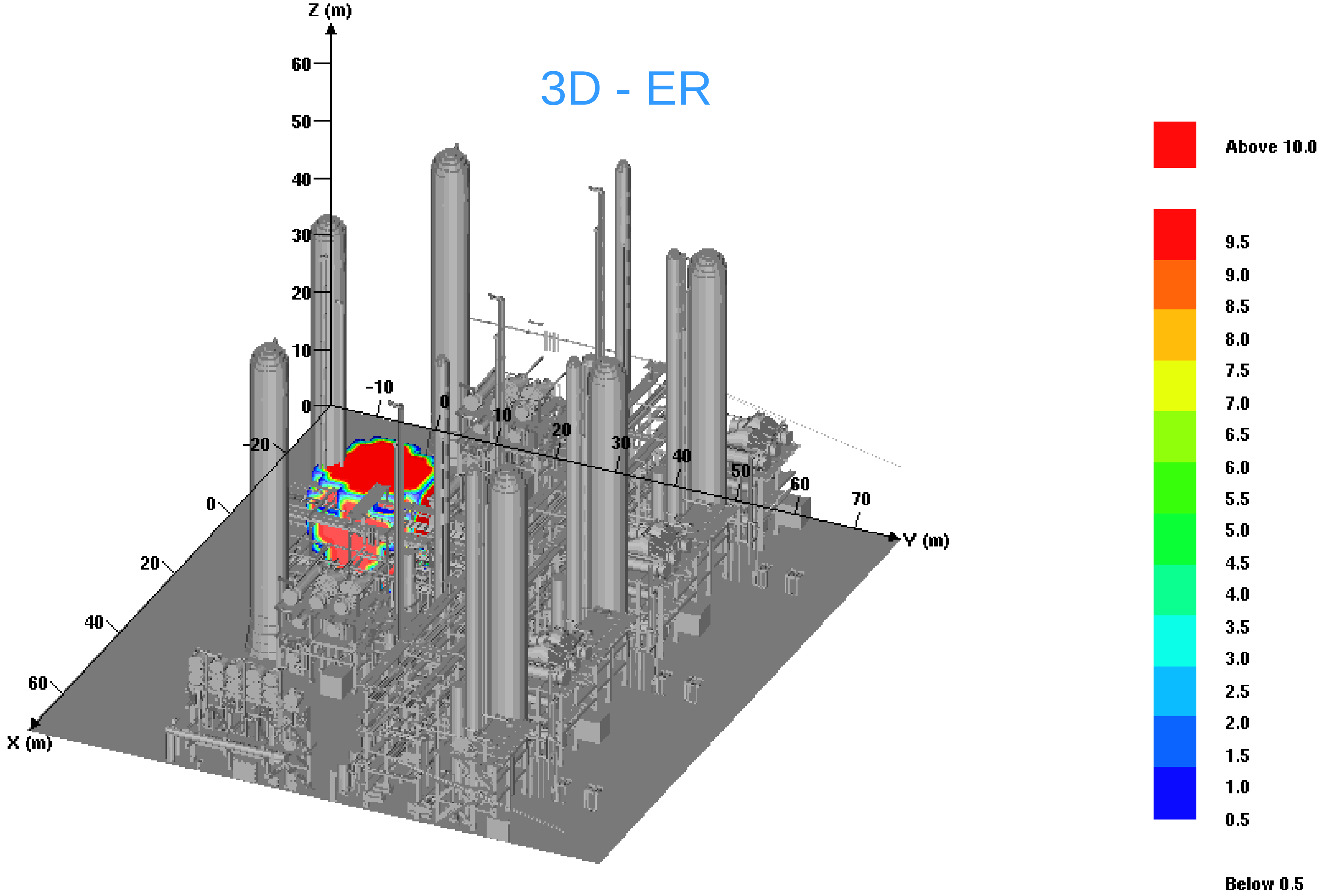
- D-403 reflux tank rupture followed by the ignition of static electricity
- The released chemical contains 100% propylene and forms a 15 m diameter, 100% concentrated spherical gas cloud.
- Cases 2 discuss the deflagration accident without water spray mitigation system.



Event 2: gas cloud & ignition point

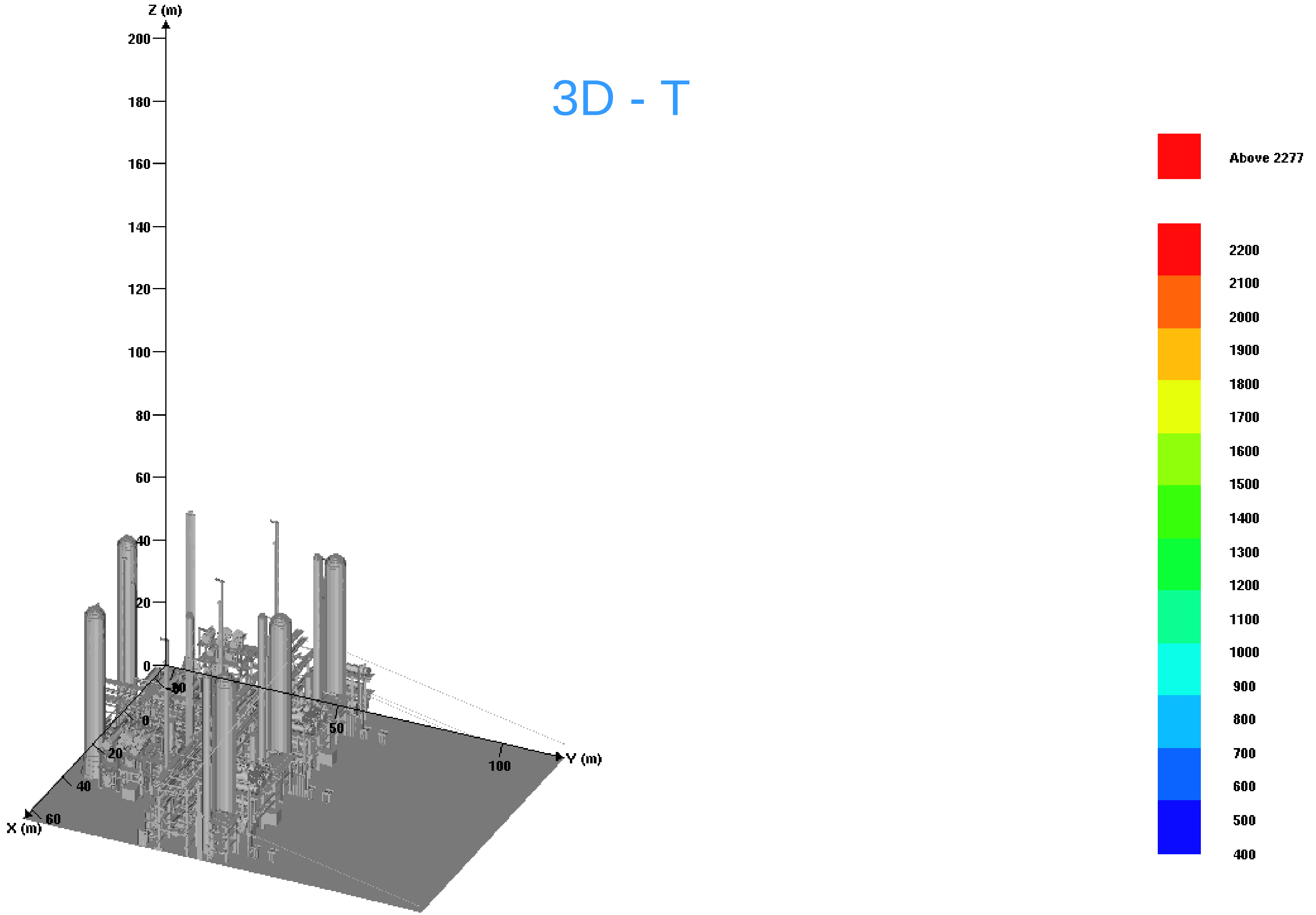


3D - ER

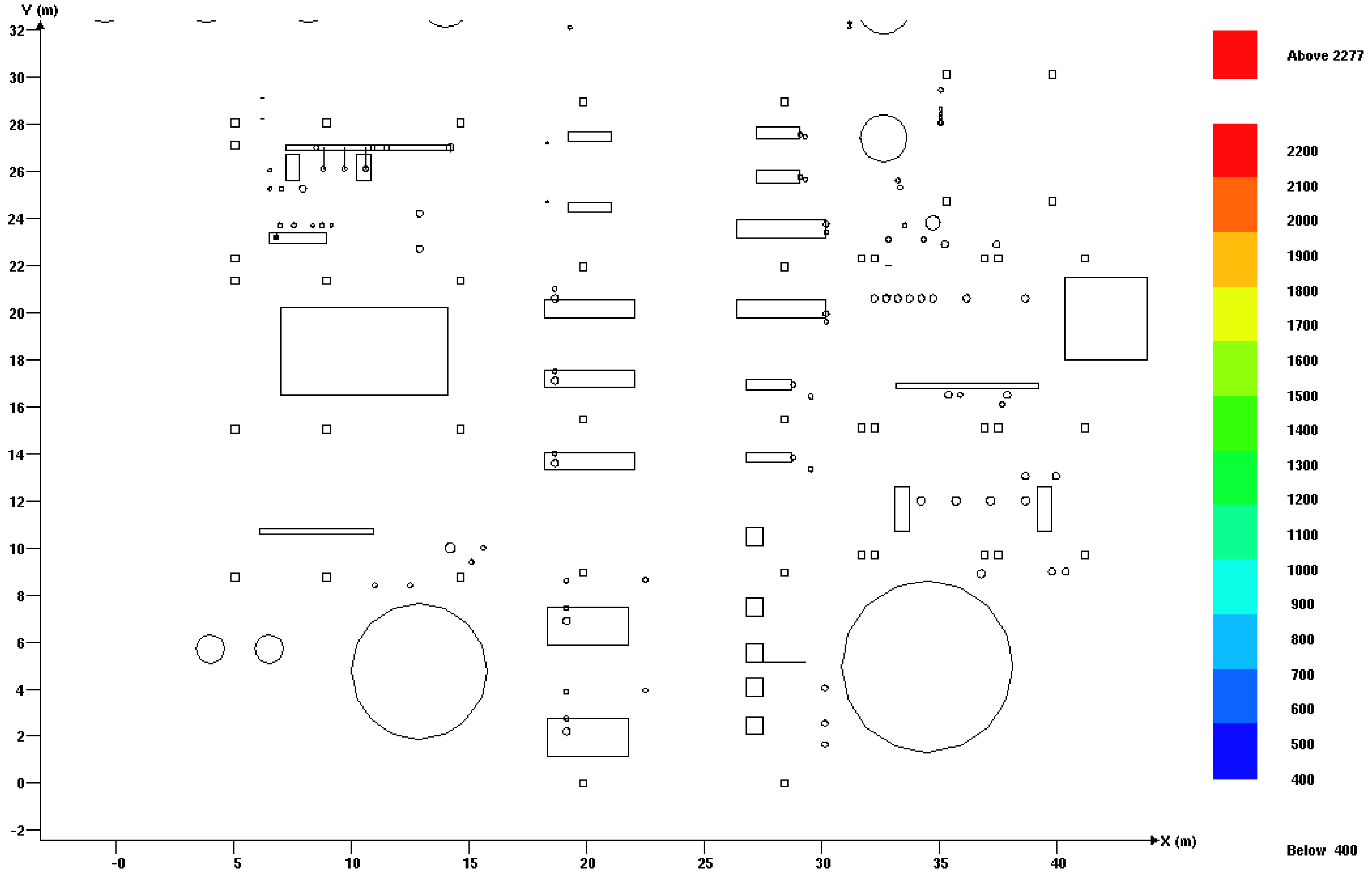


Job=020100. Var=ER (-). Time= 120.016 (s).
X=-32 : 69, Y=-15 : 73, Z=1 : 62 m

3D - T



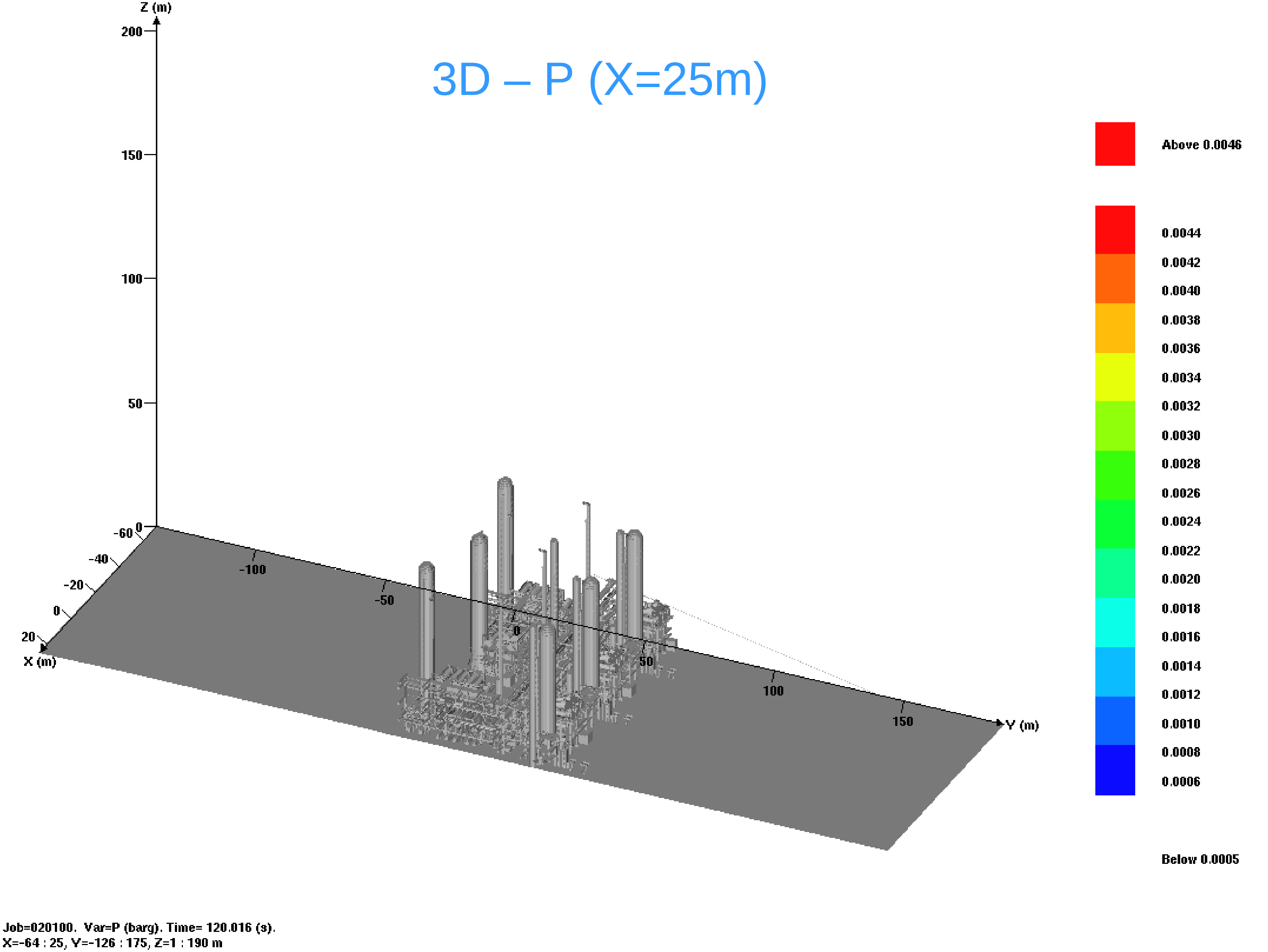
Job=020100. Var=T (K). Time= 120.016 (s).
X=-24 : 62, Y=-1 : 111, Z=1 : 190 m



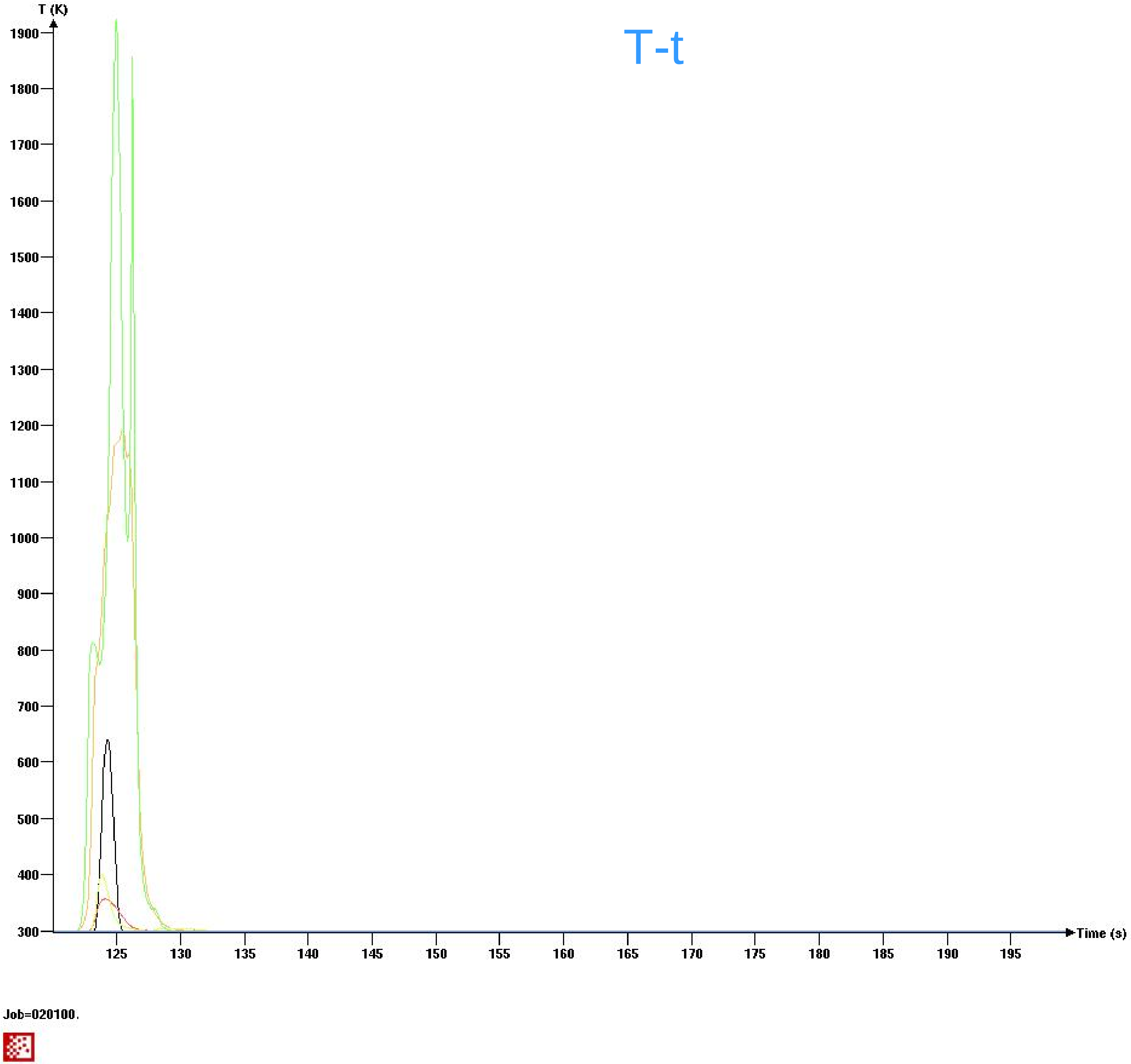
Job=020100. Var=T (K). Time= 120.016 (s).
XY plane, Z=1 m

2D – T (Z＝1m)

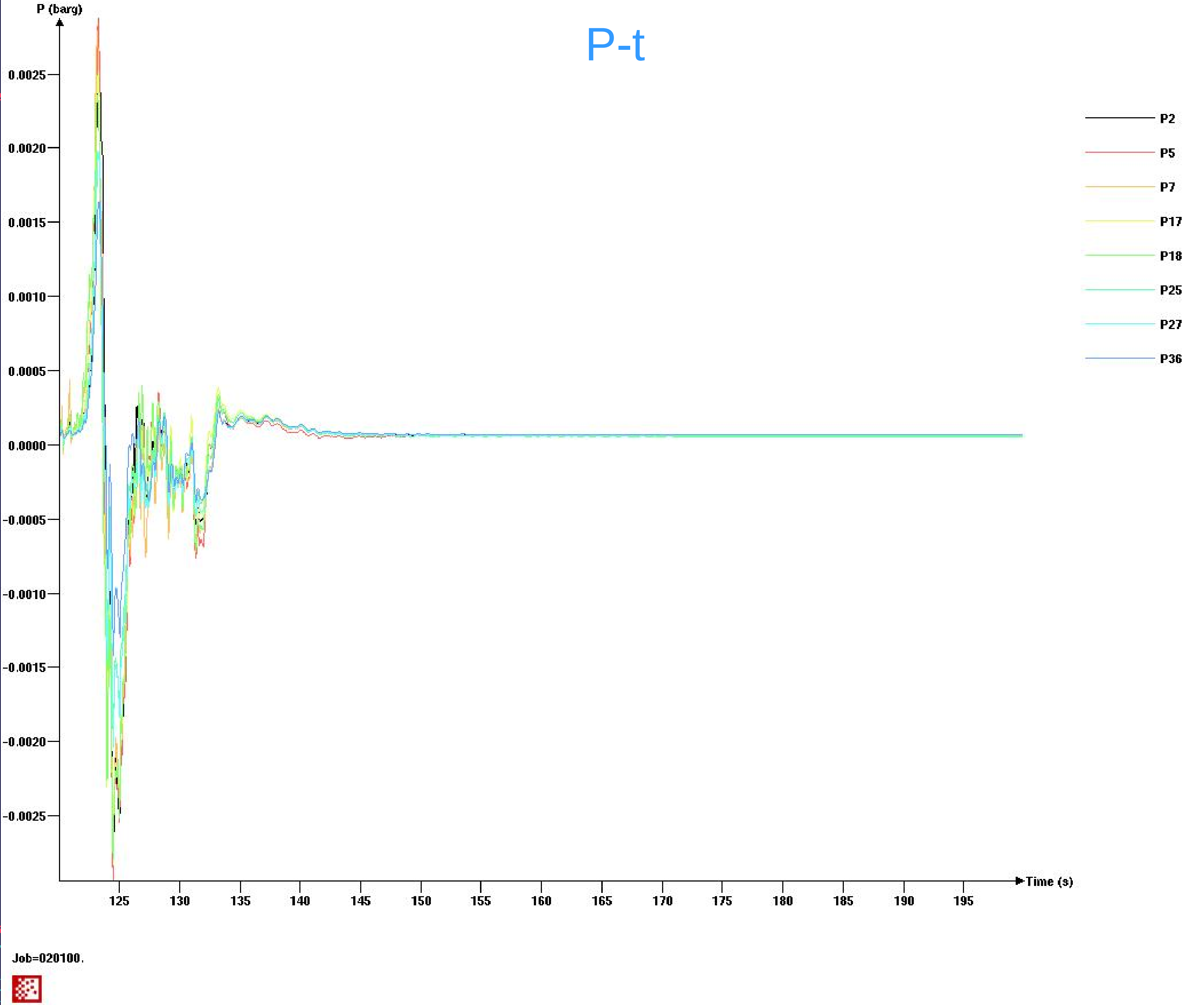
3D – P (X=25m)


Z (m)
200
150
100
50
0
-60
-40
-20
0
20
X (m)
-100
-50
0
50
100
150
Y (m)
Above 0.0046
0.0044
0.0042
0.0040
0.0038
0.0036
0.0034
0.0032
0.0030
0.0028
0.0026
0.0024
0.0022
0.0020
0.0018
0.0016
0.0014
0.0012
0.0010
0.0008
0.0006
Below 0.0005
Job=020100. Var=P (barg). Time= 120.016 (s).
X=-64 : 25, Y=-126 : 175, Z=1 : 190 m

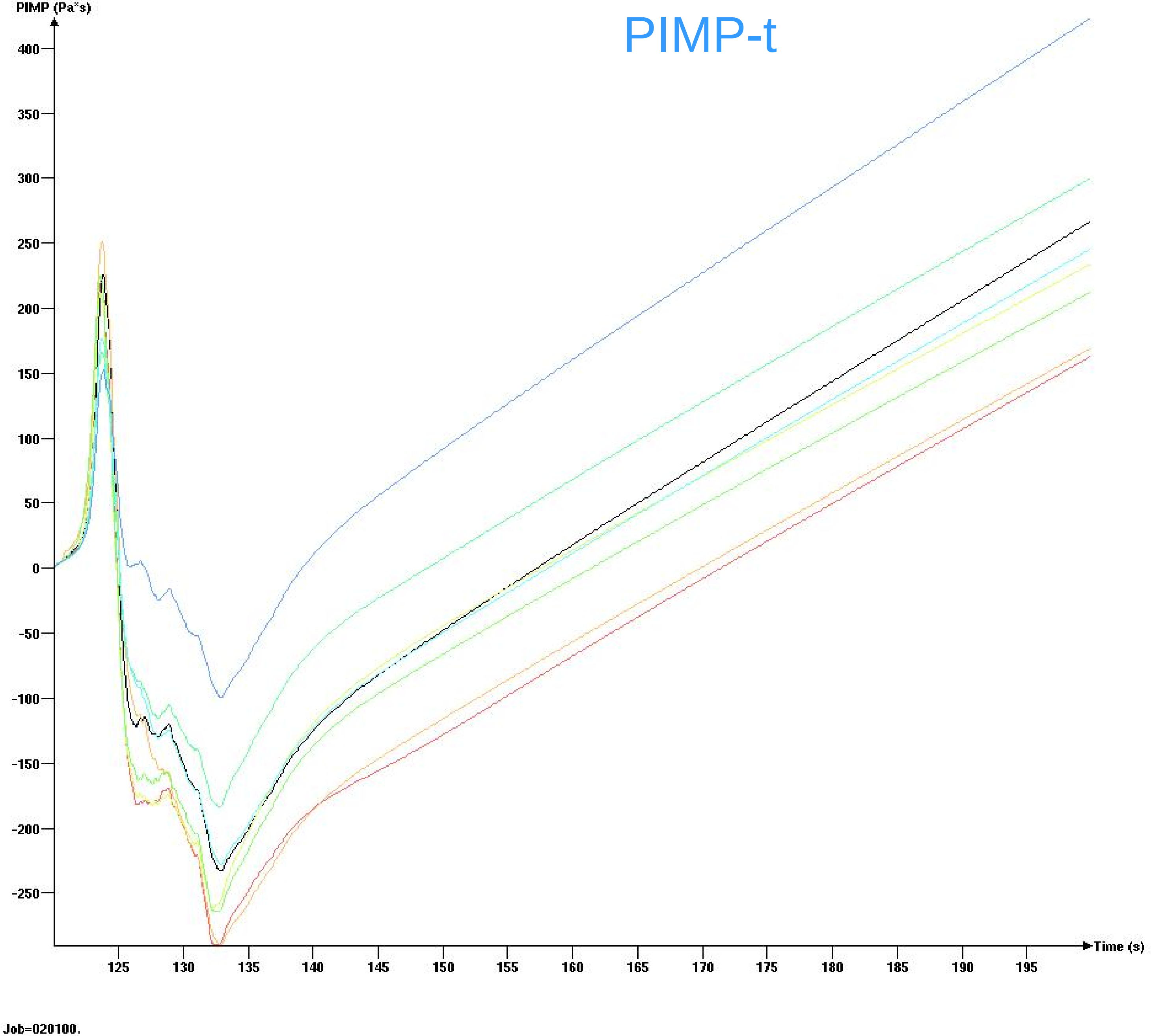
T-t


T (K)
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
Time (s)
P2
P5
P7
P17
P18
P25
P27
P36
Job=020100.

P-t

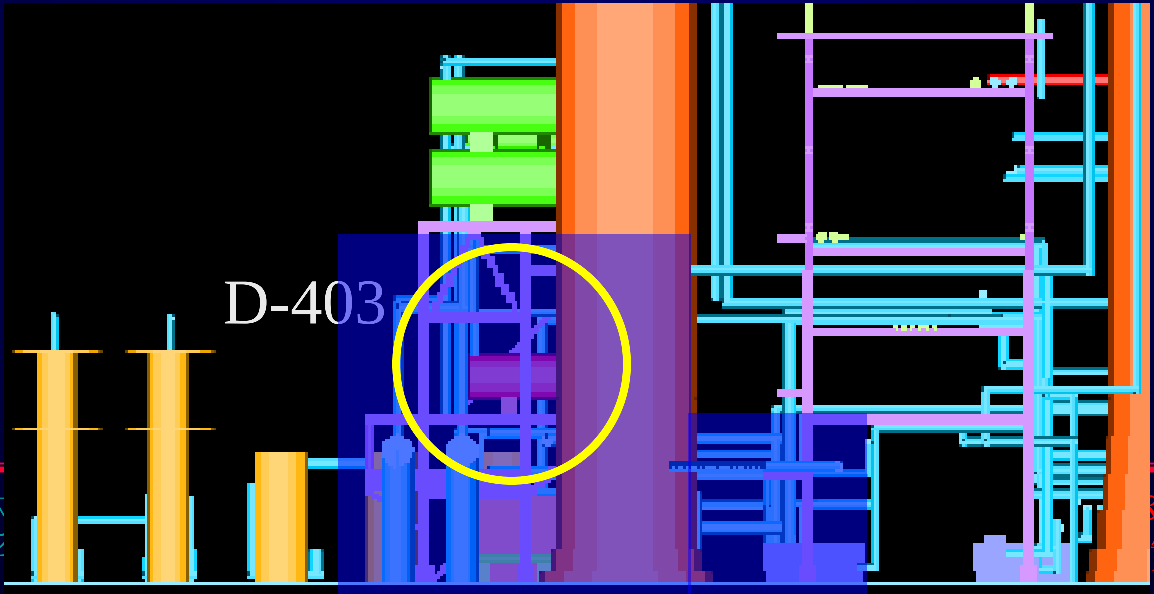

P (barg)
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
-0.0005
-0.0010
-0.0015
-0.0020
-0.0025
125 130 135 140 145 150 155 160 165 170 175 180 185 190 195
Time (s)
P2
P5
P7
P17
P18
P25
P27
P36
Job=020100.

PIMP-t

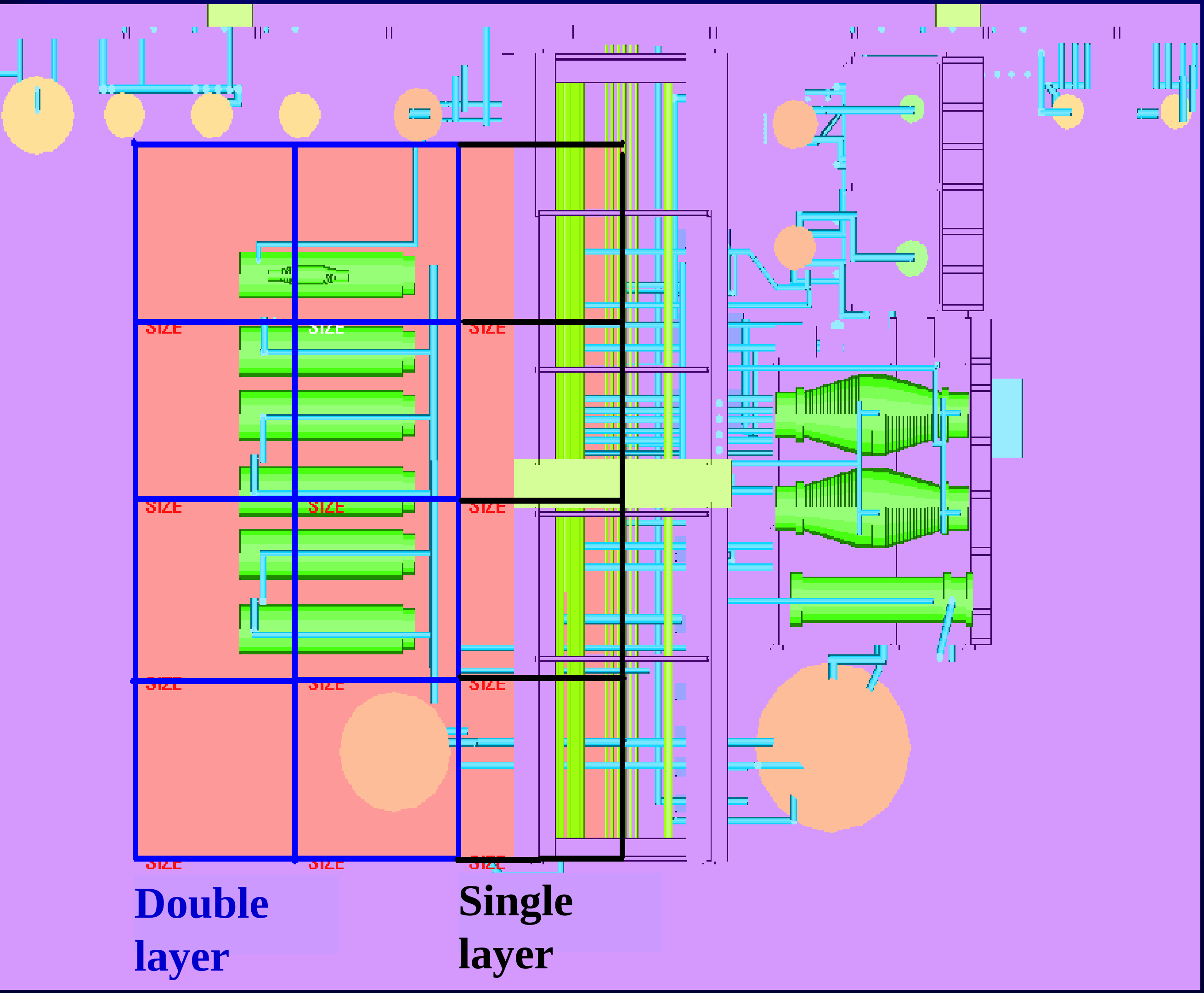

PIMP (Pa*s)
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
Time (s)
P2
P5
P7
P17
P18
P25
P27
P36
Job=020100.

Case 3: reflux tank rupture with water spray

- D-403 reflux tank rupture followed by the ignition of static electricity
- The released chemical contains 100% propylene and forms a 15 m diameter, 100% concentrated spherical gas cloud.
- Cases 3 discuss the deflagration accident with water spray mitigation system.

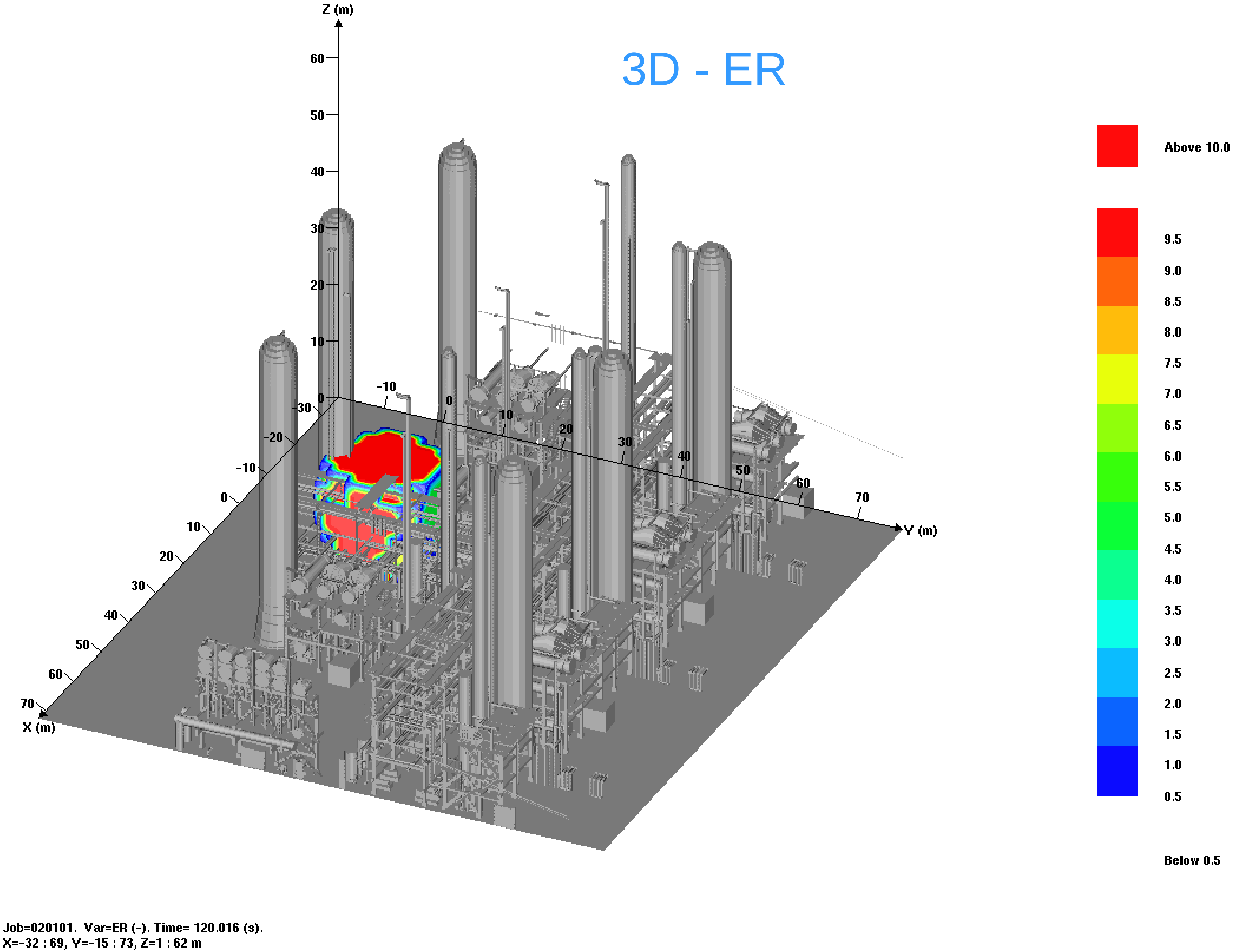


Location of water spray (total: 20)

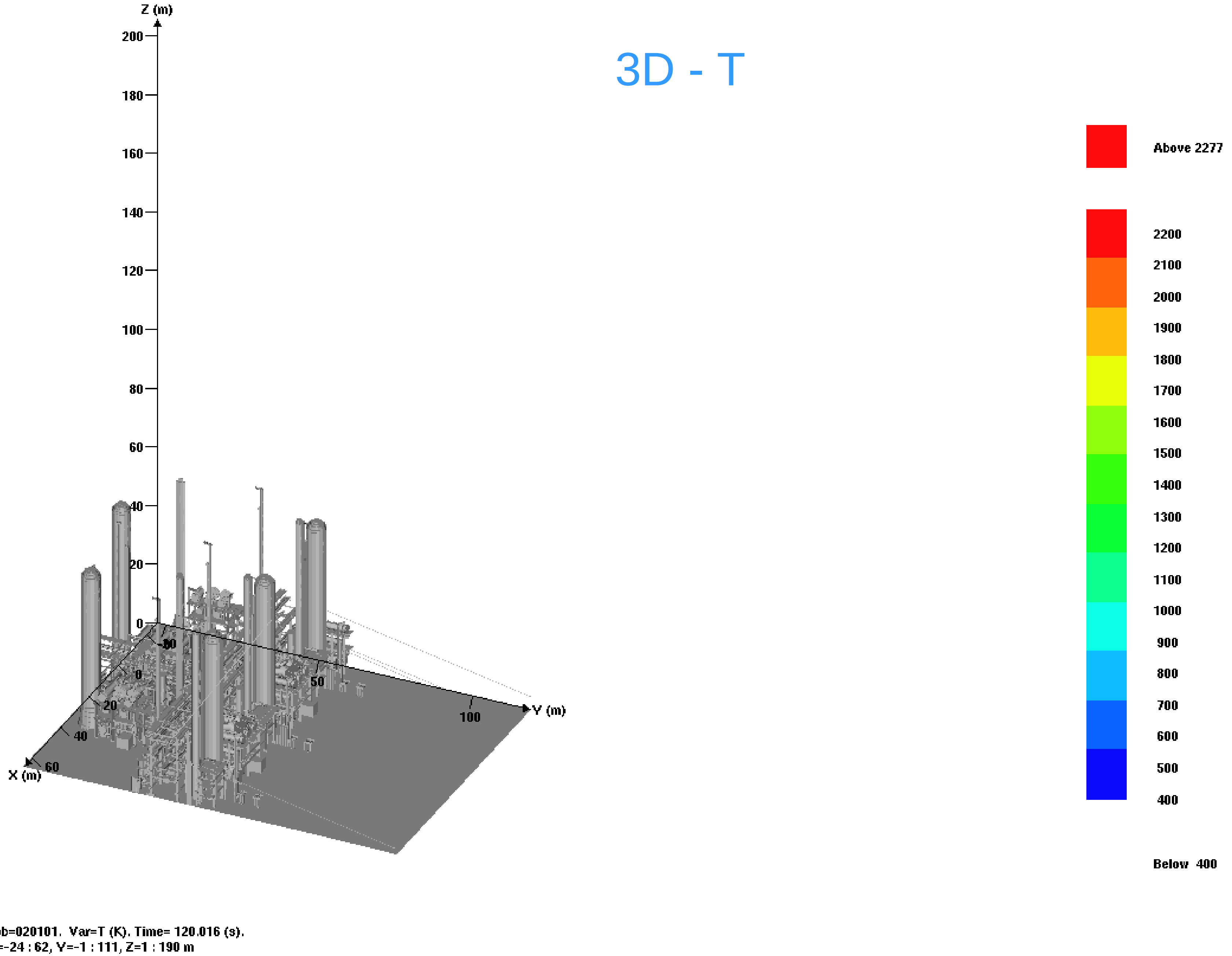


- Drop diameter:
  846 μm
- System vol.:
  8 m × 8 m × 8 m
- Volume coeff.:
  0.2 ‰

3D - ER

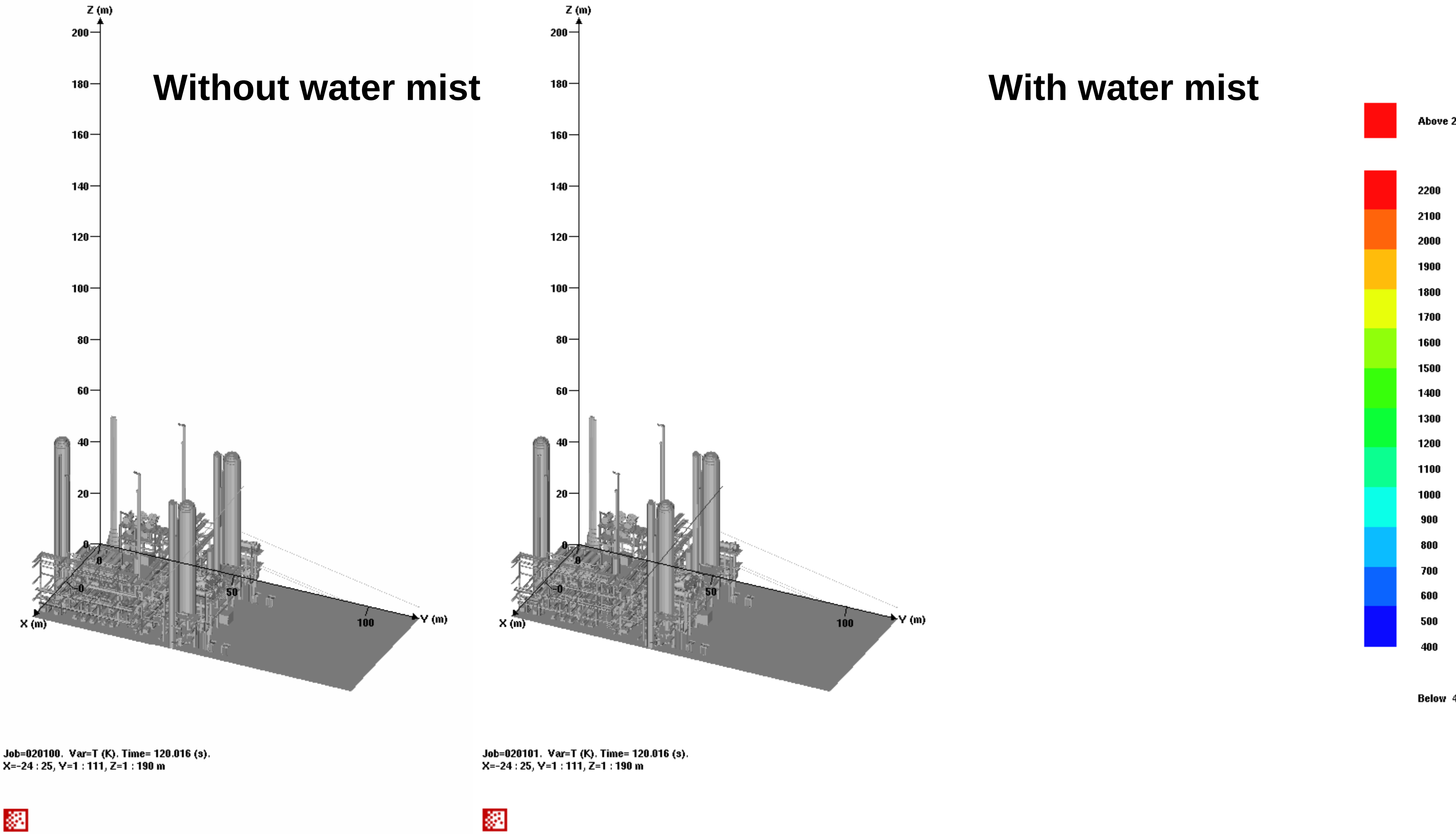

Z (m)
X (m)
Y (m)
Above 10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Below 0.5
Job=020101. Var=ER (-). Time= 120.016 (s).
X=-32 : 69, Y=-15 : 73, Z=1 : 62 m

3D - T



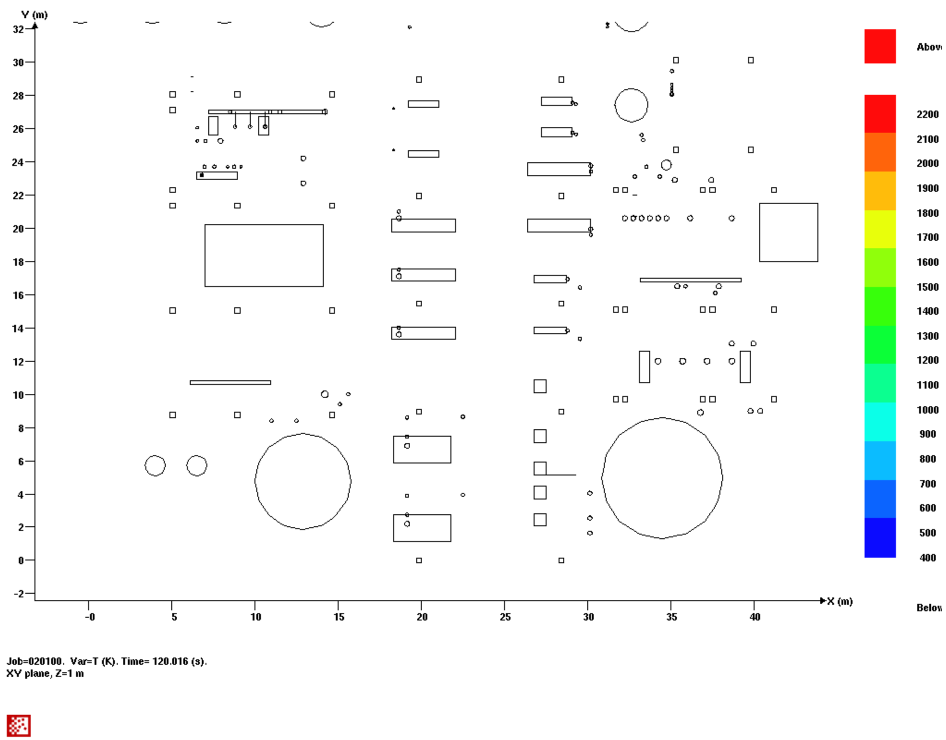
Z (m)
200
180
160
140
120
100
80
60
40
20
0
-20
0
20
40
60
X (m)
50
100
Y (m)
Above 2277
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
Below 400
Job=020101. Var=T (K). Time= 120.016 (s).
X=-24 : 62, Y=-1 : 111, Z=1 : 190 m

3D – T (X =25m)

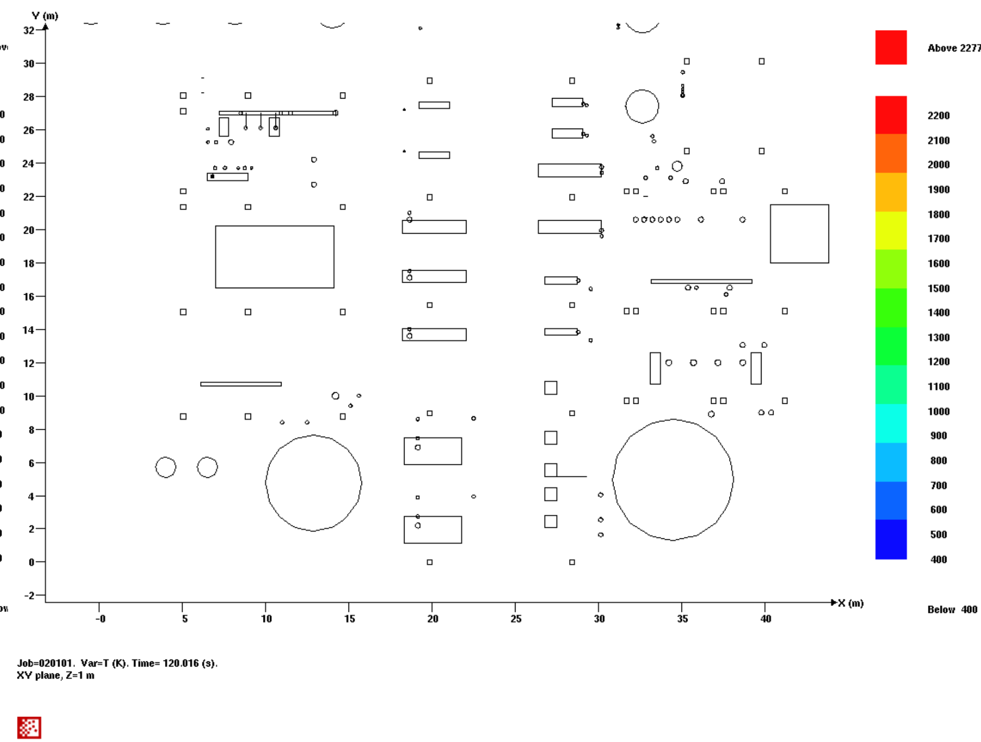

Without water mist
With water mist
Z (m)
200
180
160
140
120
100
80
60
40
20
0
X (m)
Y (m)
50
100
Above 2
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
Below 4
Job=020100. Var=T (K). Time= 120.016 (s).
X=-24 : 25, Y=1 : 111, Z=1 : 190 m
Job=020101. Var=T (K). Time= 120.016 (s).
X=-24 : 25, Y=1 : 111, Z=1 : 190 m

2D – T (Z=1m)

Without water mist

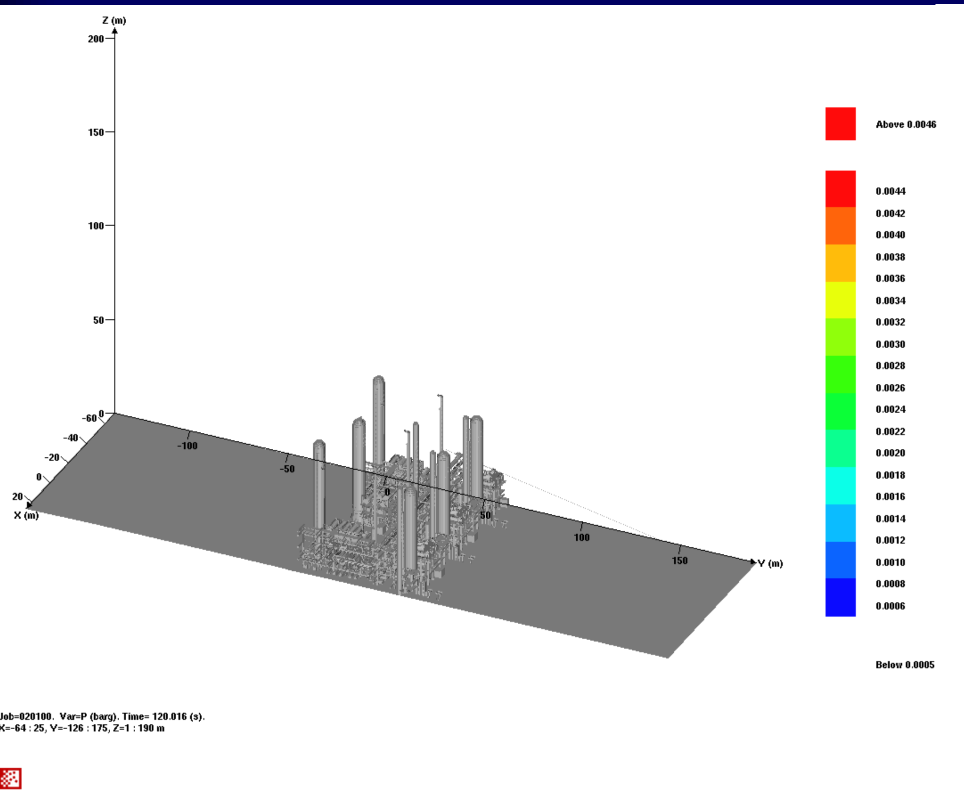


With water mist

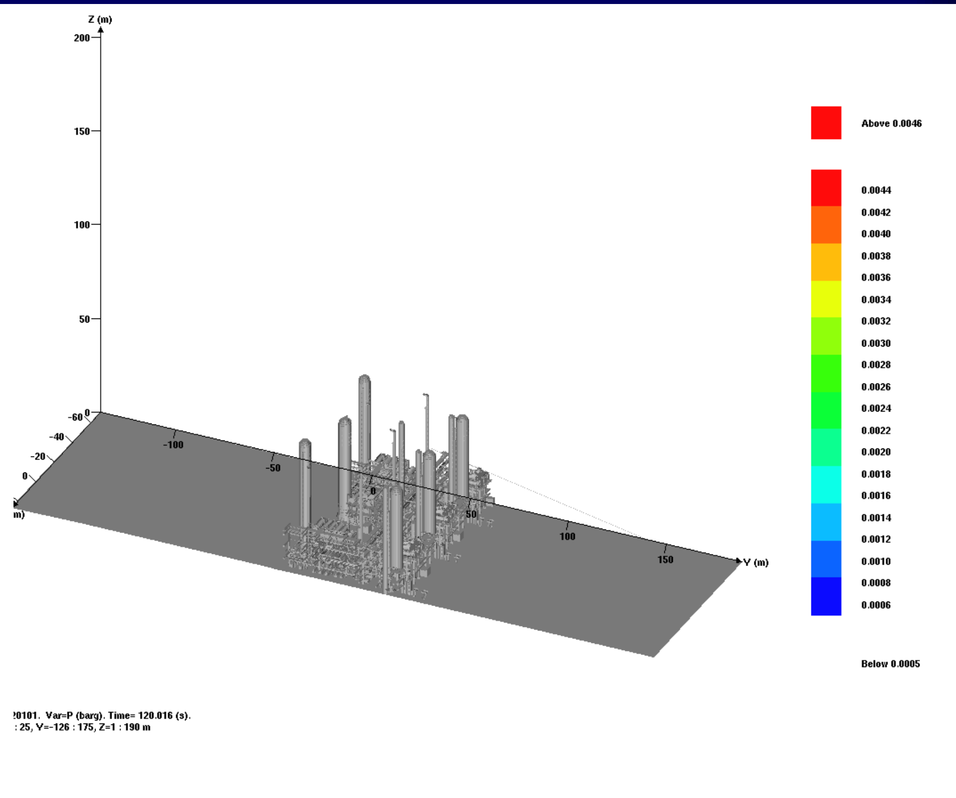


Overpressure

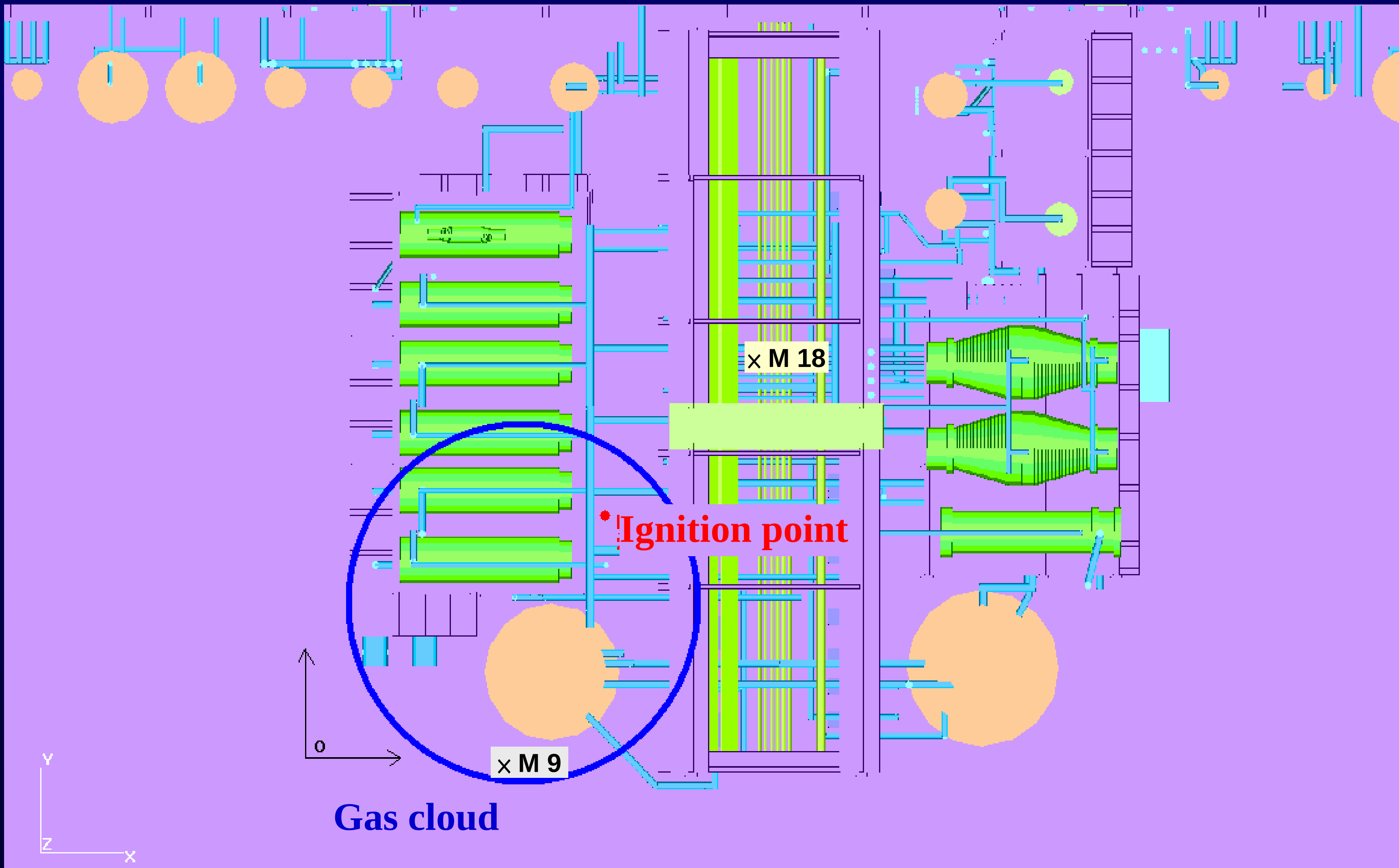
Without water mist

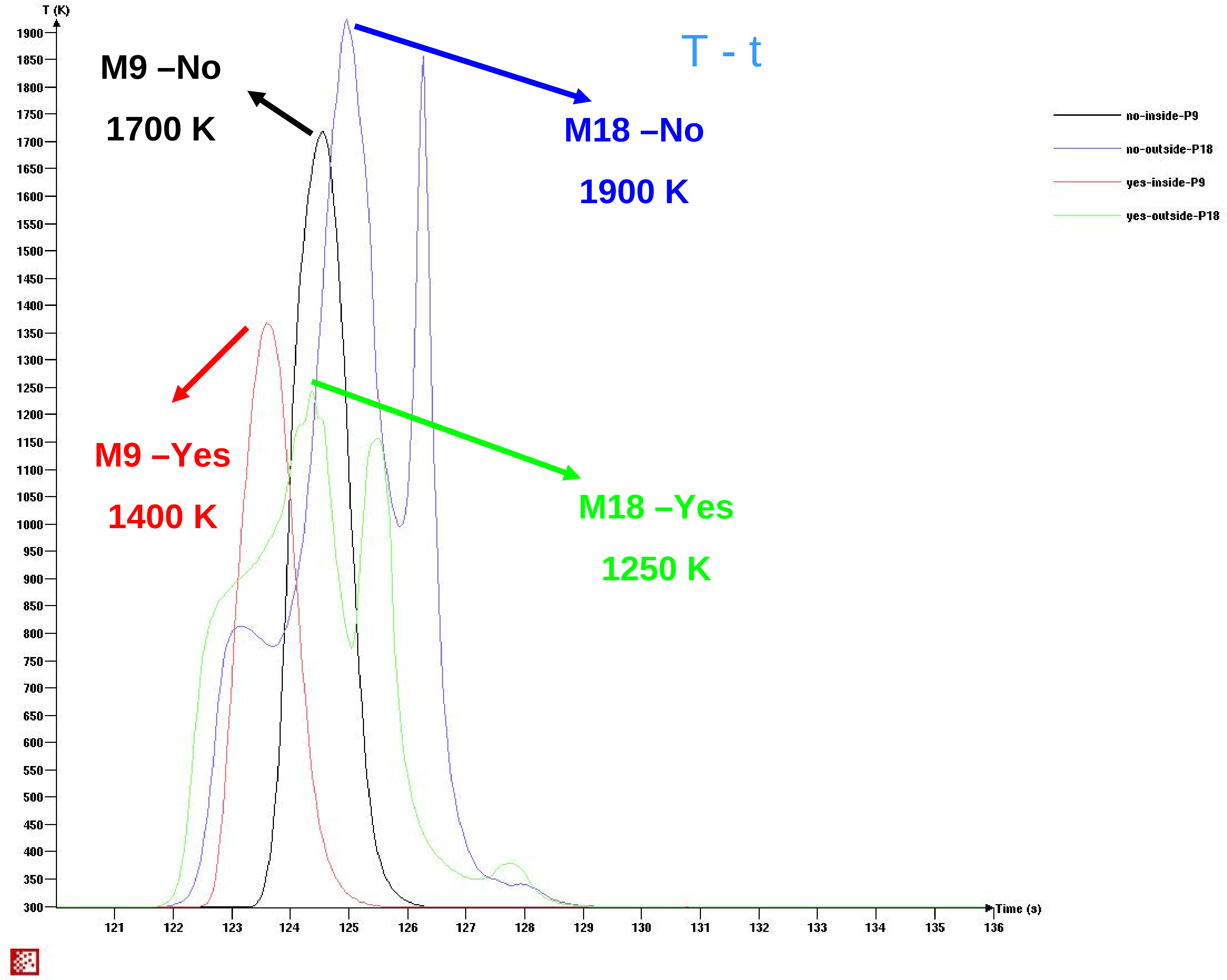


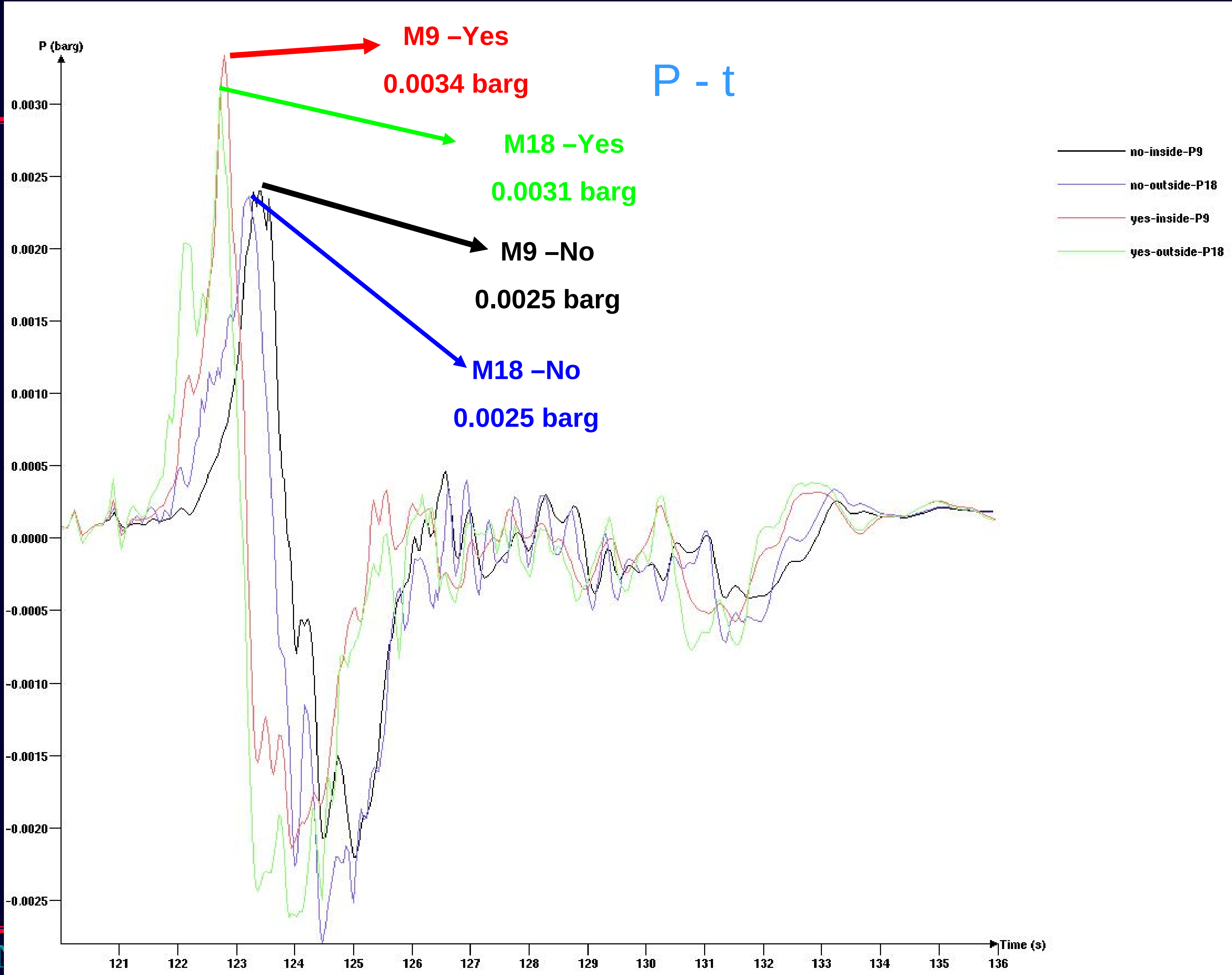
With water mist

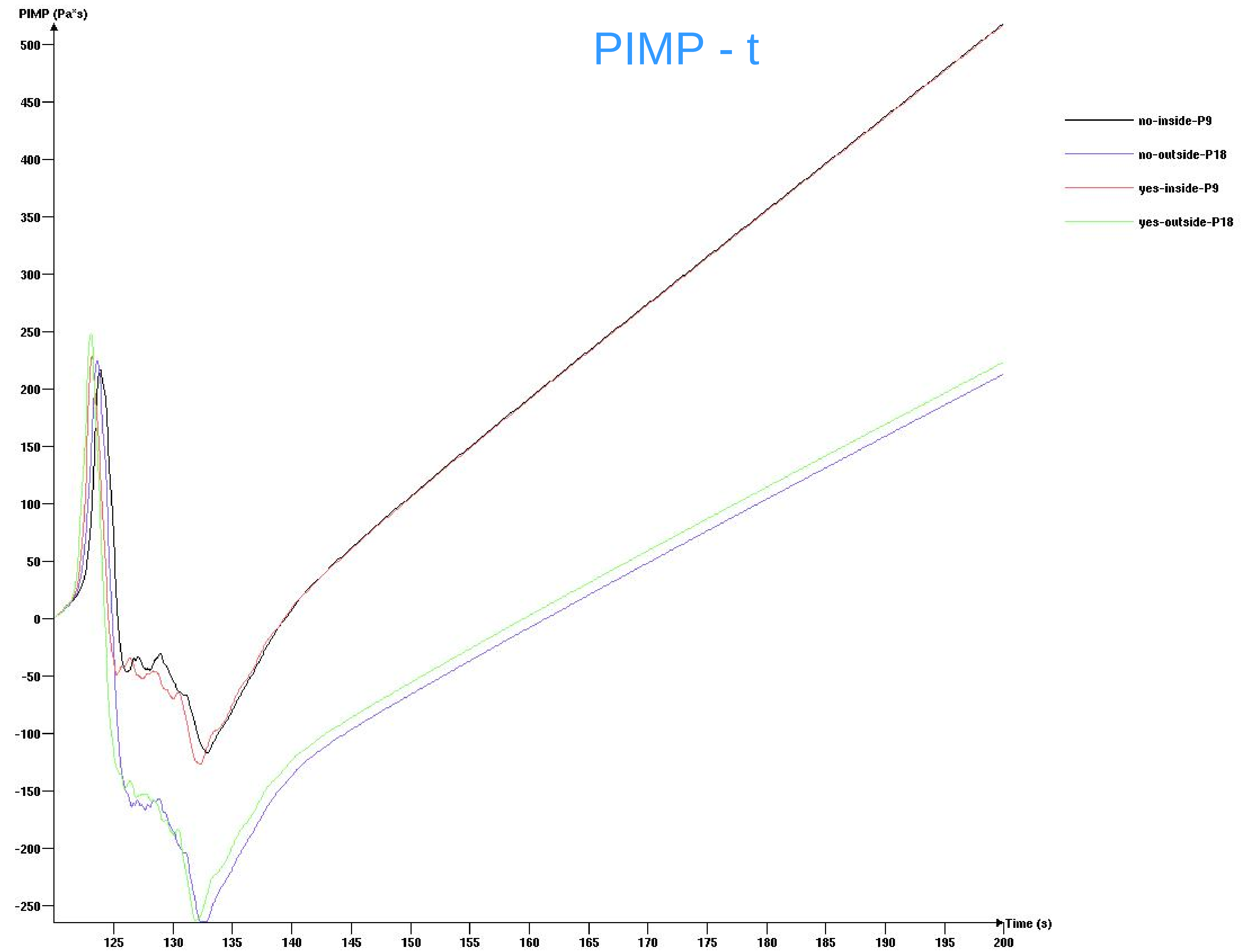


Comparison the results of M9 & M18




T - t
T (K)
Time (s)
M9 –No
1700 K
M18 –No
1900 K
M9 –Yes
1400 K
M18 –Yes
1250 K
no-inside-P9
no-outside-P18
yes-inside-P9
yes-outside-P18
1900
1850
1800
1750
1700
1650
1600
1550
1500
1450
1400
1350
1300
1250
1200
1150
1100
1050
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
300
121
122
123
124
125
126
127
128
129
130
131
132
133
134
135
136


M9 –Yes
0.0034 barg
P - t
M18 –Yes
0.0031 barg
M9 –No
0.0025 barg
M18 –No
0.0025 barg
P (barg)
Time (s)
no-inside-P9
no-outside-P18
yes-inside-P9
yes-outside-P18


PIMP - t
PIMP (Pa*s)
Time (s)
no-inside-P9
no-outside-P18
yes-inside-P9
yes-outside-P18
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
200

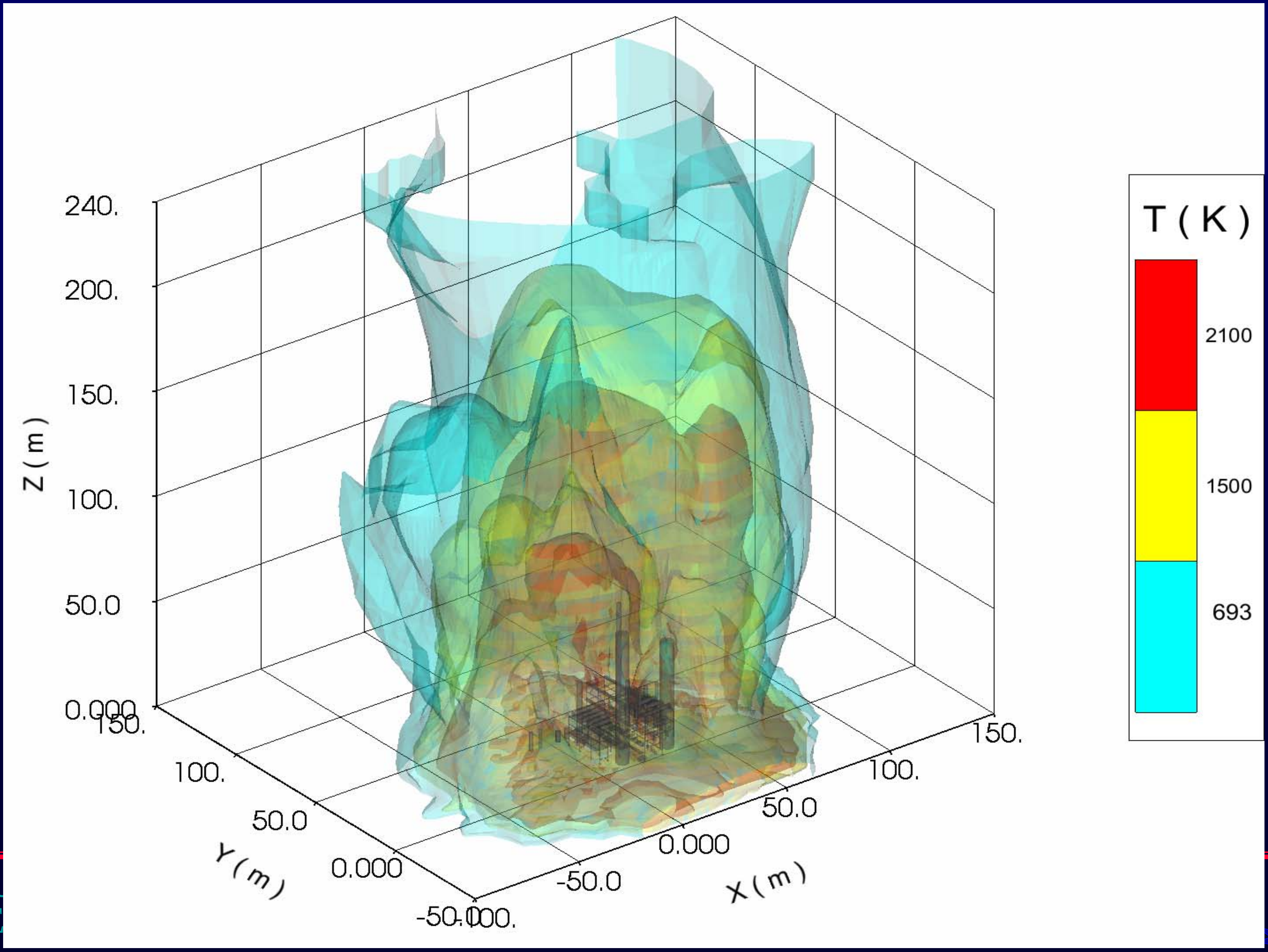
Summary of FLACS simulation

Case No.	Vapor cloud vol.(m^3)	Peak temp (K)	Peak overpress. (barg)	Peak impulse press. (Pa*s)
1	28,730	2,351	0.02265	3,233
2	1,767	2,277	0.00458	2,055
3	1,767	2,277	0.00508	2,061

Isosurface threshold of risk analysis module

Hazardous factor	Threshold	Unit	Comments
Overpressure	0.02	barg	Window glass damage (Clancey, 1972)
	0.069	barg	Partial damage to the house
	1.6	barg	Major damage to the house structure
Impulse pressure	18,000	Pa*s	Death threshold of IP (Eisenberg, 1972)
	37,300	Pa*s	30% death via impulse pressure
	49,700	Pa*s	95%death via impulse pressure
Temperature	700	K	The highest temp human can endure
	1,500	K	Flame temperature
	2,100	K	
Death rate	1	%	
	50	%	
	90	%	

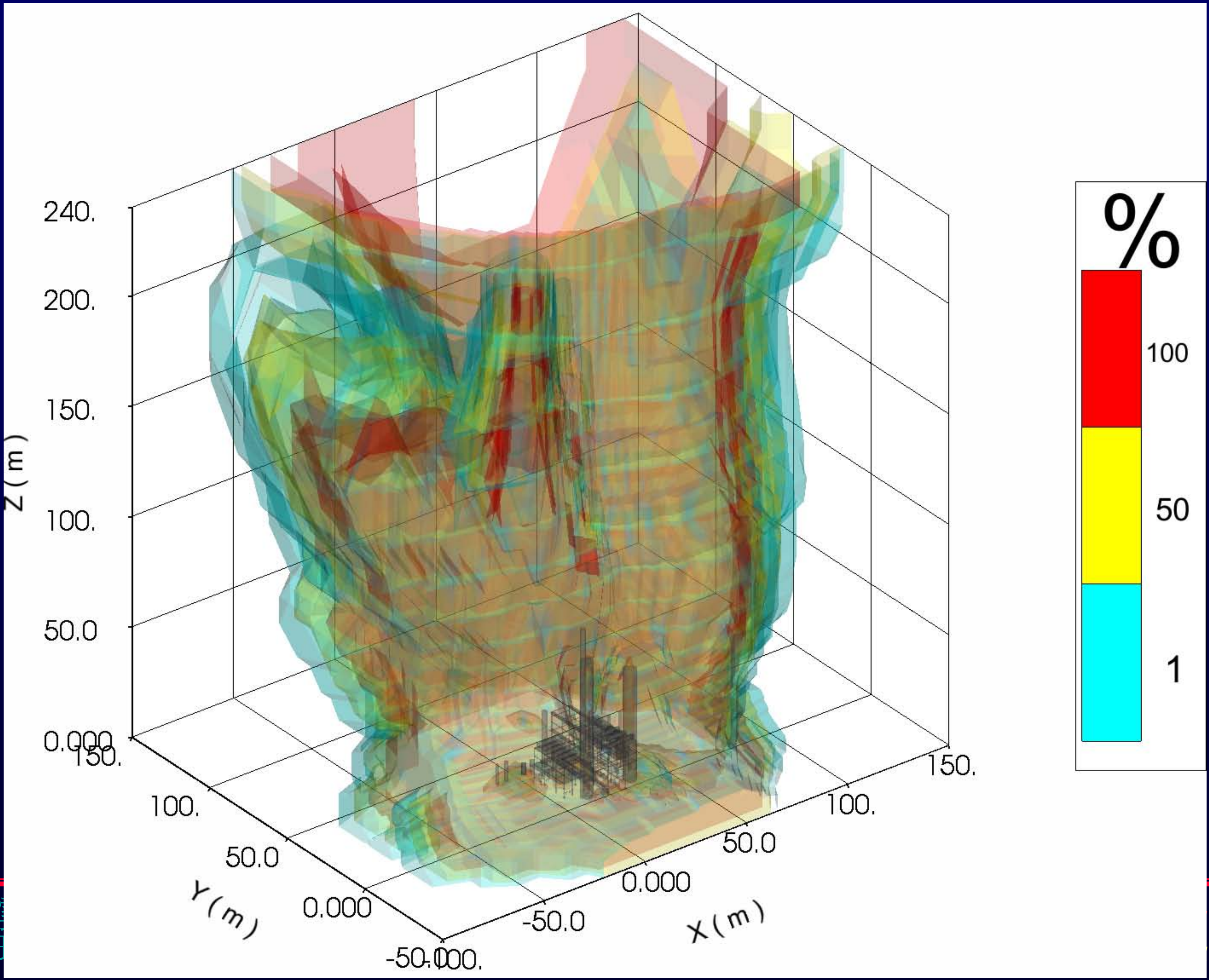
Case1: isosurface of max. thermal radiation



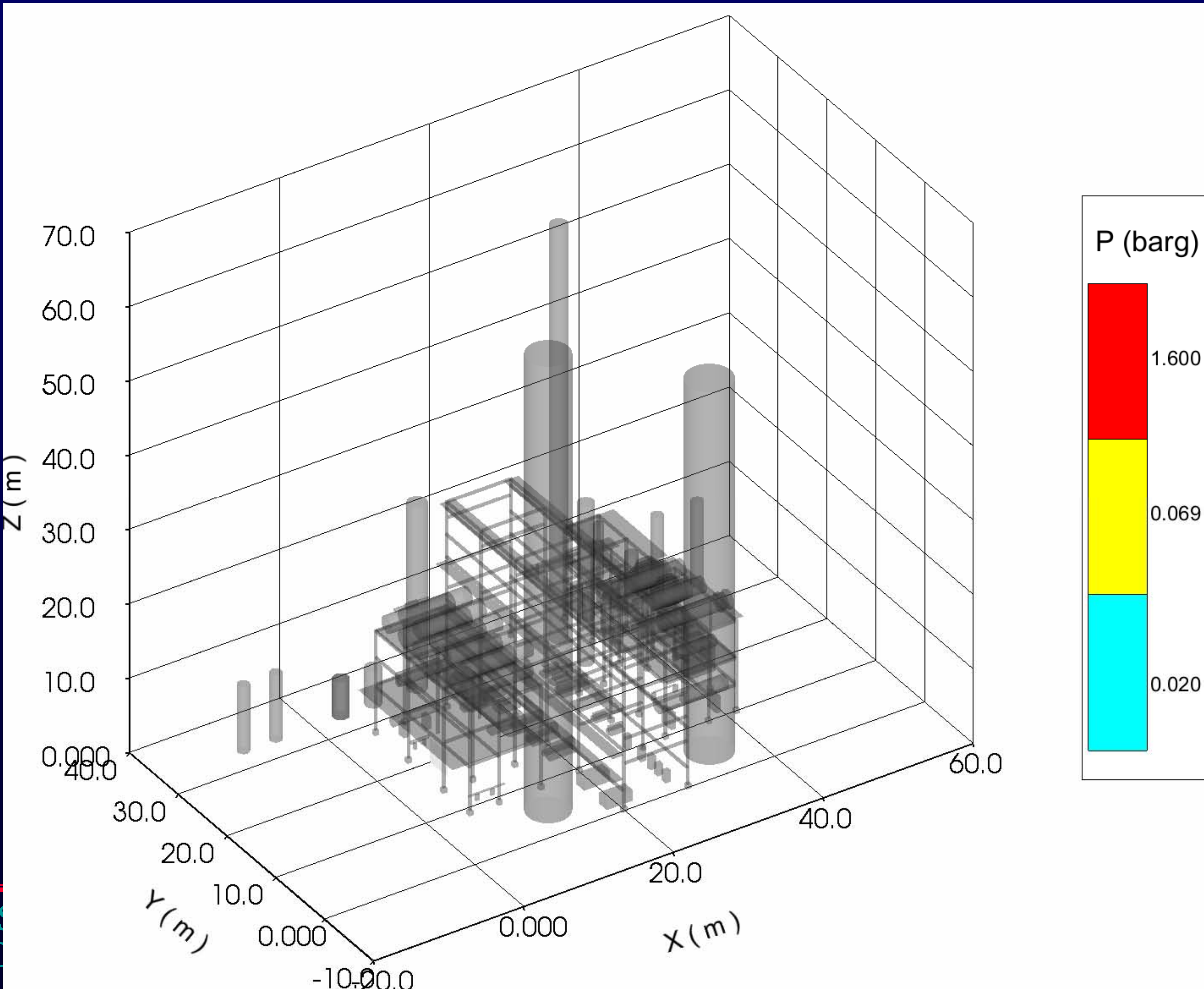
NYU
SHE

CPR Lab

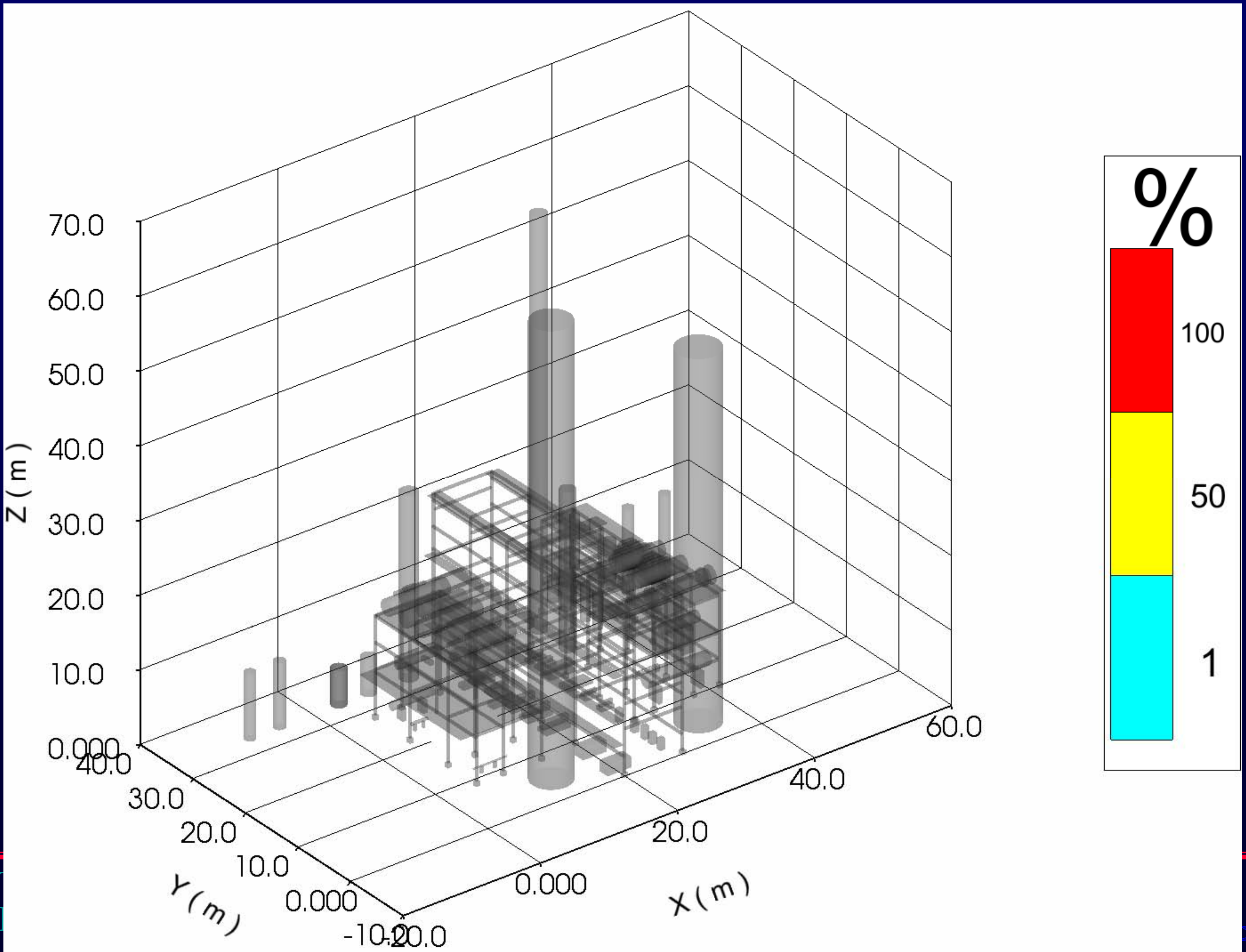
Case1: isosurface of death probability (TR)



Case1: isosurface of max. overpressure



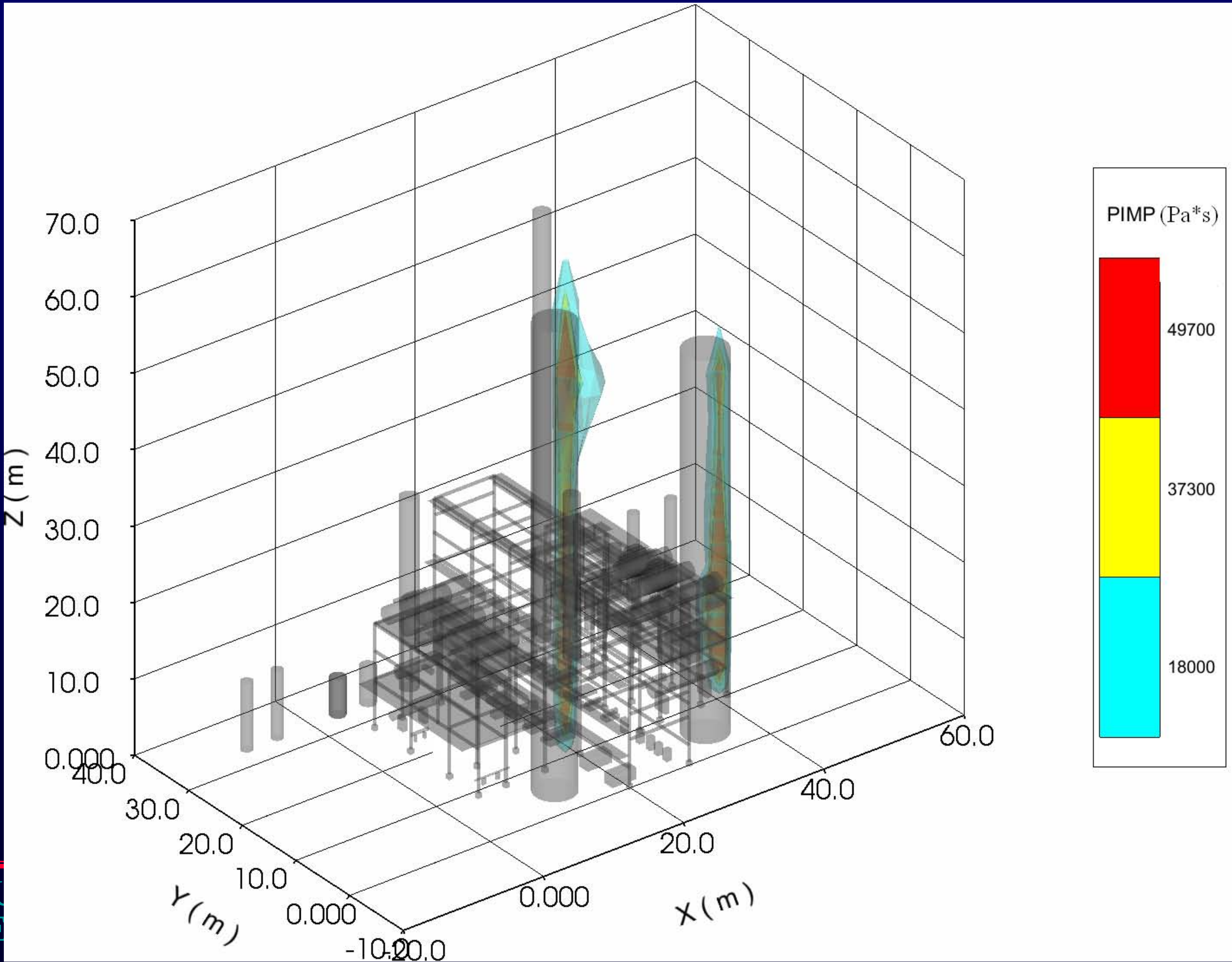
Case1: isosurface of death probability (OP)



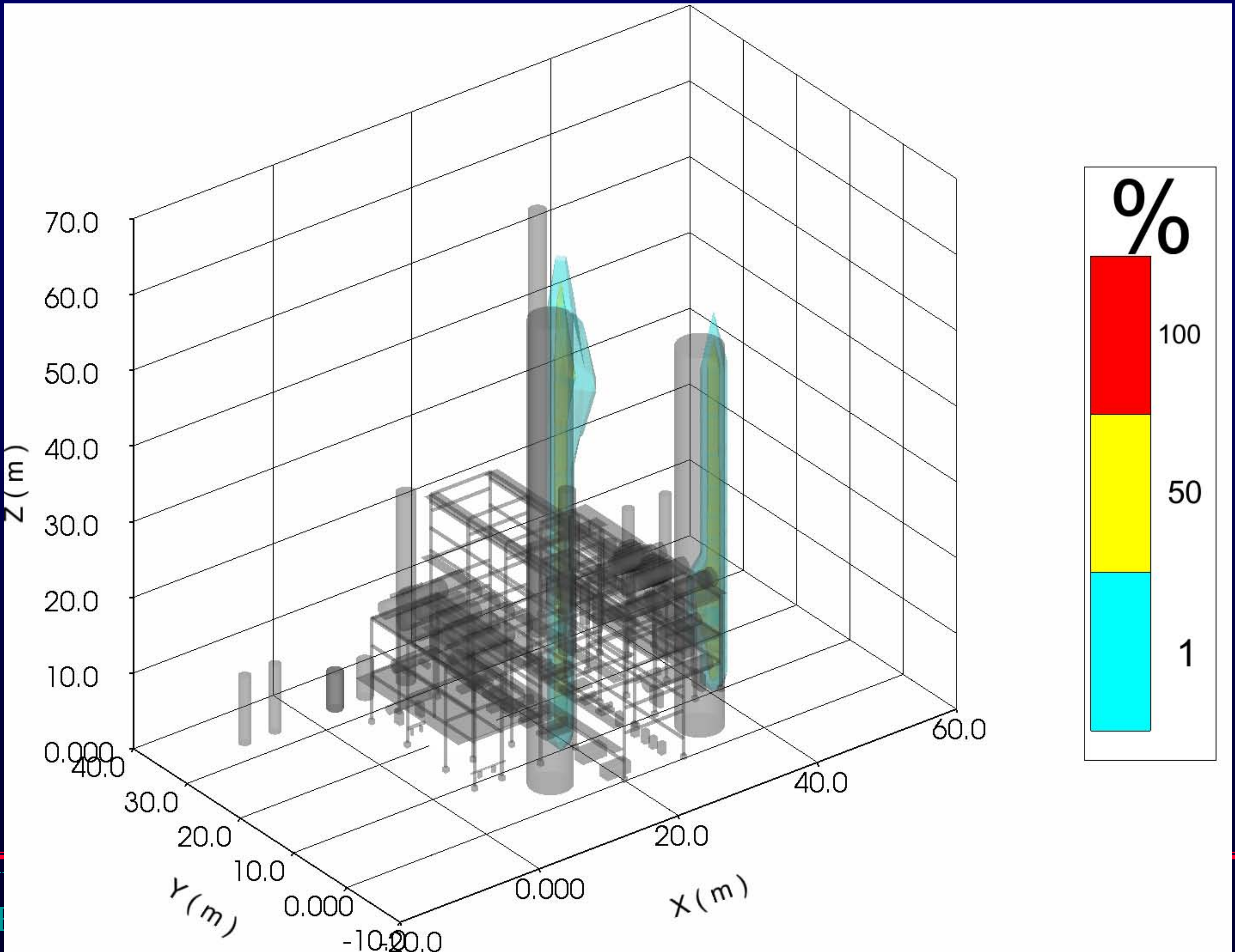
NY
SH

CPR Lab

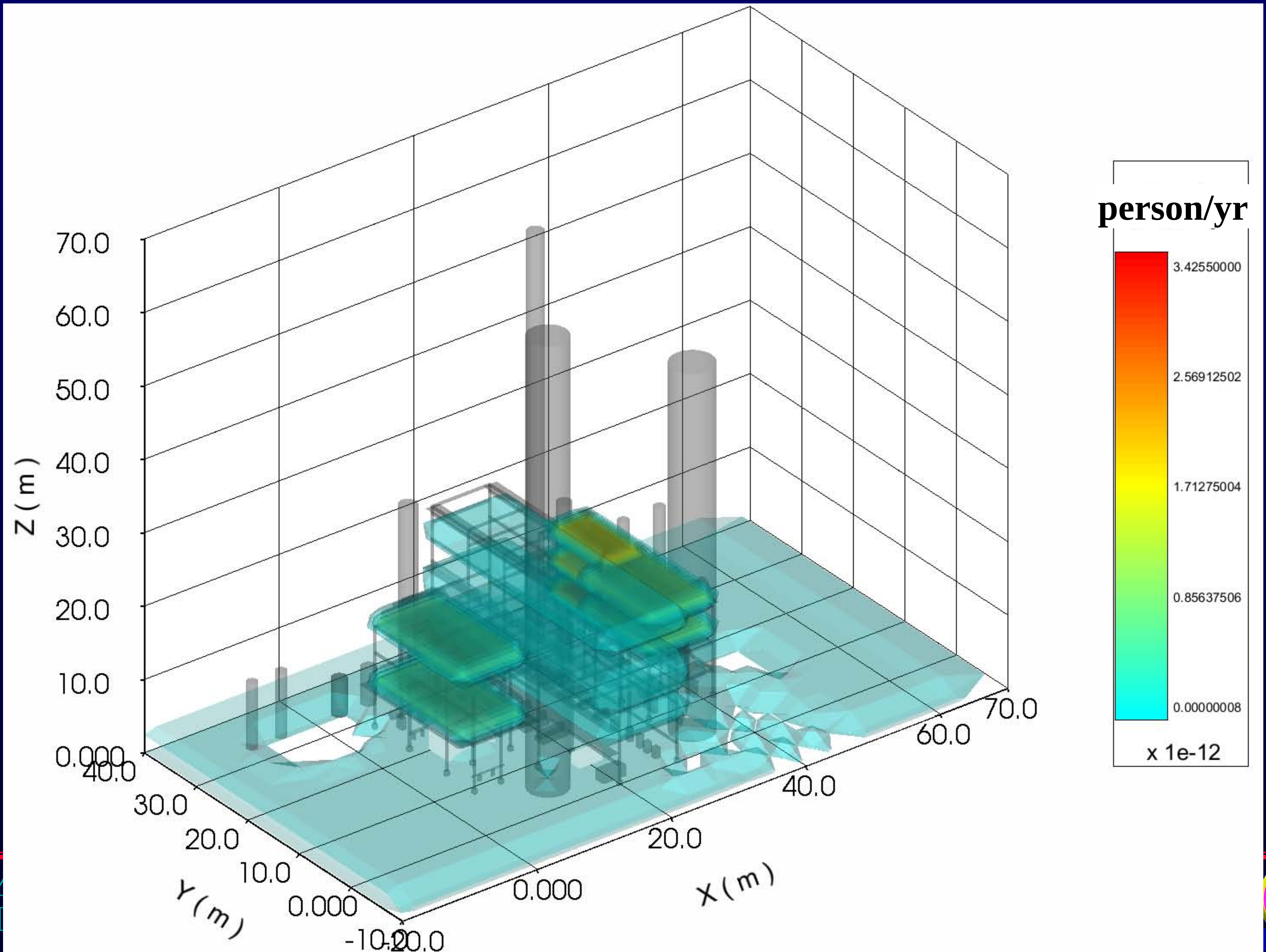
Case1: isosurface of max. impulse pressure



Case1: isosurface of death probability (IP)



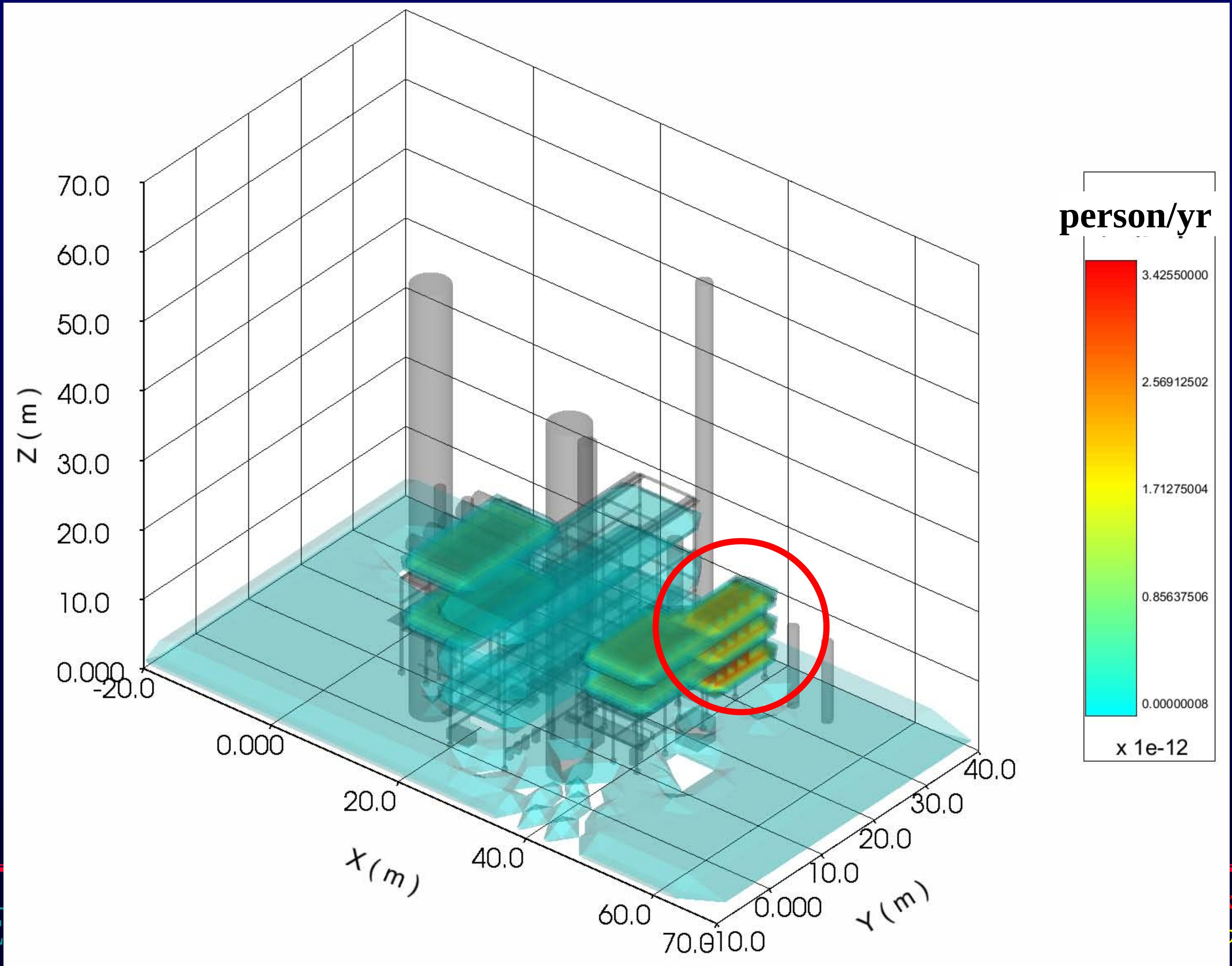
Case1: isosurface of individual risk (left front)



NY
SH

CPR Lab

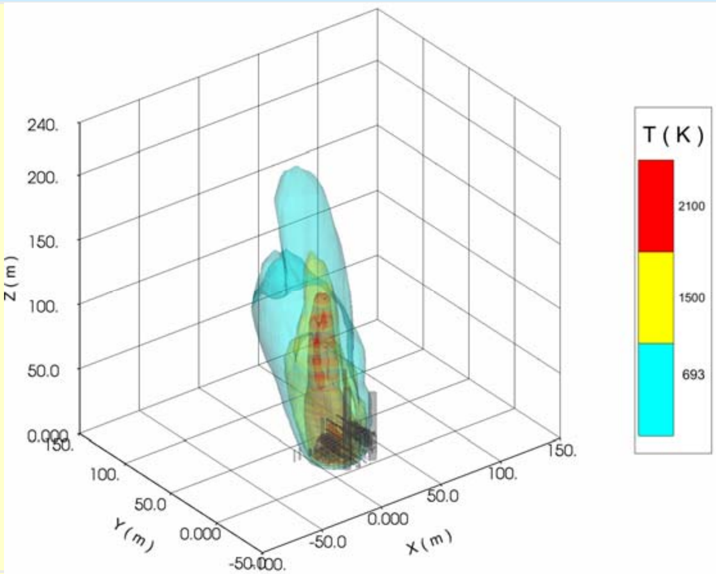
Case1: isosurface of individual risk (right front)



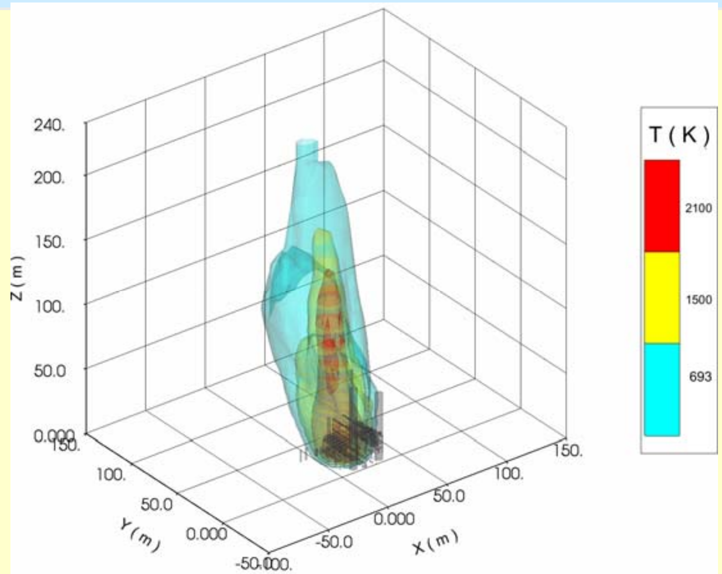
Comparison of thermo radiation

Case 2

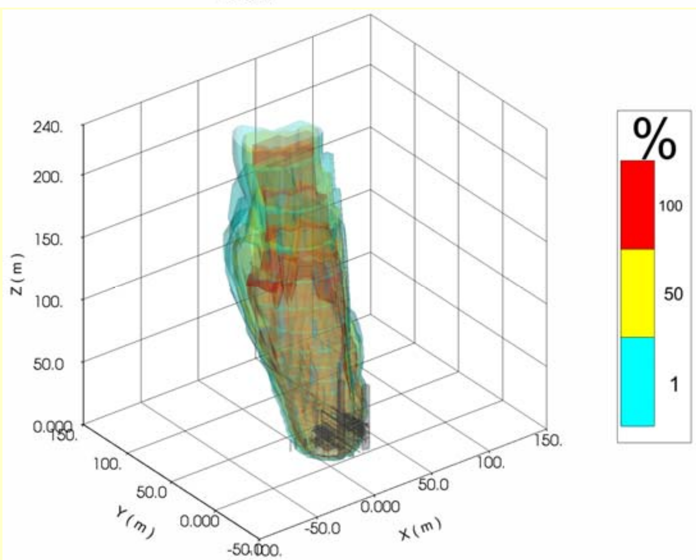
max. physical effect

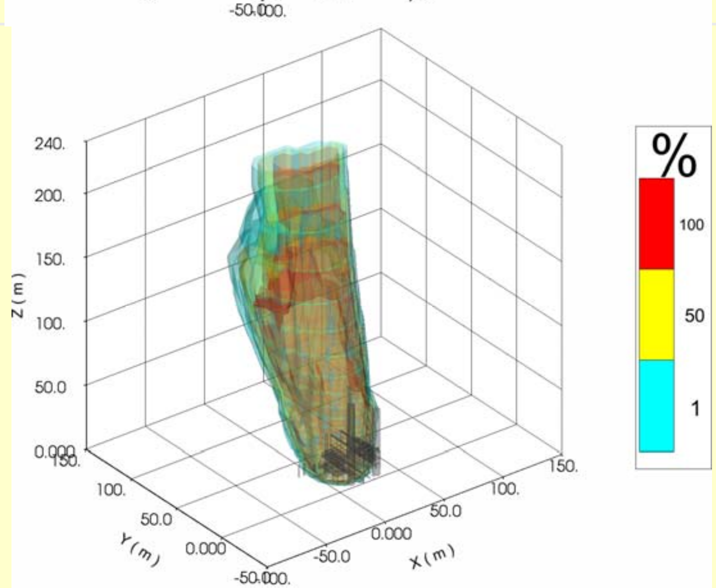


Case 3



death probability

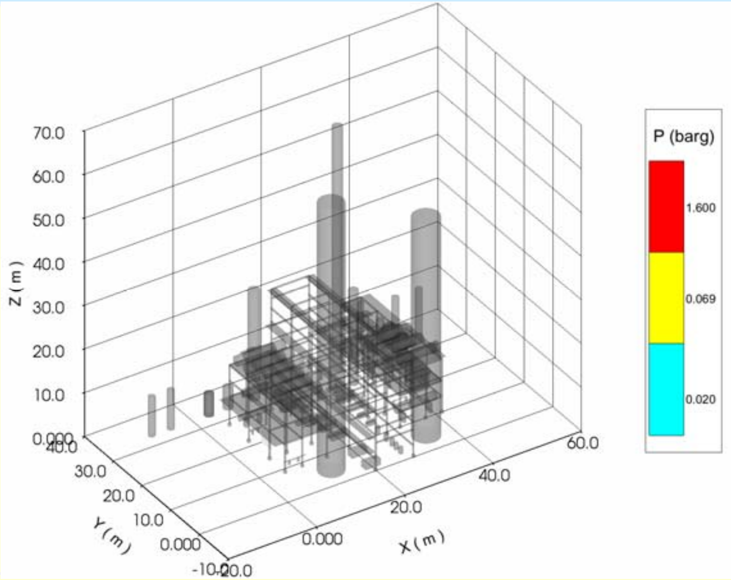




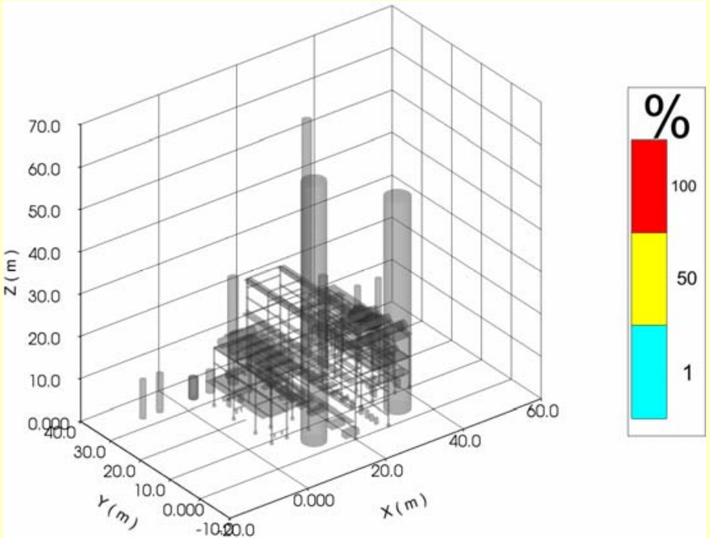
Comparison of overpressure

Case 2

max. physical effect

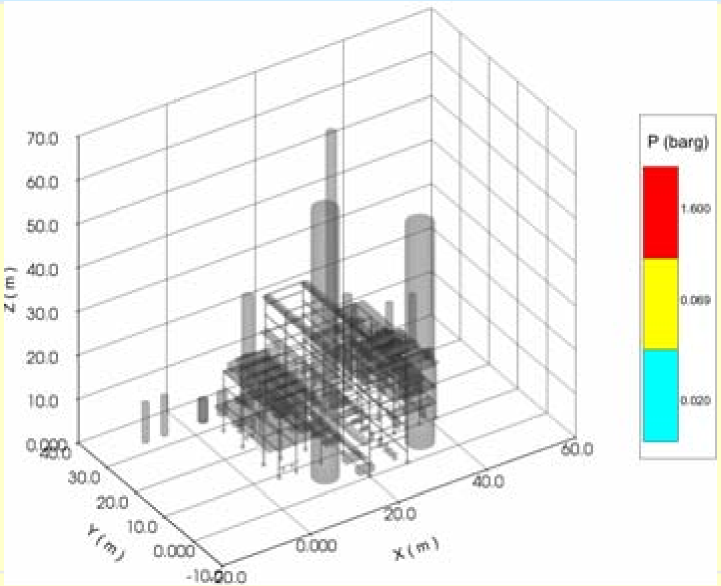


death probability

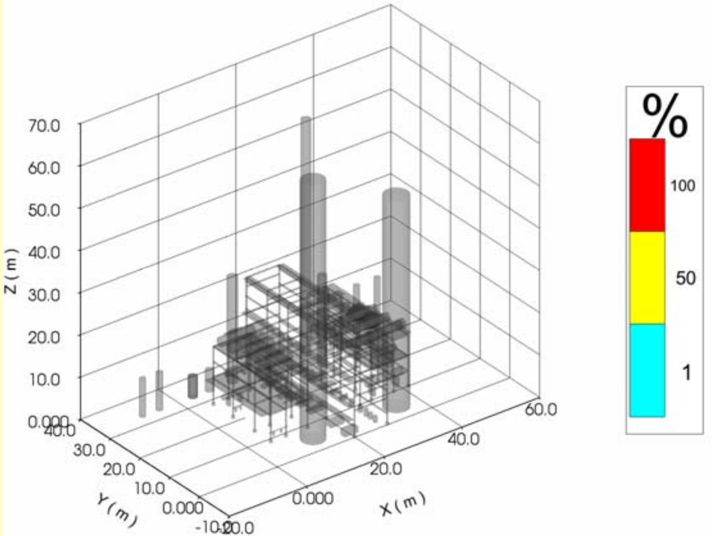


Case 3

max. physical effect



death probability

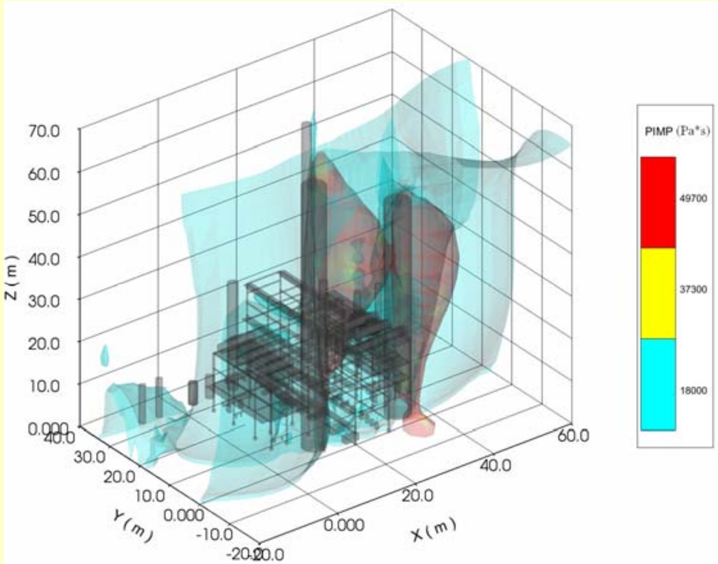


Comparison of pressure impulse

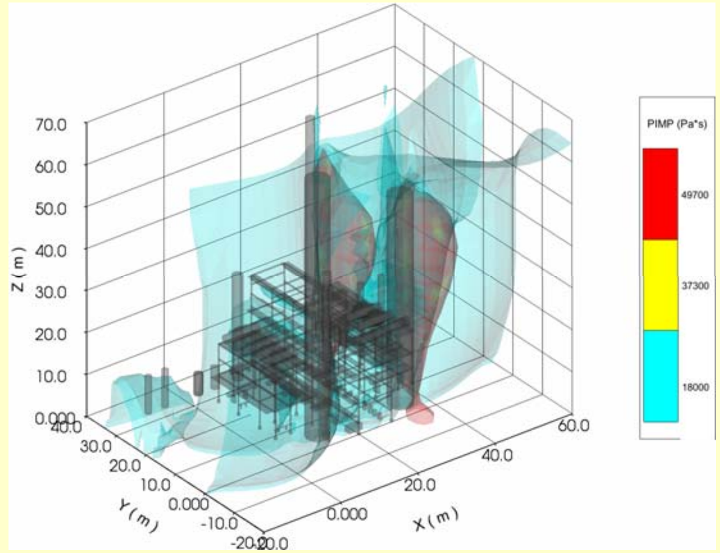
	Case 2	Case 3

max. physical effect

Case 2

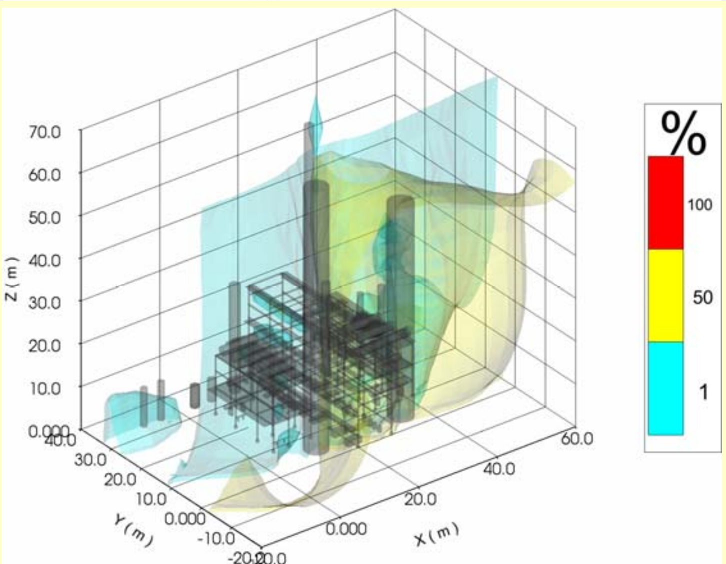


Case 3

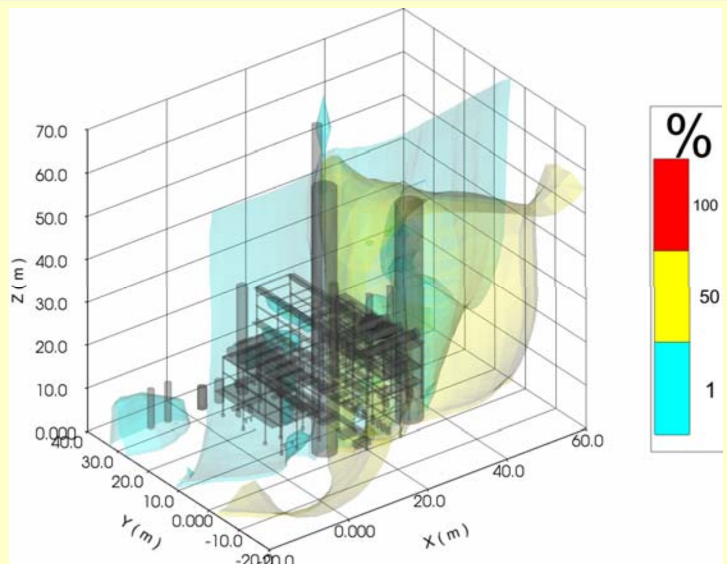


death probability

Case 2



Case 3

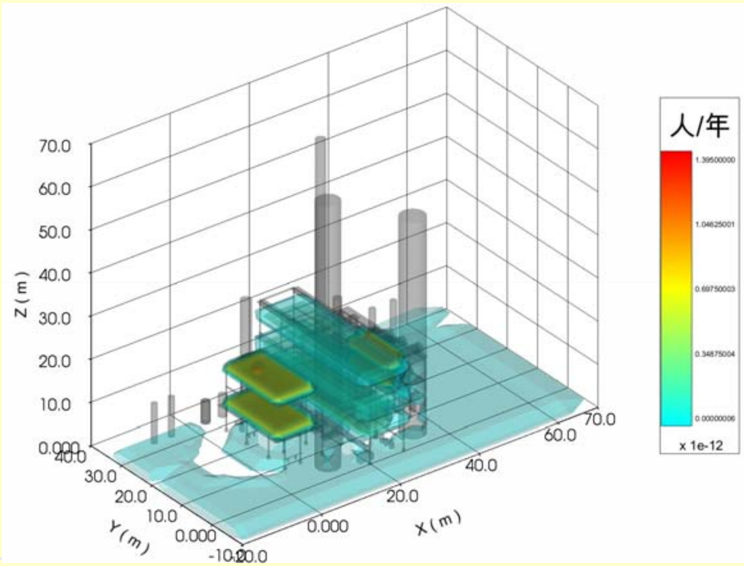


Comparison of individual risk

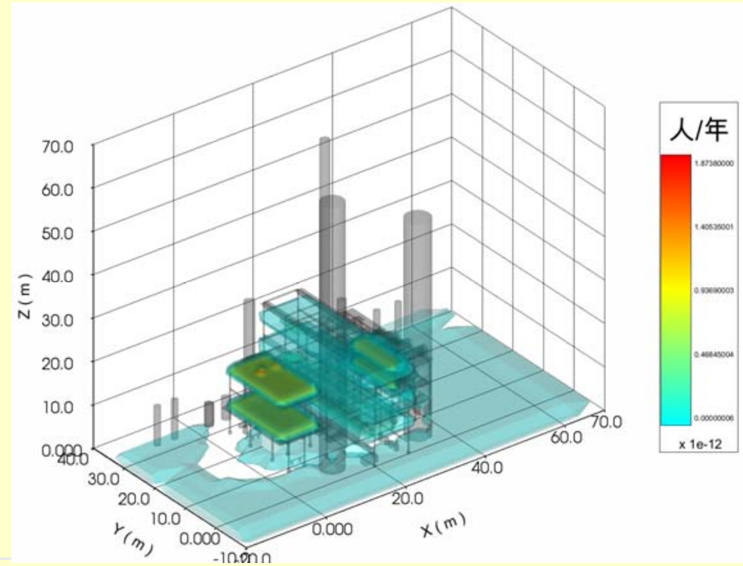
Case 2 — **Case 3**

Left front side

Case 2:

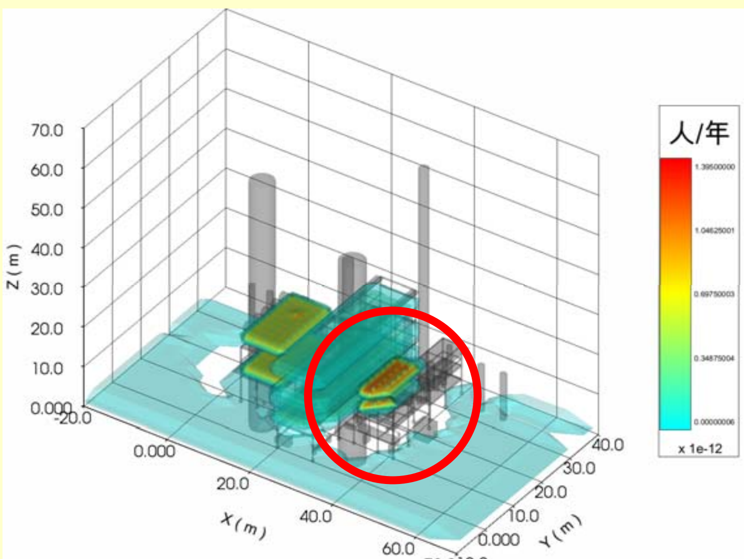


Case 3:

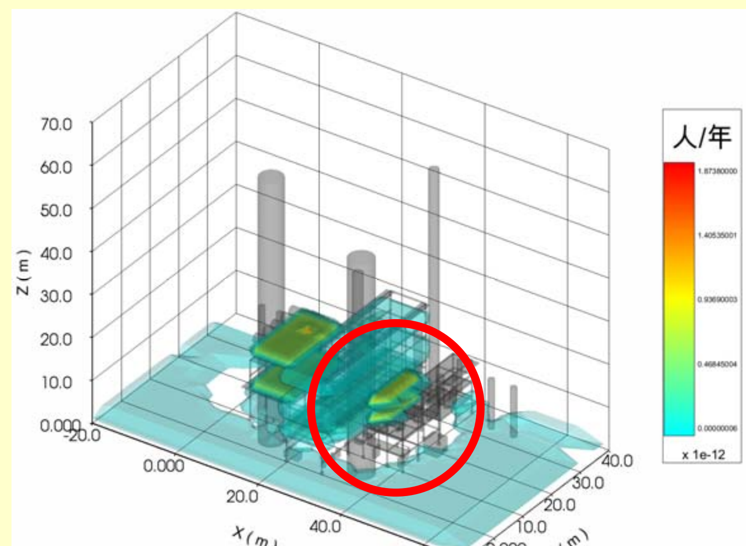


Right front side

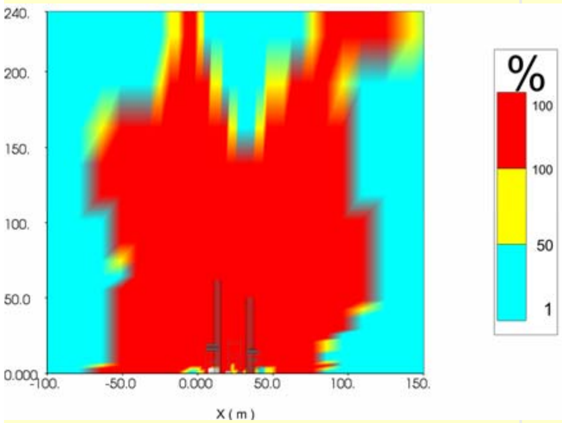
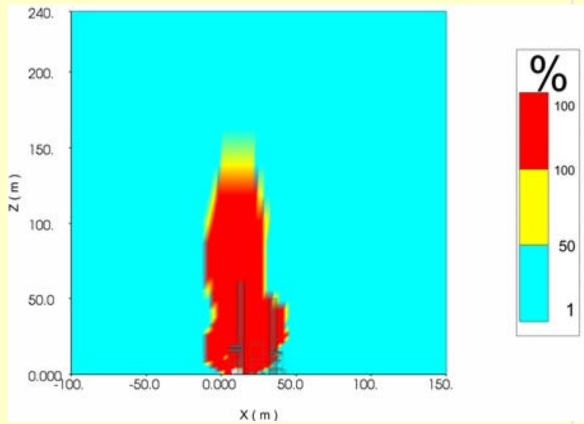
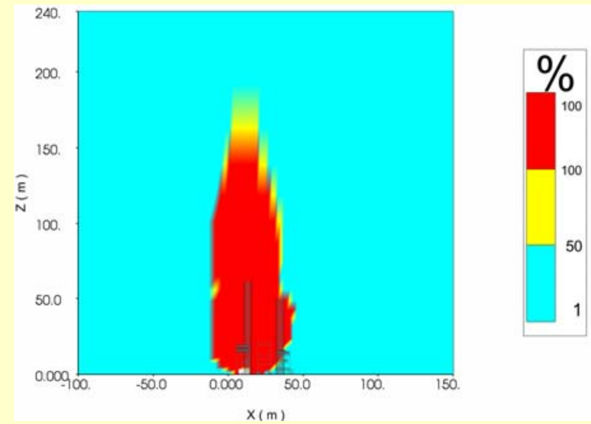
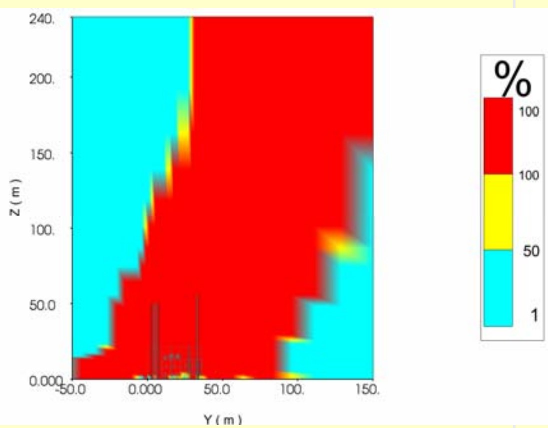
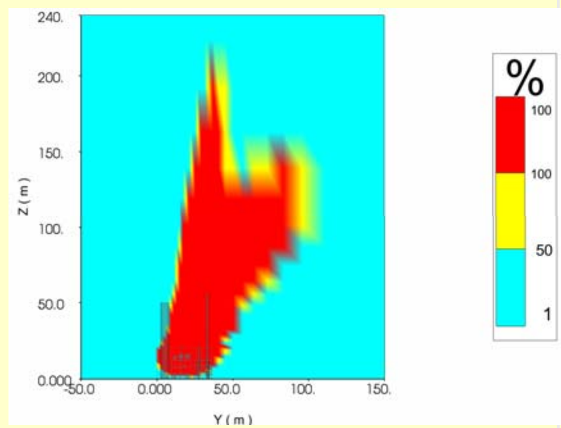
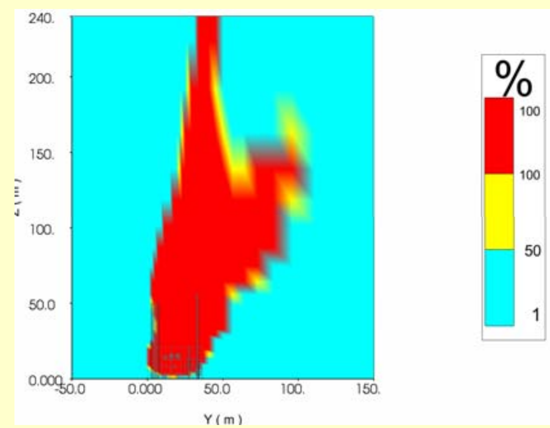
Case 2:



Case 3:



Comparison of cross-sectional view of death probability isosurface

	Event 1	Event 2	Event 3
front side			
Right side			

Simulation Results of Risk Analysis Module

Location	Case 1	Case 2	Case 3
ground areas	8.0E-20	6.0E-20	6.0E-20
P-2 area	5.7E-13	7.0E-13	6.0E-13
P-3 area	5.7E-13	7.0E-13	6.0E-13
R-2 area	5.7E-13	1.4E-12	1.0E-12
R-3 area	5.7E-13	1.4E-12	1.0E-12
R1-2 area	3.4E-12	0	0
R1-3 area	3.4E-12	0	0
R1-4 area	3.4E-12	0	0
M-2 area	8.0E-20	6.0E-20	6.0E-20
M-3 area	8.0E-20	6.0E-20	6.0E-20
M-4 area	8.0E-20	6.0E-20	6.0E-20
vacant lots	8.0E-20	6.0E-20	6.0E-20

Simulation Results of Risk Analysis Module (cont.)

Case No.	Total population (person)	Thermal radiation death (person)	Overpressure death (person)	Impulse pressure death (person)	Total death (person)	Death rate (%)
1	2.72	2.70	0	0	2.70	99.5
2	2.72	1.47	0	0.02	1.49	54.8
3	2.72	1.40	0	0.03	1.43	52.4

Conclusions

- In this research, a conceptual ***3D risk analysis technique*** was proposed via the combination of the CFD simulation results with self-developed codes for calculating effect model and individual risk. This technique has been successfully implement on the fire & explosion risk analysis task within a petrochemical plant's process area.
- The ***3D risk analysis technique*** can not only improve the drawback of the traditional methods which usually neglect the terrain, the obstacle, and concentration fluctuations effects but also extend the risk analysis region from 2D into 3D domain

Conclusions (cont.)

- The simulation results show that employees at high levels would receive higher risk (3.4×10^{-12} person/yr), while the risk values on the ground areas and vacant lots would be the lowest (6.0×10^{-20} person/yr). Therefore, an apparent risk difference exists between different heights at the same location.
- This study also investigates whether the fire and explosion hazard can be mitigated by installing water spray system. According to the simulation results, water spray activation really has the potential to reduce individual risk. However, its turbulent effect can also shorten the initiation time of explosion and increase the overpressure.
- The 3D risk analysis technique proposed in this research can not only used in chemical industry but can also be extended to other industries (aerial, submarine, or ever space risk analysis) where height (depth) has a critical meaning with them.

Thank you for your attention!

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