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date: 11 June 2007
to: E. D. Vugrin
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from: A. E. Ismail 6/11/07
subject: Errors in input files for NUTS for CRA-2004 PABC calculations

While preparing files for the Waste Isolation Pilot Plant Performance Assessment (WIPP PA) calculations carried out as part of Analysis Plan AP-132 (Vugrin and Nemer 2007), two sets of typographical errors were detected in the input files used for the codes NUTS and ALGEBRACDB as part of the calculations determining Salado transport:

1. In the input files for NUTS, NUT_*_CRA1BC_R*_S*.INP, located in class CRA1BC-0 of library LIBCRA1BC_NUT, three of the BRAGFLO grid coordinates defining the north Rest of Repository area were incorrectly specified: the coordinates (35, 10, 1), (35, 11, 1), and (35, 12, 1) were listed instead of (36, 10, 1), (36, 11, 1), and (36, 12, 1).

2. In the ALGEBRACDB post-processing scripts used after each stage of NUTS in the WIPP PA, a number of calculation statements included one of the following commands:

   IFGT0(FLUXJM1[E:1197],FLUXJM1[E:1297],0.)
   IFGT0(FLUXJM1[E:1198],FLUXJM1[E:1298],0.)
   IFGT0(FLUXJM1[E:1199],FLUXJM1[E:1299],0.)

   instead of the correct forms

   IFGT0(FLUXJM1[E:1197],FLUXJM1[E:1197],0.)
   IFGT0(FLUXJM1[E:1198],FLUXJM1[E:1198],0.)
   IFGT0(FLUXJM1[E:1199],FLUXJM1[E:1199],0.)

   The former, incorrect statements replaced the correct fluxes in the DRZ with fluxes measured far away from the repository, where nuclide transport would presumably be much smaller. However, because the indicated fluxes are in the *y*-direction from just above the repository into the cells directly above those, it is unclear what effect correcting this error will have on total releases. The most likely effect of the change is to increase the number of pathways that lead to the borehole; however, since those paths are through regions of possibly lower permeability, the total releases will likely decrease.

These errors were corrected, and the NUTS calculations from the 2004 Compliance Recertification Application Performance Assessment Baseline Calculations (CRA-2004 PABC) were re-run, as outlined in Kanney and Leigh (2005) and Long and Kanney (2005), to assess the impact of the errors. To determine the effect of releases to the Culebra on the overall release probabilities, CCDFGF was also run, incorporating the results from the corrected NUTS calculations. All files were generated and stored in the Code Management System (CMS) as outlined in Long and Kanney (2005), except files were saved in the class CRA1BC-1 instead of CRA1BC-0.

As discussed below, results from runs carried out with these corrections indicate that the nuclide releases to the borehole-Culebra interface (element 1845 in the current BRAGFLO grid) are approximately the same as the values reported in the analysis reports submitted for the original Compliance Recertification Application (CRA) (Lowry 2003) and the subsequent CRA baseline calculations (Lowry 2005). However, the impact of these

changes on the overall complementary cumulative distribution functions (CCDF's) computed using CCDFGF is negligible as transport of nuclides through the Culebra is sufficiently hindered that little, if any, of the nuclides present will reach the land withdrawal boundary (LWB) within the 10,000-year horizon covered by WIPP PA.

The results for the maximum releases to the Culebra for the isotope calculation runs [designated ISO in Long and Kanney (2005), Section 5.1.6.3] are summarized in Table 1. These runs model radionuclide transport in the Salado formation following E1 and E2 intrusions at 350 yr and 1000 yr. The data for the CRA1BC-0 and CRA1BC-1 results were taken from the SUMMARIZE files for NUTS stored in the CMS repository, library LIBCRA1BC_SUM, classes CRA1BC-0 and CRA1BC-1, respectively. The data were analyzed using a Perl script, *find_max.pl*, executed on a Mac workstation running OS X (see Appendix A for a code listing). Visual inspection of the results of the script in comparison to the original data files were used to validate the performance of the script.

Comparison of the present runs (CRA1BC-1) to the older runs (CRA1BC-0) show that, except for one case (Th-230 in an E2 intrusion at 1000 yr), the maximum releases to the Culebra for the original calculations are greater than or equal to the releases obtained for the corrected calculations. Note that each value in Tables 1 and 2 represents the maximum across all three replicates; moreover, the different values for a given row may come from different vectors; thus, the "Total" column may not be equal to the sum of the individual isotope maxima.

Table 1 Maximum total releases to the Culebra for the isotope (ISO) runs carried out as part of the original CRA-2004 PABC calculations (CRA1BC-0) and the corrected CRA-2004 PABC calculations (CRA1BC-1). The results are shown for each of the four major isotopes present, as well as the total releases. All results are in EPA units.

Int. Type	Time	Version	Am-241	Pu-239	U-234	Th-230	Total
E1	350 yr	CRA1BC-1	29.9	36.3	0.0608	0.135	43.0
		CRA1BC-0	36.6	43.1	0.0667	0.145	50.4
	1000 yr	CRA1BC-1	13.3	30.3	0.0515	0.125	31.0
		CRA1BC-0	16.2	30.3	0.0515	0.134	31.2
E2	350 yr	CRA1BC-1	1.12	2.87	0.00820	0.000361	4.00
		CRA1BC-0	1.49	2.93	0.00820	0.00152	4.42
	1000 yr	CRA1BC-1	0.320	1.53	0.00724	0.00145	1.53
		CRA1BC-0	0.320	1.53	0.00724	0.00139	1.53

Table 2 Maximum total releases to the Culebra for the time-intrusion (INT) runs carried out as part of the corrected CRA-2004 PABC calculations. The results are shown as a function of time for each of the four major isotopes present, as well as the total releases. All results are in EPA units; CRA1BC-0 values are taken from Table 4 of Lowry (2005).

Intrusion	Time	Version	Am-241	Pu-239	U-234	Th-230	Total
E1	100 yr	CRA1BC-1	34.0	36.9	0.0386	0.136	52.6
		CRA1BC-0	42.4	43.7	0.0676	0.146	62.6
	3000 yr	CRA1BC-1	1.15	24.7	0.0452	0.109	24.8
		CRA1BC-0	21.4	24.7	0.0509	0.116	29.1
	5000 yr	CRA1BC-1	0.122	18.4	0.0384	0.0907	18.4
		CRA1BC-0	0.155	10.6	0.0384	0.0959	18.4
	7000 yr	CRA1BC-1	0.0166	10.6	0.0312	0.0720	10.6
		CRA1BC-0	0.0208	10.6	0.0313	0.0748	10.6
	9000 yr	CRA1BC-1	0.00247	5.40	0.0173	0.0401	5.44
		CRA1BC-0	0.00280	4.94	0.0183	0.0409	4.99
E2	100 yr	CRA1BC-1	1.63	2.85	0.00861	0.00163	4.49
		CRA1BC-0	2.16	3.06	0.00567	0.00159	5.22
	3000 yr	CRA1BC-1	0.00810	0.701	0.00389	0.000941	0.701
		CRA1BC-0	0.00834	0.376	0.00389	0.000408	0.376
	5000 yr	CRA1BC-1	0.000891	0.168	0.00227	0.000486	0.169
		CRA1BC-0	0.000918	0.249	0.00227	0.000408	0.250
	7000 yr	CRA1BC-1	0.000111	0.00699	0.00153	0.0000263	0.00702
		CRA1BC-0	0.000115	0.00699	0.00155	0.0000239	0.00702
	9000 yr	CRA1BC-1	0.00000419	0.00494	0.00125	0.00000314	0.00495
		CRA1BC-0	0.00000437	0.00629	0.00125	0.00000314	0.00629

Comparing the results for the time-intrusion calculations (INT), we find that the results are roughly equal for the original and corrected CRA-2004 PABC calculations (Table 2; Figures 1 and 2). We find that the complementary cumulative distribution function (CCDF) shown in Figure 3 for releases from the Culebra remains virtually unchanged between the original and corrected CRA-2004 PABC calculations. According to Figure 3, a release from the Culebra of 0.0001 EPA units occurs with a probability of approximately 0.001; such a release, however, is five orders of magnitude lower than the 10 EPA unit limit at that probability. Similarly, the mean release from the Culebra is four orders of magnitude below the mean direct brine release for $p = 0.001$. Thus, it is reasonable to conclude that there is no adverse effect on the correctness of the estimates of total releases obtained from the CRA-2004 PABC calculations.

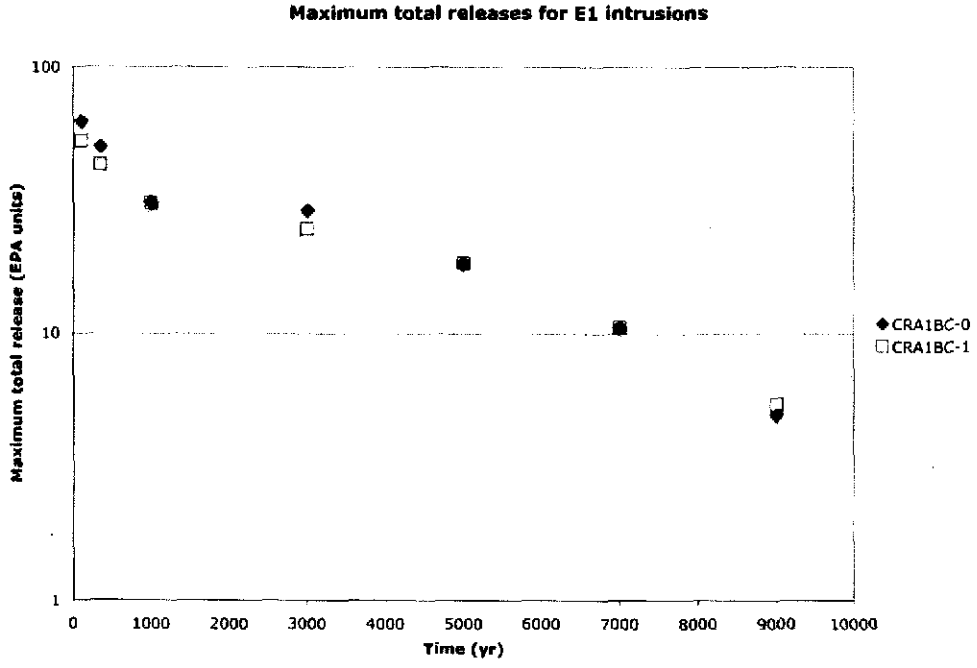

Figure 1 Comparison of maximum total releases for the original (CRA1BC-0) and corrected (CRA1BC-1) KANNEY AND LEIGH calculations for intrusions of type E1 among all three replicates.

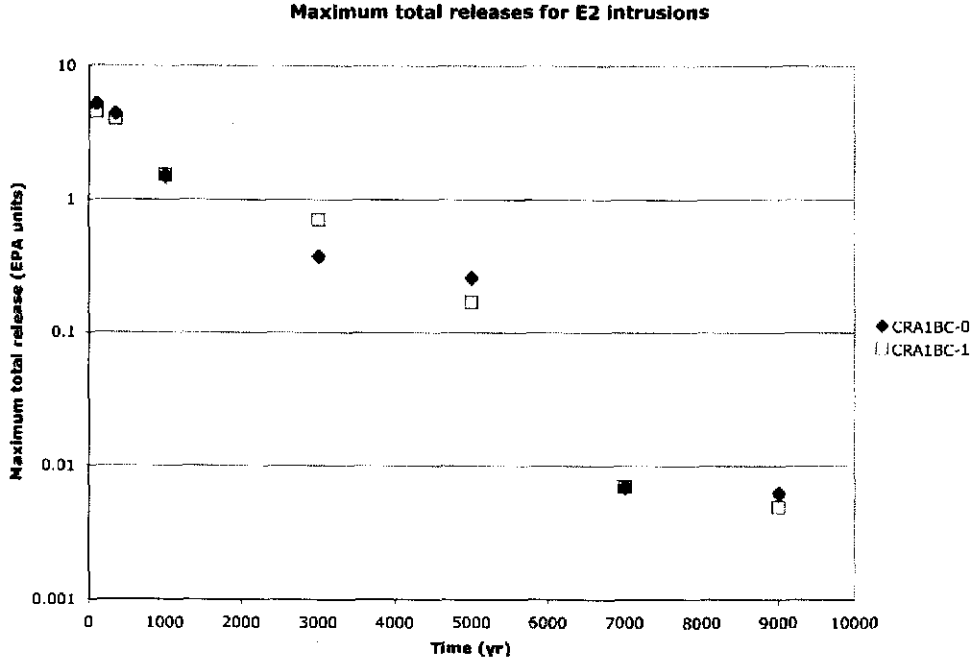

Figure 2 Comparison of maximum total releases for the original (CRA1BC-0) and corrected (CRA1BC-1) CRA-2004 PABC calculations for intrusions of type E1 among all three replicates.

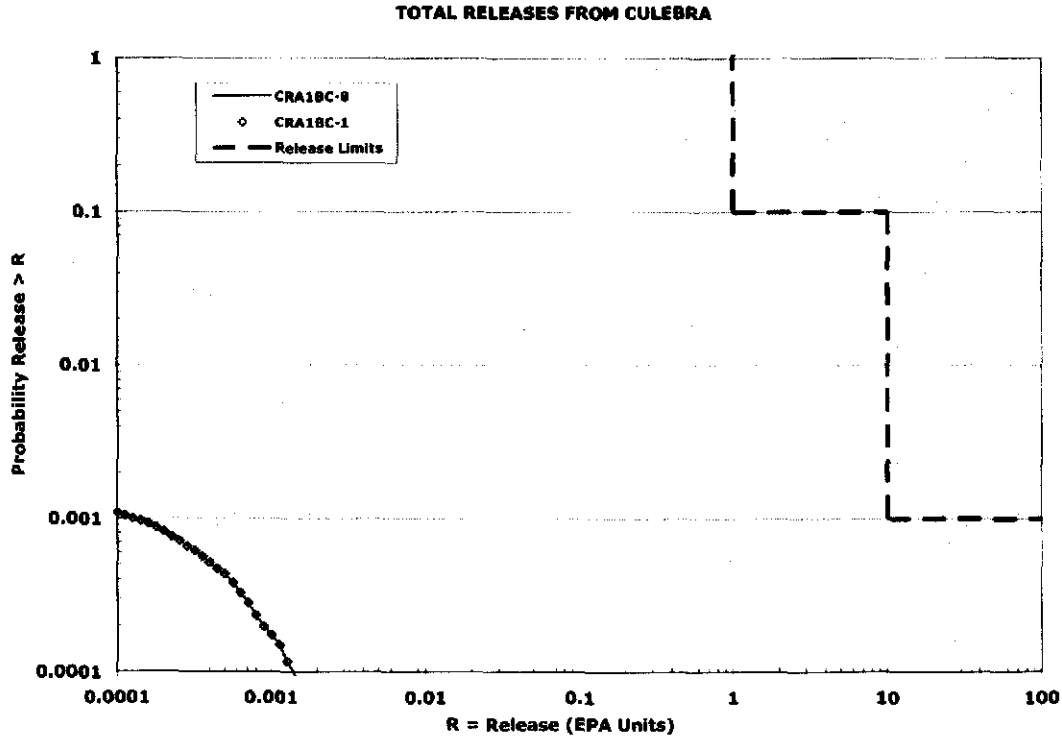

Figure 3 Complementary cumulative distribution function (CCDF) for total releases from Culebra for the original CRA-2004 PABC (line) and corrected CRA-2004 PABC (diamond) calculations. EPA limits are represented by dashed line at right of figure. CCDF is shown only for a single replicate (R2).

References

Kanney, J. F. and Leigh, C. D. (2005) Analysis Plan for POST CRA PA Baseline Calculations. AP-122, Revision 0. Carlsbad, NM: Sandia National Laboratories. ERMS 539624.

Long, J. J. and Kanney, J. F. (2005) *Execution of Performance Assessment Codes for the CRA-2004 Performance Assessment Baseline Calculation.* Carlsbad, NM: Sandia National Laboratories. ERMS 541394.

Lowry, T. S. (2003) Analysis Package for Salado Transport Calculations: Compliance Recertification Application. Carlsbad, NM: Sandia National Laboratories. ERMS 530164.

Lowry, T. S. (2005) Analysis Package for Salado Transport Calculations: CRA-2004 PA Baseline Calculation. Carlsbad, NM: Sandia National Laboratories. ERMS 541084.

Vugrin, E. D. and Nemer, M. B. (2007) Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment. AP-132, Revision 0. Carlsbad, NM: Sandia National Laboratories. ERMS 545496.

Appendix A: Code listing for *find_max.pl*

```
#!/usr/bin/perl

# A. E. Ismail
# 5/13/07

# find_max.pl: Determines maximum for each species and for all species
# for a given replicate.

use strict;

# Run algorithm for each routine individually.
&find_max($_) for (@ARGV);

sub find_max {
  my $file = $_[0];
  my $handle = substr(lc($file), 0, -6);
  my $output = $handle . ".sum";
  my $summary = $handle . ".dat";

  # Open data and output files
  print "Processing $file...\n";
  open IN, "<$file" or die "Could not open input $file.\n";
  open OUT, ">$output" or die "Could not open output $output.\n";
  open SUM, ">$summary" or die "Could not open summary $summary.\n";

  # Vectors to store maximum activities and PA vector numbers.
  my @max = (0., 0., 0., 0., 0., 0., 0.);
  my @loc = (0, 0, 0, 0, 0, 0, 0);

  # Discard header from input file
  <IN> for (1 .. 4);

  while (<IN>) {
    # Parse each line. Determine if current activity is greater than the
    # maximum currently stored; if so, replace existing value with the new
    # maximum. Also update loc vector, which stores the ID of the PA vector.
    my @array = split;
    next if (!@array);
    my $row = 0;
    # Determine total activity. Am, Pu, U are normalized by 232; Th by 23.2
    # to convert Ci to EPA units.
    for my $q (2 .. 5) {
      my $term = $array[$q] / (($q != 5) ? 232 : 23.2);
      $row += $term;
      $max[$q - 1] = $term, $loc[$q - 1] = $array[0]
      if ($term > $max[$q - 1]);
    }
    $max[5] = $row, $loc[5] = $array[0] if ($row > $max[5]);
    $max[6] = $array[6], $loc[6] = $array[0] if ($array[6] > $max[6]);
    # Print results for each PA vector to output for creation of figures.
    printf SUM "%3d  %10.5g  5  %10.5g  4  %10.5g  3  %10.5g  2  %10.5g  1\n",
      $array[0], $array[2] / 232, $array[3] / 232, $array[4] / 232,
```

```
      $array[5] / 23.2, $row
        if ($array[1] > 9999);
  }

  # Print overall replicate maxima to output file.
  for (1 .. 6) {
    printf OUT " %12.6g   %3d\n", $max[$_], $loc[$_];
  }

  close IN;
  close OUT;
  close SUM;
}
```