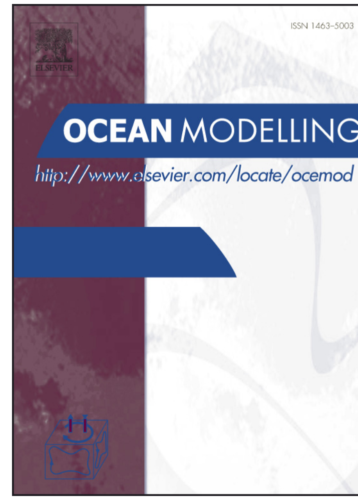
Accepted Manuscript



Short communication

Problems in *RMSE*-based wave model validations

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PII: S1463-5003(13)00141-8
DOI: http://dx.doi.org/10.1016/j.ocemod.2013.08.003
Reference: OCEMOD 841

To appear in: *Ocean Modelling*

Received Date: 11 May 2013
Revised Date: 9 August 2013
Accepted Date: 11 August 2013

Please cite this article as: Mentaschi, L., Besio, G., Cassola, F., Mazzino, A., Problems in *RMSE*-based wave model validations, *Ocean Modelling* (2013), doi: http://dx.doi.org/10.1016/j.ocemod.2013.08.003

Problems in *RMSE*-based wave model validations

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Abstract

In order to evaluate the reliability of numerical simulations in geophysical applications it is necessary to pay attention when using the Root Mean Square Error (*RMSE*) and two other indicators derived from it (the Normalized Root Mean Square Error *NRMSE*, and the Scatter Index *SI*). In the present work, in fact, we show on a general basis that, in conditions of constant correlation coefficient, the *RMSE* index and its variants tend to be systematically smaller (hence identifying better performances of numerical models) for simulations affected by negative bias. Through a geometrical decomposition of *RMSE* in its components related to the average error and the scatter error it can be shown that the above mentioned behavior is triggered by a quasi-linear dependency between these components in the neighborhood of null bias. This result suggests that smaller values of *RMSE*, *NRMSE* and *SI* do not always identify the best performances of numerical simulations,

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and that these indicators are not always reliable to assess the accuracy of numerical models. In the present contribution we employ the corrected indicator proposed by Hanna and Heinold (1985) to develop a reliability analysis of wave generation and propagation in the Mediterranean Sea by means of the numerical model WAVEWATCH III®, showing that the best values of the indicator are obtained for simulations unaffected by bias. Evidences suggest that this indicator provides a more reliable information about the accuracy of the results of numerical models.

Keywords: Model validation, *RMSE*, Scatter Index, WAVEWATCH III®, Mediterranean Sea

1. Introduction

Discussion and analysis of the behavior of statistical indicators employed for the evaluation of the performances of numerical models is often neglected due to their apparent simplicity. In some circumstances, anyway, their use can lead to conflicting and inconsistent results in trying to reproduce physical phenomena such as atmosphere dynamics or ocean wave generation and propagation (e.g. Willmott and Matsuura, 2005). Mentaschi et al. (2013) showed that some problem related to performances evaluation may occur if the analysis is based on the widespread indicator *NRMSE*, defined as

$$NRMSE = \sqrt{\frac{\sum_{i=1}^{N} (S_i - O_i)^2}{\sum_{i=1}^{N} O_i^2}} \tag{1}$$

where S_i is the ith simulated data, O_i is the ith observation and N is the number of observations available for the analysis. The problem arose clearly during a validation procedure of the wave model WAVEWATCH III®(WWIII, Tolman, 2009) for storm conditions in the Mediterranean Sea. The model has been run employing different parameterizations in order to find the optimal set for wave simulations in an enclosed basin. Namely, the source terms of wave growth-dissipation introduced by Ardhuin et al. (2010) have been used in its standard parameterizations BJA (Bidlot et al., 2007) and ACC350 [1]. Hence a sensitivity analysis has been performed in the parameters space in the neighborhood of the default values of ACC350 parametrization, varying each parameter keeping the others at their reference value. Source terms of growth-dissipation proposed by Tolman and Chalikov (1996), hereinafter TC, have been also used. An overall number of 43 different parameterizations have been tested on 17 different case studies corresponding to wave storms in the Mediterranean Sea. Simulated data have been compared against measurements obtained by 23 buoys belonging to the Rete Ondametrica Nazionale (RON, Italy) and to Boyas Puertos del Estado (Spain).

Figure 1: Comparison between significant wave height data measured by La Spezia buoy and those simulated by WWIII (ACC350 and TC parameterizations; February 1990 storm).

Results obtained in the framework of this research reported an underestimation of about 11% for significant wave height, and of about 8% for mean

[1] The acronym ACC350 refers to the authors F. Ardhuin, F. Collart and B. Chapron, who developed a term describing the long swell decay, based on a study of Synthetic Aperture Radar observations (Ardhuin et al., 2008, 2009)

period when the TC parameterization was used. Conversely the ACC350 parameterization led to results relatively unaffected by bias, overestimating the significant wave height of about 2%, and the mean period of about 1.5% (see table 2). As an example of this trend, figure 1 reports the observations of La Spezia buoy for significant wave height together with TC and ACC350 results, for February 1990 storm.

Values of correlation coefficient ρ were roughly the same for the two parameterizations, revealing a similar scatter component of the error. Therefore an indicator combining information on the average and the scatter error, like $NRMSE$, was expected to identify ACC350 as the best overall parameterization. However the value of $NRMSE$ hinted at better results for TC than for ACC350 (see table 2 where the overall value of normalized bias $NBI = \left(\bar{S} - \bar{O}\right)/\bar{O}$, correlation coefficient ρ and $NRMSE$ are reported for the two parameterizations).

In the present contribution we show that this issue can be extended generally to the $RMSE$ error indicator, defined as

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(S_i - O_i\right)^2} \tag{2}$$

and to its normalized form ($NRMSE$). Furthermore, subtracting the average component of the error we obtain the Scatter Index SI defined here as

$$SI = \sqrt{\frac{\sum_{i=1}^{N}\left[\left(S_i - \bar{S}\right) - \left(O_i - \bar{O}\right)\right]^2}{\sum_{i=1}^{N} O_i^2}}. \tag{3}$$

where $\bar{S}$ and $\bar{O}$ are the average simulation and observation values respectively.

In the next section the drawback of $RMSE$ is analysed using a synthetic serie of data and then analytically, presenting a systematic approach to outline and define the problem. A geometrical decomposition of $RMSE$ in its scatter and bias components is provided to better understand the dependency between these components and the proof of the shortcoming and the relative inaccuracy for SI, $NRMSE$ and $RMSE$ is developed. Section 4 is dedicated to show how to improve the evaluation of the performances by means of the corrected indicator introduced by Hanna and Heinold (1985), hereinafter HH from the name of the authors. Finally conclusions are drawn in section 5.

2. The idealized problem

The drawback of using the $RMSE$ as an indicator of the performances of a numerical simulation can be easily reproduced using an idealized time series. Let us for example consider an observation series given by:

$$O_i = 1 + \sin t_i, \qquad 0 < t_i < \pi \tag{4}$$

where t_i represents the time discretized in 120 time steps. We define a first mock simulation, given by

$$S_i^u = O_i + [\mathrm{mod}(i, 2) * 1.4 - 0.7] \tag{5}$$

where the function $\mathrm{mod}(i, 2)$ vanishes when i is even and it is equal to one when i is odd. The first mock simulation is thus given by the observation series plus a sawtooth function, and is clearly unaffected by bias, since the number of time steps is even (the superscript u in S_i^u stands for unbiased). We then define a second mock simulation multiplying the first one by a factor 0.87: $S_i^b = 0.87 \cdot S_i^u$. Simulation S_i^b has the same correlation coefficient as the observation series O_i and S_i^u, but is affected by a strong negative bias. The two mock simulations are shown in figure 2, together with the observation series. The black continuous line represents the observation series O_i, the blue line corresponds to the unbiased simulation S_i^u while the red line represents the biased simulation S_i^b. Clearly the best simulation between S_i^u and S_i^b is the unbiased one, S_i^u. Nonetheless the computation of $NRMSE$ and SI returns better values for S_i^b, as shown in table 1 where the values of correlation coefficient and bias are also reported.

Figure 2: (a) Unbiased mock simulation S_i^u and (b) biased mock simulation S_i^b represented against observations (black lines).

Simulation	ρ	NBI	$NRMSE$	SI
S_i^u	0.407	0 %	0.421	0.421
S_i^b	0.407	-13 %	0.389	0.367

Table 1: Statistical error indicators of S_i^u and S_i^b relative to O_i.

3. Formulation of the problem

Let us consider a set of N observations O_i of a measurable quantity (in our case the significant wave height and the mean wave period) and the corresponding values obtained by numerical model simulations. The use of different parameterizations for the numerical models results in different sets of N simulated values S_i, characterized by varying statistical parameters such as mean, standard deviation and higher order moments. Therefore the observations and their statistical parameters can be considered as invariant of the problem, while simulation results and their statistical parameters are the system variables. In order to measure the accuracy of the simulations we use the following statistical indicators:

- the bias
$$BI = \bar{S} - \bar{O} \tag{6}$$
which is an index of the average component of the error. A value closer to zero identifies a better simulation;

- the correlation coefficient
$$\rho = \frac{1}{N} \frac{\sum_{i=1}^{N} \left(S_i - \bar{S}\right) \left(O_i - \bar{O}\right)}{\sigma_S \sigma_O} \tag{7}$$
where σ_S and σ_O are the standard deviations of the simulations and the observations respectively. This quantity, which ranges between -1 and 1, is an index of the scatter component of the error, and a value closer to 1 indicates a smaller scatter of the simulated values around the observed ones.

The correlation coefficient has been chosen as the main indicator of the scatter component of the error since it remains roughly constant for all the simulations, outlining a constant behavior of the random error in our experiments. In the rest of the manuscript we therefore assume that changes in the parameters of the model do not alter the correlation coefficient. The behaviour of other indicators will be analysed varying the bias in the neighborhood of null bias.

The *RMSE* indicator combines informations on the average and on the scatter components of the error since it can be expressed in terms of bias and correlation coefficient

$$RMSE^2 = BI^2 - 2\rho\sigma_S\sigma_O + \sigma_S^2 + \sigma_O^2 \quad . \tag{8}$$

The behavior of *RMSE* in the neighborhood of null bias is not immediately arguable from (8) because the average and the standard deviation of the simulation are not independent. The dependency arises once the correlation coefficient is assumed to be constant. A set of simulations with constant ρ is obtained multiplying an unbiased simulation S_0 by an amplification factor $\alpha = (1 + NBI)$,

$$S_i = (1 + NBI)S_{0i} \tag{9}$$

$$\bar{S} = (1 + NBI)\bar{O} \tag{10}$$

$$\sigma_S = (1 + NBI)\sigma_{S0} \tag{11}$$

where σ_S is the standard deviation of S, σ_{S0} is the standard deviation of the corresponding unbiased simulation and *NBI* has been defined in the introduction.

Validity of (9)-(11) implies a constant value of ρ and, vice versa, a constant ρ implies the validity of (10) and (11). Let us assume a generic linear relationship between σ_S and $\bar{S}$ in the neighborhood of null bias:

$$\sigma_S = k\bar{S} + c \tag{12}$$

where k and c are arbitrary constants. We can now demonstrate that a constant value of ρ requires a zero value of the coefficient c, showing that σ_S and $\bar{S}$ are proportional. This proportionality means that relations (10) and

(11) must hold. To this purpose, if we consider two different simulations, S'_i and S''_i, such that their average values are related by a coefficient α, $\bar{S}'' = \alpha\bar{S}'$ and $\overline{S''O} = \alpha\overline{S'O}$, employing (12) it is possible to rewrite the standard deviation of S''_i as a function of $\bar{S}'$:

$$\sigma_{S''} = k\alpha\bar{S}' + c. \tag{13}$$

Using the above assumptions and the fact that $\overline{SO} = \bar{S}\bar{O} + \rho\sigma_S\sigma_O$, we find that a constant value of ρ requires a null coefficient c in relationship (12). Hence in the neighborhood of zero bias we obtain $\sigma_S = k\bar{S} \Rightarrow \sigma_S/\bar{S} =$ constant .

Using relationships (10) and (11) in (8) and differentiating with respect to NBI one finds a positive value of $\left.\frac{\partial RMSE}{\partial NBI}\right|_{NBI=0}$, meaning that $RMSE$ does not present a minimum for null bias, but decreases together with NBI. This fact shows the drawback of using the $RMSE$ as an indicator of the simulation performances, since for a constant value of the correlation coefficient the $RMSE$ attains lower values for simulations that underestimate the average (negative bias).

3.1. RMSE geometrical decomposition

The $RMSE$ indicator can be decomposed in its components proportional to the average deviation between simulations and observations and to the scatter of the values around the average. This decomposition provides a geometrical insight into the fact that the described drawback is due to a dependency between the two components. Let us define the scatter component SC_{RMSE} as the root mean square deviation between the simulation and the

Figure 3: $RMSE$ represented as a vector in $SC_{RMSE} - BI$ Cartesian space.

observation series subtracted of their average values

$$SC_{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} [(S_i - \bar{S}) - (O_i - \bar{O})]^2}{N}} \quad . \tag{14}$$

In the case of an unbiased simulation, SC_{RMSE} and $RMSE$ coincide. If simulations and observations have the same standard deviation and their correlation coefficient is equal to 1, SC_{RMSE} vanishes. It can be easily shown that the $RMSE$ can be expressed as the quadratic sum of the scatter component and the bias BI

$$RMSE^2 = SC_{RMSE}^2 + BI^2 \quad . \tag{15}$$

Expression (15) shows that from a geometrical point of view the two contributions are orthogonal and $RMSE$ can be represented as a vector in $SC_{RMSE} - BI$ Cartesian space (see figure 3). Moreover, the Scatter Index SI can be written in terms of the SC_{RMSE} as:

$$SI^2 = \frac{\sum_{i=1}^{N} [(S_i - \bar{S}) - (O_i - \bar{O})]^2}{\sum_{i=1}^{N} O_i^2} = \frac{SC_{RMSE}^2}{\overline{O}^2 + \sigma_O^2} \quad . \tag{16}$$

It is easy to derive a relationship analogous to (15) for $NRMSE$:

$$NRMSE^2 = SI^2 + BC_{NRMSE}^2 \tag{17}$$

where BC_{NRMSE} is the bias component of the $NRMSE$, proportional to the NBI

$$BC_{NRMSE} = NBI \sqrt{\frac{\overline{O}^2}{\overline{O}^2 + \sigma_O^2}} \quad . \tag{18}$$

Expression (17) provides a representation of $NRMSE$ as a vector in $SI - BC_{NRMSE}$ space. It is useful to remark that $RMSE$ and its variant $NRMSE$ present the same behavior in all respects, and the drawbacks of $RMSE$ are identically shared by $NRMSE$.

Figure 4: Panels (a) and (b): correlation coefficient versus normalized bias for significant have height and mean period. Panels (c) and (d): BC_{NRMSE} versus SI for significant have height and mean period. Blue lines represent expression (21). Red triangles represent the sensitivity analysis in the neighborhood of ACC350.

3.2. Scatter Index, NRMSE and RMSE systematic deviation

SI and BC_{NRMSE} appearing in expression (17) are orthogonal but not necessarily independent and a relationship can be found for a set of simulations presenting a constant value of ρ.

The scatter component of $NRMSE$, SI, can be expressed in terms of the standard deviations of observation and simulation

$$SI^2 = \frac{\sigma_S^2 + \sigma_O^2 - 2\rho\sigma_O\sigma_S}{\overline{O}^2 + \sigma_O^2} \quad . \tag{19}$$

Hence using (10) and (11) SI can be expressed as a function of NBI, and assuming that $\sigma_{S0} \sim \sigma_O$, i.e. the standard deviations of the unbiased simulation and of the observation series are roughly equal, it is possible to write

$$SI^2 \sim \frac{\sigma_O^2}{\overline{O}^2 + \sigma_O^2}\left[NBI^2 + 2(1-\rho)NBI + 2(1-\rho)\right] \quad . \tag{20}$$

The first derivative of SI^2 with respect to NBI in the neighborhood of null NBI is always positive, hence SI is not minimum for null bias. A first order expansion of SI in the neighborhood of $NBI = 0$ returns

$$SI \sim SI_0\left(1 + \frac{1}{2}NBI\right) \tag{21}$$

where SI_0 is the Scatter Index of the unbiased simulation.

Figure 5: Hypothetical unbiased simulation versus minimum $NRMSE$ simulation in $SI - BC_{NRMSE}$ Cartesian space. Given expression (21) (the blue line), minimum $NRMSE$ simulation is affected by negative bias.

Relationship (21) fits quite well the results of our experiments as shown in figure 4, where each point represents a different parameterization: blue ones refer to ACC350, black ones to TC and the red ones represent the results of the sensitivity analysis in the parameter space in the neighborhood of ACC350 (see section 1).

In panels (a) and (b) the correlation coefficient ρ is plotted versus the NBI for both significant wave height and mean period, showing that ρ is roughly constant as required by the considerations done in section 3. In panels (c) and (d) results are plotted in the $SI - BC_{NRMSE}$ space revealing that they lie roughly on the blue line which represents expression (21). Quite surprisingly the parameterization most affected by negative bias, i.e. TC, is the one with the best value of the Scatter Index for both significant wave height and mean period. This finding reveals that, under the assumptions outlined in section 3, the Scatter Index tends to be systematically better for simulations characterized by a negative bias. Furthermore, it is well evident that $NRMSE$ is affected by the same drawback since the latter can be represented as a vector in the $SI - BC_{NRMSE}$ space. Indeed the simulation with the best possible value of the $NRMSE$ is not the unbiased one but the one perpendicular to the line of the points in $SI - BC_{NRMSE}$ space satisfying relationship (21), as reported in figure 5. Considerations drawn for $NRMSE$ can be easily generalized to $RMSE$, given the correspondence between relations (17) and (15).

The behavior of $RMSE$ described in this section tends to be more pronounced when the correlation coefficient is significantly smaller than 1. This can be deduced observing that the Scatter Index, expressed by relation (20), assumes a minimum value for $NBI = \rho - 1$. Therefore the drawback of using $RMSE$ is more relevant when the scatter component of the error is large.

4. A corrected indicator

The discussion presented in section 3 clearly shows that lower values of $RMSE$, $NRMSE$ and SI are not always associated to better performances of numerical models and that those indicators are not always reliable estimators of simulations accuracy. Notwithstanding this kind of behavior their use is widespread in many scientific fields (e.g. Komen et al., 1994; Fekete et al., 2005; Persson, 2011). To overcome this problem Hanna and Heinold (1985) proposed the exploitation of a corrected statistical indicator defined as

$$HH = \sqrt{\frac{\sum_{i=1}^{N}(S_i - O_i)^2}{\sum_{i=1}^{N} S_i O_i}} \quad . \tag{22}$$

It is straightforward to show that HH can be expressed in terms of simulation and observation average values, standard deviations and correlation coefficient as follows

$$HH^2 = \frac{\overline{S}^2 + \sigma_S^2 + \overline{O}^2 + \sigma_O^2}{\bar{S}\bar{O} + \rho\sigma_S\sigma_O} - 2 \quad . \tag{23}$$

Hence HH can be expressed as a function of NBI using (10) and (11), and assuming that $\sigma_{S0} \sim \sigma_O$ we can write

$$HH^2 \sim \left(\frac{\overline{O}^2 + \sigma_O^2}{\overline{O}^2 + \rho\sigma_O^2}\right)\left(\frac{NBI^2 + 2NBI + 2}{NBI + 1}\right) - 2 \quad . \tag{24}$$

The first derivative of HH^2 with respect to NBI results

$$\frac{\partial HH^2}{\partial NBI} \sim \left(\frac{\overline{O}^2 + \sigma_O^2}{\overline{O}^2 + \rho\sigma_O^2}\right)\left(\frac{NBI^2 + 2NBI}{NBI^2 + 2NBI + 1}\right) \tag{25}$$

which vanishes for null bias. The second derivative of HH^2 with respect to NBI is

$$\frac{\partial^2 HH^2}{\partial NBI^2} \sim \left(\frac{\overline{O}^2 + \sigma_O^2}{\overline{O}^2 + \rho\sigma_O^2}\right)\left(\frac{2}{(NBI + 1)^3}\right) \tag{26}$$

which is always positive for $NBI = 0$. Therefore HH is approximately minimum when the bias is null. This finding clearly does not imply the equivalence between bias and HH because, unlike bias, HH is able to capture the scatter component of the error.

This behavior can be noticed quite clearly in some wave generation/propagation simulations in the Mediterranean Sea, as reported in figures 6 and 7 where the corrected indicator HH is plotted versus NBI for all the parameterizations employed in the sensitivity study. Indeed, numerical simulations with the lowest value of HH tend to be closer to the line of null bias, while results with higher value of HH tend to be farther away from the vanishing bias conditions (compare results obtained with ACC350 and TC presented in figures 6 and 7 and those presented in figure 4). These findings are reported quantitatively in table 2 showing the different error estimations for the corrected HH indicator and for the other statistical indicators. The use of HH allows to correctly interpret the performances of numerical model simulations and their agreement with field observed data.

	ACC350		**TC**		**BJA**	
	H_s	T_m	H_s	T_m	H_s	T_m
NBI	2.1%	1.5%	-11.9%	-8.4 %	-4.6%	1.0 %
$\boldsymbol{\rho}$	0.883	0.640	0.889	0.659	0.885	0.639
NRMSE	0.2864	0.2424	0.2798	0.2395	0.2800	0.2485
HH	0.3460	0.2505	0.3634	0.2604	0.3502	0.2574

Table 2: Results of statistical indicators for significant wave height H_s and mean period T_m obtained for parameterizations ACC350, TC and BJA. Values computed for the ensemble of all storms and all buoys (29620 observations).

Figure 6: *HH* versus *NBI* for significant wave height. Red points represent the sensitivity analysis in the neighborhood of ACC350.

Figure 7: *HH* versus *NBI* for mean period. Red points represent the sensitivity analysis in the neighborhood of ACC350.

5. Conclusions

Small values of the widespread error indicators *RMSE*, *NRMSE* and *SI* are not always associated with the best performances of a numerical model reproducing natural processes such as atmosphere dynamics, ocean circulation or wave generation and propagation. In particular *RMSE* and its variants tend to assume values typical of better performances for simulations which underestimate the measured physical quantities (i.e. wind speed, wave height...). Through a geometrical decomposition of the *RMSE* indicator in its average and scatter components it has been possible to demonstrate that the above mentioned drawback relies on a linear dependence between the two components in the neighborhood of null bias. It has also been shown that this deviation is more noticeable when the scatter component of the error is large, i.e. when the correlation coefficient is appreciably lower than unity. To overcome this issue the error indicator *HH*, introduced by Hanna and Heinold (1985) has been employed. It has been shown that *HH* attains a minimum value for null bias when $\sigma_{S0} \sim \sigma_O$ is assumed. Evidences from wave generation and propagation analysis in the Mediterranean Sea suggest that the *HH* indicator provides a more reliable and accurate information about the accuracy of a numerical simulation than the *RMSE* indicator.

Acknowledgements

The Authors would like to thank Gabriele Nardone from ISPRA, who provided us with RON buoys data, and Pilar Gil from Puertos del Estado for the Spanish buoy data. Special thanks go to Marcello Magaldi for his advices and suggestions. This work has been supported by the RITMARE Flagship Project funded by the Italian Ministry of University and Research. GB has been funded by MIUR in the framework of ”Azioni Integrate Italia-Spagna”.

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Figure 1

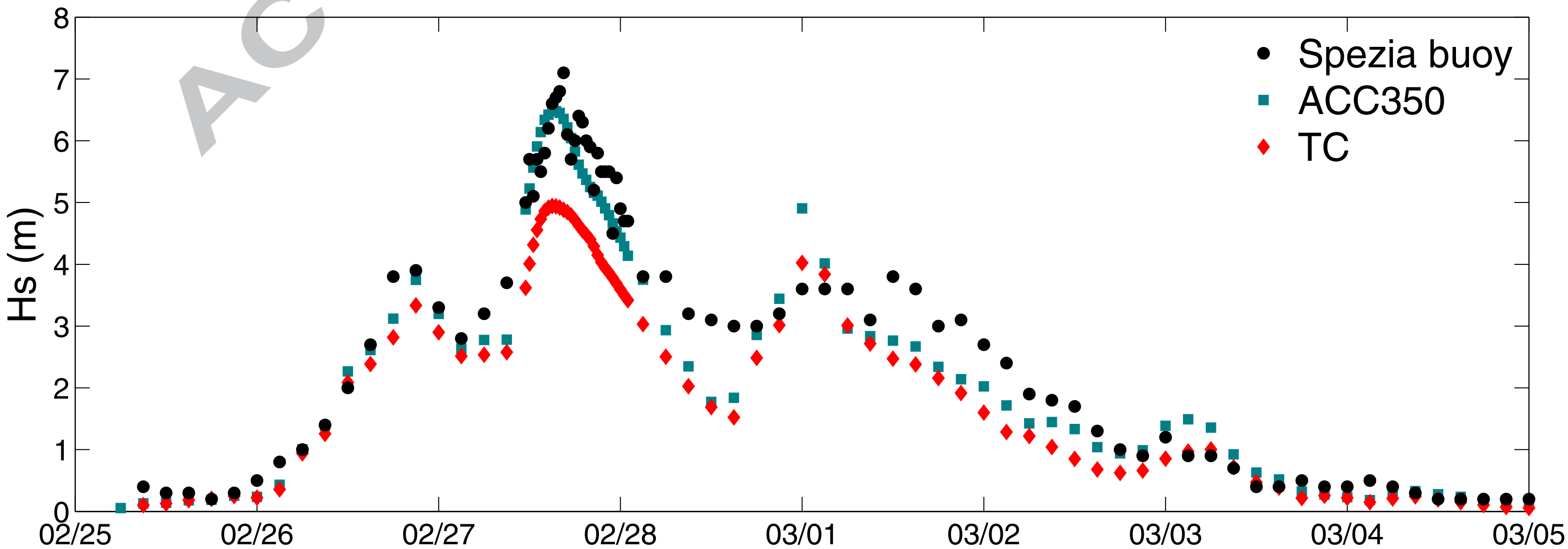
Spezia buoy
ACC350
TC
Hs (m)
0
1
2
3
4
5
6
7
8
02/25
02/26
02/27
02/28
03/01
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Figure 2 (a)

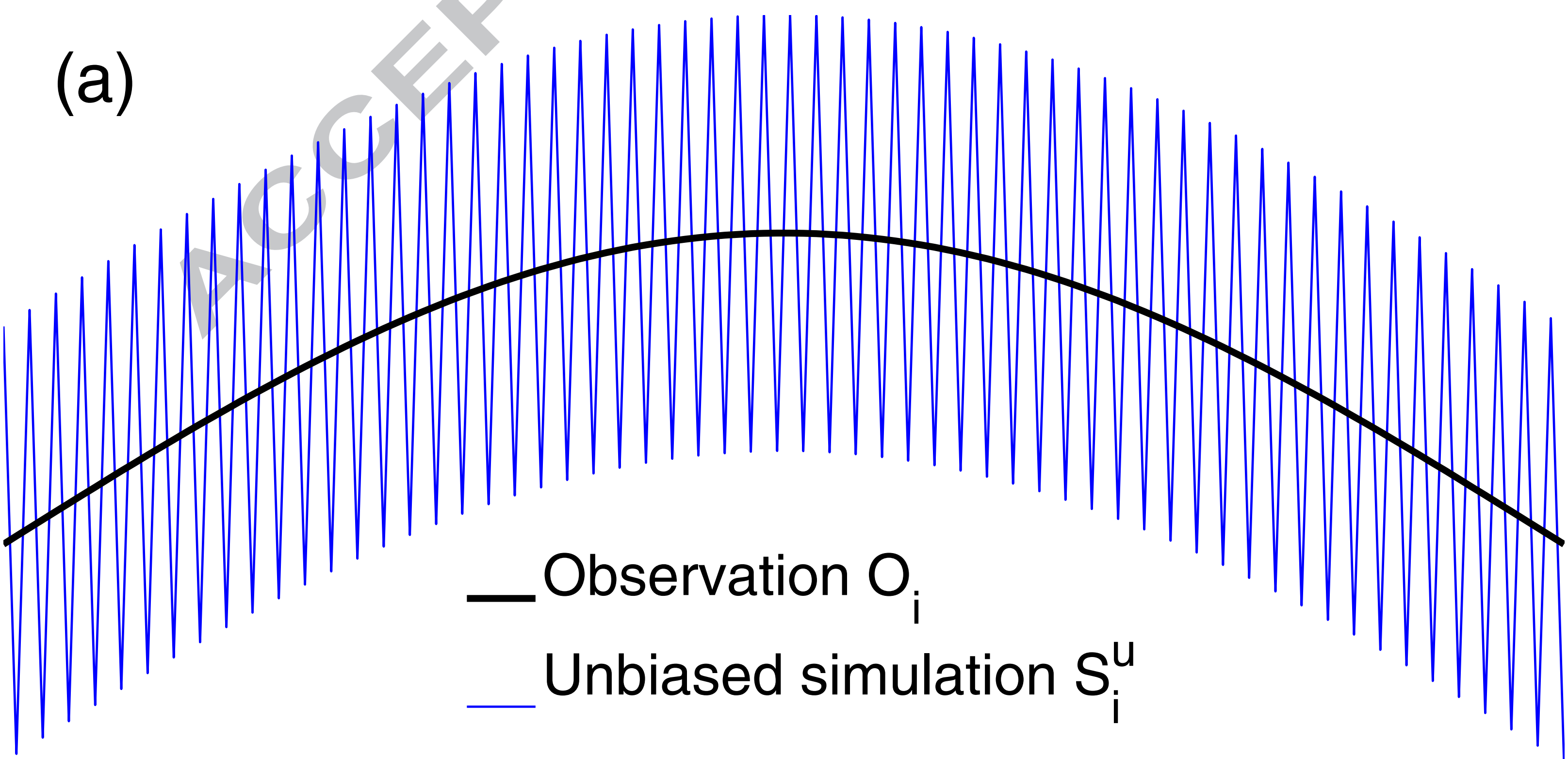


Figure 2 (b)

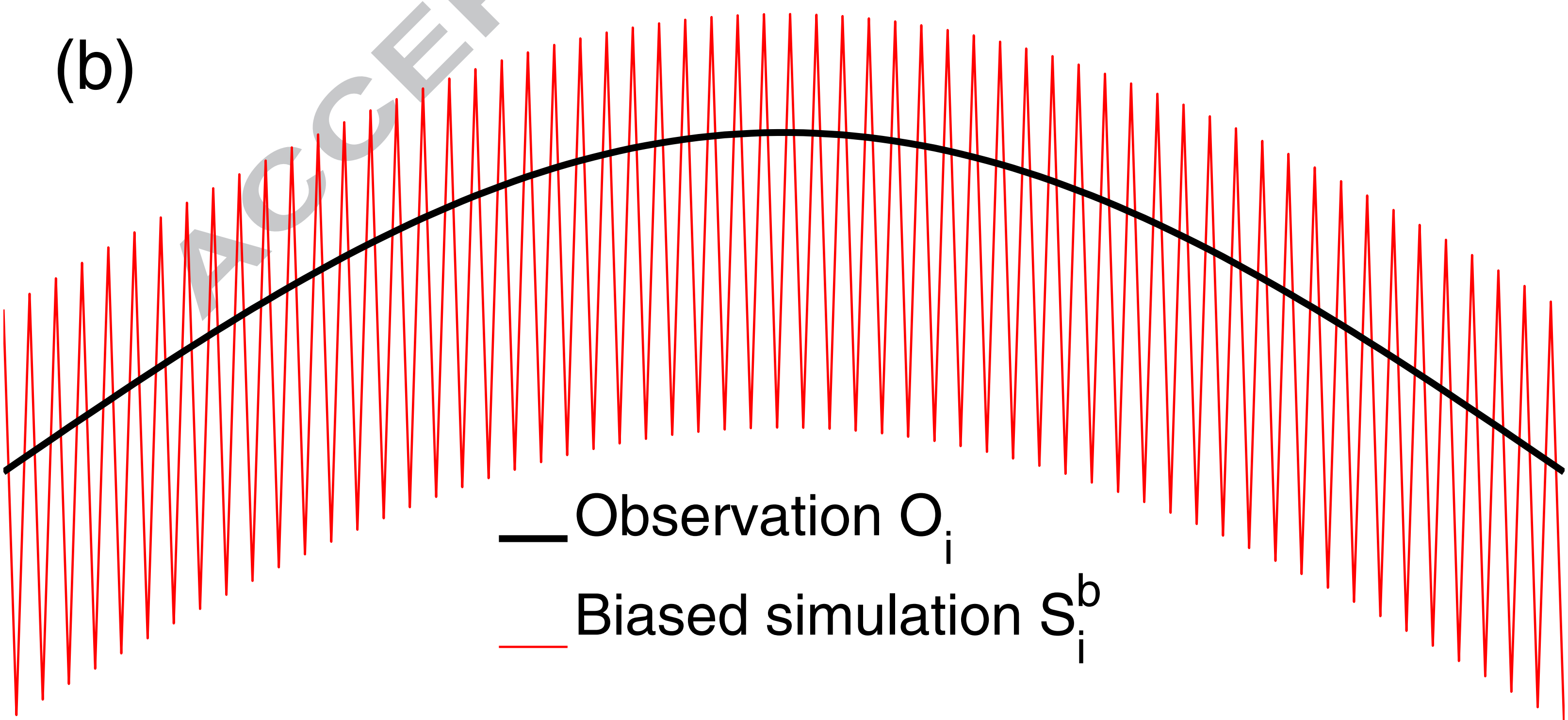


Figure 3

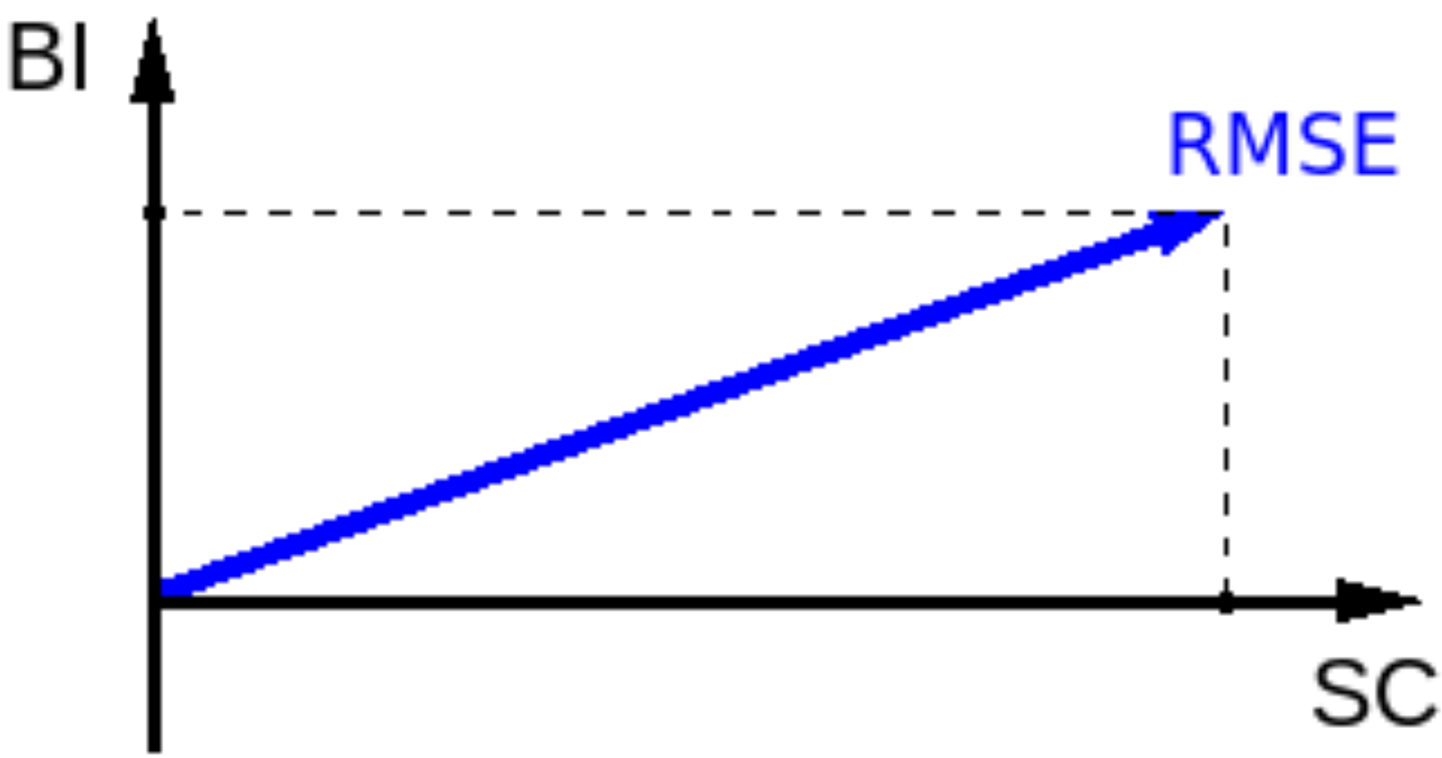
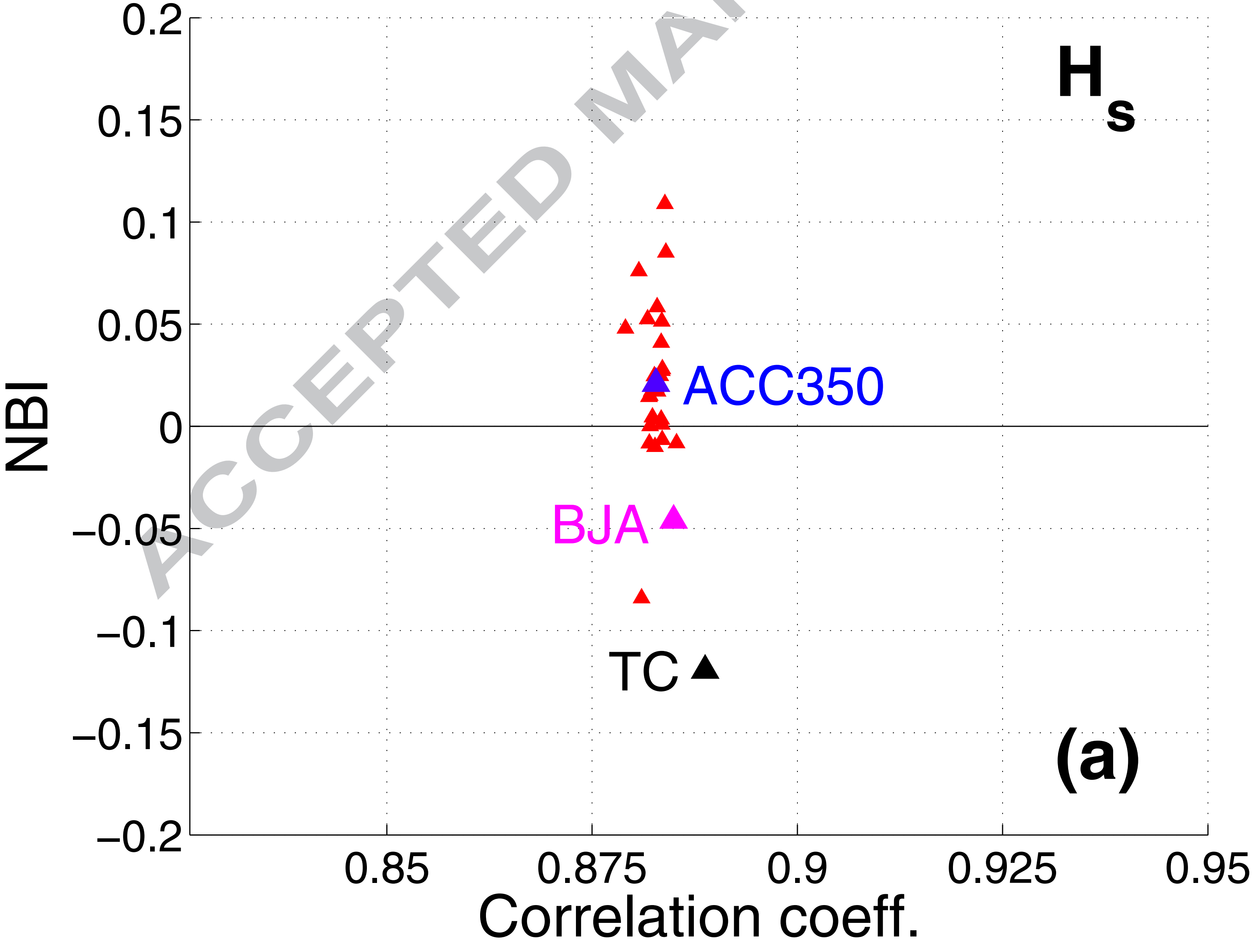
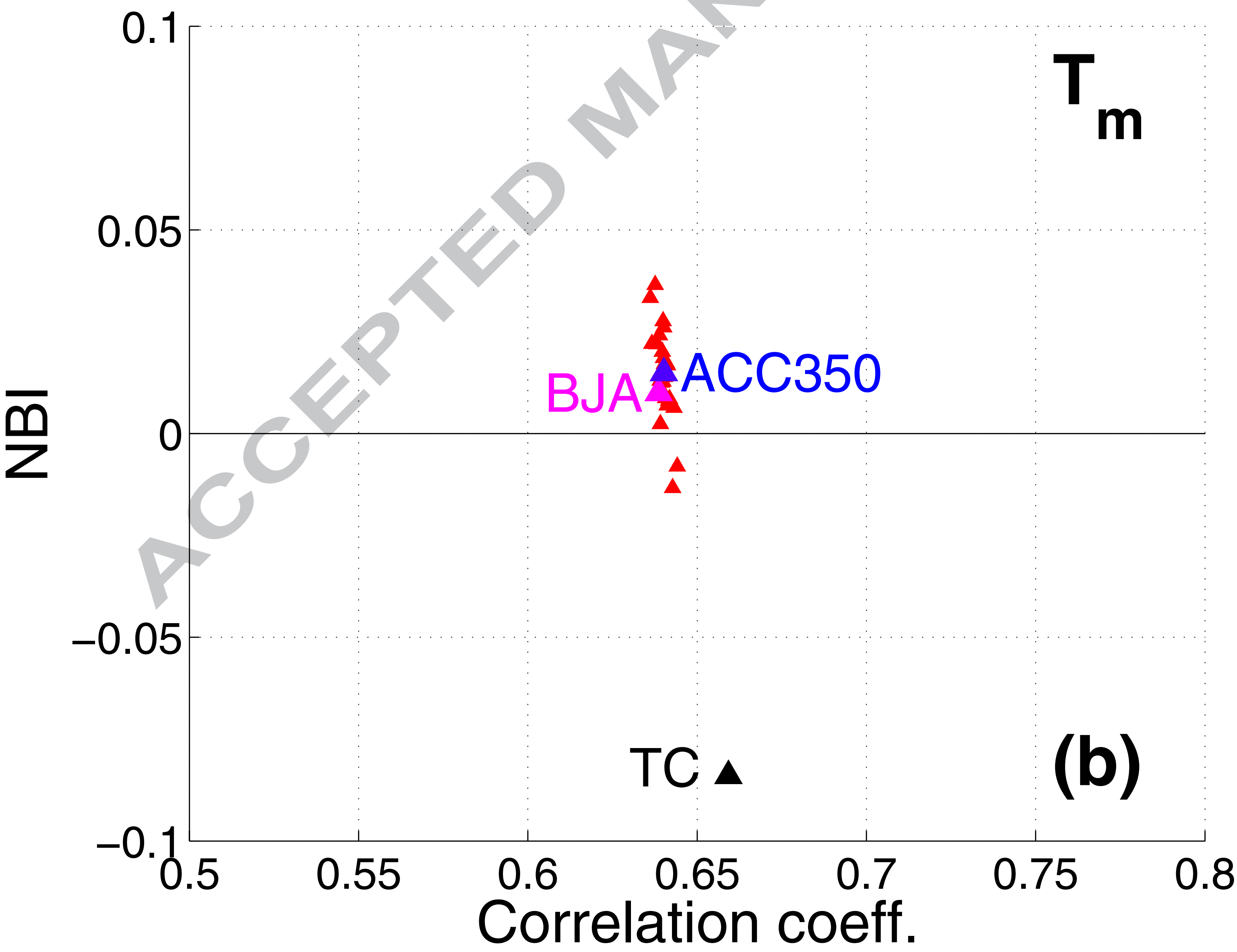


Figure 4 (a)



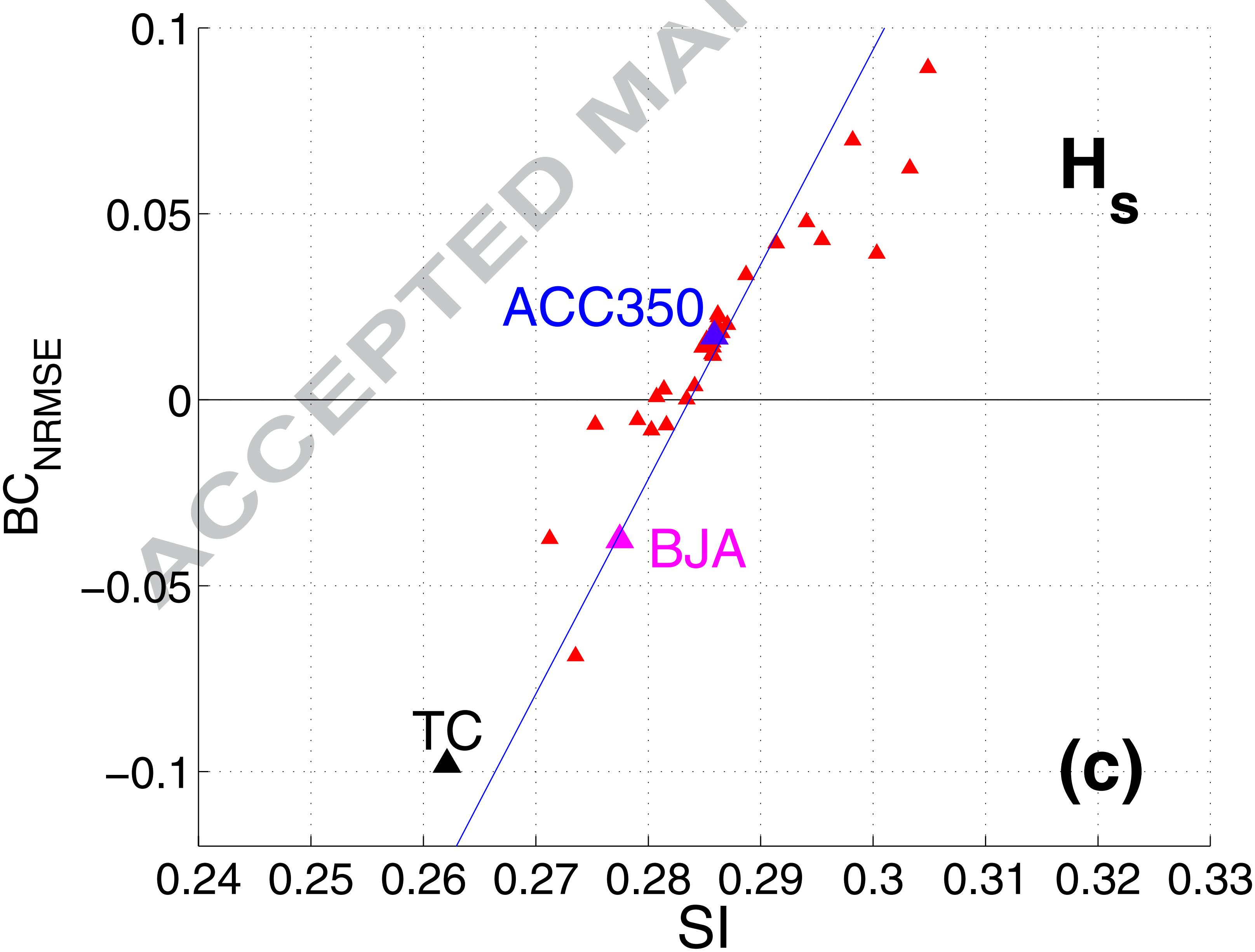
H
s
ACC350
BJA
TC
(a)
NBI
Correlation coeff.
0.2
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
−0.2
0.85
0.875
0.9
0.925
0.95

Figure 4 (b)



T_m
NBI
Correlation coeff.
0.1
0.05
0
−0.05
−0.1
0.5
0.55
0.6
0.65
0.7
0.75
0.8
BJA
ACC350
TC
(b)

Figure 4 (c)



0.1
0.05
0
−0.05
−0.1
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
0.32
0.33
SI
BC$_{NRMSE}$
H$_s$
ACC350
BJA
TC
(c)

Figure 4 (d)

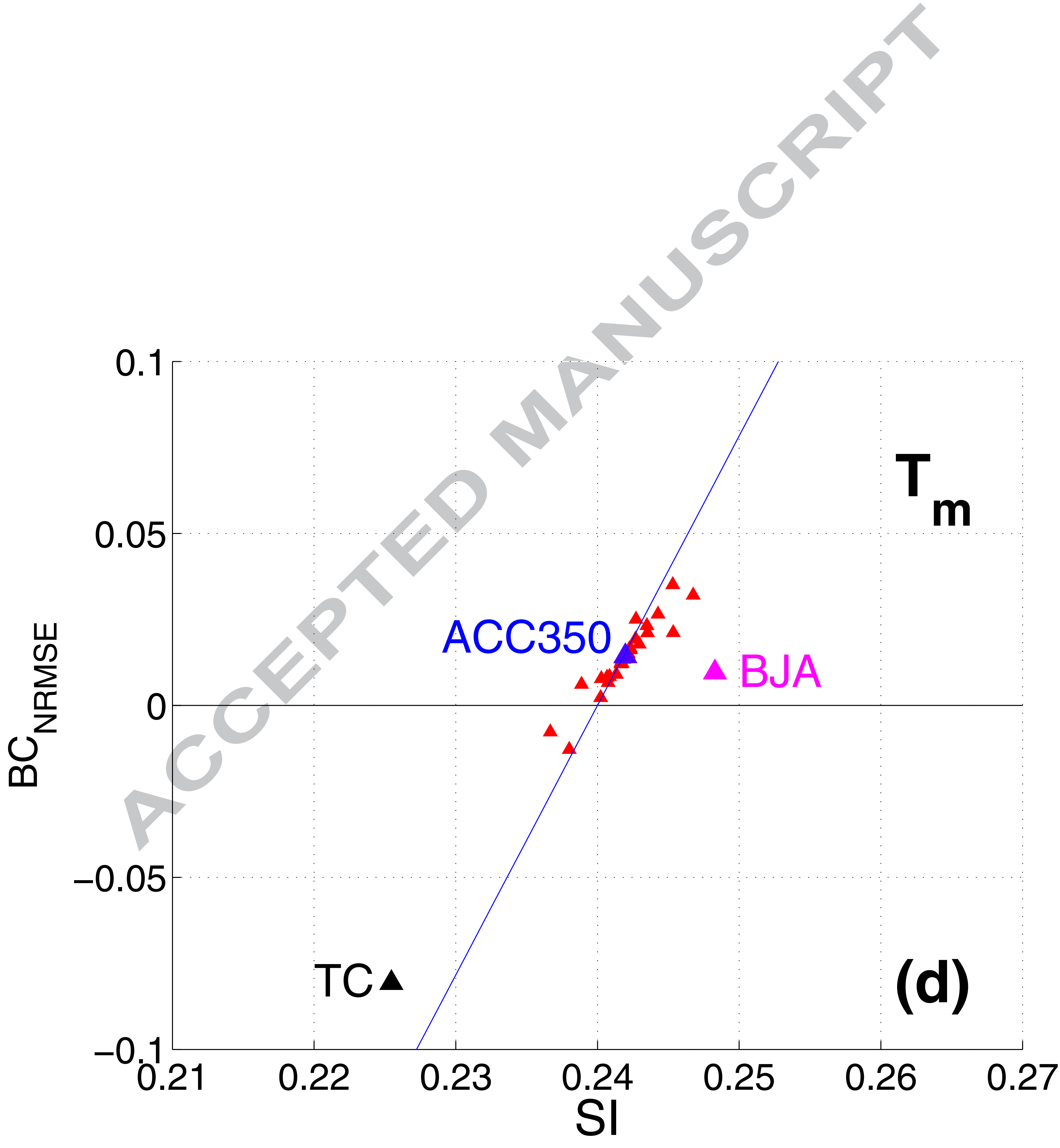

0.1
0.05
0
−0.05
−0.1
0.21
0.22
0.23
0.24
0.25
0.26
0.27
SI
BC_NRMSE
T_m
ACC350
BJA
TC
(d)
ACCEPTED MANUSCRIPT

Figure 5

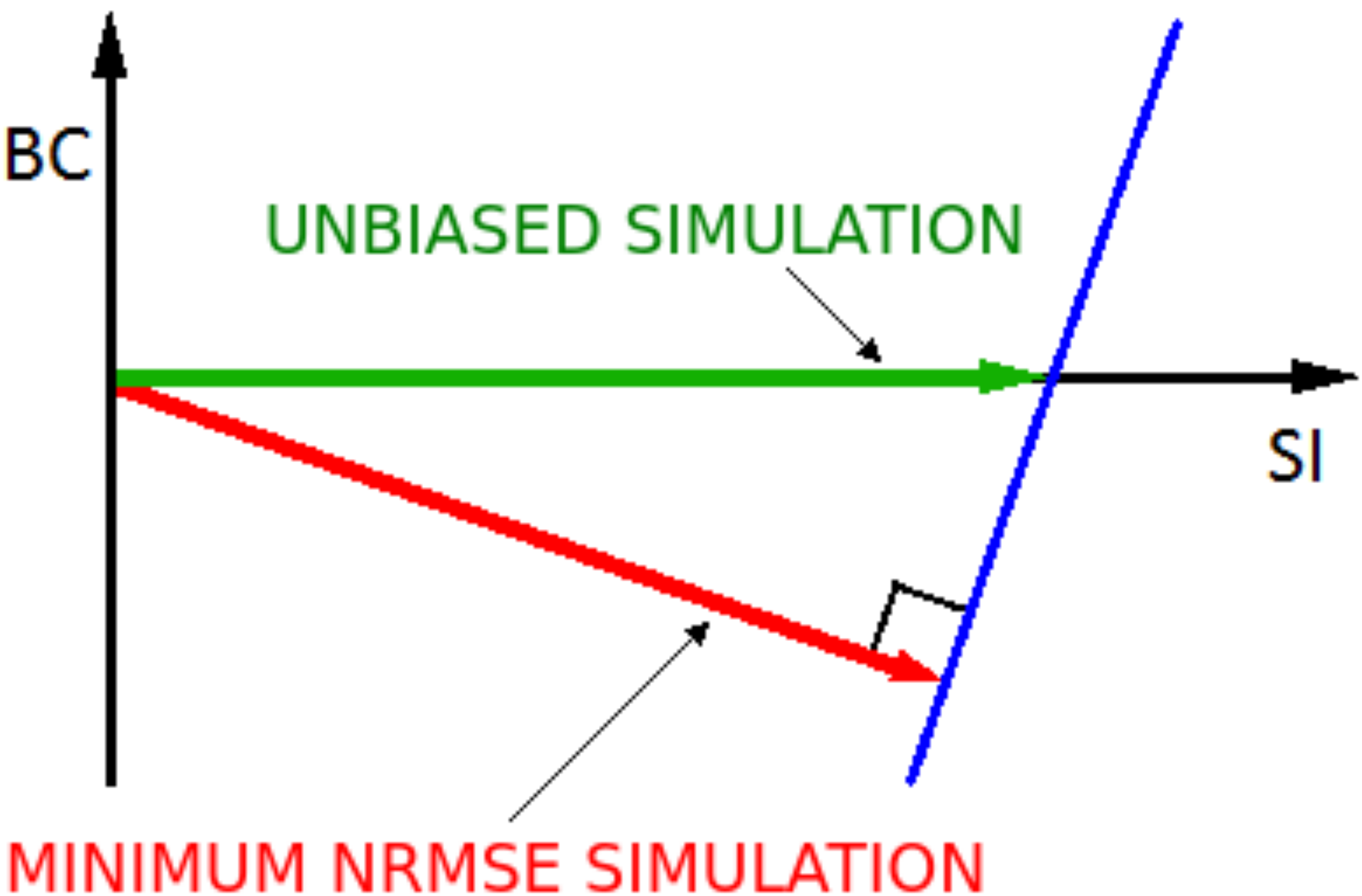
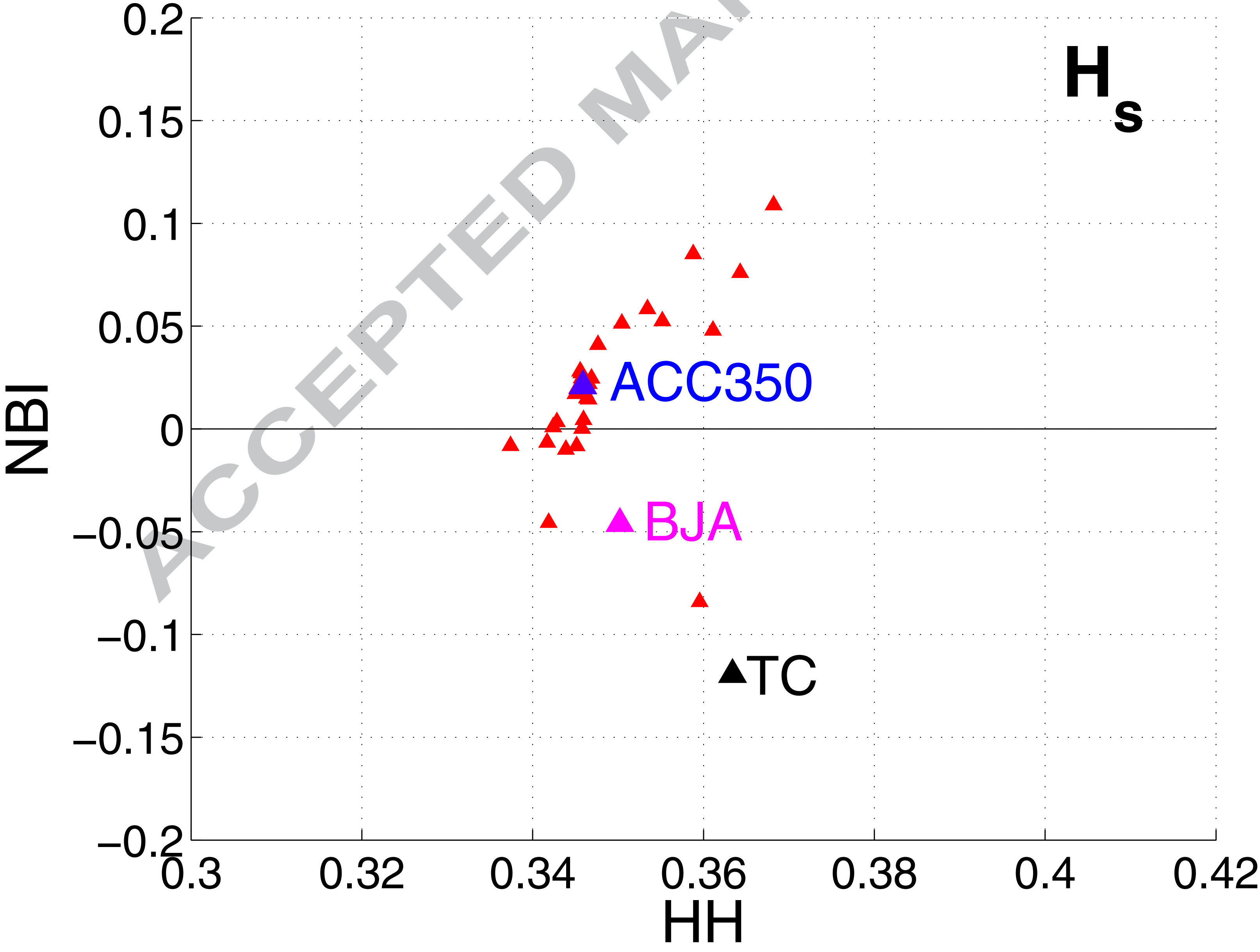
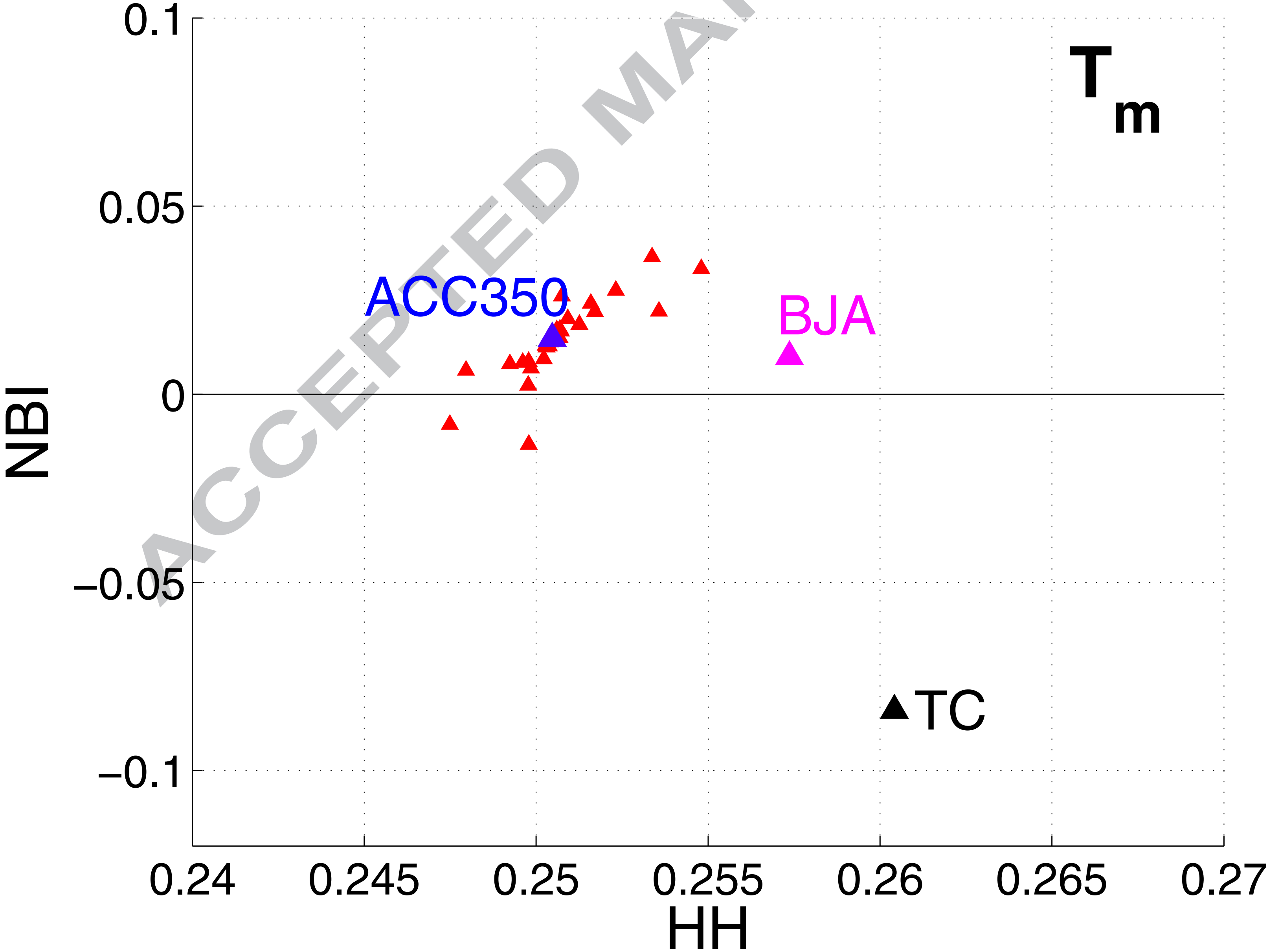


Figure 6



H
s
NBI
HH
ACC350
BJA
TC
0.2
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
−0.2
0.3
0.32
0.34
0.36
0.38
0.4
0.42

Figure 7



T_m
ACC350
BJA
TC
NBI
HH
0.1
0.05
0
−0.05
−0.1
0.24
0.245
0.25
0.255
0.26
0.265
0.27

Highlights

- RMSE tends to be better for simulations that underestimate the average.
- This trend is more noticeable when the correlation coefficient is appreciably lower than unity.
- The issue is due to a dependency of the scatter component of the RMSE on the bias.
- HH indicator provides a more accurate information on the accuracy of a simulation.