

Preparation of Simulated Waste Solutions



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PREPARATION OF SIMULATED WASTE SOLUTIONS

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SAVANNAH RIVER SITE

PREPARATION OF SIMULATED WASTE SOLUTIONS

By D. D. Walker

SUMMARY

Waste Processing Technology personnel routinely prepare 0.5 to 10 L batches of salt solutions simulating Savannah River Site (SRS) soluble waste. This report describes the compositions and preparation methods.

DISCUSSION

The simulant compositions vary by waste type (e.g., average, high hydroxide, and high nitrate) and by total sodium ion concentration (typically 3 to 7 molar Na⁺). The waste types represent the average and extreme compositions expected in the feed stream sent to the salt decontamination process.¹⁻² As such, they do not represent the extremes in composition of liquid waste currently in the SRS tank farms. Some blending is expected prior to transfer to the salt decontamination process. The two extreme compositions are called "high hydroxide" and "high nitrate" solutions. The high hydroxide solution represents tank supernate and the high nitrate solution represents dissolved salt cake. The average solution represents a blend of all soluble waste in the tank farm. For any of the three waste compositions (i.e., anion distribution), the total sodium ion concentration can be varied up to 7 molar. The nominal sodium ion concentration is 5.6 molar for the feed to the ion exchange option for salt disposition.

Table I lists the concentrations of 15 major components in the three waste types. Numerous minor components, particularly hazardous metals such as chromium, are not routinely included in simulants.

Appendix A lists the amounts and identities of chemicals used to prepare 1-L batches of each waste type at 5.6 M Na⁺. Small batches of simulants are prepared from reagent or similar purity chemicals.

When high purity chemicals are used in the preparation, typically less than 0.5 grams of solids fail to dissolve per liter of solution. Larger amounts of insoluble solids could be obtained if lower purity chemicals are used in the preparation. For most applications, the solutions are filtered if solids remain after final dilution. The solutions should be cooled to room temperature and aged for at least 24 hours before filtering.

Aluminum nitrate [Al(NO₃)₃·9H₂O] is the usual source of aluminate ion. Use of aluminum nitrate requires addition of extra sodium hydroxide and less sodium nitrate based on the following stoichiometry.



TABLE I. Composition of Simulated Waste Solutions

<u>Component</u>	<u>Concentration (molar)</u>		
	<u>Average</u>	<u>High OH⁻</u>	<u>High NO₃⁻</u>
Na ⁺	5.6	5.6	5.6
K ⁺	0.015	0.030	0.0041
Cs ⁺	0.00014	0.00037	0.00014
OH ⁻	1.91	3.05	1.17
NO ₃ ⁻	2.14	1.10	2.84
NO ₂ ⁻	0.52	0.74	0.37
AlO ₂ ⁻	0.31	0.27	0.32
CO ₃ ²⁻	0.16	0.17	0.16
SO ₄ ²⁻	0.15	0.030	0.22
Cl ⁻	0.025	0.010	0.040
F ⁻	0.032	0.010	0.050
PO ₄ ³⁻	0.010	0.008	0.010
C ₂ O ₄ ²⁻	0.008	0.008	0.008
SiO ₃ ²⁻	0.004	0.004	0.004
MoO ₄ ²⁻	0.0002	0.0002	0.0002

Aluminum nitrate yields an acidic solution in water and can react with sodium nitrite to form NO₂ gas. Thus, the preferred order of addition is to dissolve sodium hydroxide first, followed by aluminum nitrate. Sodium nitrite is added only after the aluminum nitrate is completely dissolved in excess sodium hydroxide.

If disodium hydrogen phosphate is used instead of trisodium phosphate, additional sodium hydroxide should be added to neutralize the acidic hydrogen.

Appendix B contains an example of instructions for the preparation of a 1-L batch of salt solution. Salt solutions in volumes ≤ 2 L are usually prepared in volumetric glassware so that the amount of water required need not be measured. However, the densities of the three types of salt solution have been measured and the required mass of water can be calculated. The density (g/mL) at 22 °C is calculated from the total sodium ion concentration (molar) by the following equations.³

$$\text{Average:} \quad d = 1.009 + 0.04454[\text{Na}^+]$$

$$\text{High hydroxide:} \quad d = 1.003 + 0.04302[\text{Na}^+]$$

$$\text{High nitrate} \quad d = 1.006 + 0.04725[\text{Na}^+]$$

REFERENCES

1. P. L. Rutland et al., "Bases, Assumptions, and Results of the Flowsheet Calculations for the Initial Eighteen Salt Disposition Alternatives", WSRC-RP-98-00166, 25 June 1998.
2. D. D. Walker, "Modeling of Crystalline Silicotitanate Ion Exchange Columns," WSRC-TR-98-00343, Rev.0, October 2, 1998.
3. D. D. Walker and G. K. Georgeton, "Viscosity and Density of Simulated Salt Solutions," WSRC-RP-89-1088, October 19, 1989.

Appendix A
Chemicals Required for Salt Solutions

Average Salt Solution (1-L batch)

<u>Component</u>	<u>Source</u>	<u>Molecular Weight (g/mole)</u>	<u>Target Concentration (molar)</u>	<u>Amount Required (grams)</u>
K ⁺	KNO ₃	101.1	0.015	1.517
Cs ⁺	CsNO ₃	194.92	0.00014	0.027
OH ⁻	NaOH	40.00	1.91	126.40
NO ₃ ⁻	NaNO ₃	84.99	2.14	101.55
NO ₂ ⁻	NaNO ₂	69.00	0.52	35.88
AlO ₂ ⁻	Al(NO ₃) ₃ ·9H ₂ O	375.14	0.31	116.29
CO ₃ ²⁻	Na ₂ CO ₃ ·H ₂ O	124.01	0.16	19.84
SO ₄ ²⁻	Na ₂ SO ₄	142.04	0.15	21.31
Cl ⁻	NaCl	58.44	0.025	1.461
F ⁻	NaF	41.99	0.032	1.344
PO ₄ ³⁻	Na ₂ HPO ₄ ·7H ₂ O	268.09	0.010	2.681
C ₂ O ₄ ²⁻	Na ₂ C ₂ O ₄	134.00	0.008	1.072
SiO ₃ ²⁻	Na ₂ SiO ₃ ·9H ₂ O	284.2	0.004	1.137
MoO ₄ ²⁻	Na ₂ MoO ₄ ·2H ₂ O	241.95	0.0002	0.048
Water				827.9
Total weight:				1258.

High Hydroxide Salt Solution (1-L batch)

<u>Component</u>	<u>Source</u>	<u>Molecular Weight (g/mole)</u>	<u>Target Concentration (molar)</u>	<u>Amount Required (grams)</u>
K ⁺	KNO ₃	101.1	0.030	3.033
Cs ⁺	CsNO ₃	194.92	0.00037	0.072
OH ⁻	NaOH	40.00	3.05	165.52
NO ₃ ⁻	NaNO ₃	84.99	1.08	20.37
NO ₂ ⁻	NaNO ₂	69.00	0.74	51.06
AlO ₂ ⁻	Al(NO ₃) ₃ ·9H ₂ O	375.14	0.27	101.29
CO ₃ ²⁻	Na ₂ CO ₃ ·H ₂ O	124.01	0.17	21.08
SO ₄ ²⁻	Na ₂ SO ₄	142.04	0.030	4.26
Cl ⁻	NaCl	58.44	0.010	0.584
F ⁻	NaF	41.99	0.010	0.420
PO ₄ ³⁻	Na ₂ HPO ₄ ·7H ₂ O	268.09	0.008	2.145
C ₂ O ₄ ²⁻	Na ₂ C ₂ O ₄	134.00	0.008	1.072
SiO ₃ ²⁻	Na ₂ SiO ₃ ·9H ₂ O	284.2	0.004	1.137
MoO ₄ ²⁻	Na ₂ MoO ₄ ·2H ₂ O	241.95	0.0002	0.048
Water				871.9
Total weight:				1244.

High Nitrate Salt Solution (1-L batch)

<u>Component</u>	<u>Source</u>	<u>Molecular Weight (g/mole)</u>	<u>Target Concentration (molar)</u>	<u>Amount Required (grams)</u>
K ⁺	KNO ₃	101.1	0.0041	0.415
Cs ⁺	CsNO ₃	194.92	0.00014	0.027
OH ⁻	NaOH	40.00	1.17	98.40
NO ₃ ⁻	NaNO ₃	84.99	2.84	159.42
NO ₂ ⁻	NaNO ₂	69.00	0.37	25.53
AlO ₂ ⁻	Al(NO ₃) ₃ ·9H ₂ O	375.14	0.32	120.04
CO ₃ ²⁻	Na ₂ CO ₃ ·H ₂ O	124.01	0.16	19.84
SO ₄ ²⁻	Na ₂ SO ₄	142.04	0.22	31.25
Cl ⁻	NaCl	58.44	0.040	2.338
F ⁻	NaF	41.99	0.050	2.100
PO ₄ ³⁻	Na ₂ HPO ₄ ·7H ₂ O	268.09	0.010	2.681
C ₂ O ₄ ²⁻	Na ₂ C ₂ O ₄	134.00	0.008	1.072
SiO ₃ ²⁻	Na ₂ SiO ₃ ·9H ₂ O	284.2	0.004	1.137
MoO ₄ ²⁻	Na ₂ MoO ₄ ·2H ₂ O	241.95	0.0002	0.048
Water				806.3
Total weight:				1271.

Appendix B Instructions for Preparation of Salt Solution

Note: The instructions are accompanied by a data sheet listing the chemicals required with spaces for the exact amounts used. Spaces are also provided for other quality assurance information (i.e., operator name, date, balance identification, manufacturers and lot numbers for each chemical).

1. Locate and label a clean, dry, 1-L volumetric flask. Weigh it empty and dry.
2. Weigh the NaOH into the flask. Add _____ g of water and dissolve the NaOH before continuing.

Caution: Dissolving NaOH will heat the solution. If the solution becomes too hot to handle safely, cool it before proceeding.

Note: If the solution is not prepared in a volumetric flask (e.g., if the water is added by weight rather than by filling to the line on the flask), keep the container closed as much as possible when the solution is hot to avoid evaporation of water. If using volumetric glassware, reserve a portion of the water for the final addition in step 6.

3. Add the aluminum nitrate to the flask and mix to dissolve.

Caution: Do not add sodium nitrite prior to dissolving the aluminum nitrate in excess NaOH. Poisonous red fumes of NO_2 could form.

4. Add the remaining chemicals.
5. Mix to dissolve (1-2 hours).
6. Allow the solution to cool to room temperature.

Note: If using volumetric glassware, fill to the line with water after cooling.

7. Reweigh the solution and compare to the expected weight. If the weights differ significantly, investigate for a missing component or error in weighing.
8. Allow the solution to age at least 24 hours.

Note: The solution should equilibrate long enough after preparation to avoid concerns from slow precipitation. For volumes as large as 10 L, 24 hours generally provides adequate equilibration time. The best practice will include a second hold period and a second filtration.

9. Filter the solution through any convenient filter (medium frit sintered glass is acceptable).

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K. DESCRIPTION/ABSTRACT

Waste Processing Technology personnel routinely prepare 0.5 to 10 L batches of salt solutions simulating Savannah River Site (SRS) soluble waste. This report describes the compositions and preparation methods.

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