

ELECTRICAL PROPERTIES OF OCEAN WORLDS: LABORATORY AND COMPUTATIONAL INVESTIGATIONS C. Psarakis¹, S. D. Vance², A. Kavner¹, K. Chin², T. T. Fidelis³, P. Sarker³, T. Wei³, B. Journaux⁴, M. J. Styczinski¹, A. Solomonidou² ¹Department of Earth, Planetary, and Space Sciences, University of California, Los Angeles (catherine.psarakis@ucla.edu), ²Jet Propulsion Laboratory, California Institute of Technology, ³Department of Chemical Engineering, Howard University, ⁴Department of Earth and Space Sciences, University of Washington, Seattle.

Introduction: The electrical conductivity of fluids offers an important tool for detecting and characterizing oceans in icy worlds using magnetic induction [1]. Investigations of the moons of the outer planets can use the planets' magnetic fields to determine the thicknesses and compositions of subsurface oceans [2,3]. Because conductivity depends strongly on composition and temperature—and also on pressure—adequate knowledge of ionic contributions to conductivity under ocean world conditions can improve the science return from future missions [3]. Here we review the existing measurements and models of electrical conductivity of NaCl solutions as a function of T, P, and concentration; describe our new molecular dynamics simulations of NaCl aqueous solution conductivity as a function of pressure; and report measured conductivities of NaCl solutions as a function of temperature and concentration from our newly-established impedance spectroscopy system.

Available bulk data for investigating ocean world salinity: Interpretation of geophysical data such as magnetic induction and/or radar backscatter in terms of the dielectric properties of a planet, moon, or geographic region, requires a broad set of measurements of electrical conductivity of planetary fluids at the relevant ranges of pressure and temperature, as well as the multicomponent solute conditions. While much of the existing datasets of electrical conductivity of aqueous fluids show single-solute aqueous conductivities as a function of temperature and concentration, there are far fewer measurements showing the effects of pressure. New measurements and analyses [4,5] summarize the ionic contributions to electrical conductivity for the majority of naturally occurring species at standard pressure and down to 0°C for dilute concentrations (<0.5 mol solute/kg H₂O) [4]. The corresponding measurements have a repeatability of better than 1.2% [5].

New electrical conductivity data for likely ocean world solutions have been measured for solutions of {0.12,10} wt% MgSO₄ from 200–1200 MPa and 243–295 K [6] and for {1,5,10} wt% NaCl from 212–1700 MPa and 233–295 K [7]. In tandem with measurements, this study [7] employed molecular dynamics simulations to investigate NaCl conductivity at pressures of 0.1–200 MPa not accessible by the experimental apparatus. The resulting simulations matched the corresponding measurements but both

experimental results and simulations are lower than the room pressure results by about 50% (See Figure 1).

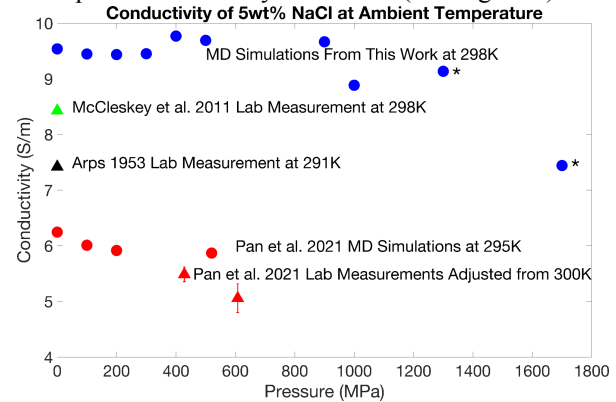


Figure 1. Results from our MD Simulations (blue). Asterisks at 1300 MPa and 1700 MPa denote possible ice–water equilibria. Also shown are published experimental data (green [5] and black [8]), and simulations (red circles [7]). High-pressure measurements (red triangles [7]) were adjusted from 300 K; only liquid data are shown.

Simulations of fluid properties: We are employing molecular dynamics (MD) simulations of aqueous solutions of NaCl to guide analyses of available data and planning of further experimental work in order to address gaps in the literature. We employ the GROMACS (version 2019.6) simulation package to compute the electrical conductivity of a 5 wt% aqueous NaCl solution in the pressure range of 0.1–1700 MPa [e.g., 3]. We use a four-point TIP4P rigid water model which has been found to be among the models most closely reproducing experimental values [9]. Our simulation box contains 157 ion pairs and 9740 water molecules, with a starting volume of 300 nm³. After running simulations that conserve *N*-particles, volume, and temperature (*NVT*), we model a pressure-conserved (*NPT*) configuration at the target pressure, keeping volume constant. The resulting output density as a function of pressure between 0.1–1700 MPa is in good agreement with the known pressure-volume equation of state for a 5 wt% NaCl aqueous fluid [10,11].

The Nernst–Einstein relation (Eq. 1) allows for the calculation of electrical conductivity from the computed values for the diffusion coefficients D_{\pm} for the dissolved cation and anion, respectively [12]:

$$\sigma = \frac{N_{pair} e^2}{V k_b T} (q_+^2 D_+ + q_-^2 D_-) \quad (1)$$

Here, N_{pair} is the number of ion pairs in the simulation box, e the fundamental electrical charge, V the average volume of the simulation box, k_b is the Boltzmann constant, T the temperature, and q_{\pm} the effective net ion charge. Our calculated electrical conductivities as a function of pressure are shown in Figure 1, along with ambient pressure measurements, and published high pressure conductivity measurements and MD simulations [7].

New measurements: To benchmark our impedance spectroscopy measurements that will be used at high pressures, we conducted new measurements of electrical conductivity of NaCl (aq) at concentrations ranging from dilute to brine 17 wt% (3 molal) at ambient pressure. We use a Gamry Interface 1010 to perform impedance spectroscopy at frequencies up to 5 MHz. Bulk electrical conductivities were determined in higher frequencies to eliminate electrode polarization using the real component of the spectrum: 10 kHz for {0.006, 0.06} wt% (1 and 10 mmol) NaCl, 50 kHz for 0.6 wt%, and 5 MHz for {5.8, 17.5} wt%. Temperature is maintained to within ± 0.5 K. A geometric cell constant was applied based on the measurements of [5] using the method of [4]. The new measurements match those previous results to within about 15%. The highest concentrations show strongly decreasing conductivity vs concentration, attributable to processes associated with solvation phenomena as suggested by MD simulations results. They consequently diverge from the extrapolation of the more dilute data by as much as 35%. Our observations of a saturation effect at high concentrations are in good agreement with existing measurements for concentrated NaCl solutions [8].

Next steps: This progress report demonstrates initial steps toward developing more comprehensive electrochemical data for investigating ocean worlds using magnetic induction. Further MD simulations are being conducted for NaCl to identify whether they may aid in the interpretation of available lab measurements. More complex ionic systems such as the doubly-charged $MgSO_4$ system are subjects for future study. Further impedance measurements are being conducted in solutions of NaCl and $MgSO_4$, with plans to examine other major ionic solutes (e.g., $MgCl_2$, $CaSO_4$) and dissolved volatiles (e.g., NH_3 , CH_4).

The measurement approach being developed at standard pressure is being adapted to fit in the bore of a new hydraulic high-pressure apparatus recently commissioned at JPL. The system, based on one already in operation for deriving thermodynamic

equations of state based on sound speeds [13], is capable of generating pressures up to 700 MPa, and sustains temperatures down to 230 K.

Acknowledgments: Part of this work is being carried out at the Jet Propulsion Laboratory, California Institute of Technology, under contract by NASA. This work was supported by JPL's Research and Technology Development program.

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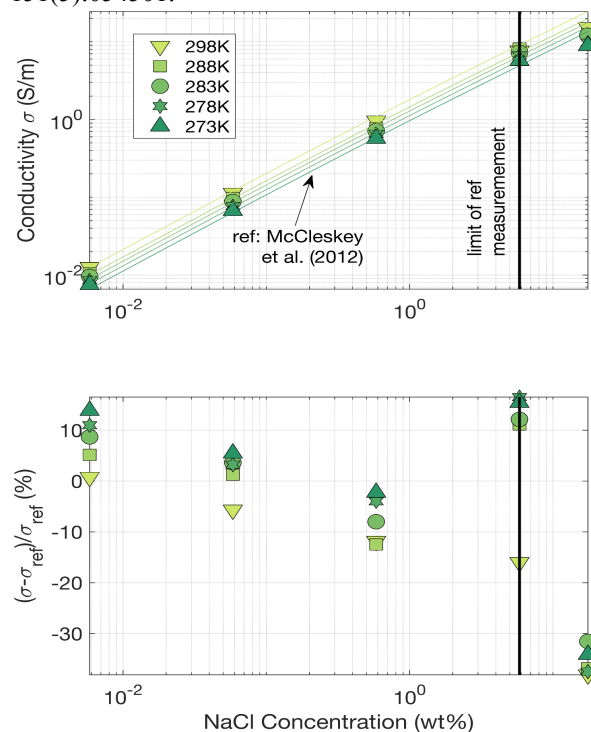


Figure 2. Measurements of bulk electrical conductivity in aqueous NaCl to 17.5 wt% at standard pressure (upper panel) and deviations (lower panel) between the measurements and the best representation of available data [4]. Symbols and corresponding colors denote temperatures in the range 273–298 K.