Assessing and correcting estimated fCO2 from carbonate chemistry models of the northeastern US

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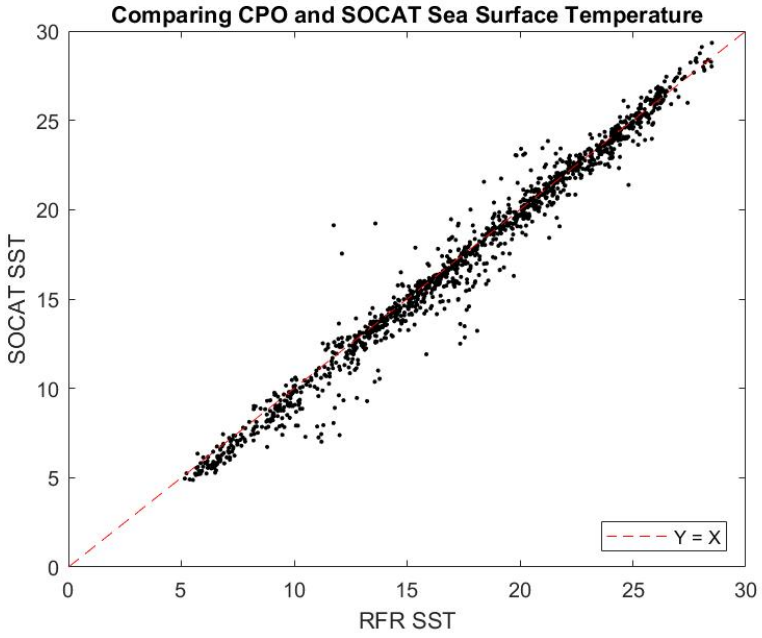
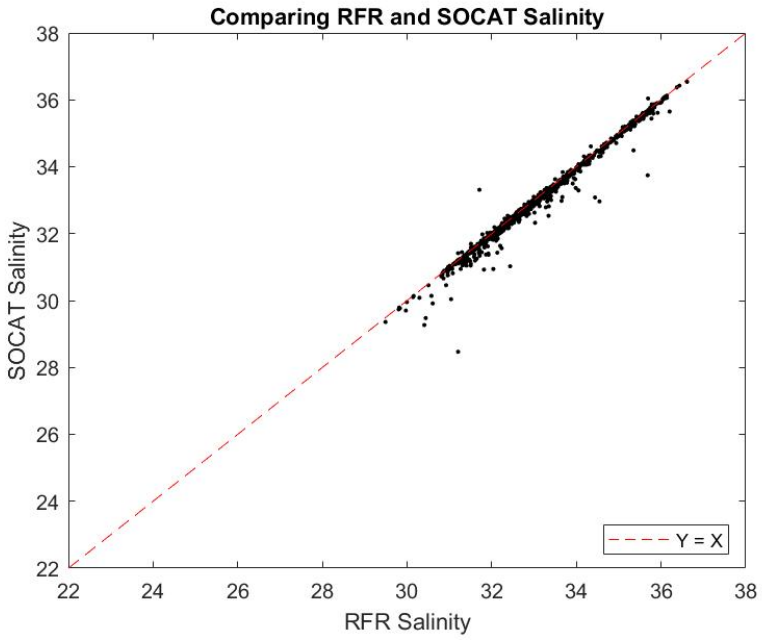
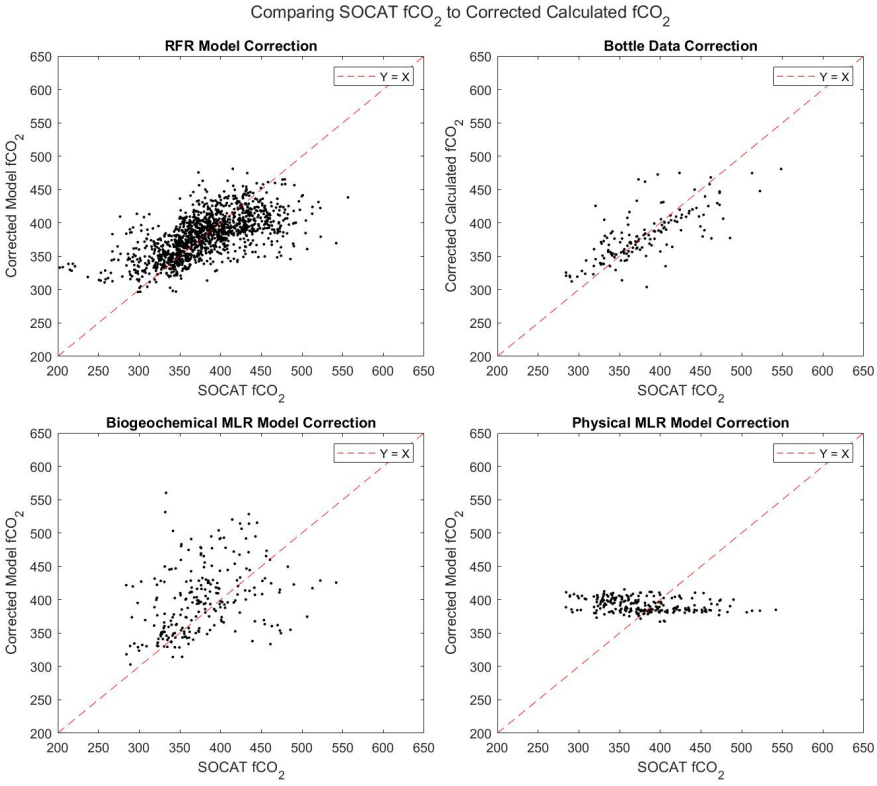
Abstract

Understanding changes in the ocean carbonate system is central to understanding ocean and coastal acidification and the effects these phenomena will have in the future. To create a more complete overview of the recent history of the carbonate system in the nearshore Northeastern United States, several recently published or in-development statistical models have used simple ocean chemistry parameters of salinity, temperature dissolved oxygen, and nitrate, or these variables plus the addition of other input parameters: sea surface temperature, chlorophyll a, sea surface height, bathymetry, and atmospheric pCO2 to generate estimates of dissolved inorganic carbon (DIC) and total alkalinity (TA). Both a Random Forest Regression model and a multiple linear regression model predicting carbonate chemistry parameters was tested for accuracy in predicting fugacity of CO2 (fCO2) by comparing them with the publicly available fCO2 data from the Surface Ocean CO2 Atlas (SOCAT) database. Comparisons revealed a bias by the models to overestimate fCO2, which was also observed when comparing the SOCAT dataset to collocated discrete observations. To resolve these biases in fCO2, a correction was fitted to the modeled datasets. This investigation suggests that models that accurately predict carbonate parameters of DIC and TA, may be limited in their ability to reproduce fCO2 conditions in coastal areas without correction. This study suggests that extrapolating ocean carbonate system models based on parameters outside their intended uses should be considered for their potential limitations.







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Introduction

Characterizing the ocean carbonate system is important in understanding ocean acidification and broader ocean chemistry. Models can help extrapolate carbonate chemistry parameters from existing chemistry data (Fig. 1)

This investigation explores the ability of a Random Forest Regression Model (RFR), a multiple linear regression model (MLR)[1] and bottle samples to predict the fugacity of CO_2 (fCO_2) in the Northeast US nearshore region from modeled or measured total alkalinity (TA) and dissolved inorganic carbon (DIC)

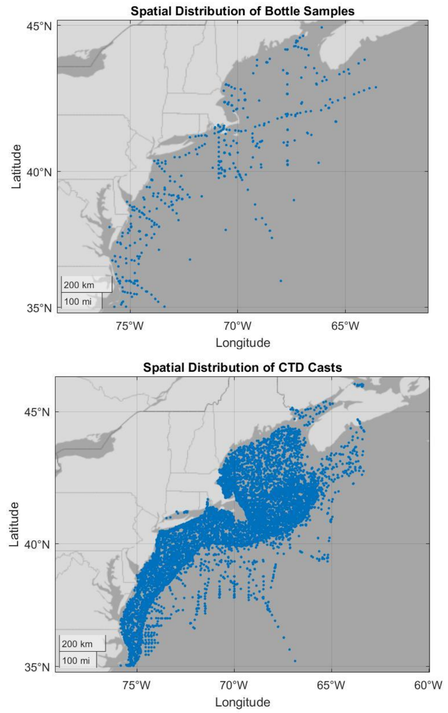

Figure 1. Spatial Distribution of Bottle Samples (Top) and CTD Casts (Bottom). Bottle samples have measures of TA and DIC, CTD cast measurements are used to model TA and DIC where measures aren't available.

Methods

To compare modeled fCO_2, the publicly available Surface Ocean CO_2 Atlas (SOCAT) was used as a source of underway fCO_2 values measured at 5m depth.

fCO_2 was calculated from measured or modeled TA and DIC using CO2SYS (v. 1.1). Surface ocean chemistry was calculated from a mean of values from a depth range.

Surface fCO_2 was then compared to SOCAT fCO_2 values by matching SOCAT datapoints within a specified radial distance and collection date range of the modeled and bottle datapoints. Multiple depth, distance and time ranges were used and compared for the best fit. fCO_2 comparisons were analyzed using Root Mean Square Error and models of linear fit.

Results

-Best fit occurred with:

- Surface depth defined as 2-8m
- Spatial Range of 1km
- Temporal Range of 3 days

-RFR and Biogeochemical MLR were biased to overestimate fCO_2 (Fig. 2)
-Calculated fCO_2 from bottle data generated a similar bias as the modeled data (Fig. 2)
-Physical MLR showed no clear relationship with the SOCAT data (Fig. 2)
-Salinity and sea surface temperature were well matched between the SOCAT data and measurements used to model

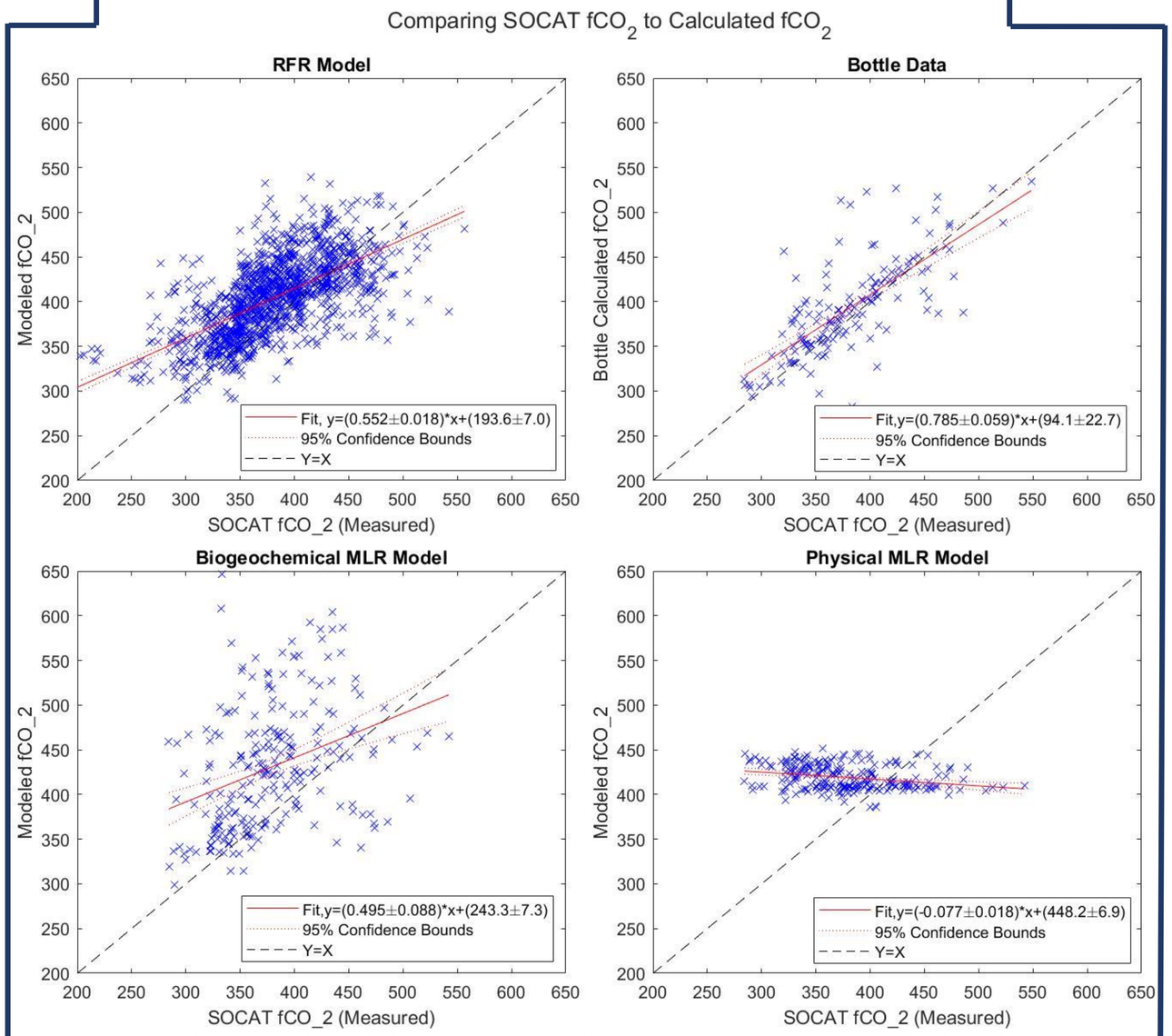

Figure 2. Direct comparisons of SOCAT fCO_2 (measured in µatm) with modeled/bottle data with linear fits.

Conclusions

Extrapolating carbonate models beyond the parameters they are intended to predict should be done with an abundance of caution.

For the Northeast US, it is suspected that CO2SYS fails to accurately predict fCO_2 due to high contributions of organic alkalinity for which CO2SYS has not accounted. As such, linear models were used to generate corrections for the models and bottle samples to make fCO_2 values extrapolated from DIC and TA closer to reality (Fig. 3)

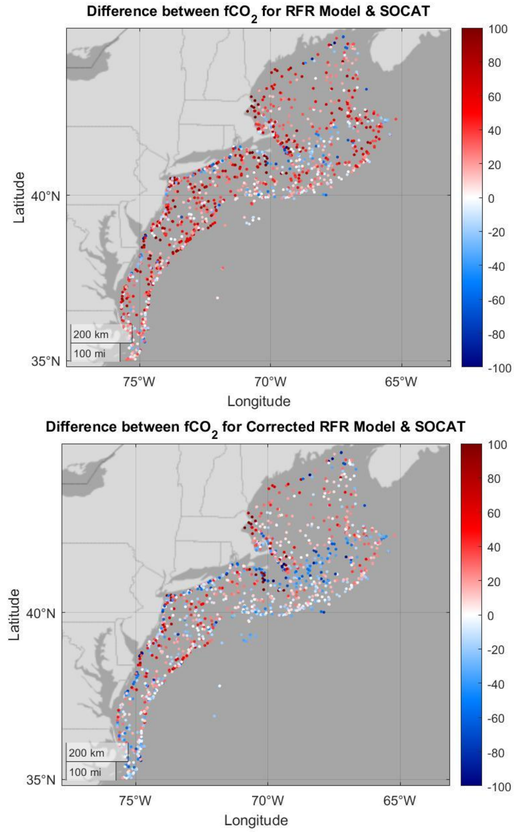

Figure 3. Spatial distribution of fCO_2 difference (Model-Measured) for model before correction (Top) and after correction (Bottom)

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[1]McGarry, K., Siedlecki, S. A., Salisbury, J., & Alin, S. R. (2021). Multiple linear regression models for reconstructing and exploring processes controlling the carbonate system of the northeast US from basic hydrographic data. *Journal of Geophysical Research: Oceans*, 126, e2020JC016480. https://doi.org/10.1029/2020JC016480