ORNL/TM-2021/1975

Density of Next-Generation Caustic-Side Solvent Extraction Solvent

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September 2021

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Cesium Removal—Next Generation Solvent Project

Density of Next-Generation Caustic-Side Solvent Extraction Solvent

Nathan P. Bessen and Bruce A. Moyer

September 2021

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LIST OF ABBREVIATED TERMS

BOBCalixC6	Calix[4]arene-bis(*t*-octylbenzo-crown-6)
Cs-7SB	Modifier 1-(2,2,3,3-tetrafluoropropoxy)-3-(4-*sec*-butylphenoxy)-2-propanol
CSSX	Caustic-Side Solvent Extraction
MaxCalix	Extractant 1,3-alt-25,27-bis(3,7-dimethyloctyl-1-oxy) calix[4]arene-benzocrown-6
MCU	Modular CSSX Unit
NG-CSSX	Next Generation Caustic-Side Solvent Extraction
NGS	Next-Generation Solvent
SRS	Savannah River Site
SWPF	Salt Waste Processing Facility
TiDG	*N*,*N*',*N*''-Tris(3,7-dimethyloctyl)guanidine
TOA	Tri-*n*-octylamine

ABSTRACT

This report recommends the appropriate modifier concentration to employ in the Next Generation Solvent (NGS) to be used in the Salt Waste Processing Facility (SWPF) at the Savannah River Site for removal of cesium from legacy tank waste. The Next Generation Caustic-Side Solvent Extraction (NG-CSSX) process employing the NGS is a marked improvement over the original Caustic-Side Solvent Extraction (CSSX) process, as it provides more effective removal of cesium from highly alkaline radioactive wastes and concentrates this removed cesium into an aqueous solution that is easy to vitrify for final disposal. Considerable effort has been devoted to optimizing the chemistry and process conditions of both systems, and their effectiveness has been demonstrated at the pilot scale at the Modular CSSX Unit (MCU). Due to the success of the demonstration and pilot-scale tests, the Salt Waste Processing Facility (SWPF) has been built to process larger volumes of waste with the CSSX process. To accelerate the waste-processing rate of the SWPF beyond its design throughput, plans call for the replacement of the CSSX process by the NG-CSSX process. To implement the NG-CSSX process in equipment optimized for CSSX, adjusting the density of the NGS to match the CSSX solvent density of 0.851 ± 0.0008 g/mL is considered advisable to obtain comparable hydraulic performance. Toward this objective, the density of the NGS has been measured at different temperatures and modifier concentrations to determine that a concentration of 0.650 M Cs-7SB modifier provides the best match for the desired density.

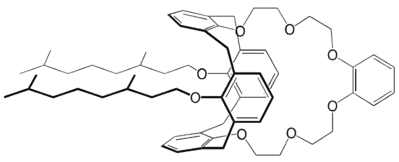
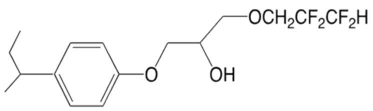
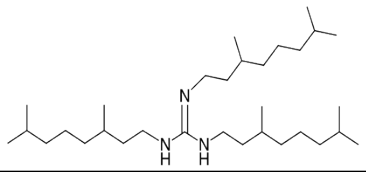
1. INTRODUCTION

This report presents new results on the density characteristics of the Next Generation Solvent (NGS) used in the Next Generation Caustic-Side Solvent Extraction (NG-CSSX) process for removing cesium from highly alkaline radioactive wastes. The results will enable an adjustment of the NGS density by increasing the modifier concentration so that the hydraulic performance of NGS can be made essentially equivalent to that of the solvent presently used in the Caustic-Side Solvent Extraction (CSSX) process.

The CSSX and NG-CSSX processes work effectively both in laboratory scale testing and in the Modular CSSX Unit (MCU) pilot plant at the Savannah River Site (SRS). The large Salt Waste Processing Facility (SWPF) has been built and has been in operation at the SRS since January 2021. It employs the CSSX process at a larger scale than that of the MCU with plans to replace CSSX with NG-CSSX following one year of operation. The equipment designs in MCU and SWPF are somewhat different [Savannah River Remediation, 2013] [Salt Waste Processing Facility Project, 2016], raising the question in a recent review as to whether the formulation of NGS as used in MCU is appropriate for deployment in SWPF [Salt Waste Processing Facility Project, 2018].

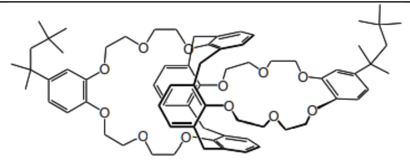
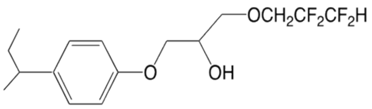
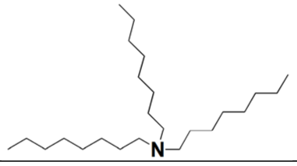
NGS uses a calixarene extractant, 1,3-*alt*-25,27-bis(3,7-dimethyloctyl-1-oxy)calix[4]arene-benzocrown-6 (MaxCalix) to extract cesium into an organic phase consisting of the isoparaffinic diluent Isopar L and the modifier 1-(2,2,3,3-tetrafluoropropoxy)-3-(4-*sec*-butylphenoxy)-2-propanol (Cs-7SB). A basic guanidine suppressor *N*,*N*',*N*''-tris(3,7-dimethyloctyl)guanidine (TiDG) is also added to enable efficient stripping of the cesium into a weakly acidic boric acid based aqueous phase. Structures and concentrations of these components are listed in Table 1. The NG-CSSX process was deployed in the MCU in the period 2013 to 2019, processing 3.4 million gallons of salt feed solution [Hommel, 2020].

Table 1. NG-CSSX Solvent Components Used in the Modular CSSX Unit

Component	Name	Chemical Name	Structure
Extractant	MaxCalix	1,3-*alt*-25,27-bis(3,7-dimethyloctyl-1-oxy)calix[4]arene-benzocrown-6 MW 955.36 0.0500 M	
Modifier	Cs-7SB	1-(2,2,3,3-tetrafluoropropoxy)-3-(4-*sec*-butylphenoxy)-2-propanol MW 338.35 0.500 M	
Suppressor	TiDG	*N*,*N*',*N*''-tri(3,7-dimethyloctyl)guanidine MW 479.89 (516.35 for HCl salt 0.003 M	
Diluent	Isopar L	C_{12}-isoparaffinic hydrocarbon balance	

The forerunner of NG-CSSX, CSSX is similar in composition but uses a different calixarene extractant, calix[4]arene-bis(*t*-octylbenzo-crown-6) (BOBCalixC6), with the same diluent and modifier. A less basic suppressor, tri-*n*-octylamine (TOA), is used. Structures and concentrations of these components are listed in Table 2. The CSSX process was deployed in the MCU in the period 2008 to 2013, processing 4.1 million gallons of salt feed solution [Hommel, 2020]. It is also being deployed for the startup year of the SWPF beginning January 2021 with the goal of processing 6 million gallons of feed.

Table 2. CSSX Solvent Components

Component	Name	Chemical Name	Structure
Extractant	BOBCalixC6	Calix[4]arene-*bis*-(*t*-octylbenzo-crown-6) MW 1149.5 0.007 M	
Modifier	Cs-7SB	1-(2,2,3,3-tetrafluoropropoxy)-3-(4-*sec*-butylphenoxy)-2-propanol MW 338.35 0.750 M	
Suppressor	TOA	Tri-*n*-octylamine MW 353.67 0.003 M	
Diluent	Isopar L	C_{12}-isoparaffinic hydrocarbon balance	

To minimize the hydraulic impact of replacing the CSSX solvent with NGS, the purpose of the present report is to determine the concentration of the Cs7-SB modifier in NGS that would produce the same density of the CSSX solvent. NGS typically has a higher extractant concentration and a lower modifier concentration than the CSSX solvent, which causes NGS to have a lower density of 0.835 g/mL than the CSSX solvent with a density of 0.851 g/mL. Ordinarily, this would be considered a potential improvement, as a greater density difference between aqueous and organic phases accelerates phase disengagement, other factors being equal. Given the design of SWPF equipment specific to CSSX, however, the option of density matching of NGS to the CSSX solvent offers a logical approach to facilitating the transition to NGS with least risk. Increasing the Cs-7SB modifier concentration can increase the density of the solvent to match the CSSX solvent density and thereby avoid density-related hydraulic issues with the implementation of NG-CSSX. A higher modifier concentration confers an added benefit in higher cesium distribution ratios, enabling decreased O:A ratio and corresponding increased throughput of feed in the extraction section. This report details a series of density measurements on NGS solvents at varying Cs-7SB concentrations and temperatures to determine the appropriate modifier concentration to be used in NG-CSSX to match the density of the CSSX solvent.

2. EXPERIMENTAL SECTION

2.1 MATERIALS

Solvent components were obtained from commercial sources and judged to be of adequate purity for use as received. 1-(2,2,3,3-Tetrafluoropropoxy),3-[4-(*sec*-butyl)phenoxy]-2-propanol (Cs-7SB modifier, Lot No. BSC 2330-1-0002) was obtained from Boulder Scientific Company. Calix[4]arene-bis(*t*-octylbenzo-crown-6) (BOBCalixC6, Lot No. 011116KCORNL005) was obtained from IBC Advanced Technologies. Tri-*n*-octylamine (TOA, Lot No. 09517AH, 98%) was obtained from Sigma-Aldrich. 1,3-*alt*-25,27-Bis(3,7-dimethyloctyl-1-oxy)calix[4]arenebenzocrown-6 (MaxCalix, Lot No. 79-239-1) and *N*,*N*',*N*''-tris(3,7-dimethyloctyl)guanidine (TiDG, Lot No. 82-043-1) were obtained from Marshallton Research Laboratories. Isopar L (Lot No. US67377E) was obtained from ExxonMobil.

Solutions for washing the solvents were prepared from hydrochloric acid (HCl, Lot No. Z216507 050) obtained from EMD and sodium hydroxide (NaOH, Lot No. 173021) from Fisher Chemical. HCl and NaOH solutions were prepared by dispensing the appropriate volume of the pre-made solutions into volumetric flasks and diluting to the mark using Milli-Q® water.

2.2 METHODS

2.2.1 Solvent Preparation

Solvents were prepared by weighing appropriate amounts of extractant, modifier, and suppressor into Class A volumetric flasks and diluting with Isopar L to the mark. All solutions were made at a room temperature of 22 ± 1°C and assuming 100% purity. The solvents used in the following studies were prepared using the concentrations given in Tables 3 and 4. The uncertainty listed in these tables is calculated by propagation of error using the standard uncertainty of the balance (± 0.0001 g) and the uncertainty of Class A volumetric flasks. After the solvent was prepared, the density of the dry solvent was measured. Following this measurement, the solvents were washed in the following manner: sequential contacts with an organic-to-aqueous phase ratio of 1:1 using 0.010 M HCl, H_2O, 0.3 M NaOH, 0.1 M NaOH, 0.03 M NaOH, 0.01 M NaOH, and then with H_2O until the solution was pH neutral. It was noted that the organic phases were cloudy after contact with the aqueous phase, but they almost entirely clarified upon centrifugation. Following washing, the density of the washed, wet solvent was measured.

2.2.2 Solvent Density Measurements

Solvent densities were measured pycnometrically using a calibrated Eisco Labs pycnometer with a nominal volume of 25 mL. This calibration was made by measuring the mass of water required to fill the pycnometer. All masses were measured using a Mettler Toledo MS204TS/00 balance. The balance was calibrated with Ainsworth class S check weights that have been independently calibrated by ORNL metrology to develop a correction factor prior to each series of measurements. This correction factor was within ± 0.1 mg in all instances. All temperatures were measured with a NIST traceable thermometer having a stated accuracy of ± 0.5°C.

The volume of the pycnometer was calibrated prior to each set of measurements by comparing the mass of the empty, dry pycnometer and the pycnometer filled with Milli-Q® water, removed from a temperature-controlled water bath and dried on the outside with a Kimwipe™. The volume of the pycnometer can be determined using Equation 1, where V_T is the volume at temperature T, $m_{\mathrm{H_2O},T}$ is the mass of the water filled pycnometer at temperature T, m_{empty} is the mass of the empty, dry pycnometer, and $\rho_{\mathrm{H_2O},T}$ is the density of water at temperature T.

$$V_T = \frac{m_{\mathrm{H_2O},T} - m_{\mathrm{empty}}}{\rho_{\mathrm{H_2O},T}} \qquad \text{Equation 1}$$

Once the pycnometer was calibrated, it was thoroughly cleaned and dried before filling with the sample to be measured and being placed in the same temperature-controlled water bath as used in the calibration. Care was taken to remove any bubbles that were present. After allowing the temperature to equilibrate, the pycnometer was removed from the bath, the solvent was topped off if necessary, and the outside of the pycnometer was dried. The mass of the filled pycnometer was then measured. The sample was removed, and the pycnometer thoroughly cleaned and dried for any following measurements. From the measured mass of the full pycnometer, the density can be calculated using Equation 2, where $\rho_{\mathrm{solvent},T}$ is the density of the solvent at temperature T and $m_{\mathrm{solvent},T}$ is the mass of the solvent loaded pycnometer at temperature T. Triplicate measurements made using this method gave a standard deviation of ± 0.0005_8 g/mL which is slightly greater than the uncertainty of ± 0.0004_9 calculated through propagation of error or the ± 0.0002_9 from ± 0.5°C uncertainty of the temperature measurement. For this reason, the uncertainty of the triplicate measurement was assumed to be representative of the precision of this method rather than propagation of error or temperature and has been applied to all density measurements.

$$\rho_{\mathrm{solvent},T} = \frac{m_{\mathrm{solvent},T} - m_{\mathrm{empty}}}{V_T} \qquad \text{Equation 2}$$

3. RESULTS AND DISCUSSION

3.1 SOLVENT DENSITY

The densities of the solvents listed in Tables 3 and 4 were measured, and the results are presented in Tables 5, 6, and 7 and Figure 1. These tables and the figure also include the densities after the addition of a correction factor to calculate the density at 25.0°C and account for temperature variations between different samples. Section 3.3 describes how this correction factor was determined. With this correction, the dry and wet CSSX solvents have respective densities of 0.8519 ± 0.0006 and 0.8516 ± 0.0006 g/mL, which is within error of the expected density of 0.851 ± 0.008 g/mL [Parsons, 2019]. The standard NGS solvent with a Cs-7SB concentration of 0.5 M has a density of 0.8361± 0.0006 when dry and 0.8338 ± 0.0006 when wet. This density is a good match to the previously measured value of 0.835 [Salt Waste Processing Facility Project, 2013]. There is a linear relationship between Cs-7SB concentration and density, and the wet and dry solvents have nearly the same density.

Table 3. NGS Compositions Tested

Nominal [Cs-7SB] (M)	Volume (mL)	Cs-7SB Grams	Cs-7SB Conc. (M)	MaxCalix Grams	MaxCalix Conc. (mM)	TiDG•HCl Grams	TiDG•HCl Conc. (mM)	Isopar L Grams
0.40	25.00 ± 0.03	3.3892 ± 0.0001	0.4007 ± 0.0005	1.1927 ± 0.0001	49.93 ± 0.06	0.0377 ± 0.0001	2.918 ± 0.009	15.8554 ± 0.0001
0.50	25.00 ± 0.03	4.2229 ± 0.0001	0.4992 ± 0.0006	1.1956 ± 0.0001	50.06 ± 0.06	0.0369 ± 0.0001	2.856 ± 0.009	15.3402 ± 0.0001
0.64	25.00 ± 0.03	5.4342 ± 0.0001	0.6424 ± 0.0008	1.1942 ± 0.0001	50.00 ± 0.06	0.0401 ± 0.0001	3.106 ± 0.009	14.6061 ± 0.0001
0.65	25.00 ± 0.03	5.5076 ± 0.0001	0.6511 ± 0.0008	1.1935 ± 0.0001	49.97 ± 0.06	0.0377 ± 0.0001	2.920 ± 0.009	14.5006 ± 0.0001
0.65	100.00 ± 0.08	22.0245 ± 0.0001	0.6509 ± 0.0005	4.7766 ± 0.0001	50.00 ± 0.04	0.1554 ± 0.0001	3.010 ± 0.003	58.2424 ± 0.0001
0.68	25.00 ± 0.03	5.7559 ± 0.0001	0.6805 ± 0.0008	1.1940 ± 0.0001	49.99 ± 0.06	0.0412 ± 0.0001	3.192 ± 0.009	14.3816 ± 0.0001
0.75	25.00 ± 0.03	6.3818 ± 0.0001	0.7545 ± 0.0009	1.1947 ± 0.0001	50.02 ± 0.06	0.0367 ± 0.0001	2.841 ± 0.009	13.9897 ± 0.0001

Table 4. CSSX Composition Tested

Volume (mL)	**Cs-7SB**		**BOBCalixC6**		**TOA**		**Isopar L**
	Grams	**Conc. (M)**	**Grams**	**Conc. (mM)**	**Grams**	**Conc. (mM)**	**Grams**
25.00 ± 0.03	6.3401 ± 0.0001	0.7495 ± 0.0009	0.2017 ± 0.0001	7.018 ± 0.009	0.0374 ± 0.0001	4.23 ± 0.01	14.6885 ± 0.0001

To simplify implementation of NG-CSSX in equipment designed for the CSSX process, it is desirable for the NGS to match the density of the CSSX solvent. The simplest way to alter the solvent density while minimizing any changes to the extraction of cesium is to change the Cs-7SB concentration. Using the linear best-fit lines for both the wet and dry NGS densities at 25°C shown in Figure 1, the necessary Cs-7SB concentration to achieve a desired density can be calculated. To match the dry density of the CSSX solvent, 0.851_{88} g/mL, a dry NGS solvent with 0.653 M Cs-7SB is needed. To match the wet density of the CSSX solvent, 0.851_{58} g/mL, a wet NGS solvent with 0.643 M Cs-7SB is required. As the precise concentration of Cs-7SB is expected to vary during operation of the NG-CSSX process due to degradation, washing into the aqueous phase, and evaporation of Isopar L, it is proposed that the desired Cs-7SB concentration be 0.650 M to approximate both the wet and dry CSSX solvent densities. The 90% confidence interval of the density of the 0.650 M Cs-7SB solvent includes the measured densities of both the dry and wet CSSX solvents.

Table 5. Measured CSSX Densities

Condition	**Temperature (°C)**	m_{empty} **(g)**	$m_{\text{H}_2\text{O},T}$ **(g)**	V_T **(mL)**	$m_{\text{solvent},T}$ **(g)**	$\rho_{\text{solvent},T}$ **(g/mL)**	$\rho_{\text{solvent},25}$ **(g/mL)**
Dry	22.8 ± 0.5	25.6999 ± 0.0001	48.8367 ± 0.0001	23.1917 ± 0.0001	45.4999 ± 0.0001	0.8538 ± 0.0006	0.8519 ± 0.0006
Wet	22.7 ± 0.5	25.6999 ± 0.0001	48.8367 ± 0.0001	23.1917 ± 0.0001	45.4948 ± 0.0001	0.8535 ± 0.0006	0.8516 ± 0.0006

Table 6. Measured Dry NGS Densities

[Cs-7SB] (M)	**Temperature (°C)**	m_{empty} **(g)**	$m_{\text{H}_2\text{O},T}$ **(g)**	V_T **(mL)**	$m_{\text{solvent},T}$ **(g)**	$\rho_{\text{solvent},T}$ **(g/mL)**	$\rho_{\text{solvent},25}$ **(g/mL)**
0.4007 ± 0.0005	22.7 ± 0.5	22.9040 ± 0.0001	47.2992 ± 0.0001	24.4537 ± 0.0001	43.0332 ± 0.0001	0.8232 ± 0.0006	0.8249 ± 0.0006
0.4992 ± 0.0006	22.7 ± 0.5	22.9040 ± 0.0001	47.2992 ± 0.0001	24.4537 ± 0.0001	43.3082 ± 0.0001	0.8333 ± 0.0006	0.8361 ± 0.0006

0.6424 ± 0.0008	23.0 ± 0.5	22.9044 ± 0.0001	47.2961 ± 0.0001	24.4519 ± 0.0001	43.7296 ± 0.0001	0.8517 ± 0.0006	0.8534 ± 0.0006
0.6511 ± 0.0008	23.0 ± 0.5	22.9044 ± 0.0001	47.2961 ± 0.0001	24.4519 ± 0.0001	43.7423 ± 0.0001	0.8522 ± 0.0006	0.8539 ± 0.0006
0.6805 ± 0.0008	23.0 ± 0.5	22.9044 ± 0.0001	47.2961 ± 0.0001	24.4519 ± 0.0001	43.8399 ± 0.0001	0.8551 ± 0.0006	0.8579 ± 0.0006
0.7545 ± 0.0009	22.7 ± 0.5	22.9040 ± 0.0001	47.2992 ± 0.0001	24.4537 ± 0.0001	44.0763 ± 0.0001	0.8647 ± 0.0006	0.8675 ± 0.0006

Table 7. Wet NGS Densities

[Cs-7SB] (M)	**Temperature (°C)**	m_{empty} **(g)**	$m_{\mathrm{H_2O},T}$ **(g)**	V_T **(mL)**	$m_{\text{solvent},T}$ **(g)**	$\rho_{\text{solvent},T}$ **(g/mL)**	$\rho_{\text{solvent},25}$ **(g/mL)**
0.4007 ± 0.0005	23 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	44.7814 ± 0.0001	0.8227 ± 0.0006	0.8215 ± 0.0006
0.4992 ± 0.0006	23 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	45.0659 ± 0.0001	0.8349 ± 0.0006	0.8338 ± 0.0006
0.6424 ± 0.0008	23.2 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	45.4704 ± 0.0001	0.8528 ± 0.0006	0.8517 ± 0.0006
0.6509 ± 0.0005	25 ± 0.5	22.9013 ± 0.0001	47.2813 ± 0.0001	24.4523 ± 0.0001	43.7202 ± 0.0001	0.8514 ± 0.0006	0.8514 ± 0.0006
					43.7112 ± 0.0001	0.8510 ± 0.0006	0.8510 ± 0.0006
					43.6926 ± 0.0001	0.8503 ± 0.0006	0.8503 ± 0.0006
0.6511 ± 0.0008	23 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	45.5027 ± 0.0001	0.8538 ± 0.0006	0.8527 ± 0.0006
0.6805 ± 0.0008	23.1 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	45.5898 ± 0.0001	0.8575 ± 0.0006	0.8564 ± 0.0006
0.7545 ± 0.0009	23 ± 0.5	25.7002 ± 0.0001	48.8365 ± 0.0001	23.1945 ± 0.0001	45.7854 ± 0.0001	0.8659 ± 0.0006	0.8648 ± 0.0006

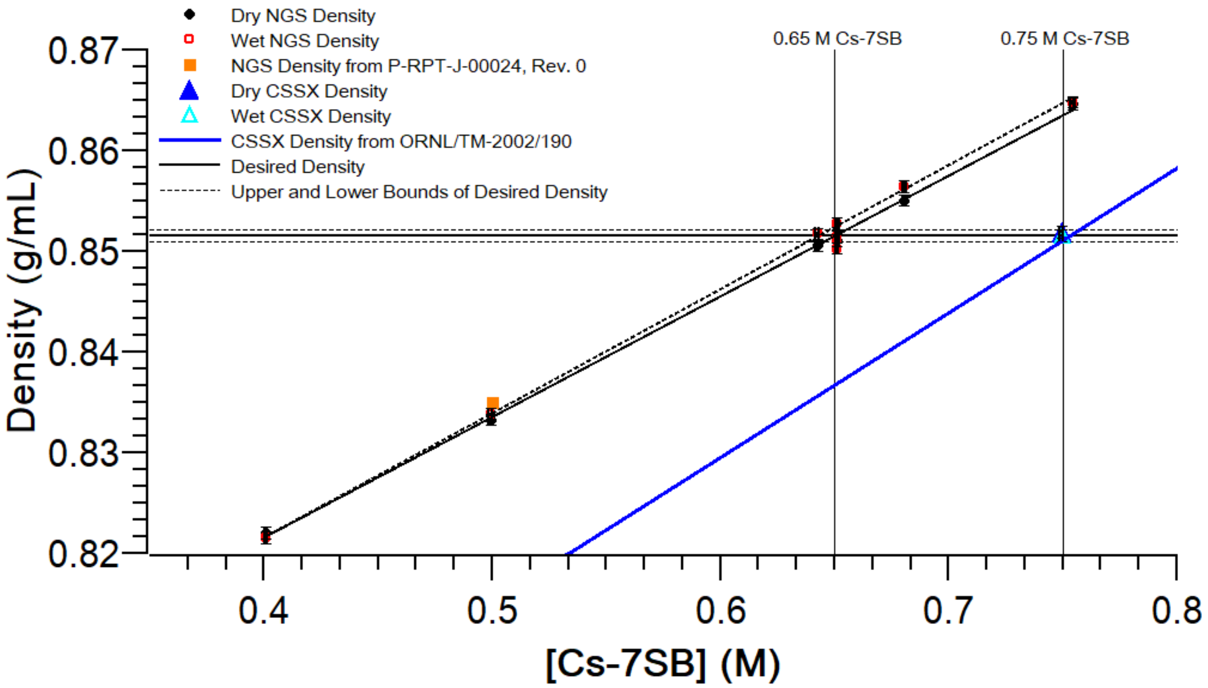


Figure 1. Density of wet and dry solvents at 25°C containing different concentrations of the Cs-7SB modifier and their linear lines of best fit. The horizontal solid and dashed lines represent the desired density of 0.8516 g/mL and the upper and lower density limits of 0.8522 g/mL and 0.8510 g/mL respectively. The blue line depicts the relationship between Cs-7SB concentration and density for the CSSX solvent as determined by Delmau et al. (2002).

As was done with the 25°C densities, correction factors can also be applied to calculate the density at 20°C. The resulting densities are shown in Figure 2. This temperature was chosen as 20°C is the temperature to be used for measuring the NGS density as specified by Parsons (2019). According to Parsons (2019), the density of dry NGS made with 0.57 M Cs-7SB should be 0.8510 ± 0.0008 g/mL. However, a linear regression of the dry solvent density reveals that the density of 0.8510 g/mL would be obtained with 0.622 M Cs-7SB. Additionally, the density of 0.8510 g/mL was chosen to match the density of the CSSX solvent to facilitate the implementation of NG-CSSX, yet the density of the CSSX solvent corrected to 20°C with Equation 4 is slightly higher at 0.856 g/mL. The density of the wet solvents is slightly higher than the dry solvent, presumably due to the extraction of water. However, this difference is not statistically significant at 1σ uncertainty.

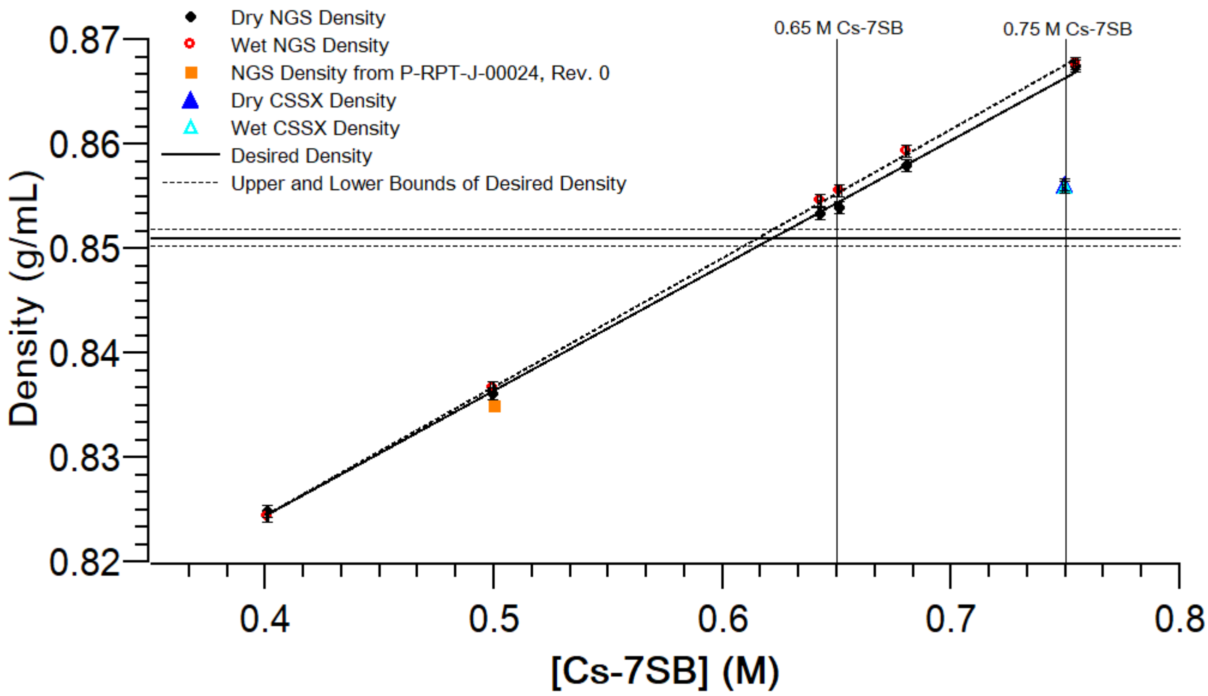


Figure 2. Density of wet and dry solvents at 20°C containing different concentrations of the Cs-7SB modifier and their linear lines of best fit. The horizontal solid and dashed lines represent the desired density of 0.8516 g/mL and the upper and lower density limits of 0.8522 g/mL and 0.8510 g/mL respectively.

3.2 SOLVENT COMPONENT DENSITIES

The densities of the liquid NGS components, Cs-7SB, and Isopar L, were measured at 25°C. The results of these measurements are shown in Table 8. Due to the high viscosity of neat Cs-7SB, it was not possible to remove several tiny bubbles from the pycnometer. Therefore, the measured density of 1.1857 g/mL is slightly under the true density and, consequently, no uncertainty is given.

Table 8. Measured Solvent Component Densities at 25°C

Component	Density (g/mL)	Molar Volume (mL/mol)
Cs-7SB	1.18	285
Isopar L	0.7582 ± 0.0006	224.6 ± 0.2[a]

[a] Calculated assuming Isopar L is entirely C_{12} isomers and has a molecular weight of 170.33.

3.3 DENSITY TEMPERATURE DEPENDENCE

The density of the NGS solvent containing 0.65 M Cs-7SB modifier was measured at different temperatures to determine the relationship between temperature and density for this solvent, as shown in

Figure 3. As there is a linear relationship between density and temperature through the temperature range studied, a linear regression can be applied and is shown in Equation 3.

$$\rho_{\text{solvent},T} = (-0.00057 \pm 0.00003) \times T + (0.8654 \pm 0.0009) \qquad \text{Equation 3}$$

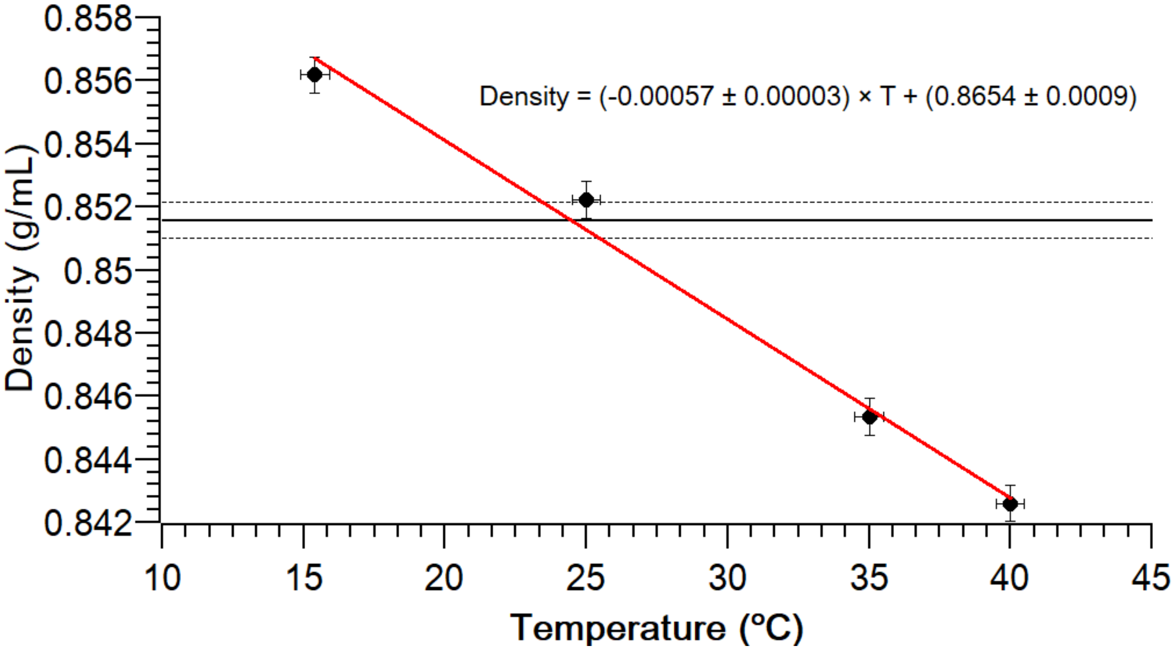


Figure 3. Density of the wet NGS solvent containing 0.65 M Cs-7SB at different temperatures. The horizontal solid and dashed lines represent the desired density of 0.8516 g/mL and the upper and lower density limits of 0.8522 g/mL and 0.8510 g/mL respectively.

A similar dataset has been collected for the CSSX solvent and is reported in by Delmau et al. (2002). A linear relationship, shown in Equation 4, was also found between CSSX solvent density and temperature. The slope of the CSSX solvent density/temperature relationship is moderately steeper than for the NGS, indicating that the NGS density is less affected by temperature

$$\rho_{\text{solvent},T} = -0.0008 \times T + 0.8714 \qquad \text{Equation 4 [Delmau et al., 2002]}$$

4. CONCLUSIONS

The density of both freshly prepared and washed NGS solvents with varying Cs-7SB modifier concentrations has been measured and compared to the density of the CSSX solvent. The density of NGS was determined to have less temperature dependence than the preceding CSSX solvent and minimal differences between the density of a freshly prepared and a washed, water-saturated solvent. Finally, it was determined that an NGS solvent with 0.650 M Cs-7SB will closely replicate the density of the original CSSX solvent to ease the implementation of the NG-CSSX process in equipment designed for CSSX.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

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QA Implementation for ORNL/TM-2021/1975

In terms of the applicable NQA-1 based criterion, Table 9 identifies the corresponding ORNL QA criterion/criteria. ORNL employs an electronic Standard Based Management System (SBMS) to deliver procedures that implement the criteria. Procedures are organized by subject areas under management systems and are implemented using a graded approach appropriate for the work. Documents that tailor the ORNL criteria to the project also appear in the table.

Table 9. NQA-1 Based Criteria

Implementing Procedures	**Document No.**	**Yes**	**No**
Organization	QAPD (criteria 1,10); QAP-X-94-CSD-001	X	
Quality Assurance Program	QAPD (criteria1,2,3,9,10) QAP-X-94-CSD-001	X	
Control of Research and Development Activities	QAP-X-94-CSD-001	X	
QA Program Requirements for Analytical Measurement Systems	QAP-X-94-CSD-001	X	
Design Control	N/A		
Procurement Document Control	QAPF (criterion 7); QAP-X-94-CSD-001	X	
Instructions, Procedures and Drawings	QAPD (criteria 4,5); QAP-X-94-CSD-001	X	
Document Control	QAPD (criterion 4); QAP-X-94-CSD-001 CSD-OP-000-AD01	X	
Control of Purchased Items and Services	QAPD (criterion 7); QAP-X-94-CSD-001	X	
Identification and Control of Items	QAPD (criteria 5,8); QAP-X-94-CSD-001	X	
Control of Processes	QAPD (criterion 5); QAP-X-94-CSD-001	X	
Control of Nondestructive Examination	N/A		
Control of Welding and Other Joining Processes	N/A		
Work Planning and Control	QAPD (criterion 5)	X	
Inspection	QAPD (criteria 8,10); QAP-X-94-CSD-001	X	
Test Control	QAPD (criteria 8,10); QAP-X-94-CSD-001	X	
Control of Measuring and Test Equipment	QAPD (criteria 5, 8); QAP-X-94-CSD-001	X	
Control of Installed Process Instrumentation	QAPD (criterion 5); QAP-X-94-CSD-001	X	
Packaging, Handling, Shipping and Storage	QAPD (criterion 5); QAP-X-94-CSD-001	X	

Notes:

QAPD – *ORNL Quality Assurance Program Description* – describes how requirements are parsed to management systems and flowed into implementing procedures through subject areas delivered by the management systems.

QAP-X-94-CSD-001 – *Chemical Sciences Division Quality Assurance Plan* – describes how the ORNL subject areas are graded within the Chemical Sciences Division. Criterion 5 includes sections that describe the documentation of research data using the registered research notebook process. The handling of registered research notebooks is described in the SBMS *Records* subject area exhibit: *Instructions for Use of this Research and Technical Notebook*. Research records are handled as permanent. CSD-OP-000-AD01 – *Administration of Chemical Sciences Division Command M*