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Interactive comment on "Estimating total alkalinity for coastal ocean acidification monitoring at regional to continental scales in Australian coastal waters" *by* Kimberlee Baldry et al.

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"The manuscript "Estimating total alkalinity for coastal ocean acidification monitoring at regional to continental scales in Australian coastal waters" by K. Baldry and co-workers reports and discusses an approach to estimate total alkalinity (TA) in coastal waters with the intention to characterize vulnerability or resilience of such waters with respect to ocean acidification. The authors employ field data of TA and of further ocean water properties to derive a suite of models to parameterize TA. In summary I have serious concerns and reservations with the paper, such that I unfortunately cannot recommend publication of the paper at its present state. I do see some potential to

improve the paper, however this would require a major overhaul of the paper. I hope the authors could make some use of my comments in order to do so. 1: In fact the paper stops, where it should start. As far as I understood the paper, the paper only takes TA and related properties to derive a suite of algorithms/models to re(!)compute TA. The following discussion then compares the TA computation with the observed TA, but nothing goes beyond the use to the variables, which have been used to train the regressions. Thus, there is no estimation of TA, so far it appears to be a recompilation only. I was searching for some time for the application of these regressions, which goes beyond training, and eventually discovered a 2-line statement about Figure 6 – which is for illustrative purposes only? Frankly, what is the usefulness of a colorful Figure for illustrative purposes? In my view this is the point where the paper should start, including detailed validation with respect to data, including data, which have not been used to train the regressions. In essence, anything prior to ïňĄgure 6 is an extended methods section."

Response: The paper aims to assess the validity of employing a uni-parameter model, relating alkalinity to salinity, for the study of the ocean carbonate system in costal areas, particularly around Australia. In no way was it suggested that the authors were characterising the biogeochemistry of the Australian coastline by constructing a distribution from empirical relationships, but rather exploring its heterogeneity and the sources of error that could arise through the use of a well accepted method due to coastal processes. This is why TA was recomputed from the algorithms, to assess if the modeled TA had a significantly different distribution to observed TA, and that variability had been captured effectively by the model. The test was bootstrapped to account for the paired data set. By employing the use of AIC values we attempt to prevent over-fitting, as the calculation for AIC has a penalty term for the addition of explanatory variables. In statistical theory, this is equivalent to minimizing the cross-validation term (CV), a common term used to choose optimum models, and the term employed by Lee et al. (2006). This is proven in Stone (1977).

Figure 6 is only intended to highlight the capabilities, if enough effort is put into understanding the empirical estimation of TA. As mentioned in the manuscript, the authors understand that unreasonable extrapolation is performed in constructing this figure, particularly as the heterogeneity around the coastline is larger than the number of points sampled, and the distance around which the algorithms hold has not been explored due to the absence of data. The authors agree that this plot can be easily misinterpreted and draw attention away from the main objectives; hence it has been removed in the revised manuscript.

We thank the reviewer for their concerns regarding the objectives of the manuscript. The review process has given us the opportunity to expand the analysis. . A new draft manuscript is attached in the author comments of the main discussion for your consideration. However, the authors respectfully feel that any further discussion on the distribution and drivers of TA in the coastal waters of Australia would be too speculative, as we have shown that the heterogeneity around the entirety of the Australian coastline cannot be fully captured with the current sampling effort.

"2: The application of the newly obtained regressions to independent data is particularly relevant to such an approach, as the causal relationship between TA and the regression properties is not clear or even not given. The extrapolation of pure empirical relationships, i.e., regression coefficients, bears the massive risk, that these only hold true within their framework of training, or trained data. It might well be the case that the extrapolation does work very well, it could also be the opposite. Figure 6 should have been the first step to open this discussion. Along these lines the justification or even explanation of regression parameters falls short, specifically with respect to the non-conservative parameters: A: Amongst the most powerful characteristics of TA is its temperature INDEPENDENCE. Open ocean TA vs. temperature relationships are not much more than masked TA-depth relationships, if at all. If you refer to temperature as (partial) TA proxy, please explain and justify, why it is used. What about seasonality, and which processes does such a relationship mimic? B: In a similar manner the used

of Chl-a as partial TA proxy should be discussed. What thought does support this? Why are water column inventories used rather than actual concentrations? The satellites do not sense the water column inventory of Chla, they "see" the upper most layer? Also an important point to be considered here are the problems of remotely sensed Chl-a values in coastal waters (case 1 vs case 2 waters). The authors mention initially that Australia's coastlines pans 33 degrees in latitude, which likely causes vastly different organic matter composition of such coastal waters. C: The use of nitrate should be justified here as well. What does it stand for, maybe as runoff proxy, or proxy for biological metabolism?"

Response: Thank you for raising this query, the authors felt that enough literature around the use of chosen variables had been published and widely accepted, and that the introduction to the manuscript explained the reasoning behind variable choice, however this is evidently not the case. We have included a section for model justification in the methods as a result. Please also see the discussion below:

The use of a uni-parameter model for the estimation of TA in coastal area is generally inadequate as usually there are more than two water masses mixing, with e.g. upwelling and river end members having variable effects over time, which alone is enough reason for the model to fail. In a region that exhibits the mixing of n end-members, a model with at least n-1 conservative explanatory variables must be employed in order to account for all conservative variability. Temperature is a conservative variable, and yes, it does not directly effect TA, but rather it indirectly is related to TA, when a cold water mass mixes with a warmer water mass, such as when upwelling occurs, which we know has seasonal variability and is not constant (Jiang et al. 2014, Lee et al. 2006, Millero et al. 1998, Ingrosso et al. 2016). Thus, the inclusion of two conservative parameters seems relevant to model the coastal region, which most often experiences the mixing of at least three water masses (river end-member, coastal end-member, offshore end-member, upwelling water mass). The inclusion of a third explanatory variable (NO_3^- or Chl-a) offers a seasonal tracer to account for seasonal variations in TA due to primary production, or river flow (river flow can only be captured by NO3- as discussed in the manuscript). To illustrate the casual relationships of the chosen variables (S, Temp, Chl-a) more clearly we will include a conceptual graphic in the introduction. As Landimayer et al. (2016) explains, indirect linkages have been exploited to study environmental surrogates in numerous cases, and is a viable method. The complexity of the problem can be illustrated by Figure 1 which is now included in the introduction. Please find the full caption below:

Figure 1: A depiction of a two end-member mixing model that contains an open ocean end-member (O) and a variable fresh-water end member (FW). Solid lines indicate different conservative mixing lines. Point A lies in the conservative mixing region, however an arrow indicates how it can be perturbed away from conservative mixing predictions by a non-conservative change in TA to point A'. Thus, there are three distinct modes of variability; FW variability, conservative mixing, and non-conservative changes in TA. The mixing of two oceanic end members in coastal regions it also very likely, further complicating the problem, and extending the region of variability, indicated by the addition of O' in the model, and associated mixing lines (dashed lines).

"Why are water column inventories used rather than actual concentrations? The satellites do not sense the water column inventory of Chla, they "see" the upper most layer?"

The authors note that the use of a water column inventory for Chla was a mistake in the previous version and such a method would not be statistically viable, as the TA observations were taken from multiple depths within this water column, so taking the inventories decreases model power. This was also bought to the attention by Reviewer 1, and consequently the algorithms presented for Base Model 3 now use discrete Chla measurements. Please see the manuscript in the author comments for changes.

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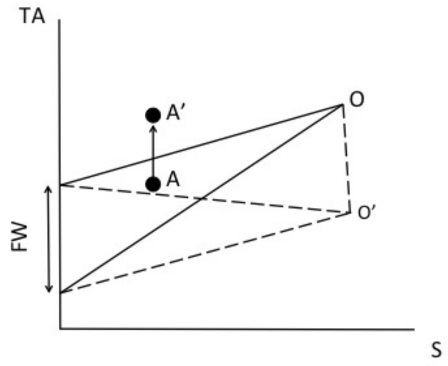

Fig. 1. A depiction of a two end-member mixing model that contains an open ocean end-member (O) and a variable fresh-water end member (FW). Solid lines indicate different conservative mixing lines.