

Appendix B

<b>NUCLEAR WASTE MANAGEMENT PROCEDURE</b> Sandia National Laboratories	<b>Parameter Problem Report (PPR)</b>	<b>Form Number: NP 9-2-2</b>  <b>Page 1 of 1</b>
Material Abbreviated Name: <u>SOLMOD3</u> Property Abbreviated Name: <u>SOLSOH</u> Associated Analysis: (CCA, PAVT, AP-159, etc.) <u>CRA19</u> Effective Date: <u>4/16/2019</u>		
<b>Description of Problem</b>  The alpha(1) terms for the binary Pitzer parameter for Ca <sup>2+</sup> / EDTA <sup>4-</sup> , Mg <sup>2+</sup> / MgEDTA <sup>2-</sup> , and the Ca <sup>2+</sup> / MgEDTA <sup>2-</sup> pairs were entered incorrectly in the EQ3/6 thermodynamic database DATA0.FM4. They were entered as 2.0 when the correct value is 1.4. While this value is NOT a direct input to PA, it did have an impact on the SOLMOD3/SOLSOH parameter value. This issue was uncovered during an extent of condition evaluation triggered by PPR 2019-003.		
<u>Paul Domski</u> <i>Shelley R. Nielsen for</i> <u>1-13-2020</u> Requester (Print, Sign and Date)  Condition Adverse to Quality? <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No (Initiate NP 16 -1 if yes)		
<b>Problem Resolution and Justification for no Condition Adverse to Quality</b>  Three analyses were performed, the first by Domski to determine if changes to the alpha(1) terms impacted any of the output PA parameters from the baseline solubility model. Domski determined that SOLMOD3/SOLSOH had been impacted which precipitated the need to evaluate downstream models which use the SOLMOD3/SOLSOH parameter. The humic colloids model uses the SOLMOD3/SOLSOH parameter to calculate PHUSIM and PHUCIM. Mariner re-calculated the humic colloids model with the updated parameters and found that there was no impact, i.e., no condition adverse to quality existed. The third model was the PA model itself, Kim ran the model with the updated SOLMOD3/SOLSOH parameter and found there was no change in the mobilized An(III), brine pressure, hydrogen gas generation rate, and transport to the Culebra. The CCDFGF plots of total release of An(III) from the repository were not impacted by the change to the SOLMOD3/SOLSOH parameter, therefore, there is no condition adverse to quality, and the WIPP PA Parameter Database will not be updated. This problem resolution and justification for no condition adverse to quality is documented in memorandum "Correction of the α1 terms of three Binary Pitzer Parameter blocks in DATA0.FM4, PPR 2019-004 through 2019-013" (Domski, 2020).		
<b>Concurrence</b>		
<u>Paul E. Shoemaker</u> <i>Paul E. Shoemaker</i> <u>01/13/2020</u> PA Manager (Print, Sign and Date)  <u>Shelley R. Nielsen</u> <i>Shelley R. Nielsen</i> <u>2019-004</u> QA Staff (Print, Sign and Date) <u>1-13-2020</u> Parameter Problem Report No. (PPR)		

**INFORMATION ONLY**