

530441



Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation

4100 National Parks Hwy
Carlsbad, NM 88220

date: July 22, 2003

to: Laurence Brush, 6822

from: Paula Sue Downes, 6821

Paula Sue Downes

Technical Review *Juanita R. Hengstenberg* Date 7.23.03

QA Review *Mano Chavara* Date 7/23/03

subject: Spreadsheet Calculations of Actinide Solubilities for the WIPP Compliance Recertification Application in support of AP-098, *Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application Analysis Plan.*

Larry,

This memo documents the method used to perform the spreadsheet calculations of the summation of Molarities for the following constituents:

- Thorium
- Neptunium
- Americium
- Boron
- Sodium
- Magnesium
- Potassium
- Calcium
- Sulfate
- Chlorine
- Bromine
- Total Inorganic Carbon
- Acetate
- Citrate
- EDTA
- Oxylate

from the FMT calculations in output files **ap098_fmt_run001** through **ap098_fmt_run030**. The original outfiles can be found on in the CMS Library called: **LIB_AP098_FMT**. The original

Information Only

output files all have an OUT extension. In this same library there are 3 Excel spreadsheets that were used to calculate the solubilities as per AP-098. All three of these spreadsheets were created under the Microsoft Windows 2000[®] operating system using Microsoft Excel 2000[®]. A cd of these files is attached to this letter for ease of use. The steps used to create these spreadsheets is located in Table 1 of this memo.

The spreadsheet titled, "Solubility results_rad.xls" contains the solubility results for thorium, neptunium, and americium. There are 60 worksheets in this file. There are 2 worksheets for each run. The first sheet for each run has the run number as the sheet name. This sheet contains the *Table of Batch Concentrations for Batch System* as imported into Excel from the original output file. The second sheet name is the run number followed by the descriptor "radionuclides". This sheet contains the solubility information for thorium, neptunium, and americium in tabular form.

The spreadsheet titled, "Solubility results_nonrad.xls" contains the solubility results for boron, sodium, magnesium, potassium, calcium, sulfate, chlorine, bromine, and total inorganic carbon. This file also contains 2 worksheets for each run for a total of 60 sheets. The first sheet for each run has the run number as the sheet name. This sheet contains the *Table of Batch Concentrations for Batch System* as imported into Excel from the original output file. The second sheet name is the run number followed by the descriptor "non-radiological". This sheet contains the solubility information for boron, sodium, magnesium, potassium, calcium, sulfate, chlorine, bromine, and total inorganic carbon in tabular form.

The spreadsheet titled, "Solubility results_internal check.xls" contains the results for acetate, citrate, EDTA, and oxylate. Because concentrations of acetate, citrate, EDTA, and oxylate are only found in those runs with organic constituents, this file only contains 30 sheets; 2 worksheets for each even numbered run. The first sheet for each run has the run number as the sheet name. This sheet contains the *Table of Batch Concentrations for Batch System* as imported into Excel from the original output file. The second sheet name is the run number followed by the descriptor "internal verification". This sheet contains the solubility information for acetate, citrate, EDTA, and oxylate in tabular form.

Table 1: Methodology for Determining Molarity Summations

Step 1	Print out original text output file for reference
	The following steps were repeated for each run
Step 2	Import table entitled <i>Table of Batch Concentrations for Batch System</i> into Microsoft Excel [®] 2000
Step 3	Label Worksheet as per the corresponding run number (e.g., 001, 002 ...)
Step 4	Create additional sheets using the naming convention of "run number, type of result". As an example the results for run number 1 would be found via the following: 1: radiological data in file "Solubility results_rad.xls" in sheet named 001 radionuclides, 2: non-radiological data in file "Solubility results_nonrad.xls" in sheet named 001 non-radiological, 3: internal verification data in file "Solubility results_internal check.xls" in sheet named 001 internal verification
Step 5	Copy Data (as values) to appropriate sheets
Step 6	Delete all rows with solid species data
Step 7	Sort data alphabetically
Step 8	Search for appropriate species
Step 9	Copy into appropriate tables
Step 10	Delete extraneous data
Step 11	Sort data based on descending order of Molarity
Step 12	Sum column titled Molarity
Step 13	Save File

Information Only

All three spreadsheets were verified by manual inspection and were reviewed by the technical reviewer who verified each step presented in the calculational methodology described in the above table for all three spreadsheets.

Enclosure: 1 cd of original output files and excel spreadsheet results

File code: WIPP:1.3.5.1.2:PA:QA-L:527285
7/28/03 RH