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Literature Review on Next Generation Solvent Isopar® L Vapor Pressure Curve and the Partitioning of its Modifier and Extractant

S. C. Hunter

March 2022

SRNL-STI-2021-00672, Revision 0

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Printed in the United States of America

**Prepared for
U.S. Department of Energy**

Keywords: *Vapor Pressure, NGS, CSSX*

Retention: *Permanent*

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Savannah River National Laboratory is operated by Battelle Savannah River Alliance for the U.S. Department of Energy under Contract No. 89303321CEM000080.



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EXECUTIVE SUMMARY

The Next Generation Solvent (NGS) is set to replace the Original Caustic Side Solvent Extractant (CSSX) at the Salt Waste Processing Facility (SWPF).

The Savannah River National Laboratory (SRNL) was requested by Savannah River Mission Completion (SRMC), formerly Savannah River Remediation (SRR), to perform a literature review on the following topics to address flammability concerns with the current solvent:

- Isopar® L vapor pressure curve for NGS,
- Partitioning ratio for the extractant MaxCalix and the modifier Cs-7SB, and
- High cesium concentration impacts on NGS radiolysis and potential solvent degradation rates in high cesium concentrations.

The following conclusions and recommendations are made based on previous experimental work and literature:

- Current SWPF flammable gas generation calculations use an Isopar® L vapor pressure curve based on experimental testing with the Original CSSX solvent. No such testing to date has been performed with NGS. It is suggested that the decrease in Cs-7SB concentration for NGS compared to the Original CSSX solvent would lead to a slightly higher vapor pressure at all temperatures in SWPF vessels. A bounding NGS vapor pressure curve has been provided; it is recommended to see if these values would challenge current flammability controls and to perform testing if needed.
- The partitioning ratio for Cs-7SB is known in the Original CSSX solvent with dilute nitric acid and caustic solutions. No tests could be found for the partitioning of Cs-7SB to dilute boric acid solutions; however, a similar partitioning ratio is expected. Due to the lipophilic alkyl chains on MaxCalix, it is expected to be even less soluble than BOBCalixC6 in the aqueous phase and should not be considered a significant contributor to the f_{organic} term. Additionally, the reaction rate of N,N',N''-Tris(3,7-dimethyloctyl)guanidine (TiDG) or its degradation products with a hydrogen radical should be estimated/determined if they are found to be significant contributors to the f_{organic} term.
- NGS is expected to see much higher Cs concentrations at SWPF in comparison to its use at the Modular CSSX Unit (MCU). These higher Cs concentrations could influence radiolytic degradation rates of the solvent. NGS appears to be fairly stable to radiolytic degradation based on previous testing and its use at MCU. However, there has not been radiolytic flammable gas generation testing with NGS to date. There is a risk that the continued use of G-values obtained for flammable gases produced from the irradiation of the Original CSSX solvent is not bounding for NGS, but this is considered a very low risk due to the similarities in the composition of the solvents, as well as the conservatism in the experimental design of the Original CSSX testing.

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LIST OF ABBREVIATIONS

BDL	Below Detection Limit
CLFL	Composite Lower Flammability Limit
Cs-7SB	1-(2,2,3,3-tetrafluoropropoxy)-3-(4-sec-butylphenoxy)-2-propanol
CSSX	Caustic-Side Solvent Extraction
DCiTG	1,3-dicyclohexyl-2-(isotridecyl)guanidine
DWPF	Defense Waste Processing Facility
ESS	Extraction, Scrub, and Strip
GC	Gas Chromatography
HLW	High Level Waste
MCU	Modular CSSX Unit
NGS	Next Generation Solvent
ORNL	Oak Ridge National Laboratory
SRMC	Savannah River Mission Completion
SRNL	Savannah River National Laboratory
SRR	Savannah River Remediation
SRS	Savannah River Site
SWPF	Salt Waste Processing Facility
TiDG	N,N',N''-Tris(3,7-dimethyloctyl)guanidine
TOA	tri-n-octylamine
TTR	Technical Task Request

1.0 Introduction

Savannah River Mission Completion (SRMC), formerly Savannah River Remediation (SRR), has identified technical gaps in the implementation of the Next Generation Solvent (NGS) at SWPF.¹ Savannah River National Laboratory (SRNL) has been requested by SRMC via a Technical Task Request (TTR) to perform a literature review on the Isopar® L NGS vapor pressure curve and partitioning ratio for MaxCalix and Cs-7SB to address flammability concerns.²

NGS has been previously used at the Modular CSSX unit (MCU, which SWPF has replaced) as a blended solvent with the Original CSSX solvent. NGS is now set to replace the Original CSSX solvent at SWPF. Table 1-1 gives the solvent compositions for both NGS and the Original CSSX solvent. The BOBCalixC6 extractant of the Original CSSX solvent has been replaced with MaxCalix in NGS, a calixarene that is more soluble in the Isopar® L diluent. The guanidine suppressor TiDG has replaced the trioctylamine (TOA) suppressor of the Original CSSX solvent. The modifier 1-(2,2,3,3-tetrafluoropropoxy)-3-(4-sec-butylphenoxy)-2-propanol (Cs-7SB) and Isopar® L diluent remain the same between the two solvent systems, but their concentrations have been adjusted.

Table 1-1. Solvent Composition Comparison

Component	Function	Original Solvent Concentration	NGS Concentration
<u>MaxCalix</u> 1,3- <i>alt</i> -25,27-bis(3,7-dimethyloctyl-1-oxy) calix[4]arenebenzo-crown-6	Extractant	-	0.05 M
<u>BOBCalixC6</u> Calix[4]arene-bis(<i>t</i> -octylbenzo-crown 6)	Extractant	0.007 M	-
<u>Cs-7SB</u> 1-(2,2,3,3-tetrafluoropropoxy)-3-(4- <i>sec</i> -butylphenoxy)-2-propanol	Modifier	0.75 M	0.65 M
<u>TiDG</u> <i>N,N',N''</i> -Tris(3,7-dimethyloctyl)guanidine	Suppressor	-	0.003 M
<u>TOA</u> Tri- <i>n</i> -octylamine	Suppressor	0.003 M	-
<u>Isopar® L</u> C ₁₂ -isoparaffinic hydrocarbon	Diluent	69 wt%	71 wt%

A vapor pressure curve for Isopar® L in NGS is needed to replace the currently-used Original CSSX Solvent Isopar® L vapor pressure data at SWPF, which will support revisions to current SWPF safety documents related to SWPF vessel purge rates and time to composite lower flammability limit (CLFL) in SWPF process vessels.³

The partitioning ratio for MaxCalix and Cs-7SB in the aqueous phase is needed for deriving the f_{organic} term used in calculating the radiolytic hydrogen generation rate in aqueous streams. An estimate of these ratios is required for understanding the impact of NGS on hydrogen generation in the SWPF and the Defense Waste Processing Facility (DWPF) aqueous waste streams.

1.1 Quality Assurance

This work was performed under a Technical Task Request (TTR).² The analysis and conclusions herein satisfy the requirements for Isopar® L vapor pressure, high Cs concentrations, and extractant and modifier

partitioning topics in Task 2 of the Task Technical and Quality Assurance Plan (TTQAP) associated with this TTR.⁴ The TTR identifies the Functional Classification as Safety Significant. Thus, this document was reviewed by Design Verification by Document Review. The requirements for performing reviews of technical reports and the extent of review are established in manual E7 2.60. SRNL documents the extent and type of review using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2.

2.0 Results and Discussion

2.1 NGS Isopar® L Vapor Pressure Curve

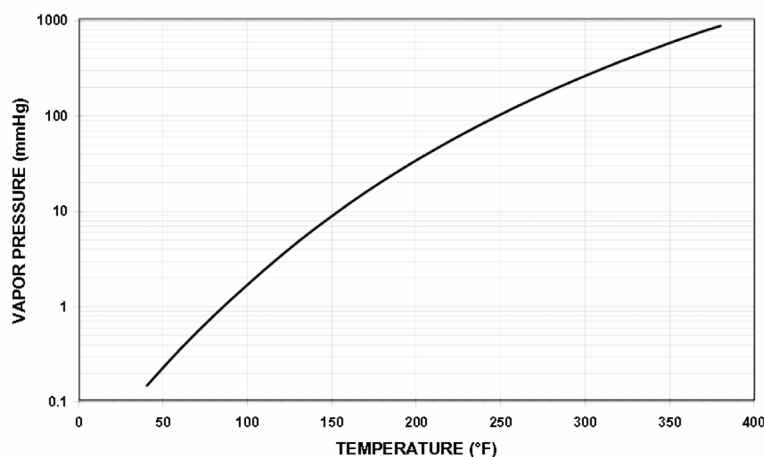
Figure 2-1 gives the vapor pressure data for pure Isopar® L, which was provided by the manufacturer, Exxon Mobil, in 2004. It should be noted that Isopar® L is a distillation fraction of aliphatic branch-chained hydrocarbon compounds ($C_{10}H_{22}$ to $C_{15}H_{32}$) and there is a potential for variability between sample lots in the compounds that compose Isopar® L as well as the ratios of these compounds within Isopar® L. In order to calculate the vapor pressure at various temperatures, the data in Figure 2-1 was fit to the Antoine Equation⁵

$$p = 10^{7.482 - \frac{1867}{T + 219.3}} \quad (1)$$

Where,

p is the vapor pressure in mmHg and
 T is the temperature in °C.

ISOPAR L



Temperature (°F)	Vapor Pressure (mmHg)
40	0.14
50	0.22
60	0.34
68	0.478
77	0.69
100	1.63
150	8.60
200	32.95
250	99.82
300	253.01

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Figure 2-1. Isopar[®] L Vapor Pressure

Current SWPF safety documents use vapor pressure data from testing at Materials and Chemistry Laboratory, Inc. with the Original CSSX solvent.⁶ This testing was undertaken to determine the vapor concentration of Isopar[®] L above the Original CSSX solvent at 16.7, 27.8, and 43.3°C by gas chromatography (GC). The resulting concentrations, shown in Table 2-1, are given in µg/mL headspace at 32mL of headspace. This data, along with testing at Oak Ridge National Laboratory (ORNL)⁷ to determine the flash temperature of the Original CSSX solvent, is used to make the following vapor pressure vs. temperature plot shown in Figure 2-2. The average flash temperature of 64.24°C for the Original CSSX solvent in the ORNL study was used to calculate the LFL (0.585%) at the flash temperature using the modified Burgess-Wheeler law.³

Table 2-1. Original CSSX Solvent Isopar[®] L Vapor in Headspace⁶

Test	Concentration in µg/mL at 16.7°C	Concentration in µg/mL at 27.8°C	Concentration in µg/mL at 43.3°C
1	2.46	5.31	11.9
2	2.48	4.64	13.3
3	2.87	5.69	14.6
4	2.42	5.32	18.8
5	3.05	5.22	111
6	2.89	5.67	11.3
7	3.88	4.43	13.3
8	3.14	5.72	15.4

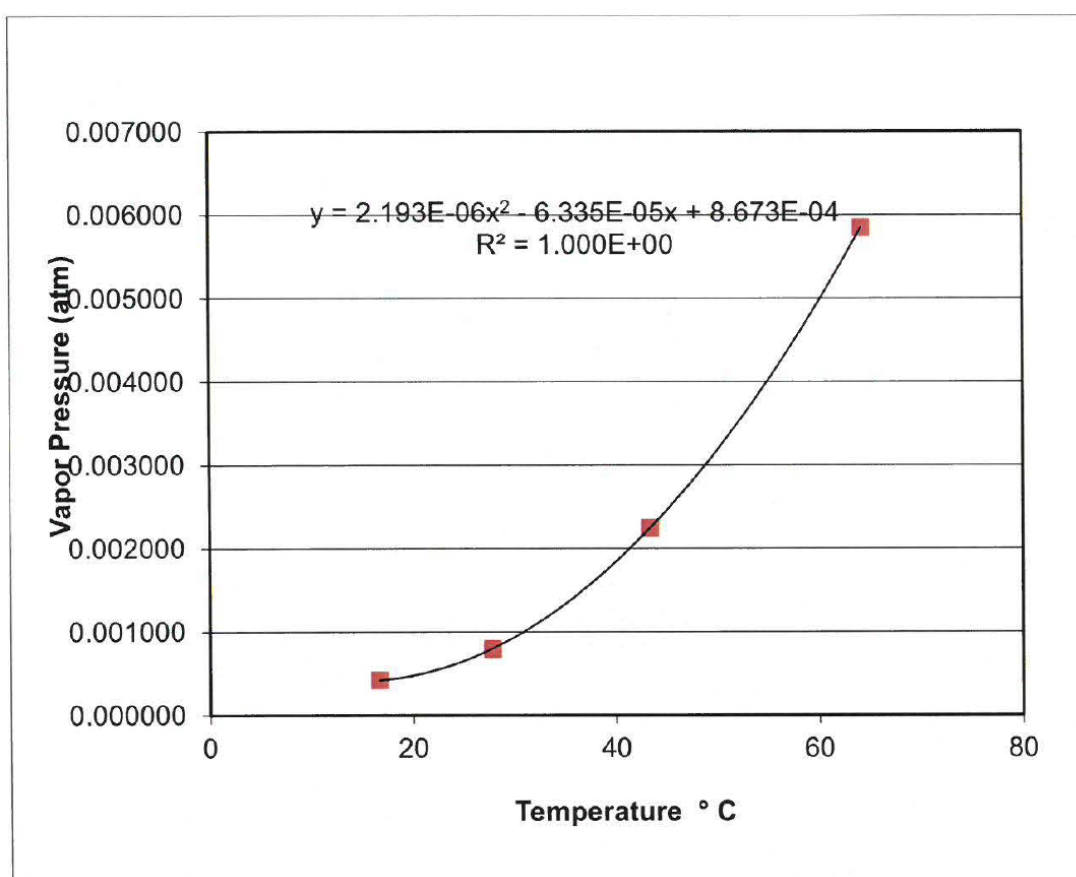


Figure 2-2. Plot of Original CSSX Solvent Vapor Pressure vs. Temperature³

Fitting the curve gives the following equation for determining vapor pressure

$$p = 2.193 \times 10^{-6} * T^2 - 6.335 \times 10^{-5} * T + 8.673 \times 10^{-4} \quad (2)$$

Where,

p is the vapor pressure (partial pressure) of CSSX solvent in atm and
 T is the temperature in °C.

Equations (1) and (2) can be used to compare the vapor pressure curves for pure Isopar[®] L and the Original CSSX solvent as shown in Figure 2-3. From Raoult's law, in an ideal solution, the partial pressure for each component would equal the vapor pressure of the pure substance multiplied by its mole fraction.

$$p_{CSSX} = x_{isopar\ L} p_{isopar\ L}^*$$

Where,

p_{CSSX} is the vapor pressure of CSSX solvent,

$x_{isopar\ L}$ is the mol fraction of Isopar[®] L in the organic phase, and

$p_{isopar\ L}^*$ is the vapor pressure of Isopar[®] L.

Using a mol fraction of 0.83 for Isopar[®] L in the Original CSSX solvent should give a vapor pressure for the CSSX solvent that is ~17% less than the Isopar[®] L vapor pressure. From the fitting of the data given in Figure 2-3, between 20-45°C the vapor pressure for the CSSX solvent was ~25-29% less than the Isopar[®] L vapor pressure. It has been suggested that Cs-7SB has a greater impact than normal on reducing the vapor pressure of Isopar[®] L in solution.⁸ When taking this into consideration, along with the reduction in Cs-7SB concentration for NGS (0.65 M vs. 0.75 M in the Original CSSX solvent) and the increase in the Isopar[®] L mol fraction for NGS (0.85), it would be probable that the NGS vapor pressure curve, if added to Figure 2-3, would fall between the calculated NGS vapor pressure curve using Raoult's law (labeled "Bounding NGS" in Figure 2-3), and the vapor pressure curve for the Original CSSX solvent.

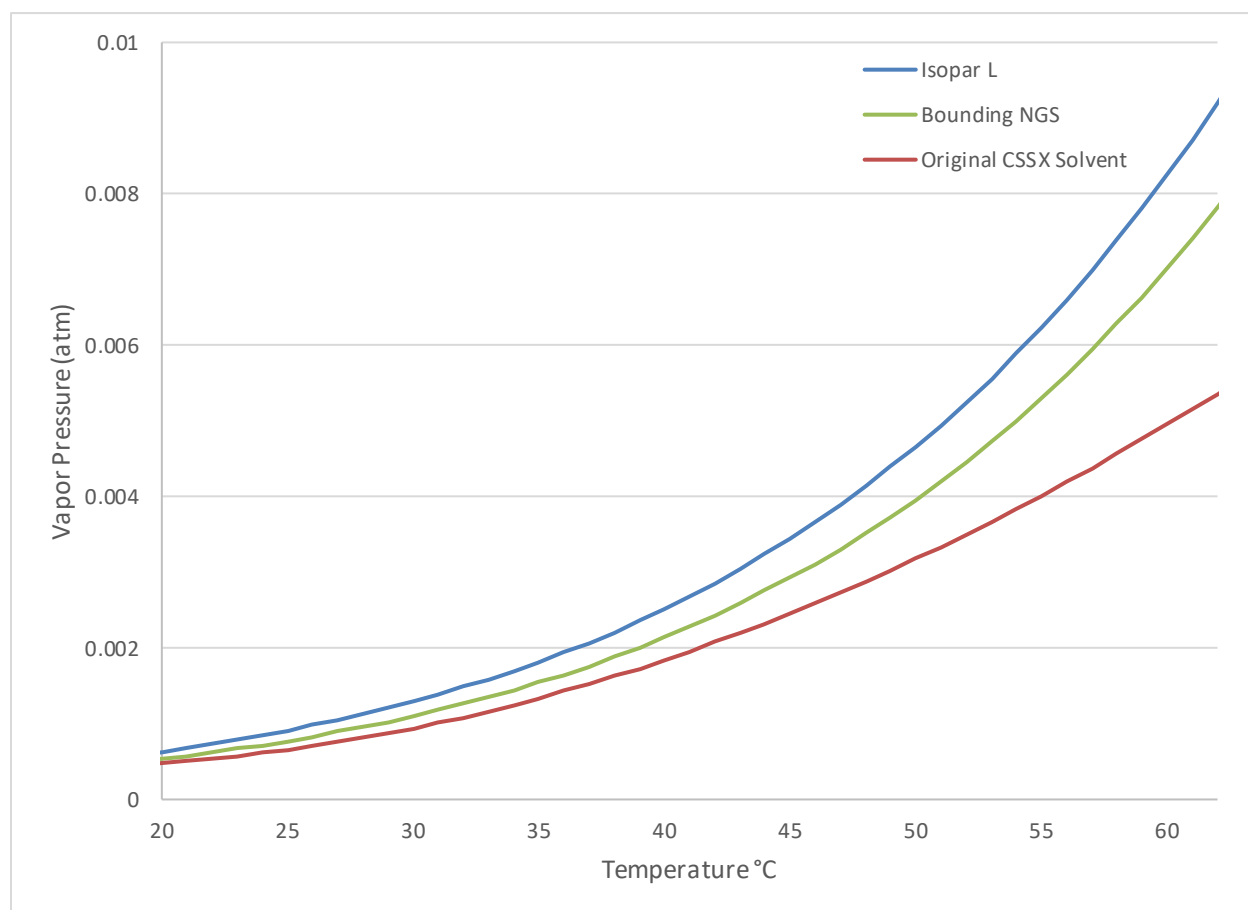


Figure 2-3. Comparison of the Vapor Pressure as a Function of Temperature of Pure Isopar[®] L, Bounding NGS Vapor Pressure Curve, and the Original CSSX Solvent

2.2 Partitioning Ratio for MaxCalix and Cs-7SB

To account for indirect radiolysis of organics in aqueous solutions by hydrogen radicals to produce H_2 , the modified radiolytic HGR equation includes an f_{organic} term, which is defined as the fraction of hydrogen radicals that react with organics instead of reacting with a scavenger. The f_{organic} term is derived from the concentration of the organic in the aqueous phase and the reaction rate for the organic with a hydrogen atom. Non-polar Isopar[®] L can be considered to be insoluble in the aqueous waste, while the other components in NGS could potentially dissolve into the aqueous phase. Therefore, an estimate of the partition ratio for these species is needed to calculate the f_{organic} term in SWPF aqueous waste streams.

In 2002, ORNL determined the partitioning ratio of the modifier Cs-7SB and the extractant BOBCalixC6 in the Original CSSX solvent.⁹ The partitioning ratio, P , is the organic-phase molarity divided by the aqueous-phase molarity of a species. The experiments were performed at 25°C with caustic simulant and various nitric acid solutions at the corresponding Organic to Aqueous Phase (O:A) ratios given in Table 2-2. As can be seen, Cs-7SB and BOBCalixC6 had very high partitioning ratios in the different experiments. The aqueous-phase concentrations were very low or below detection limit (BDL) for both species. In fact, all concentrations of the calixarene in the aqueous phase were BDL, indicating a $P > 12,500$. The actual P value for BOBCalixC6 may be much higher based on estimates of true lipophilicity of the extractant. The lowest partitioning ratio for Cs-7SB was $P > 8,000$, while it had a very high partitioning ratio in contact with the caustic simulant, $P > 50,000$. Since this testing, the nitric acid in the stripping solution has been replaced with boric acid. A partitioning ratio for Cs-7SB in contact with the boric acid strip solution that will be used at SWPF could not be found in the literature; however, boric acid is a weak acid in comparison to nitric acid and thus the partitioning ratio for Cs-7SB should be similar to what is listed below.

Table 2-2. Partitioning Ratios of Cs-7SB and BOBCalixC6¹⁰

Aq. phase	O:A	Cs-7SB Partitioning Ratio	BOBCalixC6 Partitioning Ratio
Full Simulant	1:10	$>5 \times 10^4$	$>1.25 \times 10^4$
1 mM HNO ₃	1:10	8.00×10^3	$>1.25 \times 10^4$
50 mM HNO ₃	1:10	1.31×10^4	$>1.25 \times 10^4$
H ₂ O	1:3	1.38×10^4	$>1.25 \times 10^4$
1 mM HNO ₃	1:3	8.11×10^3	$>1.25 \times 10^4$
2.5 mM HNO ₃	1:3	9.27×10^3	$>1.25 \times 10^4$
10 mM HNO ₃	1:3	2.13×10^4	$>1.25 \times 10^4$
25 mM HNO ₃	1:3	1.88×10^4	$>1.25 \times 10^4$
50 mM HNO ₃	1:3	1.83×10^4	$>1.25 \times 10^4$
100 mM HNO ₃	1:3	1.45×10^4	$>1.25 \times 10^4$

According to the manufacturer's safety data sheet for MaxCalix, it is considered insoluble in water. Partitioning ratios for MaxCalix were not found in the literature, but can be considered to be bounded by current BOBCalixC6 partitioning ratios. MaxCalix has an improved solubility in Isopar[®] L compared to BOBCalixC6 due to its long lipophilic alkyl chains. These lipophilic alkyl chains would also lower the solubility of MaxCalix in the aqueous phase in comparison to BOBCalixC6. It should be noted that the BOBCalixC6 concentration in the aqueous phase was BDL in all tests, and its actual partitioning ratio is expected to be orders of magnitude higher.

In addition to the partitioning ratio, the reaction rate for Cs-7SB and MaxCalix with a hydrogen atom would also be needed to derive the f_{organic} term. A reaction rate for Cs-7SB is known, but one for MaxCalix was not found.¹¹ However, as mentioned above, MaxCalix should be insoluble in the aqueous phase and can be

considered to not be a significant contributor to the f_{organic} term. This review did not examine TiDG or its degradation products. The degradation/partitioning of TiDG has been studied previously and current testing is underway to determine the partitioning of its major degradation products.^{12,13} As stated above, their reaction rates with a hydrogen radical would either have to be estimated or experimentally determined to be included in the f_{organic} term.

2.3 Impacts of High Cesium Concentration on NGS Radiolytic Degradation

SWPF can process aqueous salt feeds with higher Cs-137 concentrations compared to MCU. The current maximum Cs-137 concentration in SWPF aqueous feed is 2.5 Ci/gal.¹⁴ For SWPF, NGS testing by Parsons looked at O:A ratios as low as 1:15;¹⁵ the current ratio in the NGS Deployment Basis of Design has the O:A ratio of 1:10 for Cs extraction.¹⁶ Following extraction, the maximum Cs-137 concentration within the solvent at SWPF would be 25 Ci/gal, if using the current Cs-137 feed limit of 2.5 Ci/gal and 1:10 O:A ratio during the extraction stage. While 25 Ci/gal corresponds to maximum Cs-137 within the solvent, the largest dose to the solvent will be in the 203A strip contactor.¹⁷ In this contactor, Cs-137-laden strip effluent will be brought into contact with the Cs-137-loaded solvent following extraction described above. An accurate estimate of the radiation dose to the solvent would require additional details such as Cs-137 concentrations and solvent volumes throughout the CSSX process. In past irradiation testing with either the Original CSSX solvent or NGS, results are typically compared to a twenty year-old estimate of 0.073 Mrad for the yearly radiation dose to the solvent in a facility similar to SWPF.¹⁸ In 2009, SRNL estimated a maximum yearly dose to the Original CSSX solvent in SWPF of 65.4 Mrad.¹⁹ Prior to any future radiolysis testing of the solvent, a more accurate calculation of the expected dose to NGS at SWPF should be pursued, if one is not already available.

There have been a number of internal irradiation tests with the Original CSSX solvent in which there was negligible solvent degradation and no significant impact on solvent performance at high doses (16 Mrad).⁹ In a follow-up ORNL study, the degradation of the Original CSSX components as a function of dose was calculated for solvent irradiated in the presence of extraction, scrub, and stripping solutions.¹⁰ The max loss rate of Cs-7SB was calculated to only be ~20 mM/Mrad after contact with all aqueous solutions. A 2015 ORNL study examined the radiolytic stability of NGS, and it was found that the Cs-7SB radiolytic degradation losses were calculated to be 0.01% loss of Cs-7SB per year at SWPF (or ~0.7 mM/Mrad loss of Cs-7SB).¹⁸ It is noted in these radiolytic tests that the solvent degradation products remain in the system to build up or affect the chemistry of the solvent, leading to a more conservative setup.¹⁸ During typical SWPF operations, these degradation products would be continually washed from the solvent as they partition to the aqueous phase. Monthly Solvent Hold Tank samples were characterized by SRNL until MCU's shutdown in order to help with replenishing solvent components as needed. Additions were mainly due to Isopar® L evaporation and/or TiDG chemical degradation/partitioning, not due to any significant radiolytic degradation. While the higher Cs concentrations at SWPF will hasten the radiolytic degradation of NGS, overall these impacts should be secondary to Isopar® L losses to evaporation and TiDG suppressor losses to chemical degradation/partitioning. Upon implementation of NGS at SWPF, if Solvent Hold Tank samples are regularly checked, then comparing Cs-7SB concentration losses over time to MCU data would be a good indicator of NGS radiolytic stability under higher Cs concentrations.

It should be noted that no radiolytic flammable gas generation testing has been performed with NGS. Current SWPF safety documents use radiolytic G-values for flammable gases that were obtained using external gamma radiation from testing with the Original CSSX solvent. A separate literature review of the radiolytic stability of NGS was published concurrently with this report, in which it was established that there is a low risk with the continued use of the radiolytic G-values from the Original CSSX solvent. Confirmatory irradiation testing to determine the hydrogen G-value for NGS was encouraged.

3.0 Conclusions

SRNL was requested by SRMC to perform a literature review on the Isopar® L vapor pressure curve for NGS, the partitioning ratio for the extractant MaxCalix and the modifier Cs-7SB, and the high cesium concentration impacts on NGS radiolysis and potential solvent degradation rates in high cesium concentrations.

The following conclusions and recommendations are made based on previous experimental work and literature:

- Current SWPF flammable gas generation calculations use an Isopar® L vapor pressure curve based on experimental testing with the Original CSSX solvent. No such testing to date has been performed with NGS. It is suggested that the decrease in Cs-7SB concentration for NGS compared to the Original CSSX solvent would lead to a slightly higher vapor pressure at all temperatures in SWPF vessels. A bounding NGS vapor pressure curve has been provided; it is recommended to see if these values would challenge current flammability controls and to perform testing if needed.
- The partitioning ratio for Cs-7SB in the original CSSX solvent is very large for caustic and dilute nitric acid solutions. No tests could be found for the partitioning of Cs-7SB to dilute boric acid solutions; however, a similar partitioning ratio is expected. Due to the lipophilic alkyl chains on MaxCalix, it is expected to be even less soluble than BOBCalixC6 in the aqueous phase and should not be considered a significant contributor to the f_{organic} term. Additionally, the reaction rate of TiDG or its degradation products with a hydrogen radical should be estimated/determined if they are found to be significant contributors to the f_{organic} term in ongoing experiments.
- NGS is expected to see much higher Cs concentrations at SWPF in comparison to its use at MCU. These higher Cs concentrations could influence radiolytic degradation rates of the solvent. NGS appears to be fairly stable to radiolytic degradation based on previous testing and its use at MCU. However, there has not been radiolytic flammable gas generation testing with NGS to date. There is a risk that the continued use of G-values obtained for flammable gases produced from the irradiation of the Original CSSX solvent is not bounding for NGS, but this is considered a very low risk due to the similarities in the composition of the solvents, as well as the conservatism in the experimental design of the Original CSSX testing.

4.0 References

1. Jain, V.; Brass, E. A.; McNew, R. T.; Boyd, C. M.; Fink, S. D.; Peters, T. B. *Implementation of Next Generation Solvent in SWPF: Technical Gap Analysis*; SRR-SPT-2020-00008 Rev. 1; Savannah River Remediation Aiken, SC, 2020.
2. Luzzatti, A. M. *Flammability Literature Review/Analysis Related to Next Generation Solvent (NGS) for the Salt Waste Processing Facility (SWPF)*; X-TTR-J-00003; Savannah River Remediation 2021.
3. Slayer, W. D. *Time To Reach Composite Lower Flammability Limit (CLFL) for SWPF Process Vessels*; S-CLC-J-00033 Rev. 2; Parsons: 2018.
4. Peters, T. B.; Woodham, W. H.; Hunter, S. C. *Task Technical and Quality Assurance Plan for Testing Related to Implementation of the Next Generation Solvent (NGS) at the Salt Waste Processing Facility (SWPF)*; SRNL-RP-2021-04327 Rev. 0; Savannah River National Laboratory Aiken, SC, 2021.
5. Campbell, S. G. *Antoine Constants for Isopar L*; X-CLC-H-00591; Aiken, SC, 2006.
6. Hall, J. R.; Peery, A. D. *Test Plan for the Determination of Isopar L Vapor Over CSSX Solvent and the Test Results*; MCLinc Project No. ORN001950; Materials and Chemistry Laboratory, inc: Oak Ridge, TN, 2007.
7. Bonnesen, P. V.; Del Cul, G. D.; Hunt, R. D.; Ilgner, R. H.; Tomkins, B. A. *Radiolysis of CSSX Solvents for Parsons Infrastructure & Technology Group in FY 2007 in Support of the Salt Waste Processing Facility at the Savannah River Site*; ORNL/TM-2007/093; Oak Ridge National Laboratory Oak Ridge, TN, 2007.
8. Zamecnik, J. R.; Bronikowski, M. G.; Cozzi, A. D.; Eibling, R. E.; Nash, C. A. *Isopar L Release Rates From Saltstone using Simulated Salt Solutions* WSRC-TR-2005-00568 Rev. 1; Savannah River National Laboratory Aiken, SC, 2008.
9. Spence, R. D.; Klatt, L. N.; Delmau, L. H.; Sloop, F. V. J.; Bonnesen, P. V.; Moyer, B. A. *Batch-Equilibrium Hot-Cell Tests of Caustic-Side Solvent Extraction (CSSX) with SRS Simulant Waste and Internal ¹³⁷Cs Irradiation*; ORNL/TM-2001/49; Oak Ridge National Laboratory: Oak Ridge, TN, 2001.
10. Moyer, B. A.; Alexandratos, S. D.; Bonnesen, P. V.; Brown, G. M.; Caton, J. E. J.; Delmau, L. H.; Duchemin, C. R.; Haverlock, T. J.; Levitskaia, T. G.; Maskarinec, M. P.; Sloop, F. V. J.; Stine, C. L. *Caustic-Side Solvent Extraction Chemical and Physical Properties Progress in FY 2000 and FY 2001*; ORNL/TM-2001/285; Oak Ridge National Laboratory Oak Ridge, TN, 2002.
11. Swancutt, K. L.; Cullen, T. D.; Mezyk, S. P.; Elias, G.; Bauer, W. F.; Ball, R. D.; Peterman, D. R.; Riddle, C. L.; Mincher, B. J.; Muller, J. J., The Radiation Chemistry of the Cs-7SB Modifier used in Cs and Sr Solvent Extraction *Solvent Extraction and Ion Exchange* **2011**, 29.
12. Moyer, B. A.; Delmau, L. H.; Duncan, N. C.; Ensor, D. D.; Hill, T. G.; Lee, D. L.; Roach, B. D.; Sloop, F. V. J.; Williams, N. J. *Recommended Guanidine Suppressor for the Next-Generation Caustic-Side Solvent Extraction Process*; ORNL/TM-2012/625; Oak Ridge National Laboratory Oak Ridge, TN, 2013.
13. Peters, T. B. *Tris(isodecyl)guanidine Degradation in the MCU System*; SRNL-STI-2015-00372 Rev. 1; Savannah River National Laboratory Aiken, SC, 2020.
14. *SWPF Feed Waste Acceptance Criteria*; X-ESR-J-00001; 2021.
15. *Next Generation Solvent Test Report Including a Higher Concentration Waste Demonstration* P-RPT-J-00028 Rev. 0; Parsons Aiken, SC, 2015.
16. *Next Generation Solvent Deployment at Salt Waste Processing Facility Basis of Design* P-DB-J-00006 Rev. 1; Parsons: Aiken, SC, 2021.
17. *Dose Rates For Close Coupled Contactor Components* S-CLC-J-00073; Parsons: Aiken, SC, 2008.
18. Roach, B. D.; Williams, N. J.; Duncan, N. C.; Delmau, L. H.; Lee, D. L.; Birdwell, J. F. J.; Moyer, B. A., Radiolytic Treatment of the Next-Generation Caustic-Side Solvent Extraction (NGS)

- Solvent and its Effect on the NGS Process. *Solvent Extraction and Ion Exchange* **2015**, 33 (2), 134-151.
19. Poirier, M. R.; Pareizs, J. M.; Peters, T. B.; Fink, S. D. *SWPF Radiolysis and Thermolysis Test*; SRNL-STI-2009-00127 Rev. 0; Savannah River National Laboratory Aiken, SC, 2009.

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