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SRNL-STI-2019-00736, Rev. 0

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GSA Aquifer Cutouts for E-Area PA Revision Transport Simulations

Abstract

The 2018 General Separations Area (GSA) aquifer model is dissected into four refined cutouts for aquifer transport in preparation for the next E-Area Low-Level Waste Facility (LLWF) Performance Assessment (PA) revision.

The recommended refined horizontal and vertical grid sizes are 20 ft and 3 ft, respectively. The horizontal resolution appropriately represents longitudinal dispersion with dispersivity of 15.4 ft. Four cutouts (i.e., West, Center, East 1, and East 2) are selected to adequately contain tracer plumes emanating from disposal units expected in the E-Area LLWF. For feasible computation, each cutout is refined to mesh sizes much less than the PORFLOW limit of 1,024,000 nodes.

Criteria for Aquifer Cutouts

The 2019 PA revision for the E-Area LLWF requires aquifer transport simulations involving physical dispersion over a range of disposal units, giving rise to uncertainty in the appropriate dispersivity. The objective of this effort is to select the aquifer cutouts with a PORFLOW (ACRi 2018) grid resolution that accommodates the smallest scale of physical dispersion expected in deterministic simulations. Hence, the following criteria must be met for each cutout:

1. A total mesh size much less the PORFLOW limit of 1,024,000 nodes.
2. Adequately contain stream traces and plumes of all disposal units (DUs) considered by the cutout.

Criterion 1 is satisfied by selection of appropriately sized cutout geometries. Criterion 2 is satisfied by using an appropriate cutout geometry from the coarse-meshed GSA aquifer flow field, such that the tracers and concentration plumes are entirely contained within the cutout without boundary overlap.

2016 GSA Aquifer Cutouts

Based on the 2016 GSA groundwater flow model (Flach et al. 2017), a study by Flach (2018) recommended three cutouts (West, Center, and East) with a horizontal grid size of 25 ft. The resulting PORFLOW grid sizes are:

Table 1. Grid sizes of the three GSA 2016 refined cutouts.

Refined Cutout	I nodes	J nodes	K nodes	Total nodes
East	74	138	48	490,176
Center	114	106	44	531,696
West	90	106	42	400,680

Figure 1 shows three GSA 2016 refined grid cutouts.

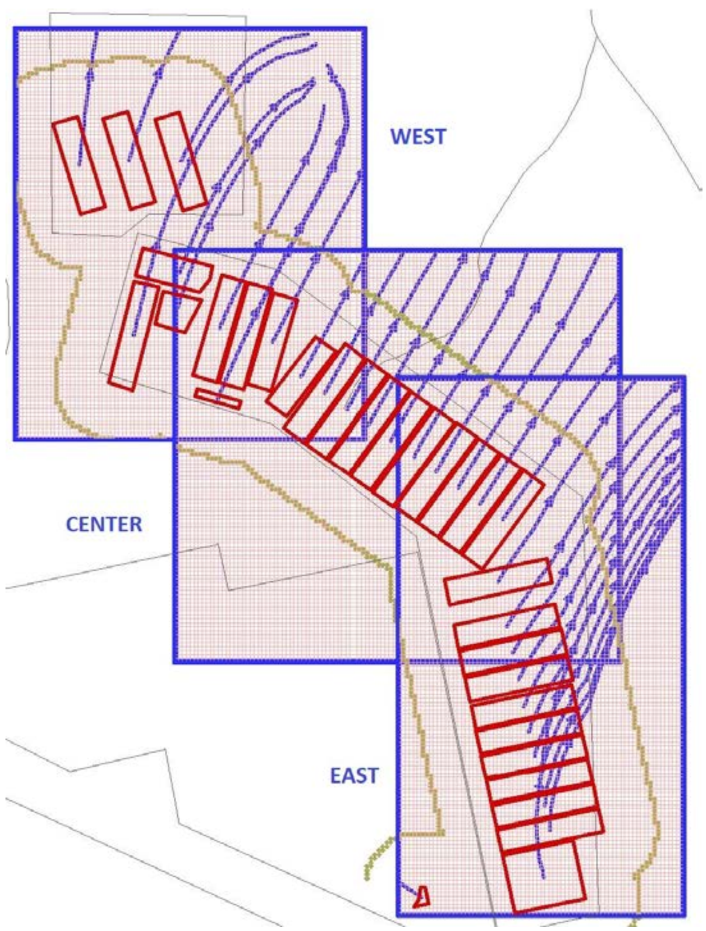


Figure 1. Refined grid cutouts of the 2016 GSA Flow Model.

These cutouts, especially the East cutout, are deemed inadequate because they did not sufficiently include all DUs and tracer plumes at the 100-meter boundary (e.g., NRCDA7E shown at the bottom left corner of Figure 2).

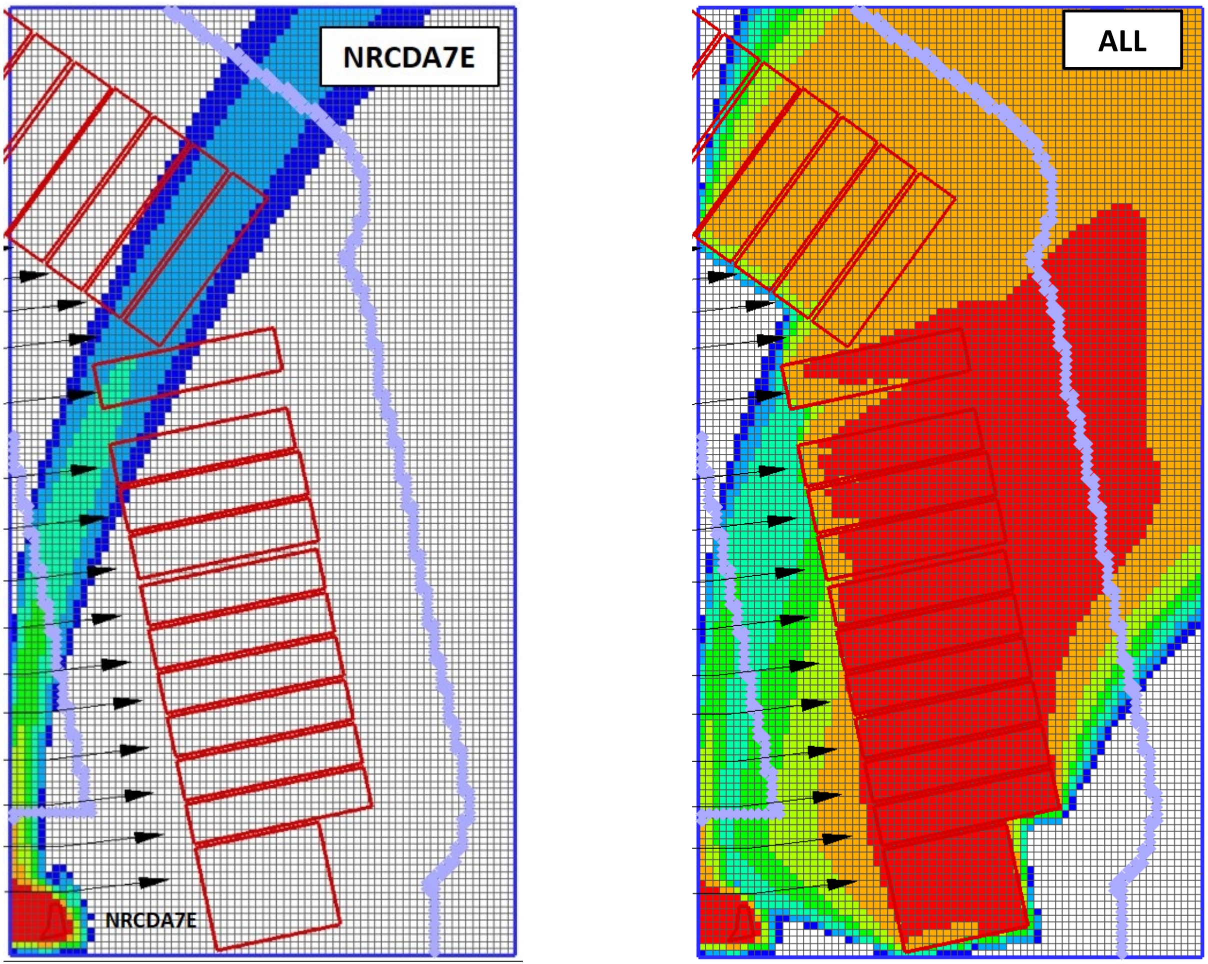


Figure 2. Tracer plumes based on 2018 GSA Flow Model in the East cutout.

<u>2018 GSA Aquifer Cutouts</u>

The 2016 GSA groundwater flow model was updated, refined and recalibrated in 2018, and is referred to as the 2018 GSA model (Flach 2019). The aquifer cutouts are therefore revised to reflect the new flow field. Recent analyses by Hamm et al. (2018 and 2019) indicate the necessity of more refined GSA aquifer cutouts to more adequately describe mechanical dispersion. Therefore, to capture all relevant spatial features and honor the PORFLOW node limit, four aquifer cutouts were created with horizontal and vertical grid sizes of 20 ft and 3 ft, respectively. The cutouts contain all DUs of interest together with their relevant 100-meter boundaries.

The cutouts are extracted from the 2018 GSA flow model using the code MESH3D Rev. 3 (Danielson 2017). Versions 1 and 2 of MESH3D were developed in Fortran. Recently the code was completely rewritten in Python resulting in Version 3.1, which provides extended capabilities to enable variable mesh refinement in all coordinate directions and supports unstructured PORFLOW grids in addition to structured grids. In the current work, input data to MESH3D are provided via a *Makefile* file. A sample of the *Makefile* to create the refined East 1 cutout is illustrated below:

```
1   SHELL = /bin/ksh
2
3   Platform = Linux
4
5   GSA_PORFLOW = ../GSA
6
7
8   cutoutindices = [[68, 41, 1], \
9                    [76, 41, 1], \
10                   [76, 59, 1], \
11                   [68, 59, 1], \
12                   [68, 41, 19], \
13                   [76, 41, 19], \
14                   [76, 59, 19], \
15                   [68, 59, 19]]
16  subdivisions = [ [68, 76, 10]], \
17                 [ [41, 59, 10]], \
18                 [ [1, 2, 2],[2, 3, 4],[3, 5, 2],[5, 10, 4],[10, 17, 2], [17, 19, 1] ] ]
19
20  GridType = Structured
21                                              .
22                                              .
23                                              .
```

The mesh is refined using the criteria given in "`cutoutindices`" and "`subdivisions`." "`cutoutindices`" specify the eight corner indices of the cutout. "`subdivisions`" applies refinement of the coarse mesh along the i, j, k directions. As shown above, the i index ranges from 68 to 76 and is subdivided into 10 refined grid cells (Line 16); the j index ranges from 41 to 59 and is subdivided into 10 refined grid cells (Line 17); the k index ranges from 1 to 19 with variably refined subdivisions using the scheme specified on Line 18. For example, [3, 5, 2] would refine the mesh such that the coarse elements along the k direction bounded by the indices [3, 4] and [4, 5] would be split in half. The grid structure in this case is structured (Line 20).

Figure 3 displays an overview of the four cutouts (i.e., West, Center, East 1, and East 2).

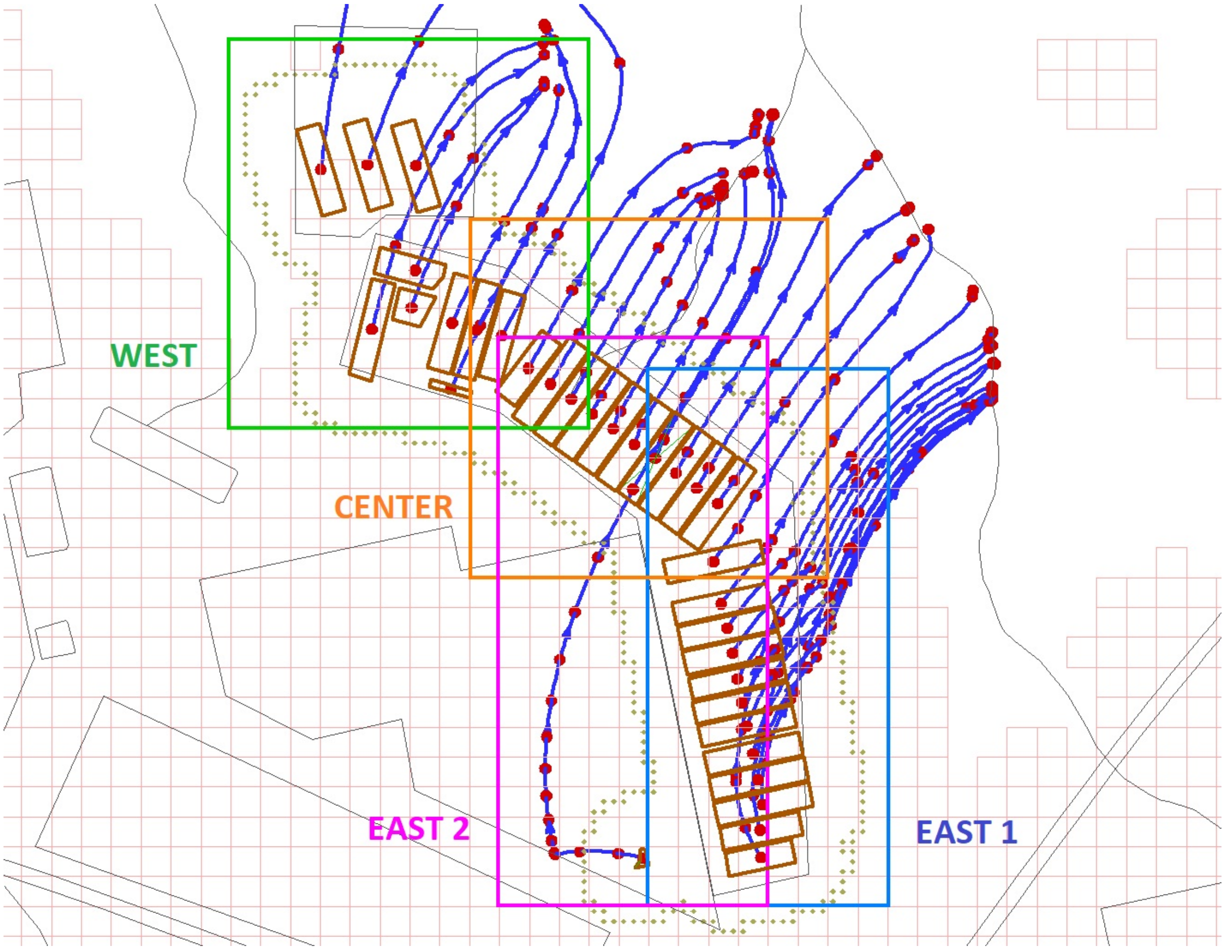


Figure 3. Four cutouts containing sections of the E-Area LLWF from 2018 GSA Flow Model.

The resulting PORFLOW grid sizes are:

Table 2. Grid sizes of four GSA 2018 cutouts.

Cutout	I nodes	J nodes	K nodes	Total nodes
East 1	10	20	20	4,000
Refined East 1	82	182	48	716,352
East 2	11	21	20	4,620
Refined East 2	92	192	48	847,872
Center	14	14	18	3,528
Refined Center	122	122	44	654,896
West	14	15	17	3,570
Refined West	122	132	42	676,368

Based on their stream traces, DUs in the E-Area LLWF are appropriately contained within the relevant cutouts as outlined in Table 3.

Table 3. Cutouts and disposal units contained within.

Cutout	Disposal Units
West	ET07, ET08, ET09, ET03, ET04, NRCDA26E, ST08, ST09, ST10, and ILV
Center	ST01 to ST07, ST11, CIG1, and CIG2
East 1	ET02, ET01, ST14, ST15, LAWV, ST16 to ST22
East 2	NRCDA7E

The following figures show individual cutouts for two flow cases: (1) without covers (Figure 4), and (2) with the final covers placed over the entire E-Area (Figure 5).

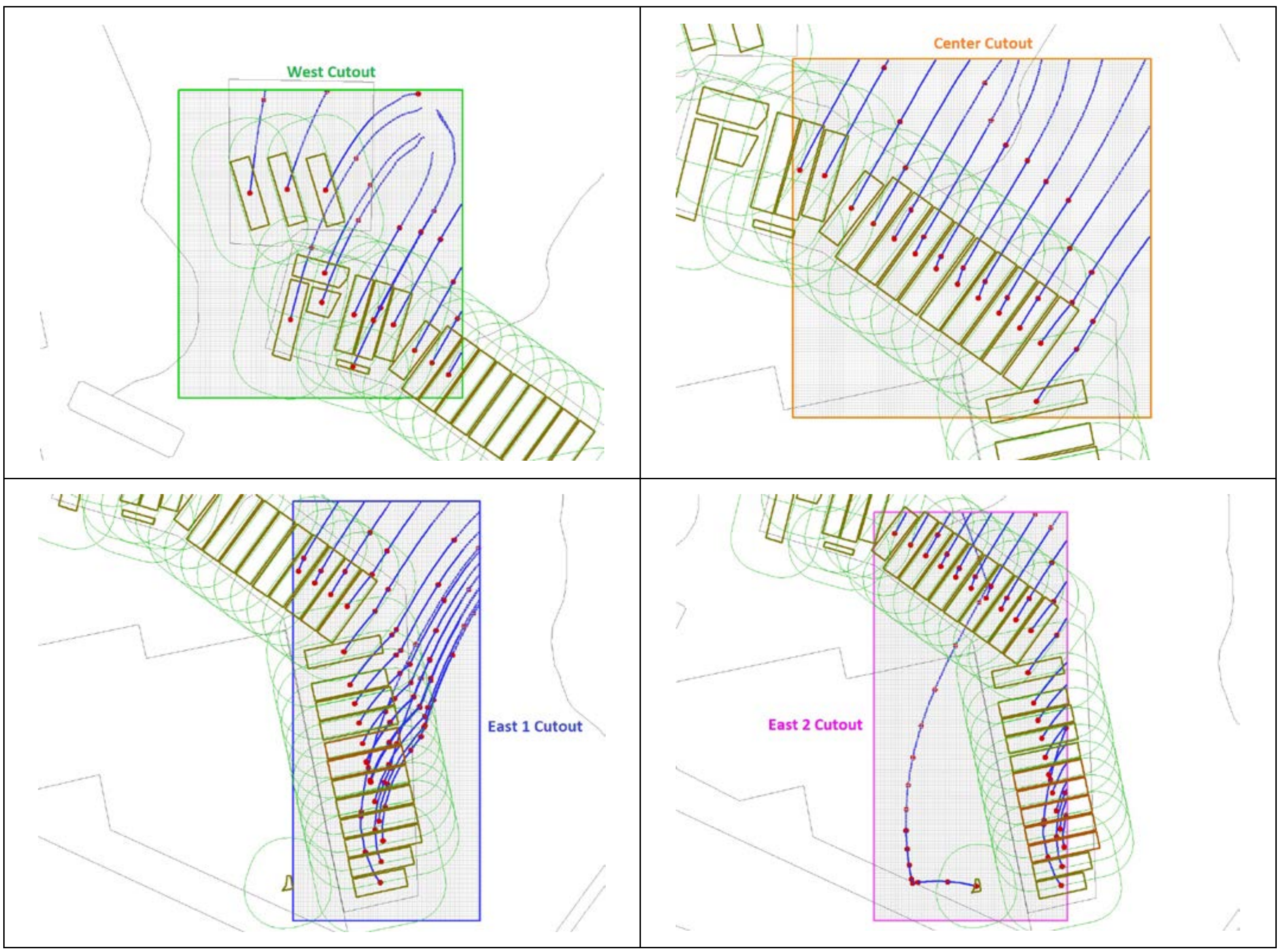


Figure 4. Refined grid cutouts of the E-Area LLWF from the 2018 GSA Flow Model (no covers).

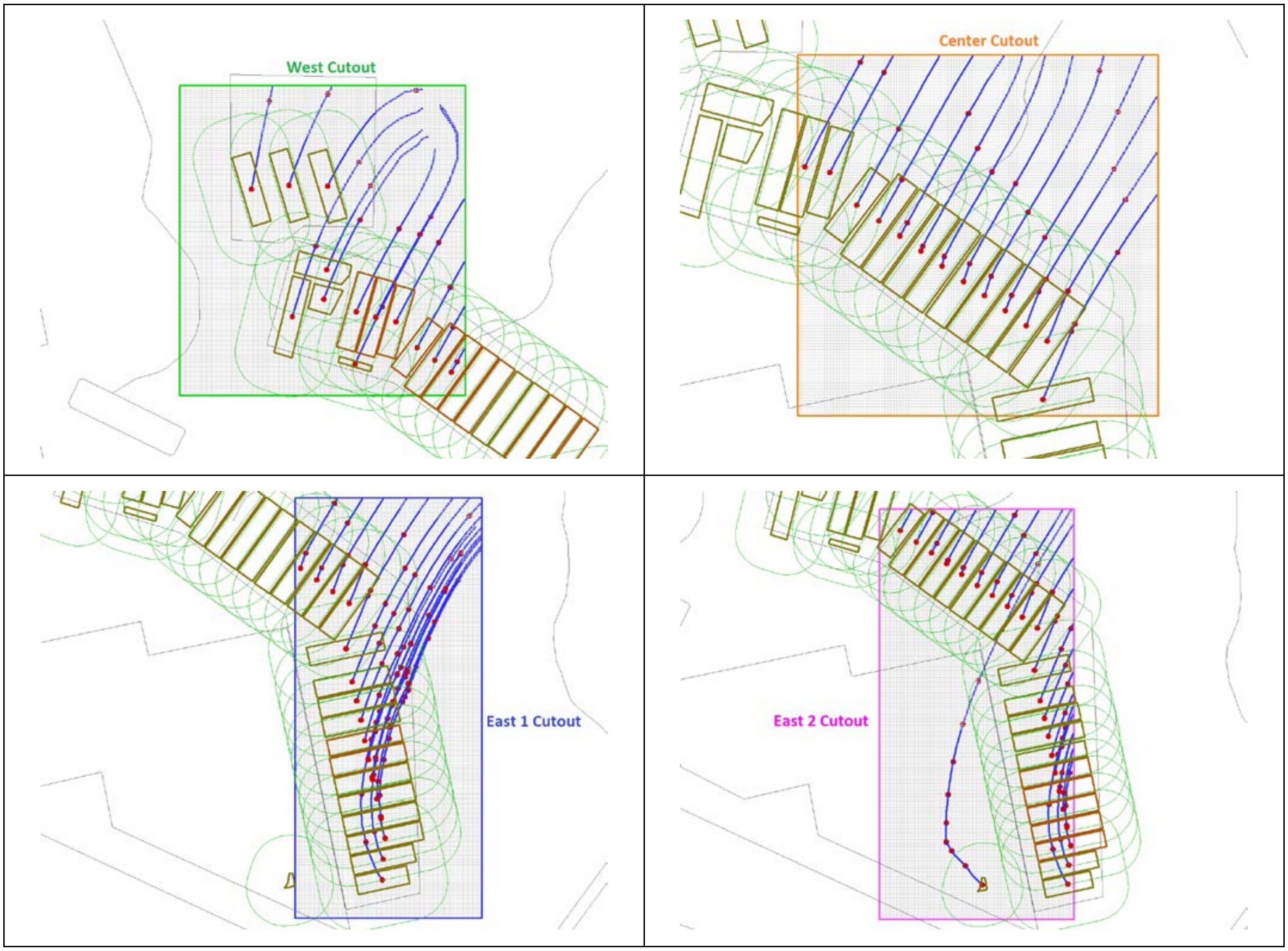


Figure 5. Refined grid cutouts of the E-Area LLWF from the 2018 GSA Flow Model (with covers).

Tracer Simulations

Tracer runs were performed for each individual disposal unit in every cutout. Two kinds of tracer runs were made:

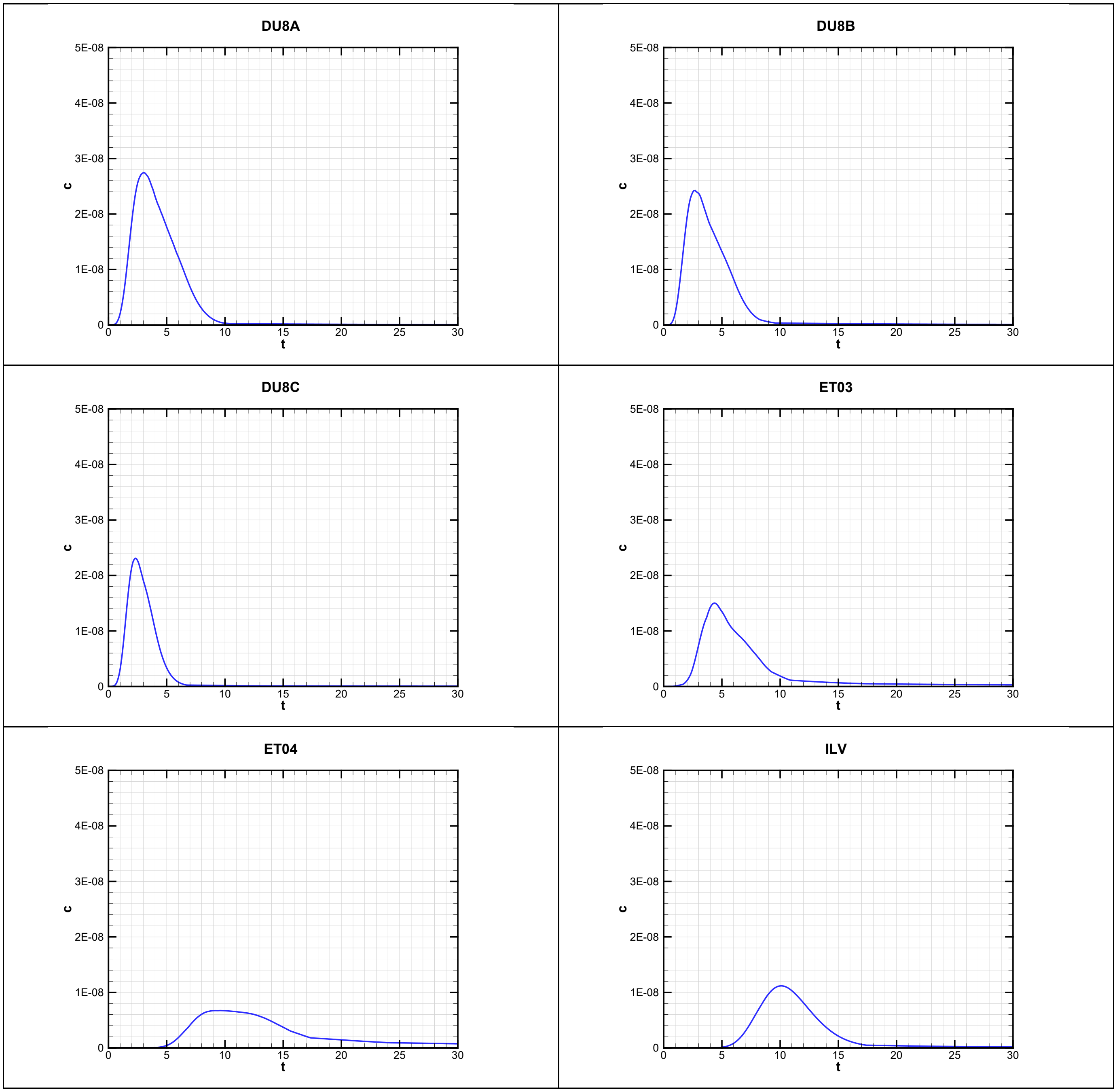
1. Transient/pulsed source: An initial inventory of 1 Ci is placed in the disposal unit. These simulations show when the maximum concentrations occur at the 100-meter boundary.
2. Steady-state source: A source is placed in the disposal unit with a constant release rate, resulting in a steady-state tracer plume around the DU of interest. To minimize mass loss, 99.9% of the tracer plume should be captured. For example, if the maximum tracer concentration at the 100-

meter boundary is 1E-8, the cutout should show the plume variation down to 1E-11. As a result, steady-state tracer runs were performed in two steps for each DU:

a. Step 1: A source with a release rate of 1Ci/yr was placed in the disposal unit.
b. Step 2: The maximum concentration at the 100-meter boundary obtained from Step 1 was normalized to 1E-8. The new resulting release rate was used in a new tracer run. This two-step process allows a quick visual inspection of the concentration plume plots to ensure the cutouts adequately contain tracer plumes emanating from all disposal units.

In these simulations, a longitudinal horizontal dispersivity aLH of 15.4ft was employed based on recommendations from a recent analysis (Hamm et al., 2019). The results of all tracer transport runs are provided below for each cutout with and without covers.

Pulsed Source Concentrations



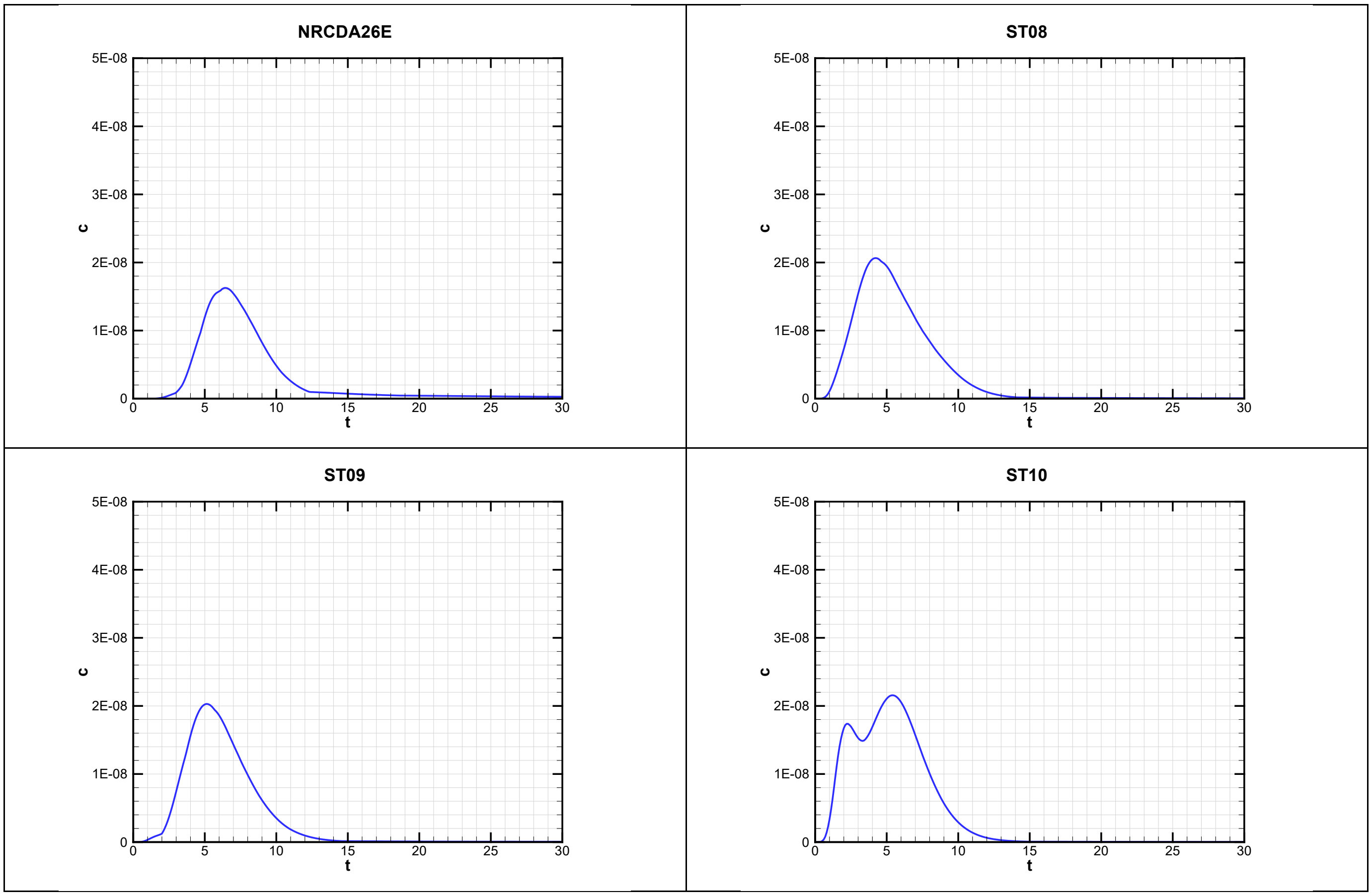
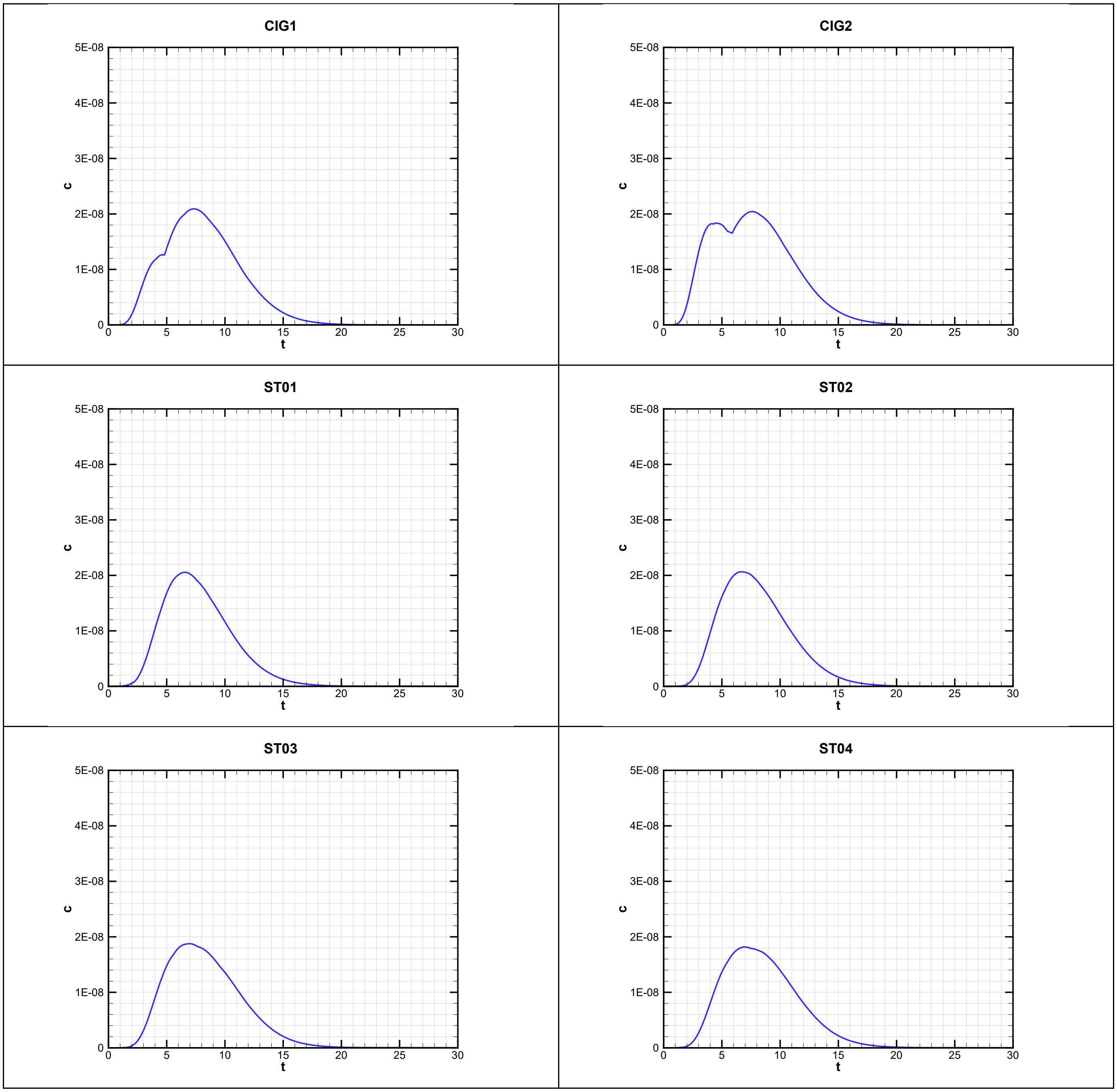


Figure 6. Disposal units in the West cutout – Pulsed tracer concentrations (no covers).


CIG1
CIG2
ST01
ST02
ST03
ST04
c
t
0
1E-08
2E-08
3E-08
4E-08
5E-08
0
5
10
15
20
25
30

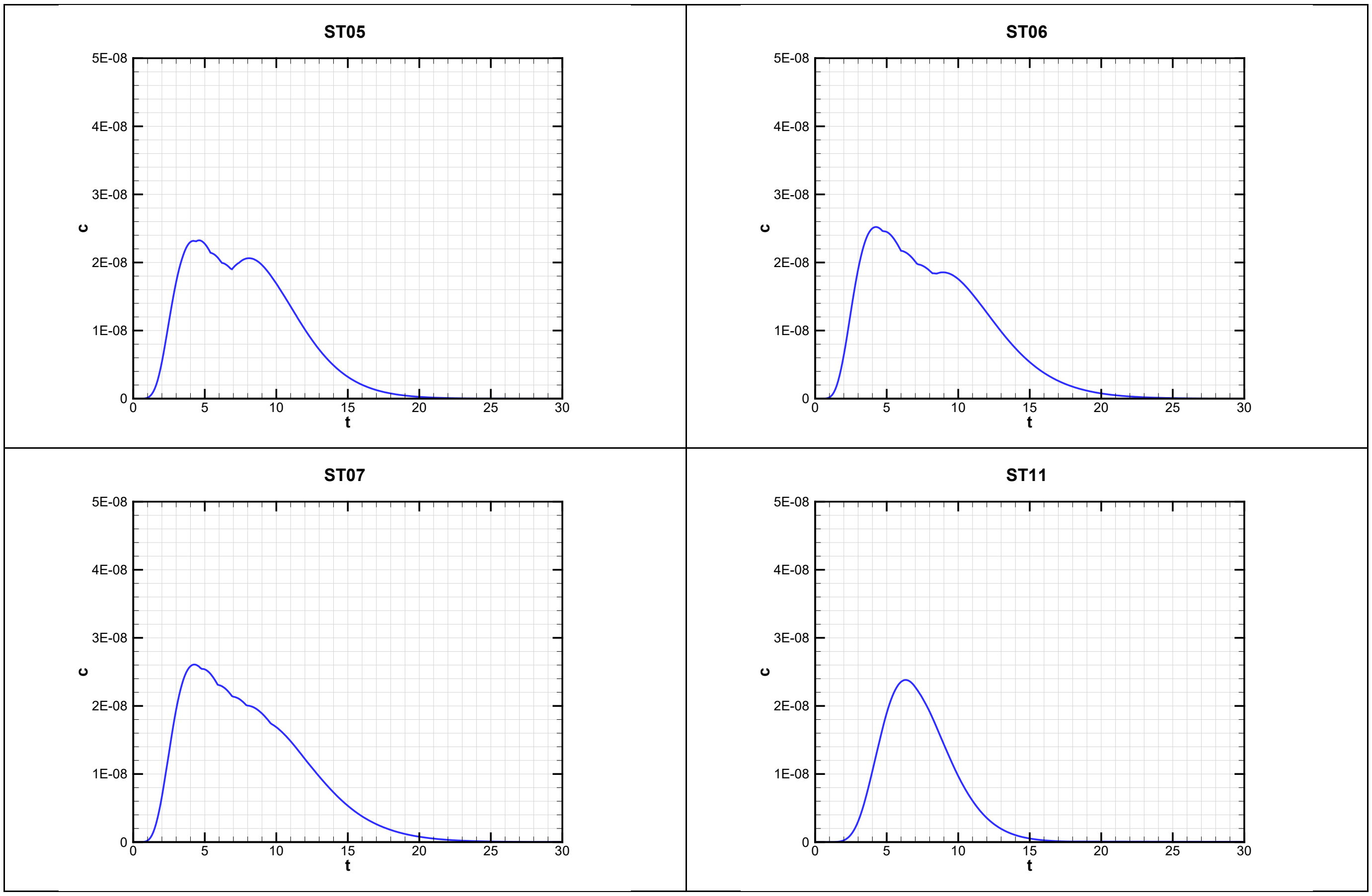
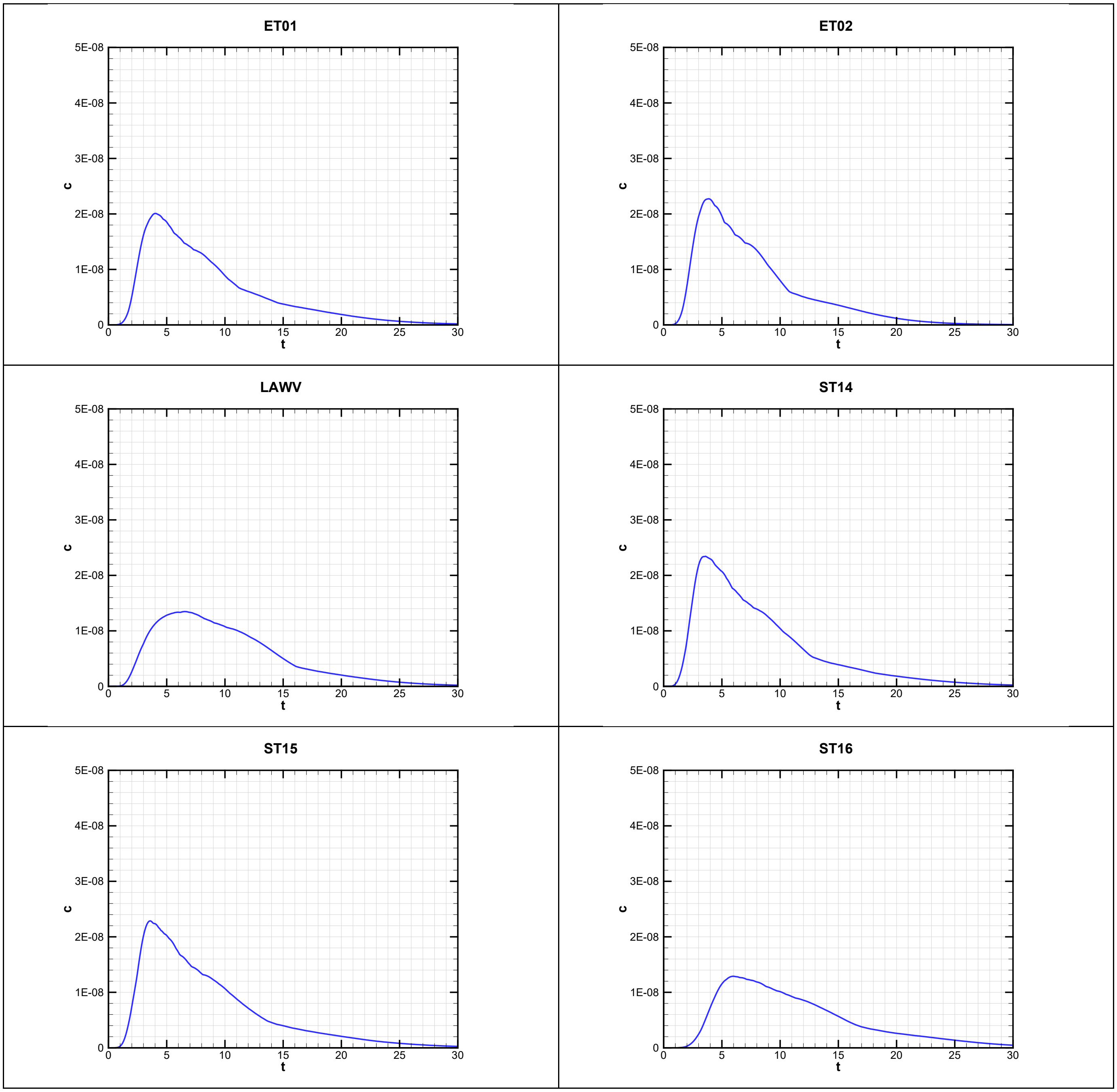


Figure 7. Disposal units in the Center cutout – Pulsed tracer concentrations (no covers).


ET01
ET02
LAWV
ST14
ST15
ST16
c
t
5E-08
4E-08
3E-08
2E-08
1E-08
0
0
5
10
15
20
25
30

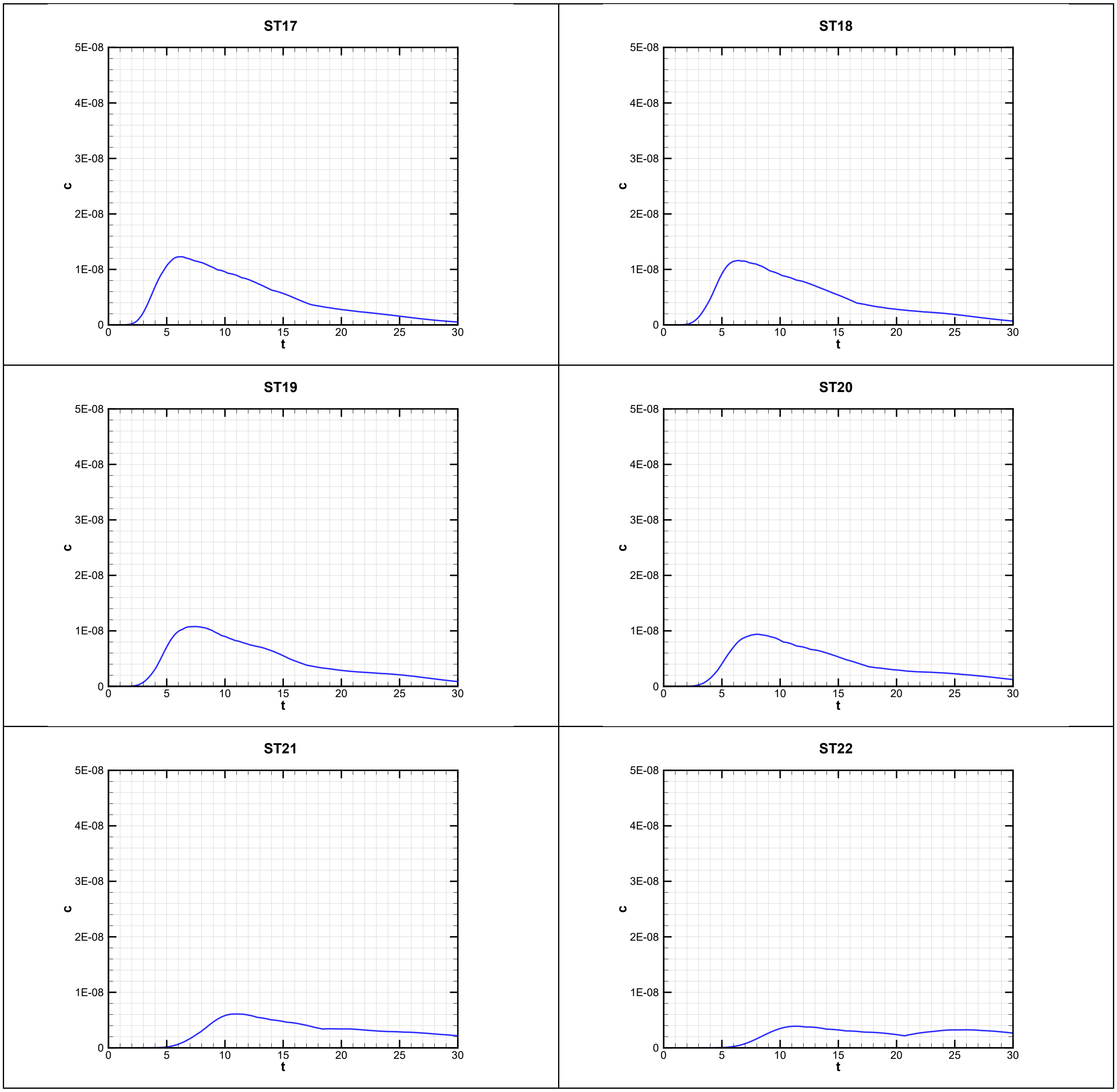


Figure 8. Disposal units in the East 1 cutout – Pulsed tracer concentrations (no covers).

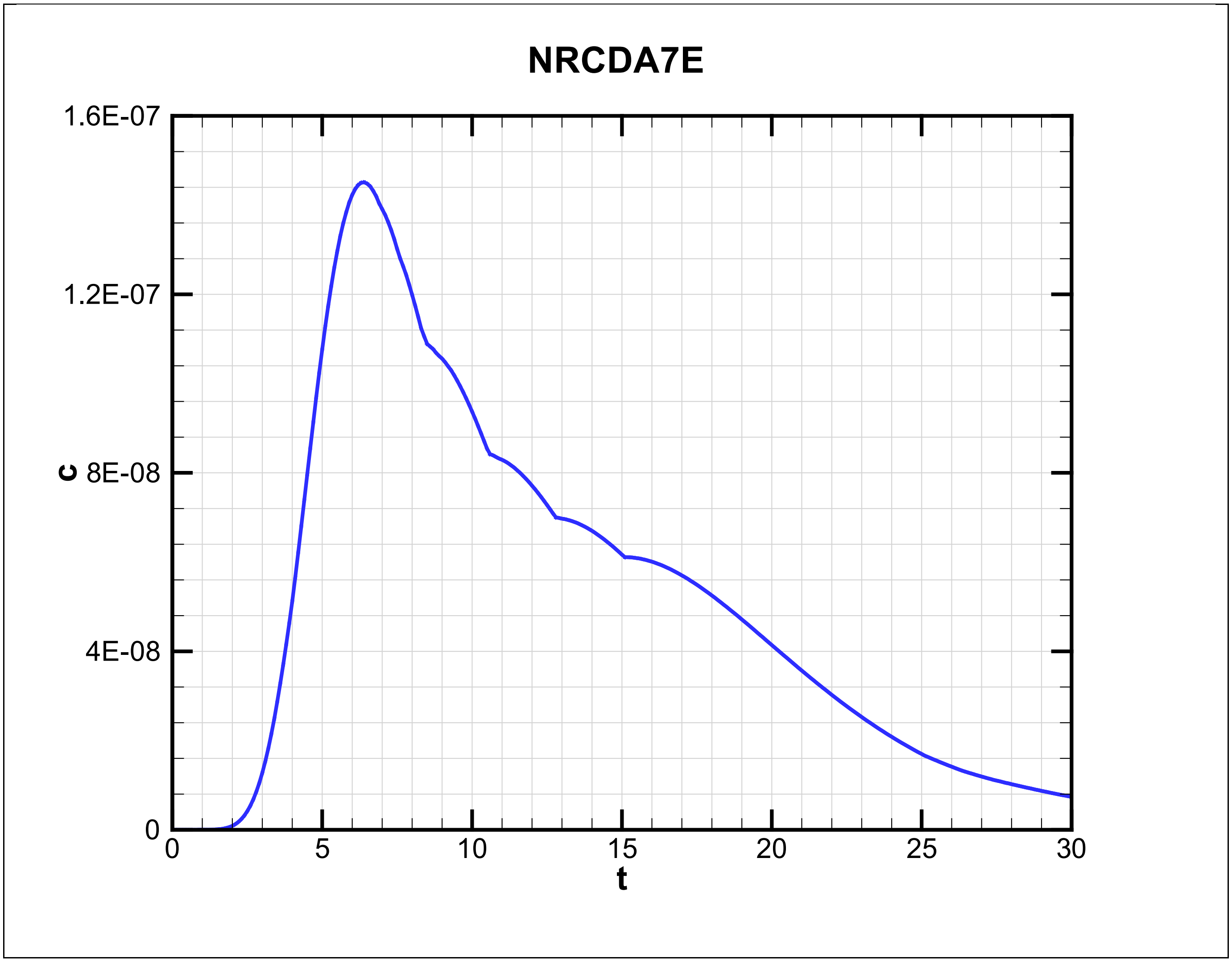
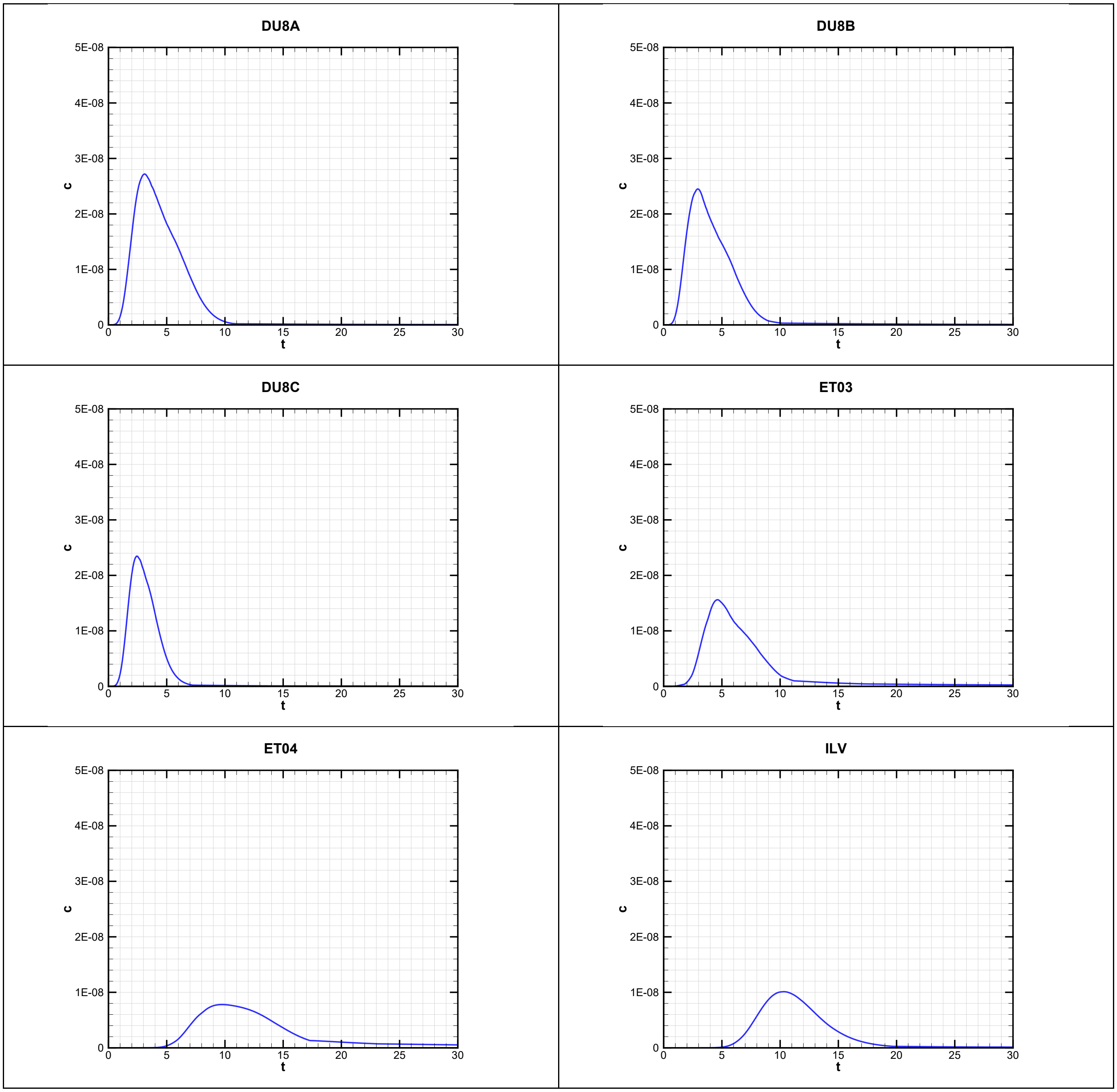


Figure 9. Disposal units in the East 2 cutout – Pulsed tracer concentrations (no covers).


DU8A
DU8B
DU8C
ET03
ET04
ILV
c
t
5E-08
4E-08
3E-08
2E-08
1E-08
0
0
5
10
15
20
25
30

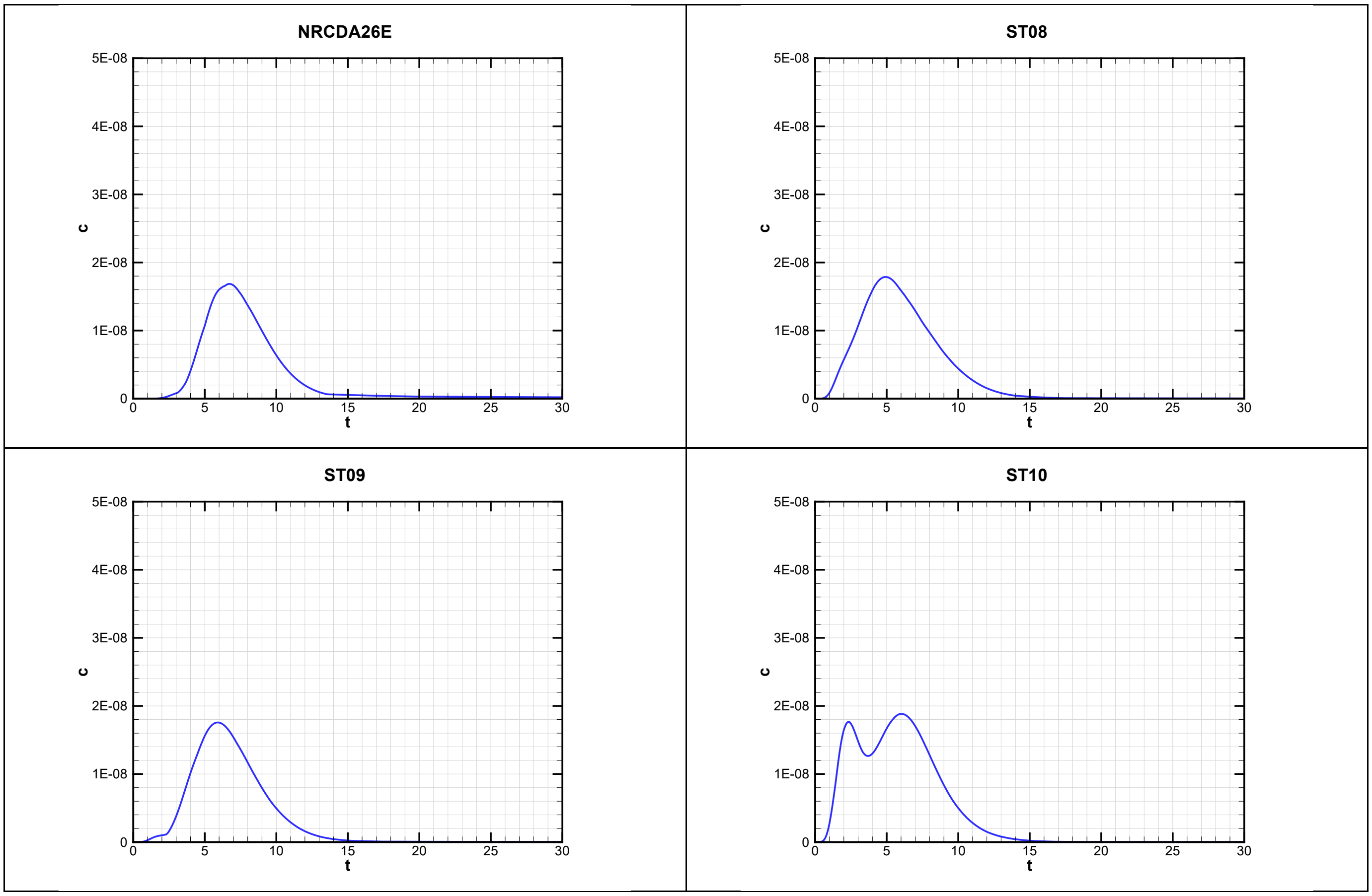
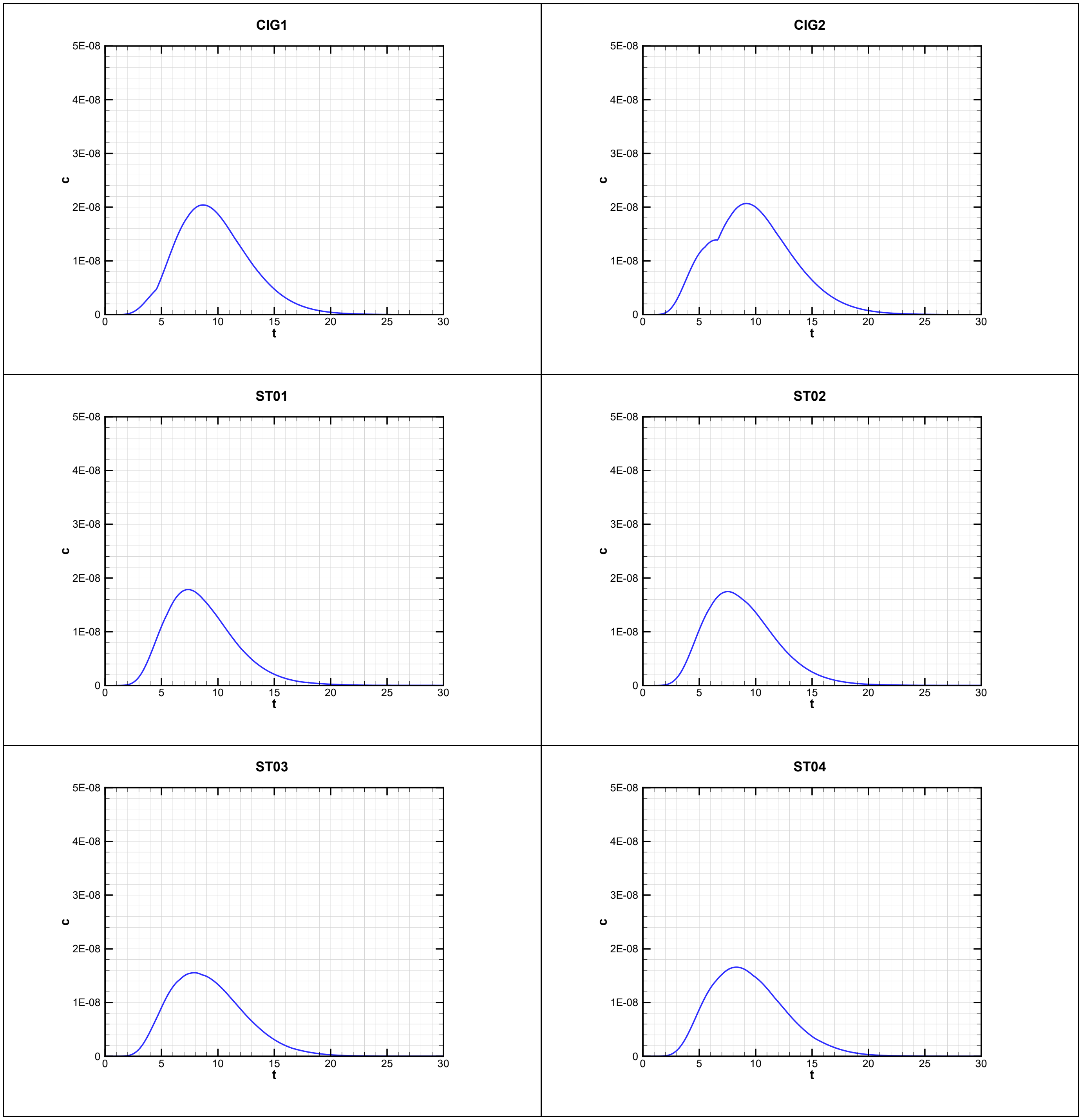


Figure 10. Disposal units in the West cutout – Pulsed tracer concentrations (with covers).


CIG1
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t
CIG2
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t
ST01
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t
ST02
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t
ST03
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t
ST04
5E-08
4E-08
3E-08
2E-08
1E-08
0
c
0 5 10 15 20 25 30
t

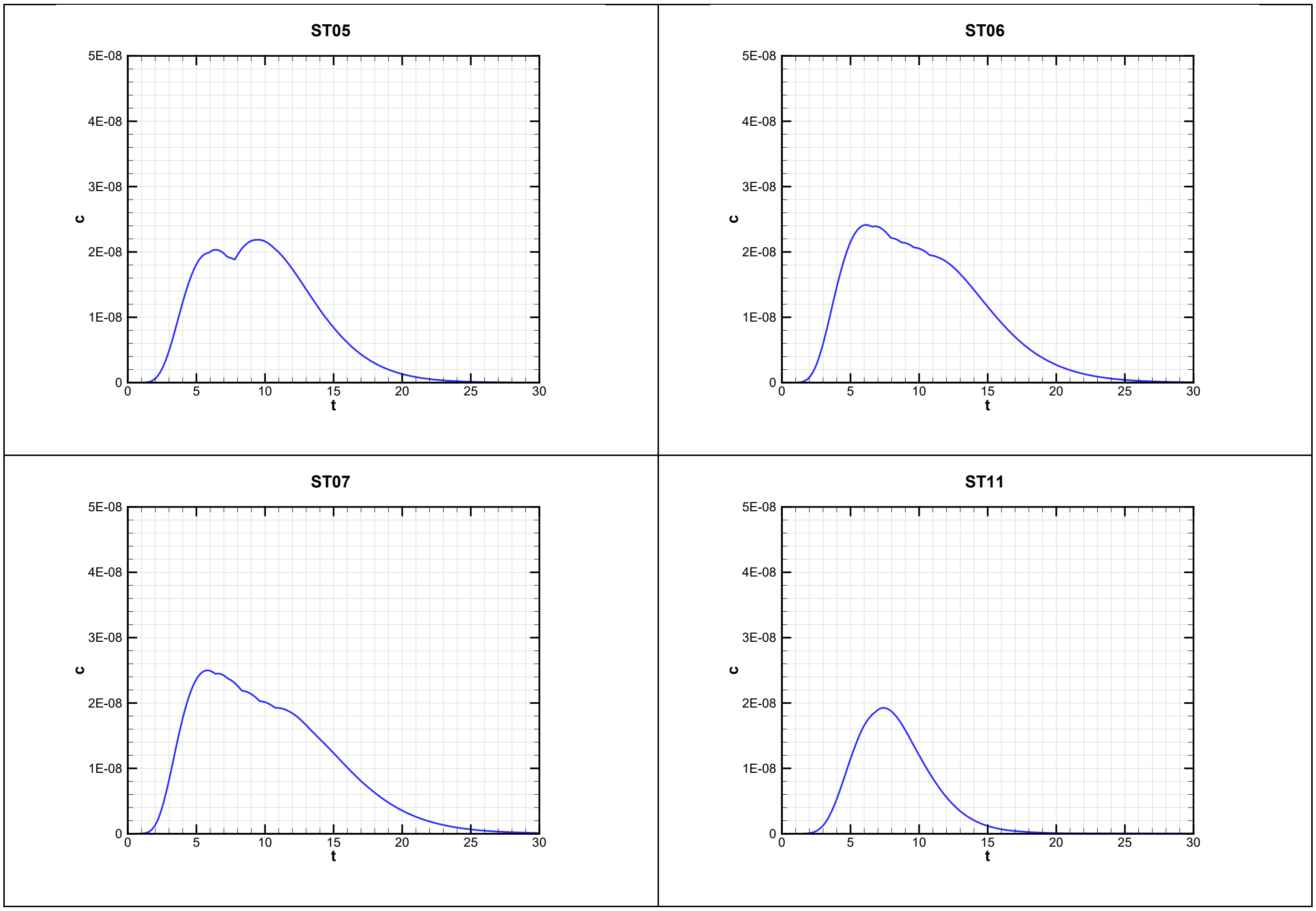
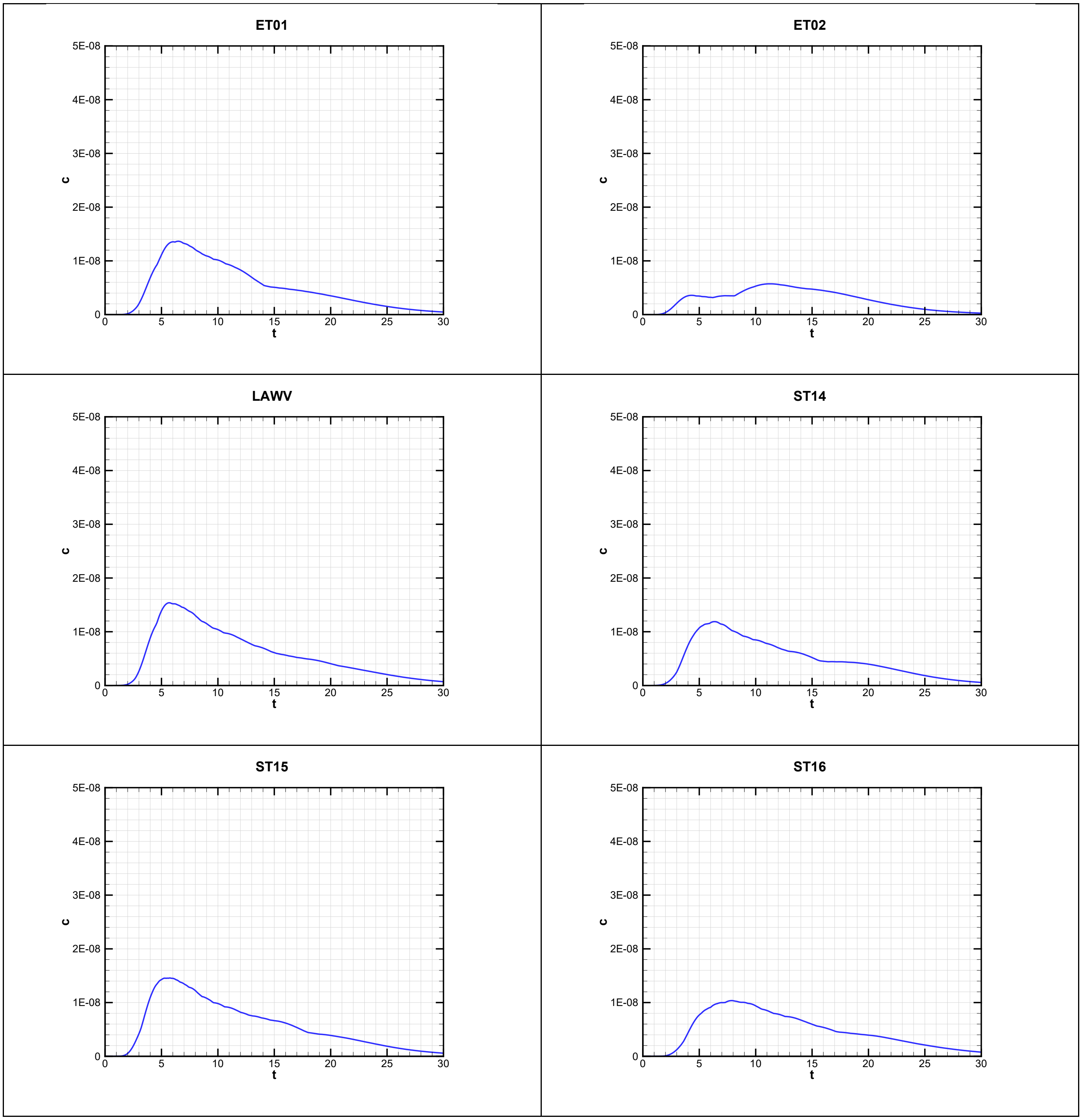


Figure 11. Disposal units in the Center cutout – Pulsed tracer concentrations (with covers).


ET01
ET02
LAWV
ST14
ST15
ST16
c
t
0
1E-08
2E-08
3E-08
4E-08
5E-08
0
5
10
15
20
25
30

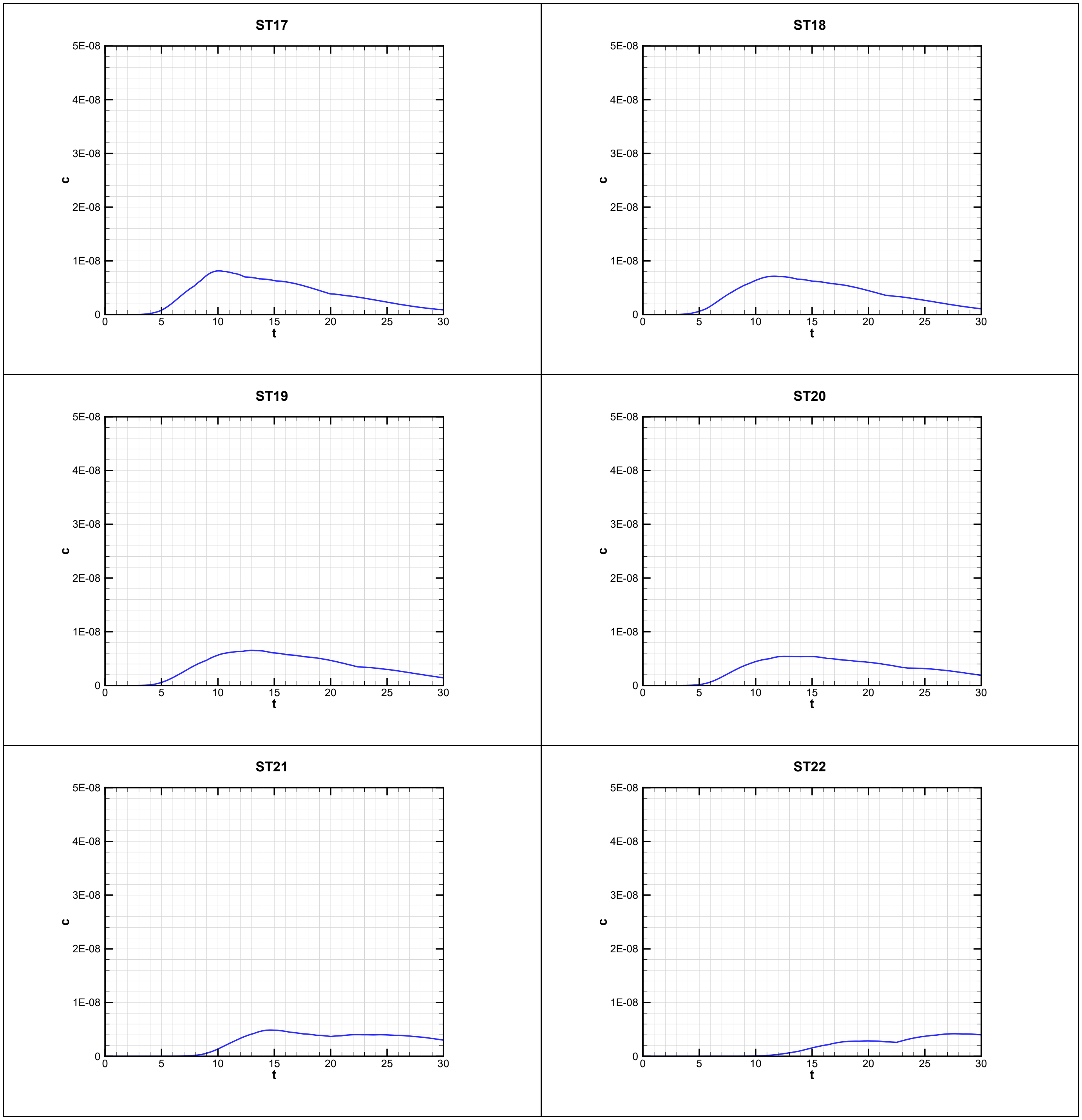


Figure 12. Disposal units in the East 1 cutout – Pulsed tracer concentrations (with covers).

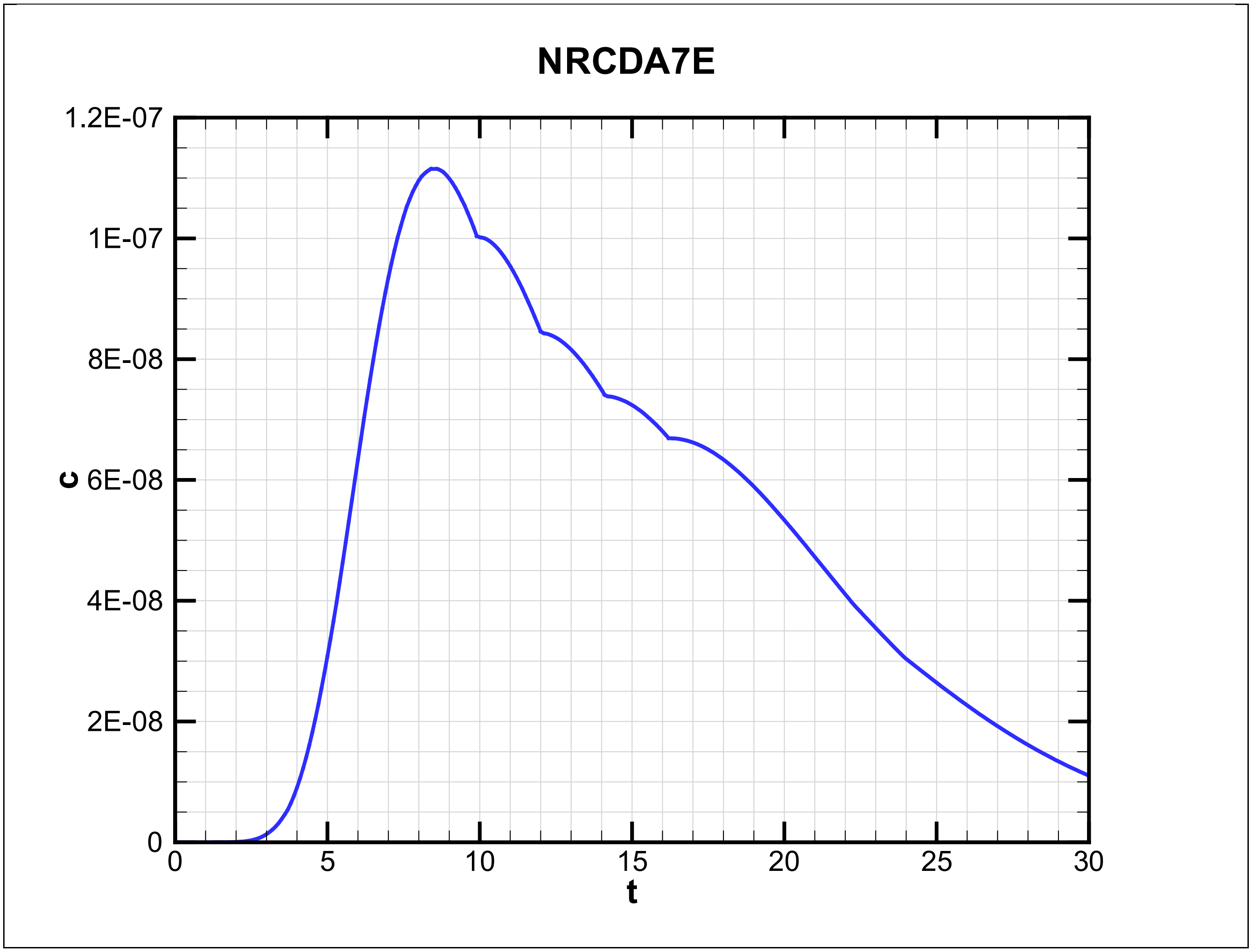
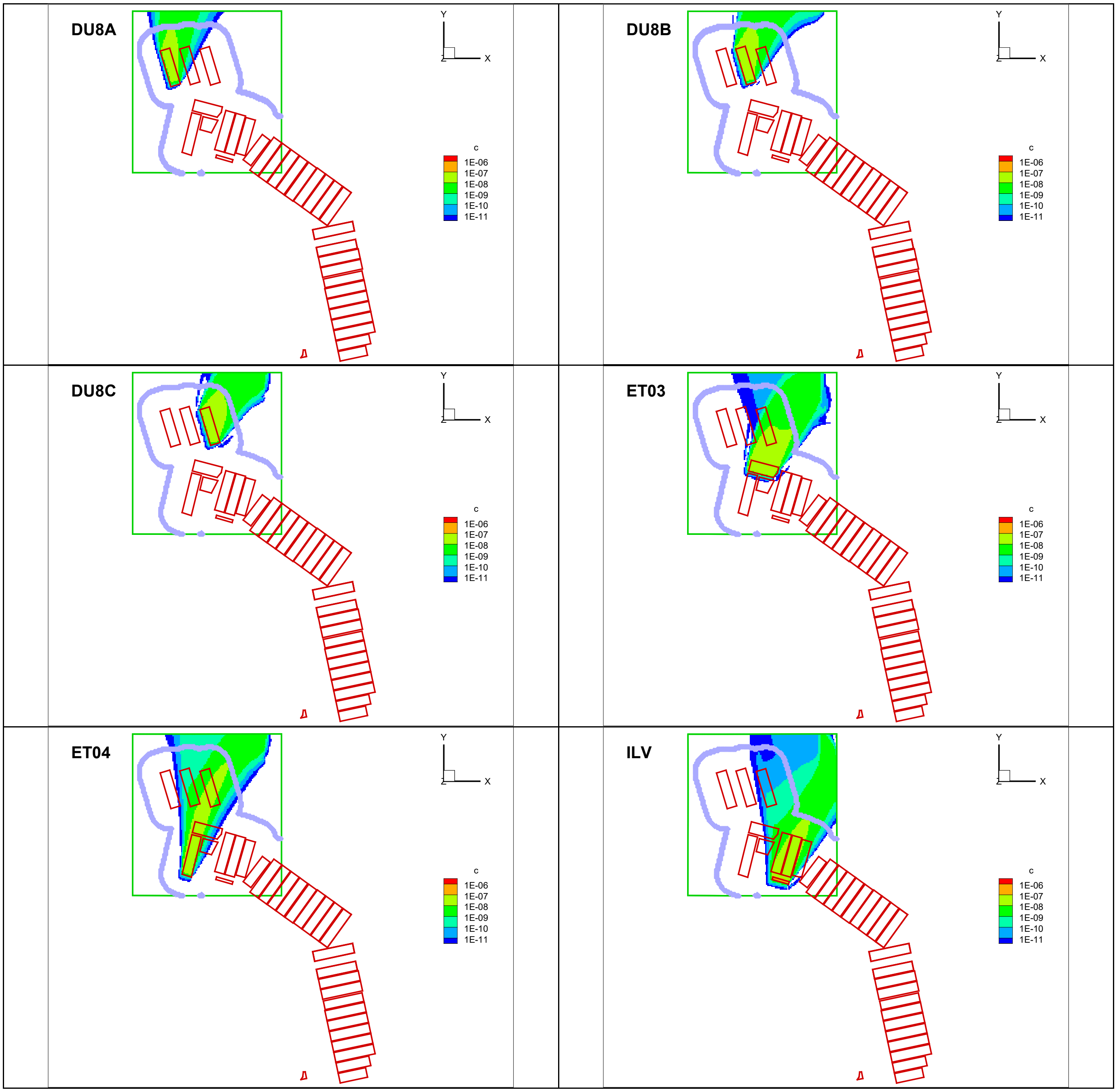


Figure 13. Disposal units in the East 2 cutout – Pulsed tracer concentrations (with covers).

Steady-State Source Concentrations



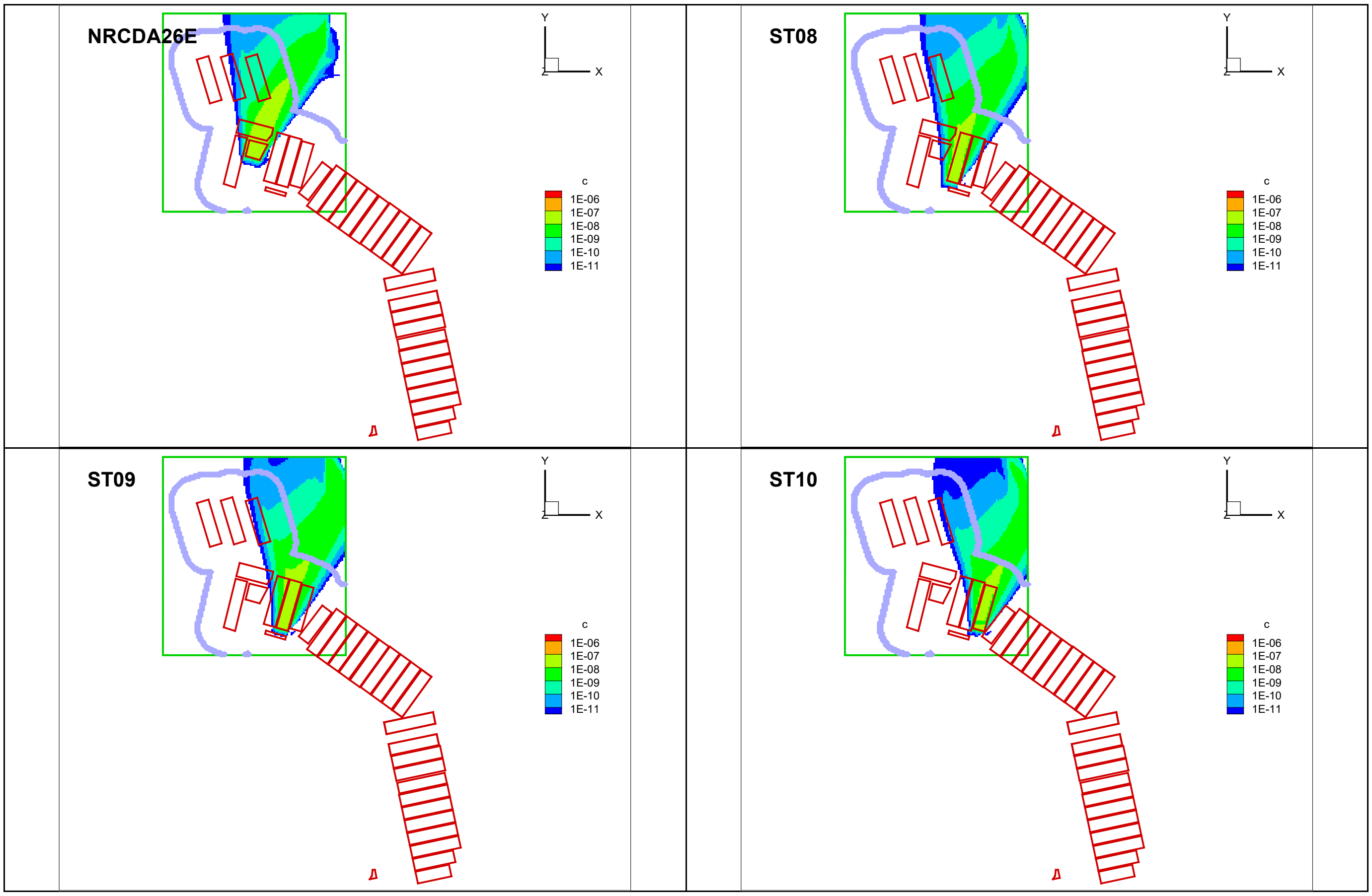
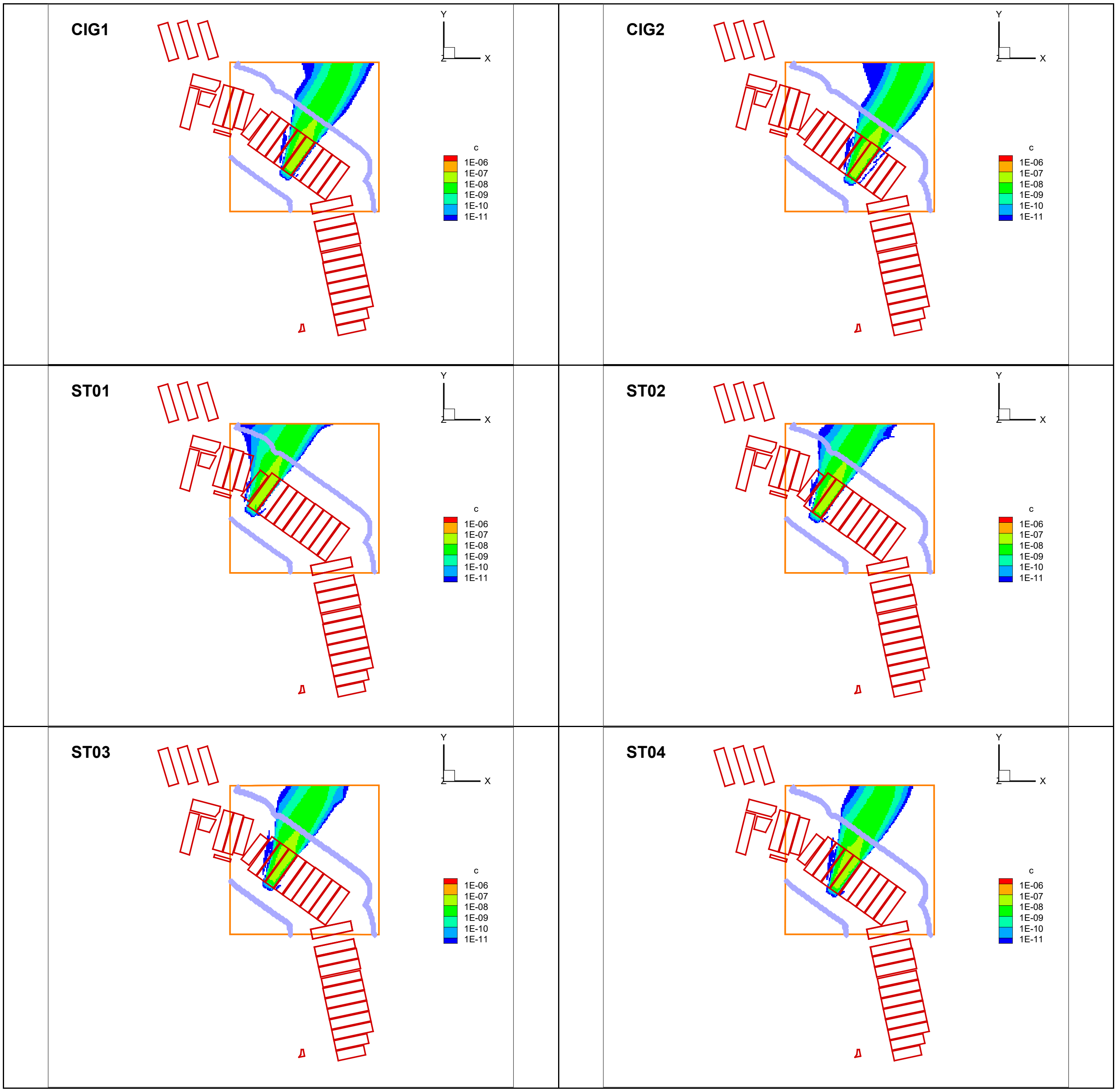


Figure 14. Disposal units in the West cutout – Steady-state tracer concentrations (no covers).


CIG1
CIG2
ST01
ST02
ST03
ST04
Y
X
c
1E-06
1E-07
1E-08
1E-09
1E-10
1E-11

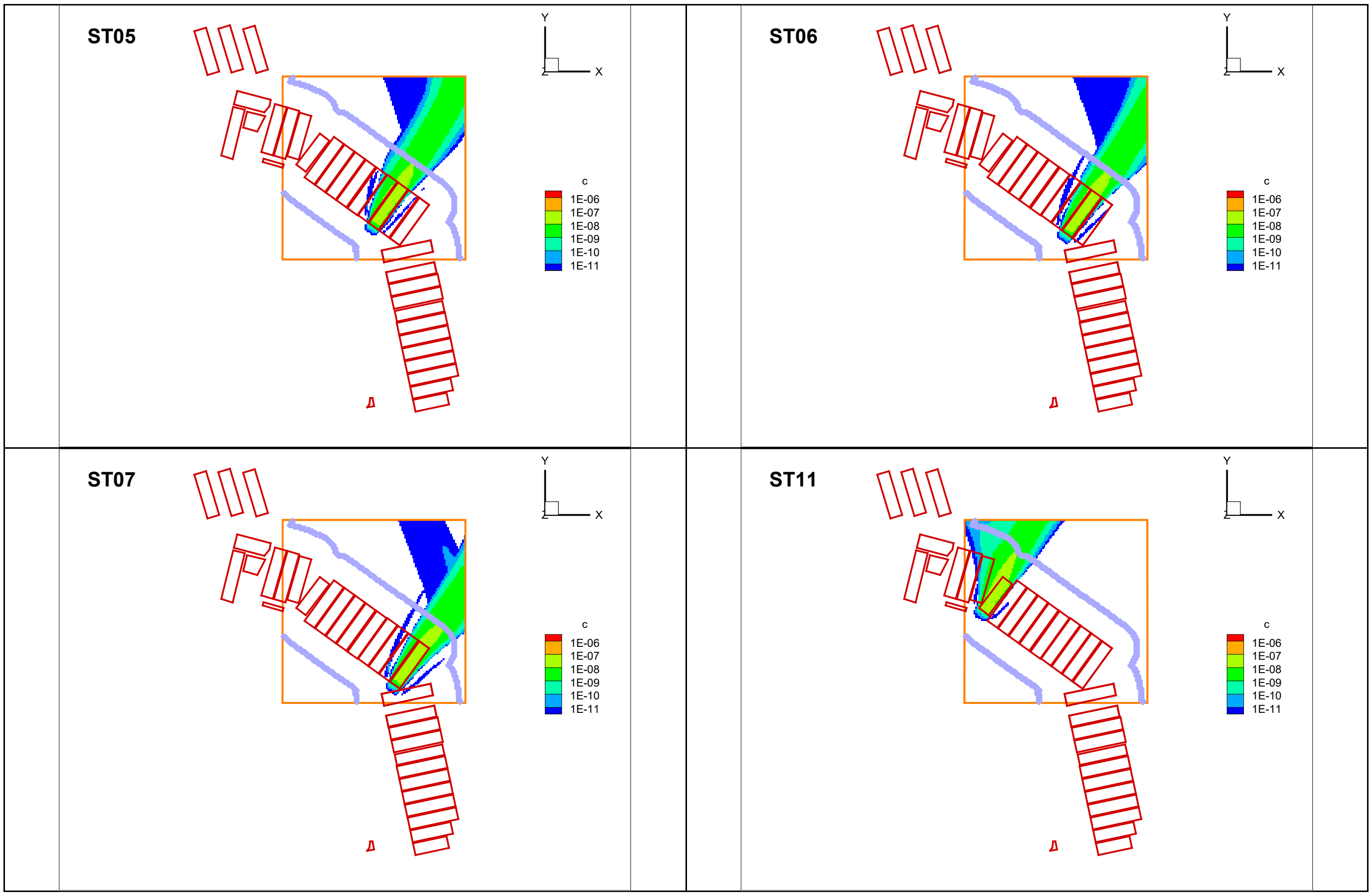
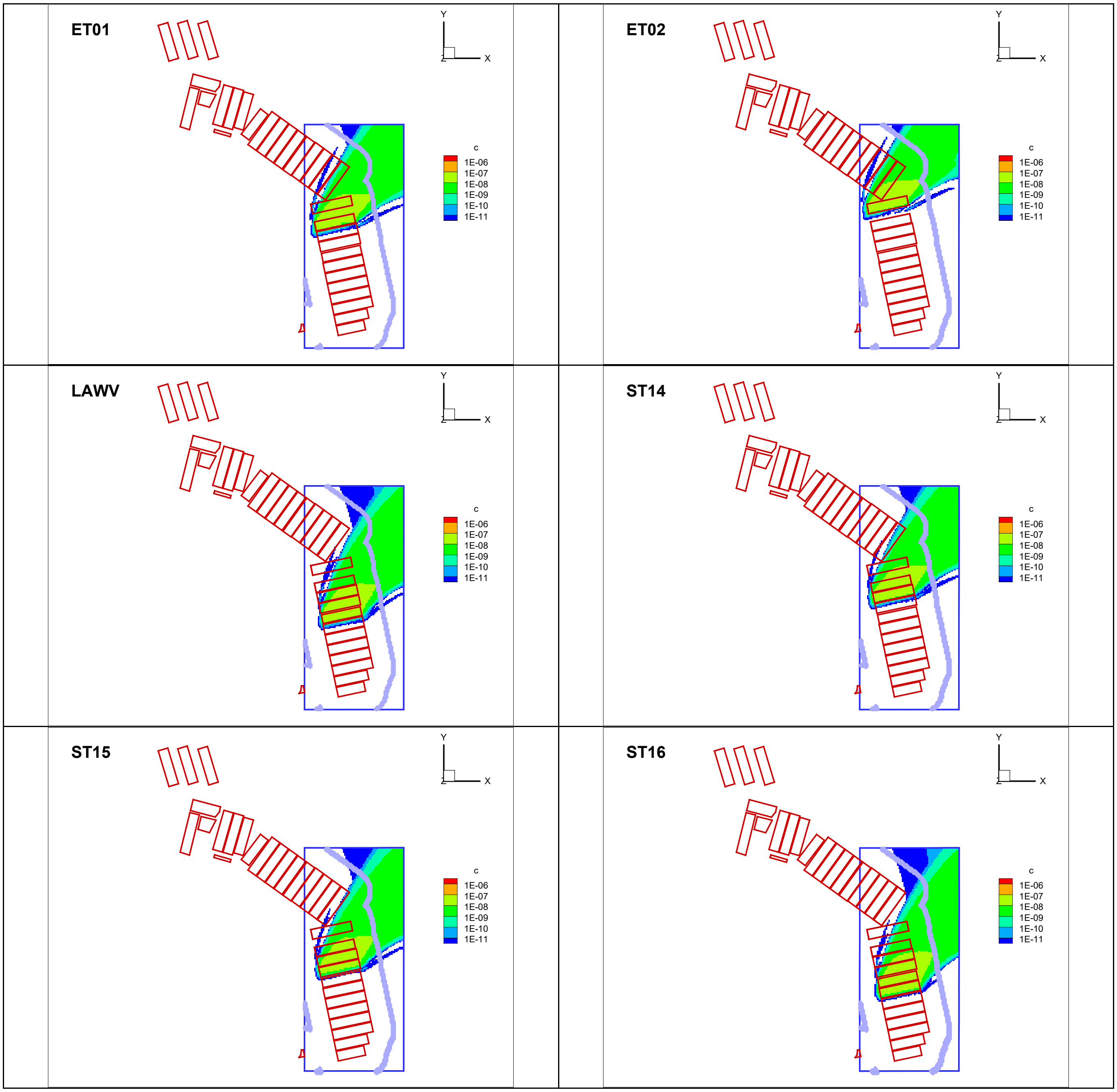


Figure 15. Disposal units in the Center cutout – Steady-state tracer concentrations (no covers).


ET01
ET02
LAWV
ST14
ST15
ST16
Y
X
c
1E-06
1E-07
1E-08
1E-09
1E-10
1E-11

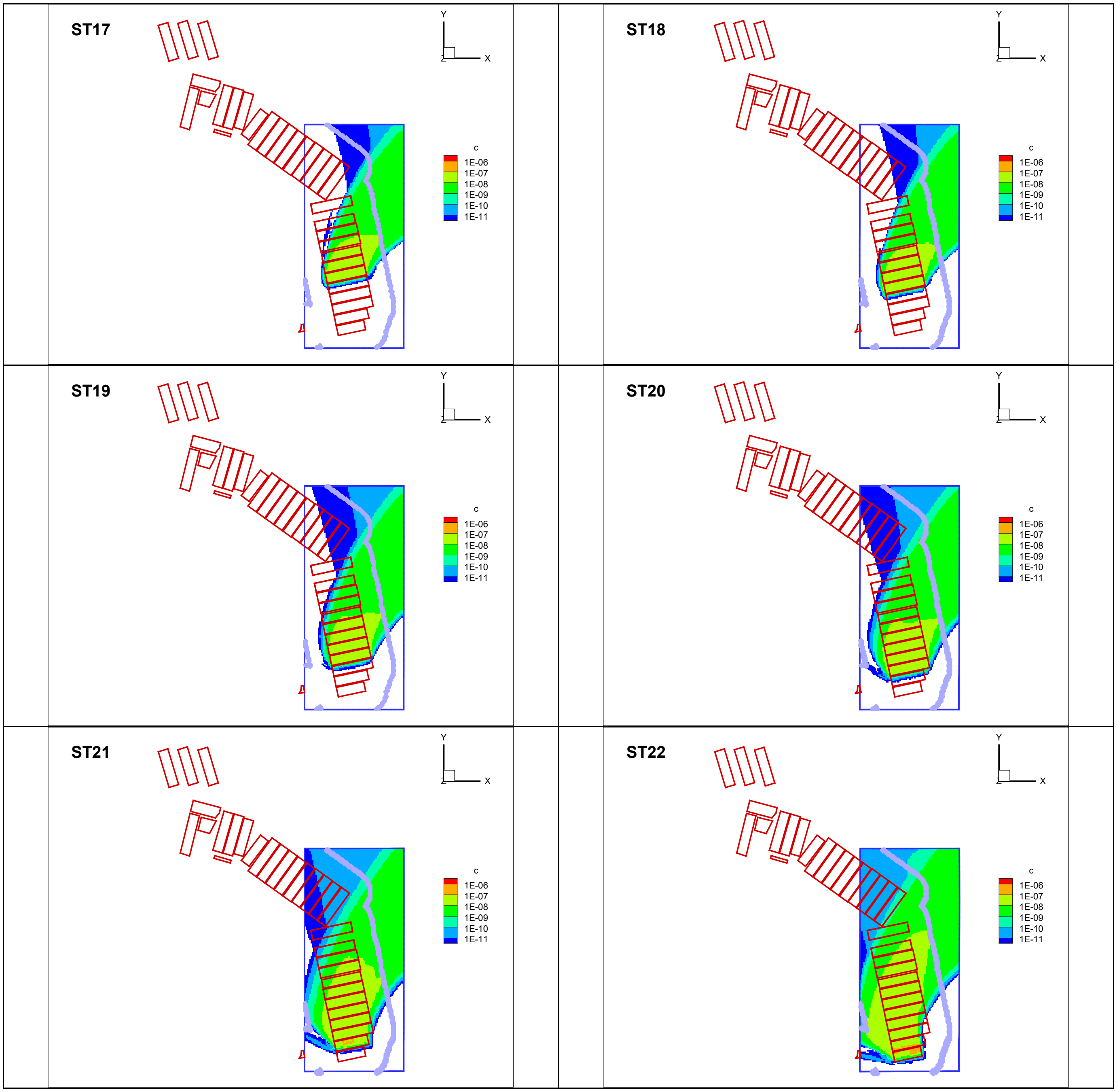


Figure 16. Disposal units in the East 1 cutout – Steady-state tracer concentrations (no covers).

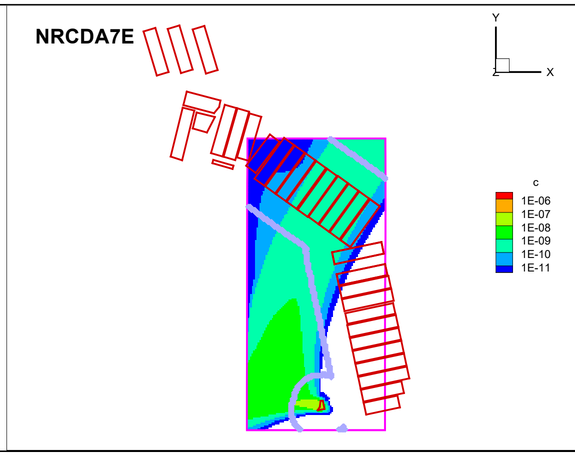
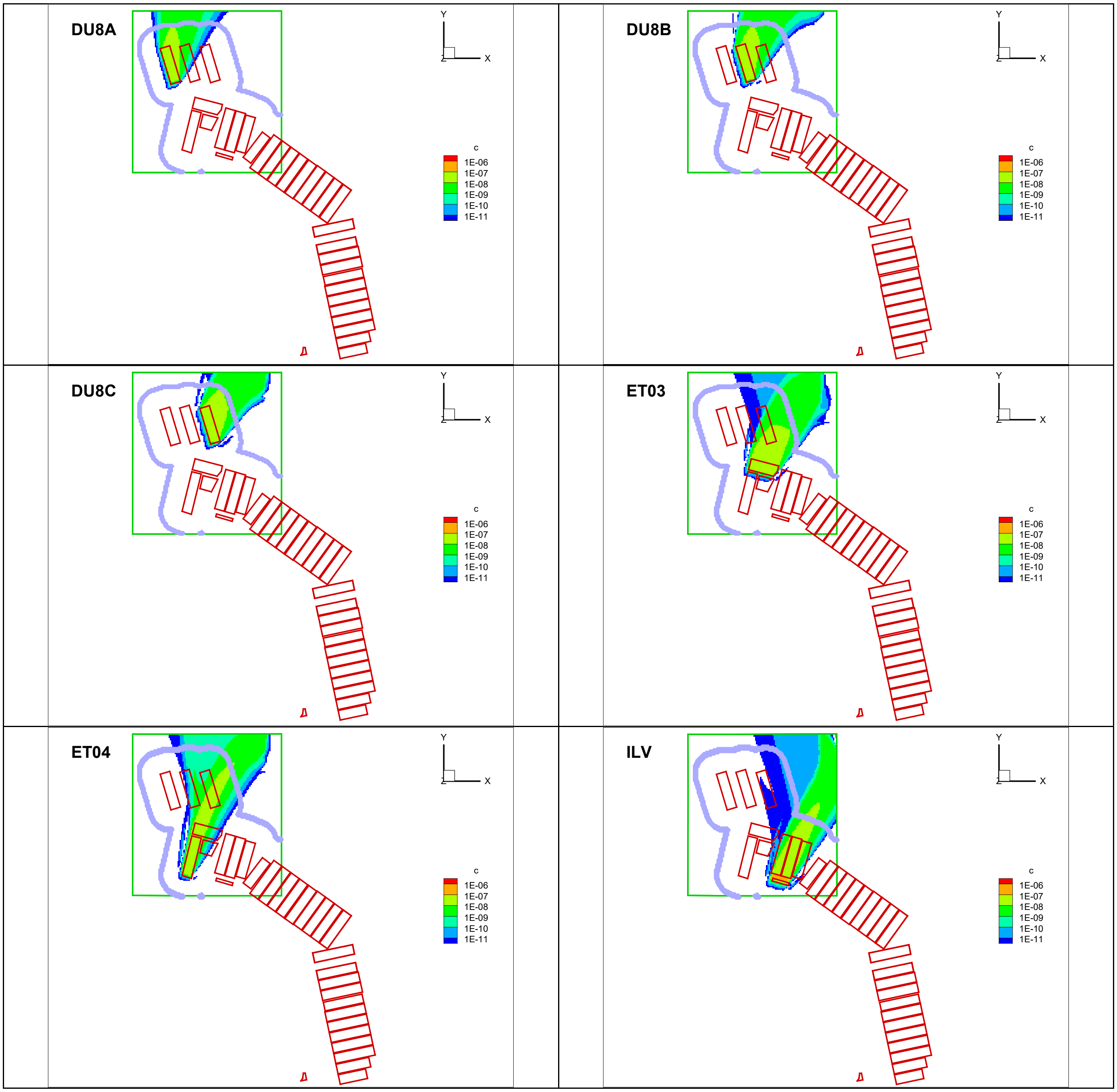


Figure 17. Disposal unit in the East 2 cutout – Steady-state tracer concentrations (no covers).


DU8A
DU8B
DU8C
ET03
ET04
ILV
Y
X
c
1E-06
1E-07
1E-08
1E-09
1E-10
1E-11

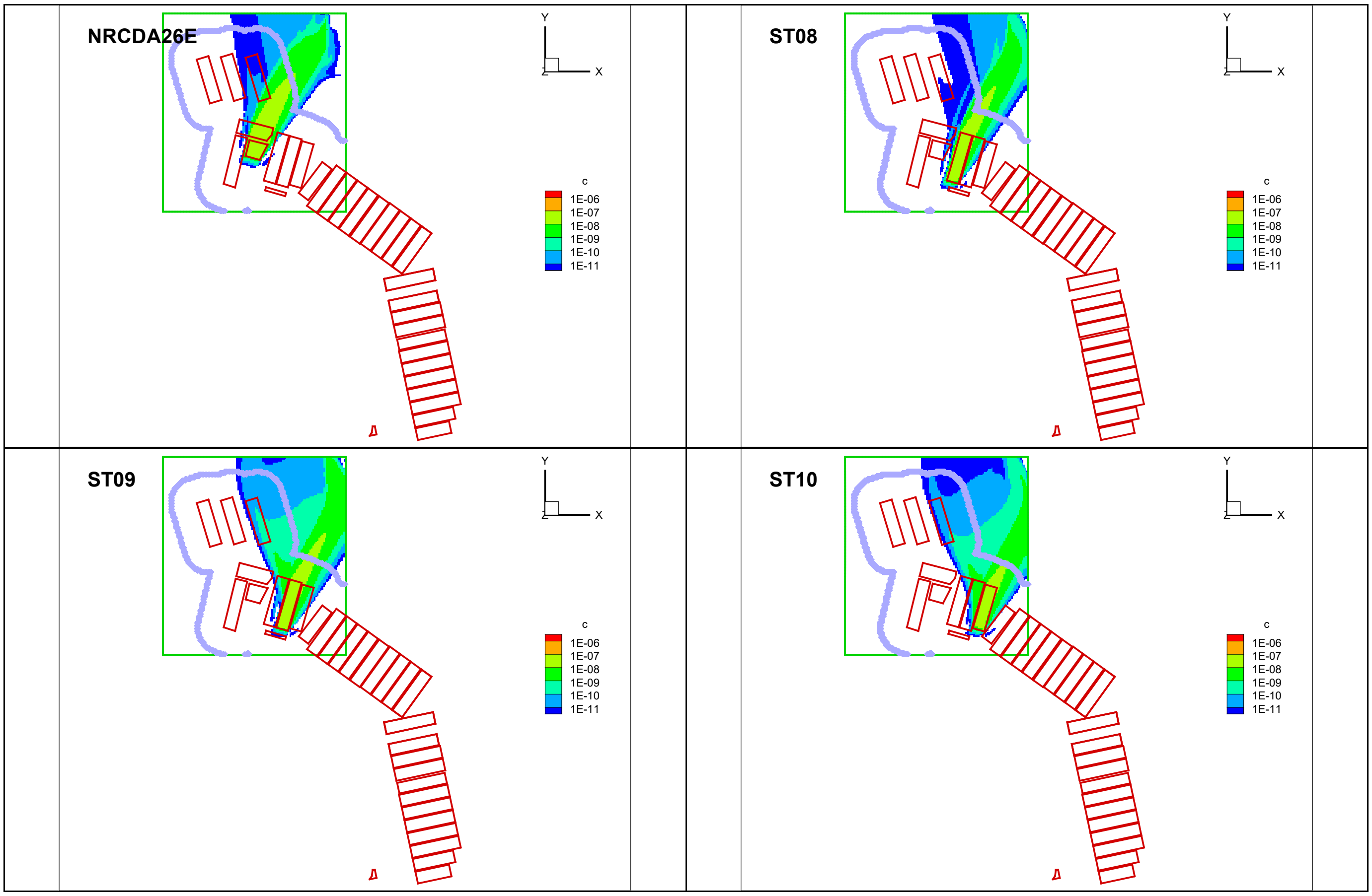
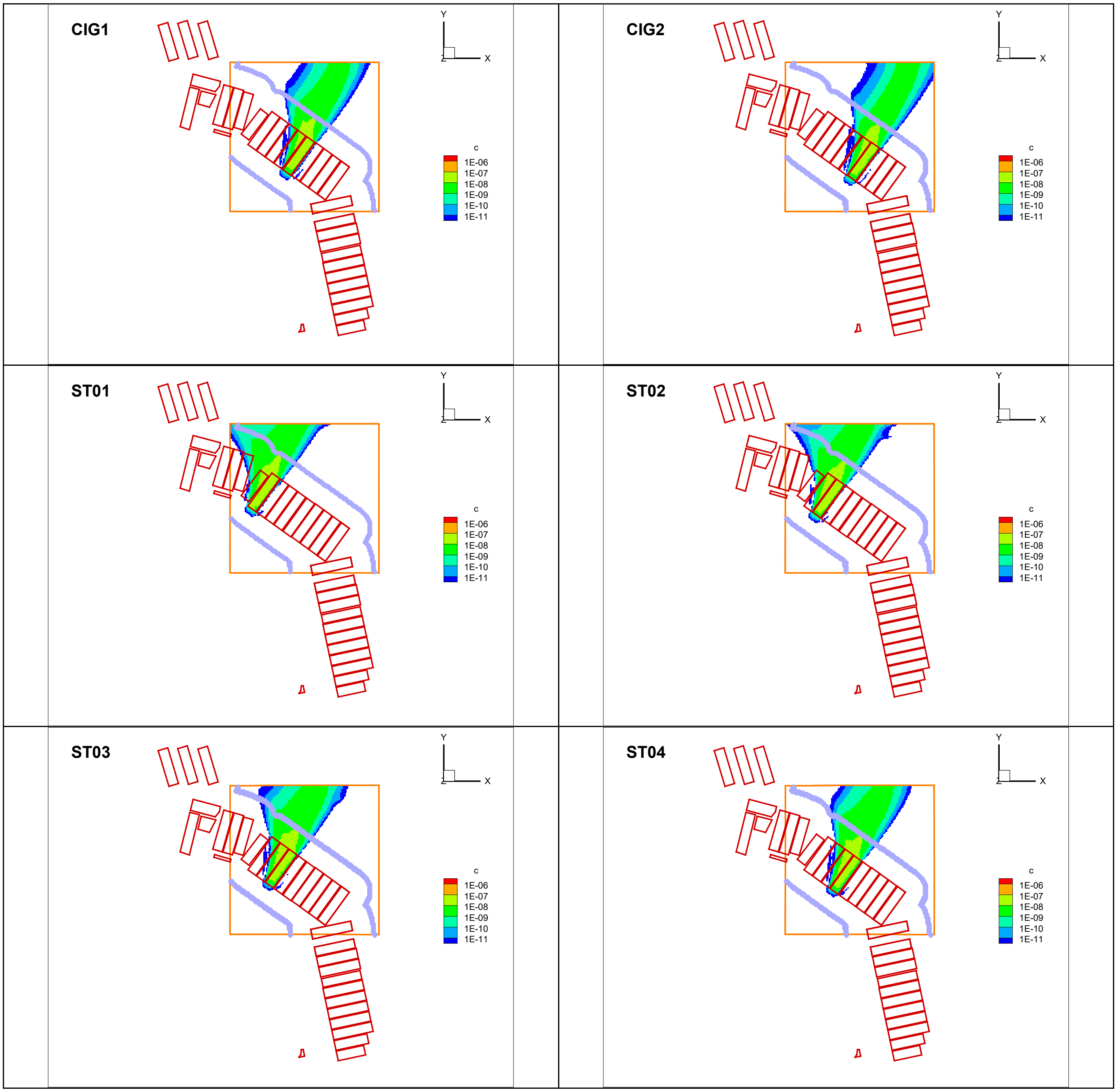


Figure 18. Disposal units in the West cutout – Steady-state tracer concentrations (with covers).


CIG1
CIG2
ST01
ST02
ST03
ST04
Y
X
c
1E-06
1E-07
1E-08
1E-09
1E-10
1E-11

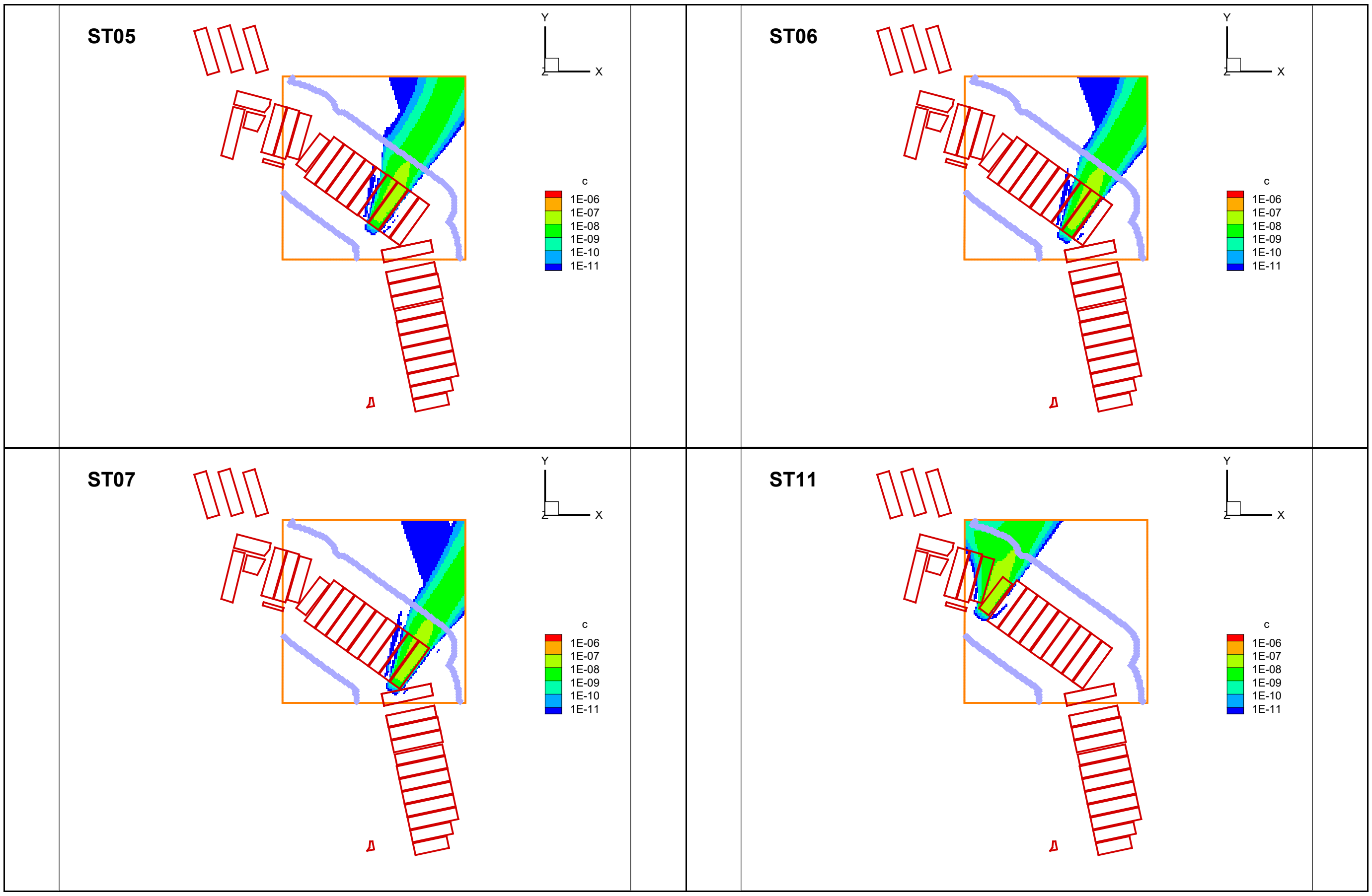
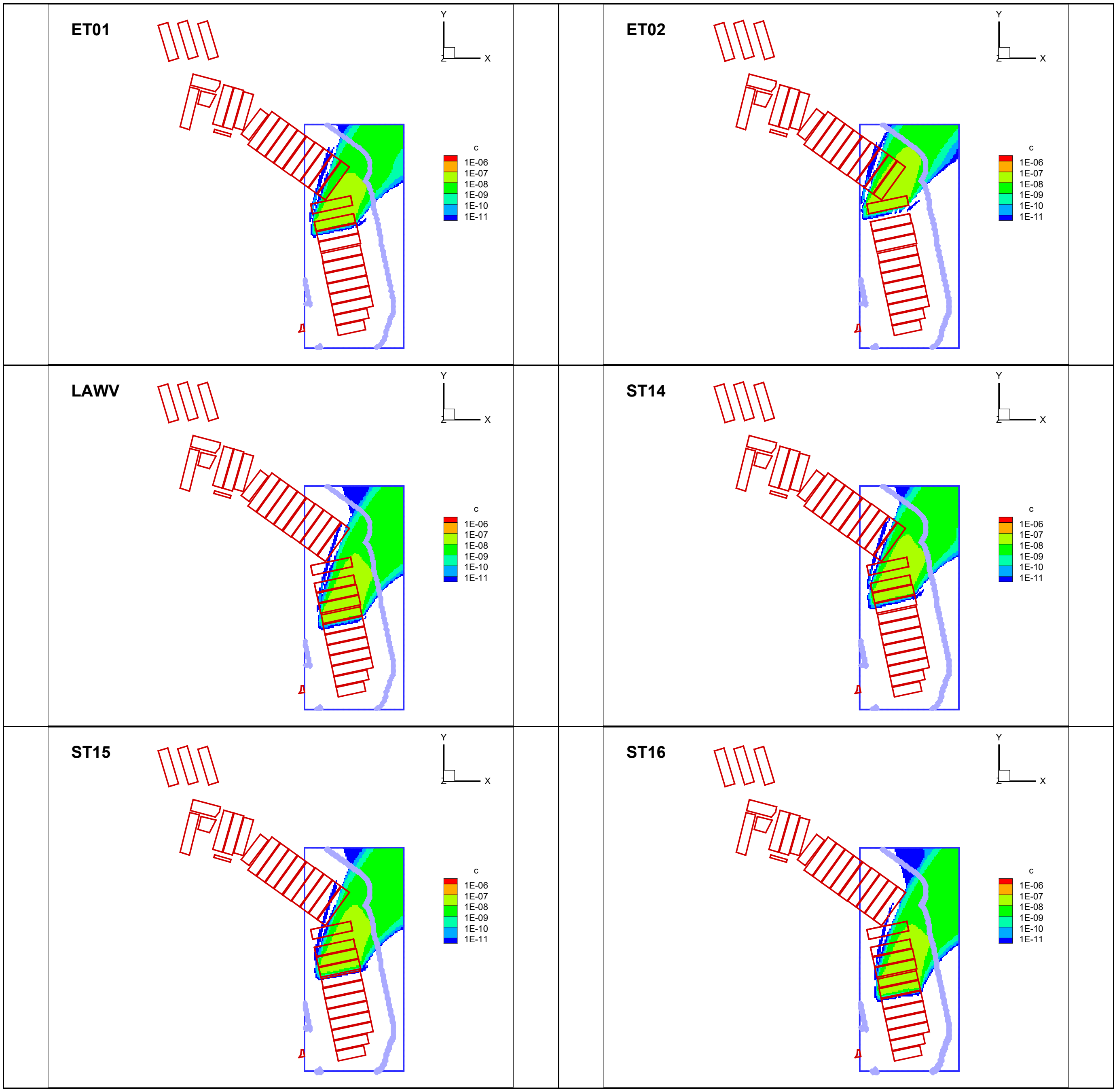


Figure 19. Disposal units in the Center cutout – Steady-state tracer concentrations (with covers).


ET01
ET02
LAWV
ST14
ST15
ST16
Y
X
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1E-07
1E-08
1E-09
1E-10
1E-11

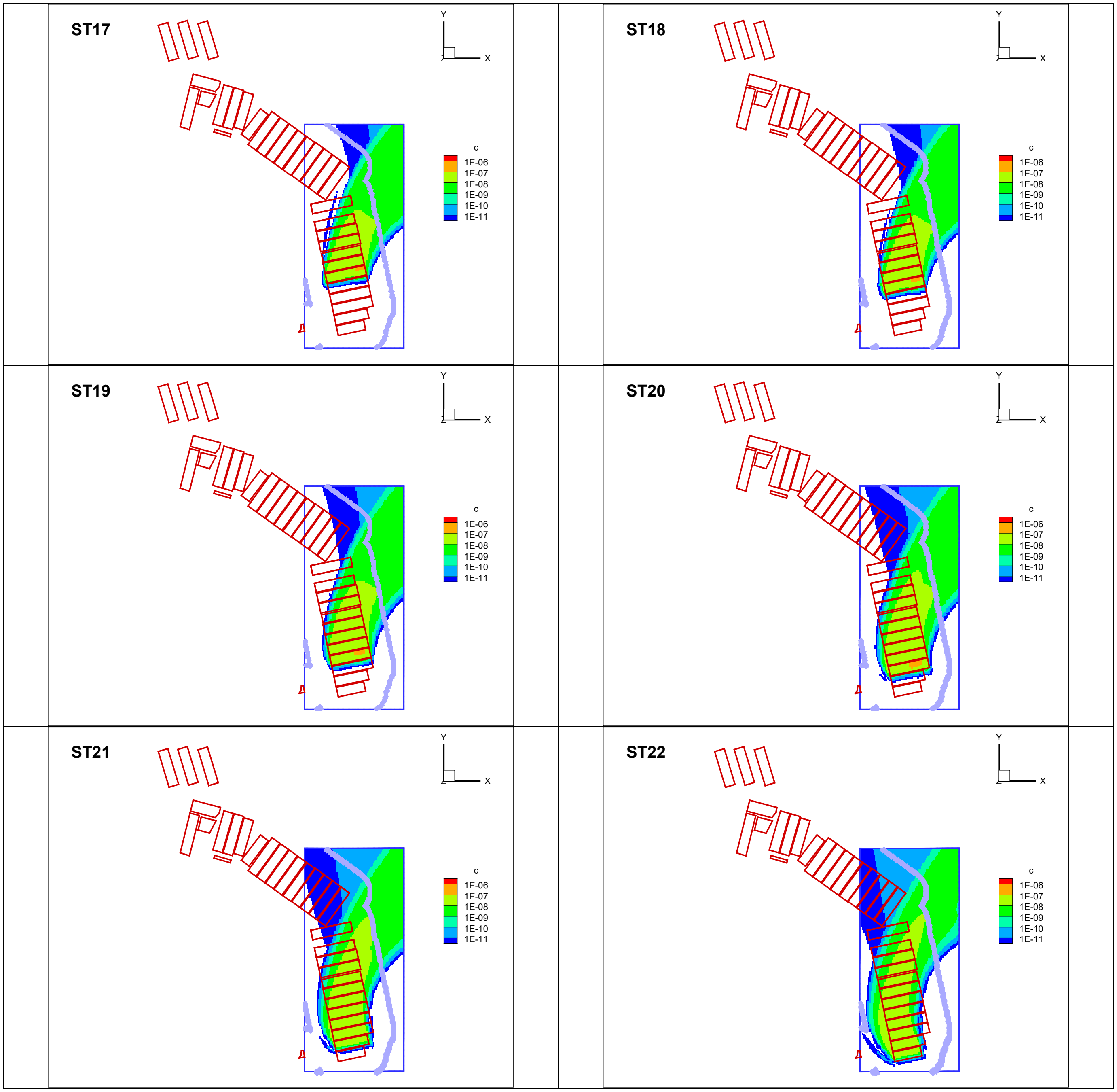

Figure 20. Disposal units in the East 1 cutout – Steady-state tracer concentrations (with covers).

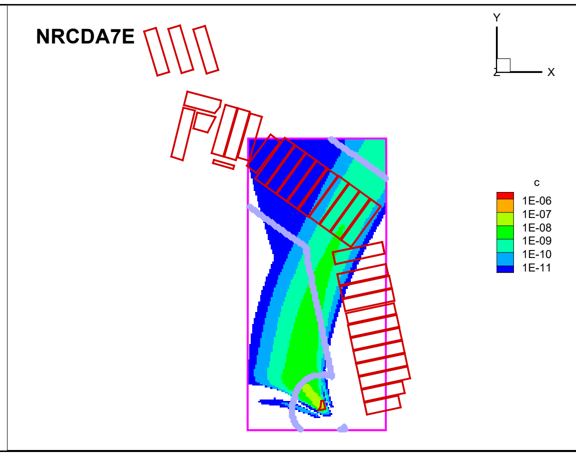

Figure 21. Disposal unit in the East 2 cutout – Steady-state tracer concentrations (with covers).

<u>Summary</u>

As shown in the previous section, the four cutouts (i.e., West, Center, East 1, and East 2) are appropriately selected to adequately contain the tracer plumes of relevant disposal units. The cutout selection minimizes the mass loss outside the cutout boundary relative to the 100-meter perimeter. Among the cutouts, the East 2 cutout has the largest size with ~850,000 nodes in order to adequately capture the NRCDA7E plume (see Figure 17 and Figure 21).

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Distribution

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