



A numerical modelling of gas exchange mechanisms between air and turbulent water with an aquarium chemical reaction [☆]



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ABSTRACT

This paper proposes a new numerical modelling to examine environmental chemodynamics of a gaseous material exchanged between the air and turbulent water phases across a gas–liquid interface, followed by an aquarium chemical reaction. This study uses an extended concept of a two-compartment model, and assumes two physicochemical substeps to approximate the gas exchange processes. The first substep is the gas–liquid equilibrium between the air and water phases, $A(g) \rightleftharpoons A(aq)$, with Henry's law constant H . The second is a first-order irreversible chemical reaction in turbulent water, $A(aq) + H_2O \rightarrow B(aq) + H^+$ with a chemical reaction rate κ_A . A direct numerical simulation (DNS) technique has been employed to obtain details of the gas exchange mechanisms and the chemical reaction in the water compartment, while zero velocity and uniform concentration of A is considered in the air compartment. The study uses the different Schmidt numbers between 1 and 8, and six nondimensional chemical reaction rates between $10^{-\infty} (\approx 0)$ to 10^1 at a fixed Reynolds number. It focuses on the effects of the Schmidt number and the chemical reaction rate on fundamental mechanisms of the gas exchange processes across the interface.

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0. Significance and novelty of this article

- This article provides a new concept and modelling strategy for a gas exchange process at a gas–liquid interface, followed by an aquarium chemical reaction. This article considers the gas exchange processes across the interface by separating this phenomenon into two physicochemical substeps; the first is a gas–liquid equilibrium of the gas at the interface, and second an aquarium chemical reaction. The modelling strategy is useful to evaluate the gas exchange rate of a highly reactive gas in water, with a lot of applicabilities in the fields of environmental sciences, atmospheric physics, chemical and mechanical engineering, and limnology.
- This article examines the effects of the Schmidt number of the gas, and the chemical reaction rate, on the gas exchange rate at the interface. The numerical data and results provided in this article are new and comprehensive, and show significant role of the chemical reaction in water on the gas exchange at the interface.

1. Introduction

Chemodynamics of a gaseous material exchanged between the air and turbulent water phases is one of the commonly observed physicochemical processes in the environment. One of the most well-known examples of the gas exchange is an

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uptake of carbon dioxide (CO₂) from the atmosphere into the ocean, and vice versa, across the ocean surfaces [1–4]. The gas exchange has been considered as one of the important processes of the global carbon cycle, and many field measurements of the gas exchange rate have been attempted to quantify the role of the ocean storage of CO₂ on the global budgets of carbon [5]. The gas exchange mechanisms between the atmosphere and river water have also been under scrutiny to clarify microbiological mass balances of CO₂ and oxygen (O₂) in the field of limnology [6,7].

Several reports have expressed concerns that CO₂ uptaken across the interface causes acidification of the seawater, since it is believed to have potential environmental and ecological impacts [8]. A series of chemical reactions of CO₂ in the seawater are expressed as [9],



The first substep indicates the gas–liquid equilibrium of CO₂ between the two phases, and the following three substeps are the chemical reactions of CO₂ into the seawater. The effect of the chemical reaction rates of CO₂ in the seawater on the gas exchange rate should be investigated carefully to clarify details and future development of the ocean acidification, and to assess possible impacts on the ecosystem in the ocean, as well as the details of the global carbon cycle.

Another example of the environmental chemodynamics of a gas exchanged between air and water with the chemical reaction is production of trifluoroacetic acid, CF₃COOH, which is known as TFA [10,11]. This substance is one of the degradation products of 1,1,1,2-tetrafluoroethane (CH₂FCF₃), or, HFC-134a, which has been used as a refrigerant of a mobile fleet [12]. A few studies on the atmospheric chemistry have pointed out that HFC-134a is broken down by a series of stratospheric photochemical reactions after it is emitted into the atmosphere [13,14], and trifluoroacetyl fluoride, CF₃COF, is one of the degradation products of the photochemical reactions [10,11]. CF₃COF is further broken down to TFA by hydrolysis in cloud moistures following the physicochemical processes with the aid of ultraviolet rays [13,14],



TFA is one of the materials having strong organic acidity, and can accumulate in a closed surface water such as a seasonal wetland after wet depositions because of its low decomposition potential in the environment [15]. Both modelling of the formation processes of TFA, and predictions of its concentration in rainwater are desired to assess the details of accumulation in closed surface waters, and the biochemical effect of TFA on aquarium ecosystem [16].

Physicochemical processes of formation of the acid rain in cloud droplets caused by, for example, sulphur dioxide (SO₂) released into the atmosphere also involve hydrolysis shown by [17]



The physicochemical processes explained above suggest that the gas exchange between air and water with an aquarium chemical reaction play an important role in determining chemodynamics of the gaseous substances in the environment.

Quantification of the gas exchange processes between air and water has been examined extensively in the fields of oceanography, and environmental sciences for the reasons expressed above. References which discuss the effect of the chemical reaction on gas transport processes into turbulent water are, however, extremely sparse. For example, many field measurements of the gas exchange rates at the atmosphere–ocean interfaces have been reported without considering the chemical reactions of CO₂ [18,19]. Also, many numerical studies on the gas exchange processes based on a direct numerical simulation (DNS) [20–24], and a large-eddy simulation technique (LES) [25–27], have not considered the effect of the aquarium chemical reactions. One of the reasons for the sparsity of references is that field and laboratory measurements on the gas exchange mechanisms with the aquarium chemical reactions are difficult, especially if the chemical reactions are fast. One of the good examples of the difficulties of measuring chemical reaction processes of the gases across the interface are indicated in a report by De Bruyn et al. [28], in which both Henry's law constants and the chemical reaction rates for several halides are obtained by several studies. Table 1 in their report [28] suggests that very large uncertainties exist in the measurements of Henry's law constant, and the chemical reaction rates of halides, resulting in considerable errors of predictions of the gas exchange rates. Another reason for the neglected effect of the aquarium chemical reactions on the gas exchange processes is that many researchers and scientist have not been aware of the critical roles of the aquarium chemical reactions on the gas exchange between air and water.

It should also be pointed out here that field and laboratory measurements of the gas exchange processes require observations of very fine-scale concentration and velocity fluctuations particularly in the near-interface turbulent boundary

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