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Miguel A. Gonzalez ; David Carrasco-Busturia ; Carlos Vega ; Jose L. F. Abascal

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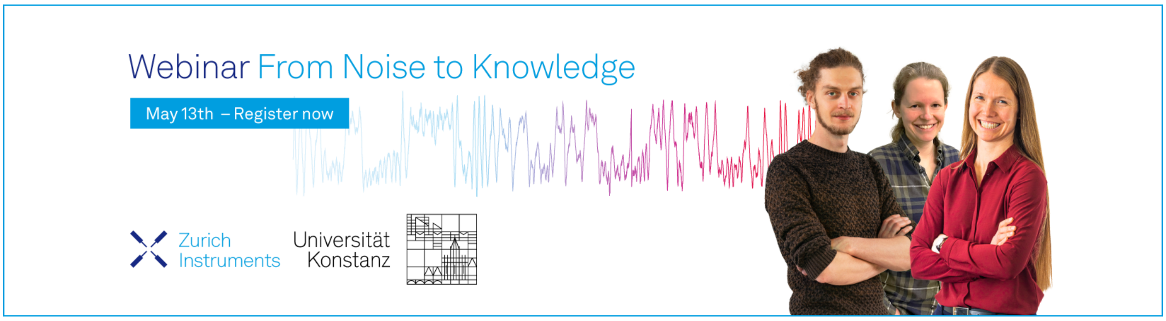

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Miguel A. Gonzalez,[a] **David Carrasco-Busturia,**[b] **Carlos Vega,** **and Jose L. F. Abascal**[c]

AFFILIATIONS

Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

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[a] **Present address:** Universidad Rey Juan Carlos, ESCET, 28933 Mostoles, Madrid, Spain.

[b] **Present address:** Division of Theoretical Chemistry and Biology, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden.

[c] **Author to whom correspondence should be addressed:** abascal@quim.ucm.es

ABSTRACT

Oceans are essentially an electrolyte solution. The experimental study of physical and chemical processes occurring in oceans remains challenging, so molecular dynamics simulations may be of great help. We have recently demonstrated that simulations using a state-of-the-art force field can accurately describe the thermophysical properties of seawater by employing a detailed chemical model of the solution. Here, we extend our previous work by investigating additional properties that require simulations on larger samples and time length scales. First, the extended time and size scales of our simulations allow for a relatively precise determination of the electrical conductivity, a fundamental property of seawater for which accurate experimental data are available, serving as a further test of the employed force field. Second, the incorporation of CO_2 into the sample enables us to evaluate its diffusion coefficient D_{CO_2}. No experimental measurements or computational simulations have yet provided estimates of carbon dioxide diffusivity at salinity levels and compositions representative of actual oceanic environments. To validate our results, we have also determined D_{CO_2} in pure water. Our simulation results show excellent agreement with experimental data in pure water, which reinforces our confidence in the predicted CO_2 diffusivity in seawater. This study provides a rigorous test of the reliability of the Madrid-2019 force field (together with TraPPE for CO_2) in saline environments. From this perspective, relevant challenges can be addressed, such as the sink of atmospheric carbon dioxide into the deeper ocean, CO_2 sequestration in deep saline aquifers, and seawater freezing (for desalination purposes).

I. INTRODUCTION

The physics and chemistry of the oceans affect human life and that of the rest of living organisms in many ways.[1,2] From a physicochemical point of view, marine waters are essentially an electrolyte solution.[3,4] Some of the processes taking place in these environments are difficult to access experimentally. Molecular dynamics has proven to be a useful tool that may help to provide reasonable predictions of physicochemical magnitudes under these conditions. All we need is a satisfactory force field describing the molecular interactions and enough computing power. Some years ago, the use of scaled charges for the ions[5] was proposed as a simple way to account for electronic polarization. Recently, it has been demonstrated that this approach leads to improved predictions for the properties of electrolytes.[6–12] In fact, our group has developed a force field—based on the TIP4P/2005 water model[13] and the charge scaling scheme—that provides a successful description of the properties of aqueous solutions.[9,10] Moreover, the so-called Madrid-2019 force field has been shown to give a very satisfactory account of the thermophysical properties of a solution mimicking the detailed composition of standard seawater.[14] However, the sample size and the simulation time length limited the accuracy of the calculations, and important properties could not be evaluated.

This work aims to complement our previous study by carrying out large-scale simulations of marine water with a dual objective. The first goal is to check the performance of the force field for the electrical conductivity. This is a relevant dynamical property of seawater. In fact, the measurement of conductivity is used as a simple and routine way to determine the salinity of a sample. Recently, it has been shown[15] that the aforementioned force field, together with an appropriate methodology, is able to describe the ionic conductivity of NaCl and KCl electrolyte solutions. Notice that a precise evaluation of the conductivity using computer simulation is quite demanding, but the experimental data are abundant and accurate. It is thus interesting to carry out extended simulations to obtain reliable predictions for the ionic conductivity as a further test of the validity of the force field in marine environments.

The other purpose of our work is to evaluate the diffusivity of CO_2 under oceanic conditions. About 30% of the increase in CO_2 in the atmosphere—mainly responsible for the increase in temperatures on our planet over the last 150 years[16,17]—has been absorbed by the oceans.[18–20] Although the sink of carbon dioxide helps mitigate the climate effects of anthropogenic CO_2 emissions, it has negative consequences, as it leads to the acidification and hypoxia of the oceans.[21–23] The ocean carbon cycle[24–26] is a very complex process. It involves the air–sea exchange at the marine surfaces,[27] the chemical CO_2–water equilibria,[28,29] the transport and diffusion of these chemical species,[26] the carbon sequestration by phytoplankton,[30] and the subsequent sedimentation of the remains of dead organisms.[22,31] Most of these processes are currently under investigation, but some are especially problematic to address. In particular, the experimental study of the diffusion of chemical species is very difficult due to the complexity of seawater and the low concentration of the solutes. Reported experimental data for the diffusion coefficients of CO_2–water mixtures are limited to pure water systems and are restricted to low temperatures and pressures. While these data are typically obtained at infinite dilution, conditions that are indeed representative of seawater, the key limitation lies in the thermodynamic conditions and the absence of measurements at salinities and compositions characteristic of oceanic environments.[32,33] On the other hand, engineering models and correlations for predicting diffusion coefficients of CO_2 in water often lack accuracy due to their empirical nature, limited validation across thermodynamic conditions, and the absence of salinity effects in their formulations.[32] We thus face an issue for which atomistic molecular dynamics simulation seems to be a good alternative. The calculation of the diffusion coefficients of CO_2 in seawater is also intensive in computer resources. Thus, we may exploit the trajectories obtained for the evaluation of the electrical conductivity in order to calculate the diffusivity of CO_2. Notice that this is the first-ever estimation of the CO_2 diffusion coefficients and their variation with temperature and pressure at the usual oceanic ranges.

II. “IN SILICO” SEASALT AND SEAWATER

The Reference Composition of Standard Seawater was *defined*[29] in 2008 to provide the best available estimate of the absolute salinity of standard seawater. It is based on the most accurate prior determination of the composition and is described in terms of the mole fractions of the solute components with a precision of $1/10^7$. The number of water molecules required to represent a seawater sample with the reference composition and a salinity of around 35 g/kg would then be of the order of 5×10^8. However, the six most abundant ions—those with an ionic mole fraction of >0.002 (chloride, sodium, sulfate, magnesium, calcium, and potassium)—represent 99.7 percent of the seasalt mole fraction. In previous work,[14] we have shown that the simulation of a solution containing only the aforementioned ions (comprising only 318 ions and ~15000 water molecules) allows a reliable comparison between simulation and experimental results for seawater. The incorporation of CO_2 into the solution complicates the problem because of its extremely low concentration, about 1/1000 of that of calcium or potassium. A sample containing just a single CO_2 molecule would require around 5×10^6 water molecules. In practice, this means that carbon dioxide is essentially infinitely diluted in seawater. An experimental study of the diffusion of CO_2 in water at 25 °C as a function of solute concentration concluded that, for all practical purposes, D_{CO_2} in water can be considered to be constant.[34] We have thus decided to increase the CO_2 concentration using a sample large enough to be practical in molecular dynamics calculations but small enough to consider CO_2 as infinitely diluted.

The solution investigated in this work is given in Table I. It includes 2500 ions, and its composition follows with excellent accuracy that of the reference composition defined by Millero *et al.*[29] From the mole fractions and the ionic charge of the six most abundant components mentioned, it is clear that the charge balance is not easily satisfied. This is related to the fact that most of the neglected constituents carry a negative charge. For simplicity, the effect of the ignored solutes has been replaced by chloride ions (seven in our sample) so that the whole system is electroneutral. The number of water molecules required to achieve a reference salinity[29] (i.e., grams of dissolved salt per kg of seawater) of $S_R = 35.166$ g/kg is 119 570. We have added 8 CO_2 molecules to our sample. Notice that, although the carbon dioxide concentration is significantly increased with respect to that in standard seawater, its mole fraction—referred to the total number of molecules, including water—is very low, around 6.5×10^{-5}. In these conditions, CO_2 can be effectively considered

TABLE I. Composition of the solution used in this work. The second column shows the number of ions, and the third column shows the mole fractions of the “seasalt,” i.e., it refers only to the ionic constituents. These reproduce with excellent accuracy the values of the Seawater Reference Composition[29] (third column) for solutes with $x > 0.002$. The number of water molecules required to get a model for seawater with a reference salinity[29] $S_R = 35.166$ g/kg is 119 570, and the last column shows the mole fraction of the species referred to the whole solution, including the water molecules. The salinity S_R is defined as the grams of dissolved salt per kg of seawater.

Component	n	x_{ion}	x_{ref}	x_{sol}
Chloride	1219	0.4876	0.4875	0.009 985
Sodium	1047	0.4188	0.4188	0.008 576
Magnesium	118	0.0472	0.0472	0.000 516
Sulfate	63	0.0252	0.0252	0.000 967
Calcium	23	0.0092	0.0092	0.000 188
Potassium	23	0.0092	0.0091	0.000 188
Minor components	7	0.0028	0.0030	0.000 057
Sum	2500	1.0000	1.0000	⋯
CO_2	8	3.2×10^{-3}	8.6×10^{-6}	0.000 065
Water ($S_R = 35.166$ g/kg)	119 570	⋯	⋯	0.979 456

as infinitely diluted, and D_{CO_2} may be calculated with reasonable accuracy.

III. METHODS

In this work, molecular dynamics simulation is used to investigate the properties of a system mimicking the composition of standard seawater. We have chosen the TIP4P/2005 model[13] to account for the interactions between the water molecules. For the ion–ion and ion–water interactions, we have used a recent parameterization[9]—the Madrid-2019 force field—based on the use of scaled charges for the ions. It includes parameters for all the ionic species present in our seawater model. For carbon dioxide, we have chosen the TraPPE[35] (Transferable Potentials for Phase Equilibria), a rigid non-polarizable model with three interaction sites representing the C and O atoms, each of them consisting of a combination of a Lennard-Jones site plus an electric point charge. The combination of the TIP4P/2005 and the TraPPE models has shown an excellent performance in describing the three phase coexistence line of CO_2 hydrates when a small deviation from the classical Lorentz–Berthelot combining rules is used for the cross CO_2–H_2O interaction.[36,37] In particular, $\epsilon_{CO_w} = 1.12 * (\epsilon_C * \epsilon_{O_w})^{1/2}$ and $\epsilon_{O_C O_w} = 1.12 * (\epsilon_{O_C} * \epsilon_{O_w})^{1/2}$. Finally, given that the average size, charge, and atomic mass of the "minor components" are similar to those of the chloride ions, we have used the latter as a simple but reasonable replacement for the interactions of the former.

The simulations have been performed using GROMACS 2016[38] with a 2 fs time step. The cutoff radii have been set to 0.9 nm for the Lennard-Jones interactions. Long range corrections to the Lennard-Jones potential energy and pressure were included. Long range electrostatic interactions have been evaluated with the smooth particle mesh Ewald method.[39,40] A rigid geometry is assumed for the water molecules and the sulfate ions using constraints, in particular the SHAKE algorithm,[41] to preserve the intramolecular distances. The Nosé–Hoover thermostat[42,43] has been applied to set the temperatures at the desired values. Most of the simulations in the isobaric–isothermal (NpT) ensemble have been done at a fixed pressure of 1 bar by means of an isotropic Parrinello–Rahman barostat.[44] Additional runs at 400 and 1000 bar have been carried out at 2 °C to analyze the effect of pressure in very deep ocean conditions. In fact, the former value is close to the pressure at the average ocean depth, and the latter one is only slightly below the pressure (1086 bar) at the deepest point in the Mariana Trench. The simulated time of the trajectories has been 120 ns.

The electrical conductivity σ has been calculated using the Einstein–Helfand relation,[45–49]

$$\sigma = \lim_{t\to\infty} \frac{d}{dt} \frac{1}{6Vk_BT} \langle [M(t) - M(t_0)]^2 \rangle, \tag{1}$$

where k_B is the Boltzmann constant and V, T, and M are, respectively, the volume, temperature, and dipole moment of the system. We only consider the ionic species for the evaluation of M. In this way, the conductivity can be easily obtained from the slope of the plot of the mean square dipole displacement vs time. This equation can be rewritten as

$$\sigma = \lim_{t\to\infty} \frac{d}{dt} \frac{1}{6Vk_BT} \left\langle \sum_i^N \sum_j^N q_i q_j [\mathbf{r}_i(t) - \mathbf{r}_i(t_0)][\mathbf{r}_j(t) - \mathbf{r}_j(t_0)] \right\rangle, \tag{2}$$

where q_i is the charge of ion i. It is important to point out that, as discussed elsewhere,[15] the nominal values of the ionic charges should be used in the calculation of σ. The above relation shows that the diffusion coefficients may also be evaluated as a by-product of the conductivity calculations.

The self-diffusion coefficients have been evaluated by means of the Einstein relation,

$$D = \lim_{t\to\infty} \frac{1}{6t} \langle [\mathbf{r}_i(t) - \mathbf{r}_i(t_0)]^2 \rangle, \tag{3}$$

where $\mathbf{r}_i(t)$ and $\mathbf{r}_i(t_0)$ are the positions of the ith particle at time t and a certain origin of time t_0. It is well known that the self-diffusion coefficients are sensitive to finite-size effects,[50,51] but the size of our samples is already large enough to avoid this problem. The uncertainties of the results for the conductivities and the diffusivities have been estimated as the standard deviation of the calculations in six runs resulting from dividing the whole 120 ns trajectories into slices of 20 ns. These estimations have been done at all the state points in the case of the conductivity. In the case of the diffusion coefficients of the ions, the uncertainties have been estimated at 15 °C.

IV. RESULTS

A. Electrical conductivity

The dependence on temperature and pressure of the electrical conductivity of seawater with salinity $S_R = 35.166$ g/kg is shown in Fig. 1. Overall, the agreement between simulation and experiment is quite satisfactory, although the predictions of the molecular dynamics data are slightly below the experimental ones. Our calculations are able to describe the substantial variation of the conductivity with the temperature. As for the dependence on pressure, the scale in Fig. 1 does not allow one to clearly perceive the small but significant increase in the conductivity at increasing pressures. This can be better seen in Fig. 2, where we represent the ratio between the conductivity at a given pressure and that at zero pressure, both calculated at 2 °C. The Madrid-2019 tends to slightly underestimate the conductivities of NaCl and KCl at low concentrations and more significantly at high concentrations.[15] However, decreasing the charge of ions in the force field (from 0.85 to 0.75 for monovalent and from 1.7 to 1.5 for divalent) may improve the agreement with the experiment. Notice that the simulation results closely follow the experimental curve.

B. Diffusivity of the most abundant ions in seawater

The experimental determination of the diffusion coefficients of solutes is never simple and becomes very tricky in the case of multicomponent solutions. In fact, reports of the diffusion coefficients of the ionic species in seawater are very scarce.[53,54] Our trajectories allow the evaluation of the diffusion coefficients of the ionic constituents of seawater and compare them to the results of our previous work[14] (see Table II). Notice that the current calculations involve about eight times more ions than the precedent ones, so the present values are more precise. The estimated uncertainty of the diffusion coefficients at 15 °C is less than 1% for the most abundant ions, i.e., chloride and sodium. The relative uncertainties of the magnesium, sulfate, potassium, and calcium ions are less than 2%, 2%, 3%, and

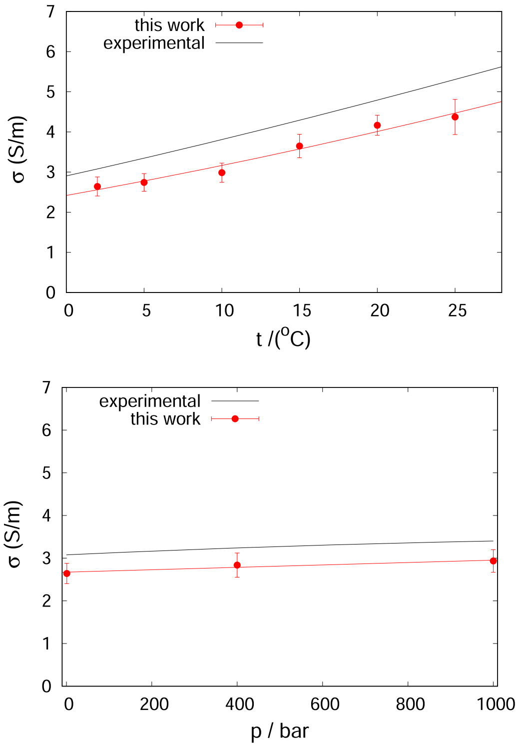

FIG. 1. Conductivity of our seawater model with salinity S_R = 35.166 g/kg as a function of temperature at p = 1 bar (upper panel) and pressure at 2 °C (lower panel). The experimental data were obtained using the TEOS-10 equation.[52]

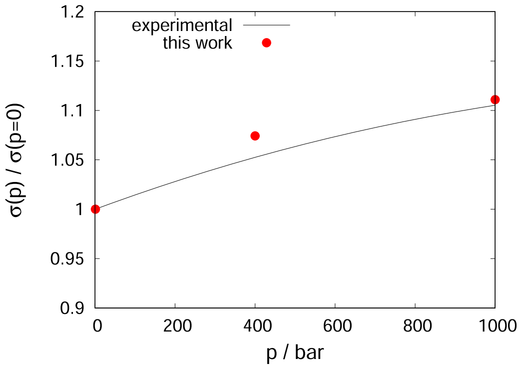

FIG. 2. Ratio between the conductivities at a given pressure and that at zero pressure. The salinity is S_R = 35.166 g/kg and the temperature is t = 2 °C.

4%, respectively. It is interesting to note that both sets of calculations are in close agreement, indicating that the conclusions of the previous work have not changed: the comparison with the scarce experimental measurements indicates that the predictions of our "*in silico*" seawater model are semiquantitative.

Since the uncertainties of the diffusion coefficients for the most abundant ions are quite small, it is possible to check more reliably the influence of pressure. Figure 3 shows that, in general, increasing pressures give rise to larger values for D_{ion}, although the magnitude of the increases is different for each ion. Within the examined pressure interval (from 0 to 1000 bar), the variation of D is evident for chloride, magnesium, and sulfate (an increase of about 10%) and slightly above the statistical error for sodium. The impact of pressure on the diffusion coefficients of the less abundant ions, calcium and potassium, cannot be assessed because of the uncertainty of the calculations.

C. Diffusivity of CO_2 in pure water

As commented above, the experimental determination of the diffusion coefficients of the solutes of a multicomponent solution is difficult. The case of CO_2 in seawater is even worse. We may find in the literature a number of data on the diffusivity of CO_2 in water.[33,55–59] However, as far as we know, there is not a single measurement of D_{CO_2} in a realistic marine environment. There are a few reports of the diffusion coefficients of CO_2 in brines, but they usually refer to a NaCl aqueous solution (see the excellent review of Polat *et al.*[33]). Certainly, the diffusivity in seawater should be quite similar to that of a NaCl solution of appropriate salinity, but it is not clear how the marine environment could be mapped onto a single-component solution. This fact motivates the use of molecular simulation to gain insight into this significant property.[33,48]

The absence of experimental data also raises an important question. If there are no experiments to check against, how reliable would

TABLE II. Self-diffusion coefficients $10^9 D/(m^2\ s^{-1})$ of solutes in our model of standard seawater with salinity S_R = 35.166 g/kg at representative oceanographic conditions. Temperatures, t, are given in Celsius degrees, and pressures, p, in bar.

t	p	CO_2	Chloride	Sodium	Magnesium	Sulfate	Calcium	Potassium
25	1	1.75	1.398	1.110	0.640	0.895	0.701	1.61
20	1	1.56	1.228	0.974	0.569	0.782	0.618	1.42
15	1	1.41	1.074	0.848	0.488	0.672	0.546	1.25
10	1	1.21	0.919	0.728	0.412	0.593	0.455	1.11
5	1	1.03	0.793	0.617	0.356	0.509	0.387	0.97
2	1	0.94	0.716	0.557	0.317	0.449	0.350	0.87
2	400	0.94	0.747	0.569	0.334	0.480	⋯	⋯
2	1000	0.93	0.790	0.577	0.355	0.504	⋯	⋯

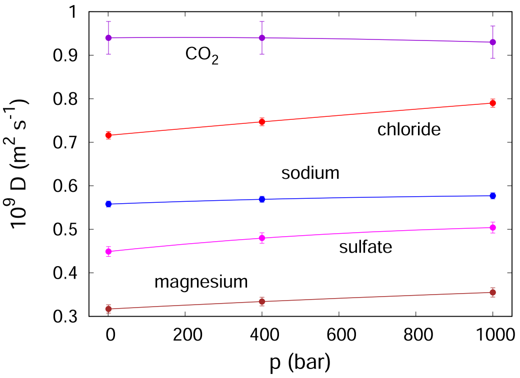

FIG. 3. Self-diffusion coefficients of the most abundant ions as a function of pressure in standard seawater with salinity $S_R = 35.166$ g/kg at 2 °C.

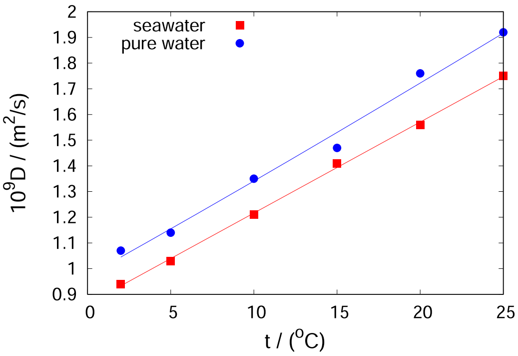

FIG. 5. Self-diffusion coefficients of CO$_2$ in pure water compared to those in standard seawater with salinity $S_R = 35.166$ g/kg at $p = 1$ bar. Points are the molecular dynamics calculations, and lines are a guide to the eye.

the simulated results then be? An indirect way to answer this question is to analyze the performance of the current force fields to evaluate the diffusivity of CO$_2$ in pure water. Given the quality of the results of the Madrid-2019 force field for a number of seawater properties,[14] if the predictions for D_{CO_2} in water are satisfactory, we may expect that the corresponding predictions for a marine environment would be reliable. Our first task should then be the calculation of the diffusivity of CO$_2$ in pure water to validate the CO$_2$–water force field. Figure 4 shows the simulated results using the TIP4P/2005 and TraPPE models for water and CO$_2$, respectively. The comparison with the experimental measurements indicates that the performance of these models is excellent. In addition, our result at 25 °C 1 bar is similar to that reported[60] by Moultos *et al.* for the same combination of water and CO$_2$ models.

D. Diffusivity of CO$_2$ in seawater

The diffusion coefficients of CO$_2$ have been obtained from the fit of the mean square displacements vs time in the interval from 50 to 400 ps. In the conditions of our study, the uncertainty of the results for D_{CO_2} is smaller than 4%. Table II shows the numeric values obtained in this work for the self-diffusion coefficients of CO$_2$ in seawater at different temperatures. Figure 5 displays a comparison of the diffusivities of CO$_2$ in pure water with those in standard seawater at 1 bar. The diffusion coefficient of CO$_2$ in seawater vs pure water just differs by a value that remains more or less constant across the range of temperatures investigated. This is certainly only due to the effect of the ions. The reduction of the diffusion coefficient of CO$_2$ in seawater with respect to pure water can be qualitatively understood by the increase in viscosity of seawater relative to pure water using the Stokes–Einstein relation.[15]

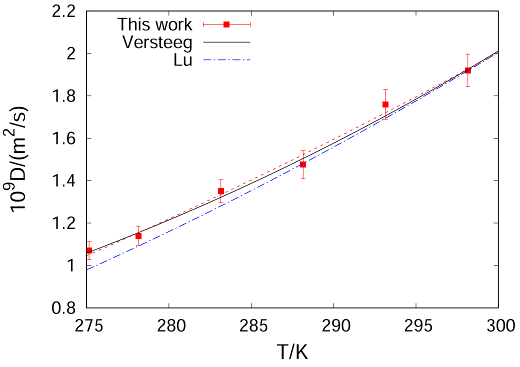

FIG. 4. Diffusion coefficients of CO$_2$ in water as a function of the temperature at 1 bar. The asterisks are the simulation results of this work, and the red dashed line is a fit of the simulation results to the function $D_0(T/T_s - 1)^m$ (which gives $D_0 = 11.6473$, $T_s = 227$, and $m = 1.551\,11$). The solid black line is the correlation of experimental measurements reported by Versteeg and Van Swaaij,[55] while the dashed-dotted blue line is the correlation of Lu *et al.*[58]

Previous studies in *pure water*[58,60,61] have shown that the dependence of D_{CO_2} on pressure is quite small. In fact, it has been reported[58] that, at 393 K, the increase of 100 bar in pressure would cause less than a 3% decrease in D and that the differences in the diffusivity of CO$_2$ are around 1%–2% for the pressure range of 140–486 bar and temperatures ranging from 298 to 423 K.[61] Our calculations for a *marine environment* (see Table II and Fig. 3) also point toward a slight decrease (about 1%) of the CO$_2$ diffusion coefficients for the range from 1 to 1000 bar. However, the variation is smaller than the uncertainty of the calculations, so the inference must be taken with some care.

V. CONCLUSIONS AND DISCUSSION

In this work, we have presented molecular dynamics calculations of the electrical conductivity of seawater at oceanic conditions (composition and thermodynamic variables). We use a detailed description of seawater with a 35.166 g/kg salinity. Apart from the water molecules, our sample includes the six most abundant ionic species (2493 ions), representing 99.7% of the reference seasalt composition. The neglected species has been replaced by 7 chloride ions so that the whole system is electroneutral. Our results, together with those of a previous study,[14] provide a stringent validation of the performance of the Madrid-2019 force field when applied to marine environments. The long scale of the simulations, both in time and sample size, also enables the first-ever estimation of the diffusion coefficients of CO$_2$ in realistic seawater conditions. Since, to the best of our knowledge, there are no experimental data to validate our computer simulation results in a marine environment, we have evaluated the CO_2 diffusion coefficients in pure water. The comparison between experiment and simulation is very satisfactory, which strongly supports the reliability of our calculations of D_{CO_2} in seawater. The saline environment decreases the diffusivity of CO_2 by a factor (around 15 percent), which remains almost constant across the investigated temperature range. In line with other studies,[58,60,61] our results suggest a small dependence of D_{CO_2} on pressure. Our more precise determinations seem to indicate that an increase in pressure translates into a slight decrease in the diffusion coefficient, although the variation is nearly within the statistical uncertainty. Considering that the pressure interval investigated in this work (1–1000 bar) is larger than that corresponding to the mean ocean depth (around 400 bar), our data suggest that changes in CO_2 diffusivity at different oceanic pressures may be barely perceptible.

In this paper, we have used a very large and detailed sample to represent seawater. The large size has been adopted to ensure that the CO_2 concentration is close to the infinite dilution limit. Both experimental work[61] and MD simulations[60] suggest that the diffusion coefficient of CO_2 is independent of the number of CO_2 molecules in the low composition regime. Fleury and Deschamps[62] have shown that the relative change in the electrical conductivity of NaCl solutions is proportional to the mole fraction of dissolved CO_2 according to $\Delta\sigma/\sigma = -6.0 x_{CO_2}$. It seems reasonable to assume that a similar relationship holds for seawater. Given that $x_{CO_2} = 6.5 \times 10^{-5}$, it is clear that the effect of the CO_2 concentration on the electrical conductivity of our system is completely negligible. Thus, it appears that a smaller sample would yield essentially the same results. Regarding the composition of the solution, we have used a six-component solute because the size of the system allows for a near-perfect match with the reference composition and because the Madrid-2019 force field incorporates parameters for these ions. However, we have shown previously[14] that a four-component seasalt already provides a good description of marine water. In particular, a sample containing about 300 ions and 15000 water molecules was able to account for several thermophysical seawater properties. An important point is whether we could further simplify the solute and represent seawater as a simple NaCl solution.[63–71] We may shed light on this question by comparing the experimental data for both solutions, trying to match the results at a given seawater salinity with those of an "equivalent" NaCl solution. Figure 6(a) shows that the experimental densities at 25 °C of marine water with salinity s are almost identical to those of halite solutions with molalities $m_{\mathrm{NaCl}} = s/53.13$. In particular, the experimental density at 25 °C of marine water with a 35.166 g/kg salinity is the same as that of a 0.662 molal (3.72 wt. %) halite solution. The small difference in salt content of both systems would not be important if the same equivalence held for other properties. Unfortunately, this is not the case when we look at the conductance measurements: the conductivity of seawater at the conditions indicated above is the same as that of a 0.584 m (3.30 wt. %) NaCl solution [see Fig. 6(b)]. The difference in "equivalence" factors arises from the fact that NaCl is a salt made of monovalent ions, but the amount of divalent ions (magnesium and sulfate) is significant in seawater. The replacement of monovalent by divalent ions affects different solution properties in a *distinct* way. For instance, it has been shown[63,72] that the presence of divalent ions significantly influences the CO_2 diffusion coefficient. In addition, it has been reported that $MgCl_2$ exhibits stronger inhibition on the growth of CO_2 hydrate than NaCl does. After all, it should not be a surprise that a multicomponent electrolyte mixture including monovalent and divalent ions could not be mapped into a simple NaCl solution. Therefore, superseding the properties of seawater with those of a NaCl solution must be done with care. This is even more so when quantitative predictions of seawater properties are required, as is the case in oceanic and environmental sciences. As illustrated in this work, it is now straightforward to determine accurately by computer simulation the properties of a solution with a composition very close to that of marine water. Use seawater to model seawater and avoid NaCl solutions as a proxy.

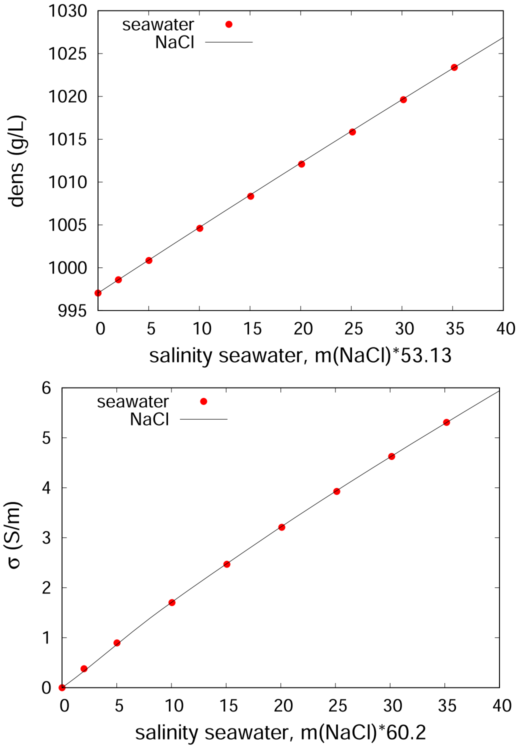

FIG. 6. Upper panel: Experimental values of the density of seawater at 25 °C as a function of the salinity, s, and of NaCl solutions as a function of the molality given by $m_{\mathrm{NaCl}} = s/53.13$. Bottom panel: Experimental values of the electrical conductivity of seawater at 25 °C as a function of the salinity and of NaCl solutions as a function of the molality given by $m_{\mathrm{NaCl}} = s/60.2$.

Our calculations may be helpful in a number of areas of marine science and related areas. The more evident one is the study of the sink of atmospheric CO_2, since we provide data that allow us to estimate the diffusion of CO_2 from the sea surface into the deep ocean. In addition, this work, together with our previous one,[14] provides a stringent test of the reliability of the Madrid-2019 and TraPPE[35] force fields in saline environments and can thus expand the interest in these types of computer calculations. For instance, a topic that may benefit from our work is that of CO_2 sequestration in deep saline aquifers.[65,67,73,74] Finally, let us cite seawater freezing,[64,66,75,76] especially in the context of freezing desalination,[68–70,76] among other relevant problems that may be tackled within this perspective.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Miguel A. Gonzalez: Conceptualization (equal); Formal analysis (equal); Investigation (equal); Validation (equal); Writing – original draft (supporting); Writing – review & editing (equal). **David Carrasco-Busturia**: Formal analysis (equal); Investigation (equal); Validation (equal); Writing – review & editing (equal). **Carlos Vega**: Conceptualization (equal); Funding acquisition (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Writing – original draft (supporting); Writing – review & editing (equal). **Jose L. F. Abascal**: Conceptualization (lead); Data curation (lead); Formal analysis (lead); Funding acquisition (supporting); Investigation (lead); Methodology (lead); Resources (equal); Software (lead); Validation (lead); Writing – original draft (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within this article.

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