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1 Meteorological and Land Surface Properties Impacting Sea Breeze Extent and
2 Aerosol Distribution in a Dry Environment

3

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15 **Key Points**

- 16 • The relative influence of a variety of environmental properties on sea breeze
17 dynamics and aerosol transport are assessed and quantified.
- 18 • Soil saturation fraction is an important factor for sea breeze properties and
19 aerosol redistribution, but is poorly represented in models.
- 20 • The results provide guidance for future improvements in numerical weather
21 prediction.

22

23 **Abstract**

24 The properties of sea breeze circulations are influenced by a variety of
25 meteorological and geophysical factors that interact with one another. These
26 circulations can redistribute aerosol particles and pollution and therefore can play
27 an important role in local air quality, as well as impact remote sensing. In this study,
28 we select eleven factors that have the potential to impact either the sea breeze
29 circulation properties and / or the spatial distribution of aerosols. Simulations are
30 run to identify which of the eleven factors have the largest influence on the sea
31 breeze properties and aerosol concentrations and to subsequently understand the
32 mean response of these variables to the selected factors. All simulations are
33 designed to be representative of conditions in coastal sub-tropical environments
34 and are thus relatively dry; as such they do not support deep convection associated
35 with the sea breeze front. For this dry sea breeze regime, we find that the
36 background wind speed was the most influential factor for the sea breeze
37 propagation, with the soil saturation fraction also being important. For the spatial

38 aerosol distribution, the most important factors were the soil moisture, sea-air
39 temperature difference and the initial boundary layer height. The importance of
40 these factors seems to be strongly tied to the development of the surface-based
41 mixed layer both ahead of and behind the sea breeze front. This study highlights
42 potential avenues for further research regarding sea breeze dynamics and the
43 impact of sea breeze circulations on pollution dispersion and remote sensing
44 algorithms.

45 **1. Introduction**

46 Sea breeze circulations are ubiquitous along coastlines in the tropics and
47 midlatitudes [Miller *et al.*, 2003]. From a basic physical standpoint, the mechanisms
48 that govern their generation and maintenance are fairly well understood. Sea
49 breezes are driven by differential daytime heating of the air over land and water
50 surfaces. In the lower atmosphere, the relatively warm air over land is associated
51 with locally low pressure and likewise the relatively cool air over ocean is
52 associated with locally high pressure. This pressure gradient induces a baroclinic
53 circulation with an inland-directed surface density current, a return flow aloft, and
54 upward motions over land that can lead to the formation of clouds and precipitation
55 if the environmental conditions are appropriate. Reviews of sea breeze dynamics
56 are provided by *Miller et al.* [2003] and *Crosman and Horel* [2010].

57 Sea breezes have generated much interest for their ability to disperse pollutants
58 that are emitted over land, and as such can be an important control on air quality
59 [e.g. *Crosman and Horel*, 2010] and remote sensing. In their review of pollutant
60 outflow from southern Asia, *Lawrence and Lelieveld* [2010] argue that sea breeze
61 circulations could be quite important for lofting pollution from the surface to higher
62 elevations where it can be transported offshore. Once lofted, pollution plumes can
63 bifurcate, and even be recirculated back into the onshore inflow layer [*Lyons et al.*,
64 1995]. Both studies conclude that a better understanding of the relationship
65 between pollution dispersion and sea breezes is necessary. To further complicate
66 the issue, other circulations such as trade winds, monsoon winds, and mountain
67 flows may occur simultaneously with the sea breeze [*Verma et al.*, 2006; *Wang et al.*,

68 2013; *Wang and Kirshbaum, 2017*] to impact pollutant transport, and the spatial
69 distribution of aerosols associated with sea breeze fronts can be heterogeneous. For
70 example, enhanced optical depths have been observed with the passage of sea
71 breeze fronts in both tropical [*Moorthy et al., 1993*] and desert [*Derimian et al.,*
72 2017] settings. For these reasons, understanding the interactions between pollution
73 and sea breezes is an active area of current research [*Loughner et al., 2014; Miao et*
74 *al., 2015; Monteiro et al., 2016; Russo et al., 2016; Mazzuca et al., 2017*].

75 The redistribution of aerosols by coastal circulations is also of interest for
76 remote sensing applications. Retrievals of quantities such as aerosol optical depth
77 are particularly difficult in coastal zones due to sudden spatial and even temporal
78 changes to land/ocean surface properties [*Anderson et al., 2013*] and due to
79 uncertainties in the vertical distribution of aerosol particles. Better understanding
80 of aerosol distribution in coastal zones could lead to improved retrievals, and also to
81 improved methods of assimilating these retrievals into numerical weather
82 prediction models.

83 Despite our basic understanding of sea breeze circulations, it can be difficult to
84 generalize the findings of single observational studies in order to understand which
85 conditions have the most control on sea breeze characteristics and pollution
86 dispersal. Generalizing previous studies is particularly challenging given that
87 properties of the land surface and atmospheric conditions can interact to impact sea
88 breeze characteristics in nonlinear ways [*Baker et al., 2001; Grant and van den*
89 *Heever, 2014*]. For example, *Grant and van den Heever [2014]* found that
90 interactions between the effects of soil moisture and aerosol concentrations can

91 lead to enhancements in precipitation greater than could be obtained by changing
92 just one of these factors alone.

93 This study is designed to determine which atmosphere and land surface
94 properties have the largest impact on sea breeze characteristics and associated
95 aerosol transport within coastal zones through the use of idealized model
96 simulations in order to better understand the general behavior of sea breezes. We
97 investigate the mean response of the sea breeze to the most important properties
98 and subsequently identify which properties most warrant further investigation.
99 Since sea breezes have been found to impact aerosol and pollution transport in both
100 humid and arid environments, we choose to begin with the relatively simple desert
101 environment. Specifically, we examine the case of a relatively dry environment that
102 does not support deep convection in order to keep the sea breeze dynamics
103 relatively simple. Subsequent studies are currently investigating the case of a moist
104 environment that does support deep convection and will address in detail how
105 these properties impact the sea breeze and aerosol transport. This research is part
106 of a larger, Multi-disciplinary University Research Initiative (MURI) funded by the
107 Office of Naval Research (ONR). The overarching goal of this project is to further our
108 understanding and forecasting abilities of aerosol properties in coastal zones by
109 bringing together expertise in satellite remote sensing, data assimilation, and high-
110 resolution modeling to address fundamental questions about the controls on the
111 spatial distribution and properties of aerosols in these areas.

112

113 **2. Methodology**

114 **2.1. Overview**

115 To address the goals of our study, we make use of a combination of idealized
116 model simulations and statistical methods. Specifically, we make use of the
117 methodological framework described in two recent studies that evaluated the
118 effects of parametric uncertainty on simulated outputs from complex atmospheric
119 models [*Lee et al., 2013; Johnson et al., 2015*]. The approach begins with the
120 identification of model parameters or initial conditions (factors) of interest, and the
121 assignment of an uncertainty range to each one in order to form a multi-dimensional
122 parameter uncertainty space over which the model is explored. A perturbed
123 parameter ensemble of model runs that optimally covers this parameter uncertainty
124 space is then generated and used to construct Bayesian statistical emulators of
125 different model output responses. Once validated, each emulator of a given model
126 output can be used to densely sample that model output response across the full
127 multi-dimensional uncertainty at a very low computational cost, enabling us to
128 explore the model output behavior over the uncertainty and to identify (and
129 quantify) key uncertainty sources.

130 In this study, we apply this framework to identify how changes in environmental
131 characteristics impact on the sea breeze characteristics and aerosol transport and
132 determine the environmental characteristics that are most influential. Our
133 perturbed parameter ensemble consists of idealized model simulations that are
134 loosely based on dry coastal environments. The simulations differ only in their
135 initial conditions. They are not meant to exactly reproduce the conditions at any one
136 time of year or location, but rather to capture representative conditions of these dry

137 coastal regions. The strength of idealized simulations is that the physical insights
138 and qualitative results gained from them are broadly applicable to many specific
139 scenarios, even if the simulations did not account for the exact evolution of every
140 geophysical variable in the specific situations.

141 We identify eleven factors (environmental characteristics) that we wish to test
142 and use to vary the initial conditions in the ensemble. To select just three values for
143 each factor and to run every combination for all eleven factors would require over
144 500,000 simulations. Since the model is computationally expensive, such a task is
145 not feasible. By using a perturbed parameter ensemble consisting of only 143
146 simulations combined with the model output emulation, we can effectively run
147 thousands of “virtual” simulations in a matter of minutes. This combination of
148 modeling and statistical techniques therefore is a powerful and effective way to
149 assess the relative importance of a large number of factors with a limited number of
150 actual simulations. The use of idealized simulations further strengthens the utility of
151 this method by making the results broadly applicable to many specific locations. In
152 the following sub-sections, we will describe the basic model set up, the factors that
153 have been chosen for investigation, how we vary these factors in the model
154 initialization, and the statistical methods used for the analysis of the resulting
155 simulations.

156

157 **2.2. Basic Simulation Set-up**

158 The model used is the Regional Atmospheric Modeling System (RAMS) [*Cotton et*
159 *al.*, 2003; *Saleeby and van den Heever*, 2013]. RAMS is a non-hydrostatic, fully

160 compressible, atmospheric numerical model that has been successfully used in
161 previous sea breeze modeling studies [e.g. *Freitas et al., 2006; Grant and van den*
162 *Heever, 2014*]. A grid spacing of 500 m in the horizontal was used. In the vertical,
163 variable grid spacing was used that was 25 m between the lowest levels and
164 stretched to 500 m after which the spacing was kept constant. There was a total of
165 57 vertical grid levels, with 17 of them within the first 1.5 km above the surface.
166 Thus, the boundary layer processes were well resolved. Model integration employed
167 a 5 second time step for 24 hours, starting at 0000LT (local time). This allowed a
168 land breeze to develop before dawn and a sea breeze to develop during the day.

169 Half of the domain used a land surface, and half used an ocean surface. The
170 LEAF-3 [*Walko et al., 2000*] land surface model was used and the land surface
171 temperature and soil moisture are prognostic variables in this scheme. We used a
172 desert surface type with sandy soil, representative of dry sub-tropical
173 environments. Finally, the sea surface temperature was kept constant throughout
174 the simulations and was varied with distance from the coast.

175 To achieve the goal of modeling sea breezes that are mostly free of moist
176 convection, we based the initial conditions on dry sub-tropical coastal
177 environments. The initial potential temperature and relative humidity profiles are
178 created from ERA-Interim data for July 2014. This month was chosen since it
179 corresponds to mid-summer when sea breezes in sub-tropical environments are
180 frequent and long-lived [*Papanastasiou and Melas, 2009; Azorin-Molina et al., 2011*].
181 The data were averaged along the North African coast between 20E and 30E (a
182 somewhat arbitrary choice) on days with cloud fraction less than 0.01. The wind

183 speed was initialized to be constant with height, and the wind direction was in the
184 cross-coast direction. All atmospheric conditions were initially horizontally
185 homogeneous. Gradients in temperature, pressure, moisture, etc. that typically form
186 and drive sea breeze circulations quickly developed after the simulation start due to
187 differing latent and sensible heat fluxes over land and ocean.

188 The *Harrington* [1997] radiation parameterization was used in all simulations.
189 The day of year selected for these idealized tests was July 15. The aerosol
190 parameterization is described by *Saleeby and van den Heever* [2013] and includes
191 dry and wet deposition, depletion by cloud droplet nucleation, and regeneration
192 upon droplet evaporation. The initial aerosol profile was horizontally homogeneous
193 and decreased exponentially with height, with a maximum concentration of 200 mg
194 ¹ at the surface. We also initialized all simulations with a passive tracer field that
195 was identical to the initial aerosol distribution. This tracer was transported by the
196 wind but otherwise was not subject to any of the physical processes that the aerosol
197 field experienced. Since most of the simulations analyzed here contained no clouds
198 by design, the tracer closely mimics the behavior and evolution of the aerosol field,
199 and is also more representative of pollution that does not serve as cloud
200 condensation nuclei (CCN).

201

202 **2.3. Factors**

203 Eleven model factors (parameters) that represent different environmental
204 characteristics were selected for evaluation within this study. The chosen factors
205 are listed with a short description in Table 1. The sea-air temperature difference

206 (SST- T_a), sea surface temperature gradient, land-air temperature difference (T_l-T_a),
207 and soil moisture content were chosen as these characteristics have the potential to
208 impact surface sensible heat fluxes. The stable layer characteristics, boundary layer
209 height, cross-coast wind speed, and Coriolis force (latitude) were chosen based on
210 the review of sea breeze modeling studies [*Crosman and Horel, 2010*] which found
211 these or related properties to be important for sea breeze dynamics. Finally, the
212 remaining factors shown in Table 1 (boundary layer potential temperature and
213 relative humidity) were included since they may have important implications for
214 aerosol transport and cloud development. While clouds do not form frequently in
215 the current study, we include these factors here for consistency with our follow up
216 study of moist sea breeze environments.

217 Table 1 also lists the plausible uncertainty range that we have assigned to each
218 factor. These selected ranges combine to produce an 11-dimensional parameter
219 uncertainty space over which we explore the behavior of the sea breeze and aerosol
220 transport in our model. The values of all factors are initial conditions for the
221 simulations, and except where noted in Table 1, the values of these factors evolve
222 during the simulations.

223 Of course, there are many other factors that we could have chosen, but which
224 have been excluded. For example, the initial conditions are horizontally
225 homogeneous in the atmosphere (see 2.2). In reality, gradients in temperature,
226 humidity, and wind almost always exist in coastal zones, and these gradients could
227 have been included as factors. We excluded these in the interest of keeping the
228 study simple and idealized. Likewise, topographical variations such as land

229 elevation and coastline curvature were also purposely excluded from this study in
230 order to keep the model set up simple, as it is the simplicity of our set up that makes
231 the results fundamental to the nature of sea breezes. That said, topographical
232 variations will certainly have an impact on the sea breeze circulation and aerosol
233 transport [e.g. *Baker et al.*, 2001] and will be addressed in separate studies.

234

235 **2.4. Use of the Factors to Initialize Simulations**

236 The factors described in Table 1 are used to vary the initial conditions for the
237 simulations. Following *Lee et al.* [2011] and *Johnson et al.* [2015], we use the
238 maximin Latin hypercube design algorithm to produce an ensemble of 143 factor
239 value combinations that provide an optimal coverage of our 11-dimensional
240 parameter uncertainty space. We then use these 143 factor value combinations are
241 used to initialize 143 RAMS simulations.

242 The application of wind speed, boundary layer and stable layer characteristics as
243 initial conditions is straightforward (see Table 1 for details). Positive wind speed
244 values correspond to initially offshore flow, and negative values correspond to
245 initially onshore flow. Above the stable layer, the relative humidity profiles were
246 identical for all simulations. The potential temperature profiles all had the same dry
247 static stability up to 200mb. At 100mb and 50mb (in the stratosphere), the potential
248 temperature is the same in all simulations. Example initial conditions for relative
249 humidity and potential temperature from three simulations are shown in Figure 1.

250 The Coriolis force is varied by changing the latitude. Latitude of course also
251 impacts the incoming solar radiation. Therefore, the latitude is set to 0°, the

252 minimum value in our allowed range for the Coriolis force, for all radiation
253 calculations in all simulations. Although this is not a sub-tropical latitude, it is
254 consistent with the value used in our follow-up study for moist environments, as is
255 the range of latitudes tested for the Coriolis force. Furthermore, the same total daily
256 insolation can be found at the highest latitudes tested in late summer, and therefore
257 the insolation is not unrepresentative of these latitudes. That said, the choice of
258 radiative latitude will have a large impact on the evolution of the sea breeze, but we
259 do not expect that choosing a different radiative latitude would qualitatively alter
260 the results of this study.

261 The use of the remaining factors as initial conditions to RAMS is fully described
262 in Table 1.

263

264 **2.5. Analysis**

265 For each model output of interest (see Sections 3.3 and 4.2), we use our
266 perturbed parameter ensemble of model runs to construct a statistical emulator
267 [O'Hagan, 2006] of the output over the parameter uncertainty space. This emulator
268 is constructed using the output of the first 121 simulations in our ensemble, using
269 the statistical software R [R Core Team, 2015], and the R package DiceKriging
270 [Roustant et al., 2012], and is validated with the remaining 22 simulations. Here, the
271 emulator model provides a mapping of the relationship between the 11-dimensional
272 parameter uncertainty space and the corresponding model output that is fast to
273 evaluate and can be used to predict the value of the output with uncertainty at any
274 combination of the factor values.

275 Using these statistical emulators, we then apply variance-based sensitivity
276 analysis techniques [*Saltelli et al., 2000*] to decompose and proportionally assign the
277 variation in each model output to the factors. Here we apply the extended-FAST
278 (Fourier Amplitude Sensitivity Test) approach of *Saltelli et al. [1999]* to compute the
279 sensitivity measures, using the R package ‘sensitivity’ [*Pujol et al., 2013*] to perform
280 the calculations. The reported percentage of variance attributed to each factor here
281 is interpreted as the direct contribution of the factor to the overall variance in the
282 given model output and does not include any contributions due to factor
283 interactions.

284

285 **3. Sea Breeze Characteristics**

286 **3.1. Sea Breeze Identification**

287 The sea breeze was objectively identified for all 143 simulations. The
288 identification algorithm is described in Appendix A. An example of a simulated sea
289 breeze from one of the model runs and the corresponding objectively identified sea
290 breeze is shown in Figure 2a. In this case, the onset of the sea breeze is at 0900 LT,
291 which is consistent with typical sea breeze onset times for the sub-tropical
292 environments [*Papanastasiou and Melas, 2009; Azorin-Molina et al., 2011*]. A weak
293 land breeze had developed before sunrise. Overall, the algorithm performs very well
294 in all cases (not shown). In addition, no sea breeze developed in 16 out of the 143
295 simulations in our ensemble. The algorithm correctly fails to identify a sea breeze in
296 all of these simulations.

297

298 **3.2. Average Behavior**

299 First, we look at the average behavior of the sea breeze in the simulations. Figure
300 3 shows the mean and standard deviation of the location of the sea breeze front and
301 the average propagation speed as a function of time. All 143 simulations in our
302 ensemble were used to create this figure. It can be seen that on average the sea
303 breeze propagates almost 150km inland in these idealized simulations that do not
304 have topographical barriers. The standard deviation of the final extent is about 50
305 km which indicates that there is a substantial amount of variability in the sea breeze
306 evolution across the ensemble. The average propagation speed increases with time
307 until about 1900 LT (1 hour after sunset). The simulated idealized sea breeze
308 acceleration is consistent with previous modeling results [e.g. *Yan and Anthes, 1987*;
309 *Sha et al., 1991*] and observations [e.g. *Simpson et al., 1977*; *Physick and Smith,*
310 1985].

311 Since one of our objectives in this study is to better understand near-surface
312 aerosol redistribution by sea breezes, we also examine the depth of the surface-
313 based mixed layer. We identified this depth as the height from the surface at which
314 the vertical potential temperature gradient first exceeds 2 K km^{-1} . Other threshold
315 values were tried, but did not qualitatively change the results. An example of the
316 evolution of the mixed layer depth is shown in Figure 2b. It is clear that the mixed
317 layer depth is strongly impacted by the sea breeze here. Ahead of the sea breeze
318 front, where the boundary layer is primarily controlled by the direct daytime
319 heating and surface fluxes, the mixed layer depth exceeds 1km. Behind the sea
320 breeze front, the mixed layer is quite shallow – in this case, less than 200m.

321 The average surface-based mixed layer depth for all simulations averaged over
322 land behind the sea breeze front (coast to the front) is shown in Figure 3c. It
323 increases until midday, slowly decreases during the afternoon, and rapidly
324 decreases after sunset.

325

326 **3.3. Sensitivity Analysis**

327 To investigate the impact of the uncertainty in our eleven factors on the sea
328 breeze, we have constructed a statistical emulator and applied the variance-based
329 sensitivity analysis method for the following three characteristics of the sea breeze:
330 the maximum extent, the difference in propagation speed during the night and day
331 (a simple measure of the sea breeze acceleration), and the surface-based mixed
332 layer depth behind the sea breeze front.

333 The daytime propagation speed was calculated as the position at 1800 LT
334 (sunset) divided by the total time that the sea breeze had been in existence, whereas
335 the nighttime propagation speed was calculated as the difference in the maximum
336 position and the position at 1800 LT divided by the time in that interval. In a few
337 cases the sea breeze exited the domain before the end of the simulation (e.g. Figure
338 A1a). In these cases, the maximum extent was estimated by extrapolating the sea
339 breeze position to 2400 LT using the nighttime propagation speed. Simulations that
340 did not produce a sea breeze were assigned values of 0 for the maximum sea breeze
341 extent and propagation speeds.

342 The mixed layer depth was taken as the maximum value in time of the average
343 depth between the coast and the sea breeze front. Simulations without a sea breeze
344 were assigned the maximum value in time of the average depth over all land.

345 The factor combinations that were used to generate each of the 22 reserved
346 validation simulations were input to the statistical emulators of the three sea breeze
347 characteristics to obtain the corresponding emulator mean predictions and 95%
348 confidence bounds on these predictions in each case. These predicted values were
349 compared to the actual simulated values from the RAMS simulations to ensure that
350 the statistical emulators are robust. Figure 4 shows this information and
351 demonstrates that the emulators for all three selected sea breeze characteristics
352 provide good predictions. With the exception of three predictions (two for the sea
353 breeze extent and one for the mixed layer depth), all other emulator predictions (63
354 in total, or 95%) agree with the RAMS modeled values within the 95% confidence
355 bounds. These results give us confidence that the emulators are accurately
356 representing the true response of each characteristic to the eleven factors under
357 study.

358 To understand which factors contribute most to the variability of the sea breeze
359 extent, the night-day propagation speed difference, and the mixed layer depth, we
360 have used the variance-based sensitivity analysis approach of *Saltelli et al.* [1999] to
361 calculate the percentage of output variance attributable to each factor. The results of
362 this analysis are shown in Figure 5 and discussed in the following subsections.

363

364 **3.3.1. Maximum extent**

365 The initial wind speed is by far the most important factor in determining the
366 maximum sea breeze extent and explains about 75% of the variance (blue bars in
367 Fig. 5). Figure 6a shows the mean response of the maximum extent to the wind
368 speed, sea-air temperature difference, and soil saturation fraction, determined
369 through simulation from the statistical emulator for this output. Over the range of
370 each factor here, the value of the mean response for the maximum extent at a
371 particular factor value (on the x-axis) is calculated as the mean of 500 predictions
372 (increasing the number of predictions minimally changes the mean) from the
373 emulator that take the given value for this factor of interest and uniformly random
374 values for all other factors.

375 In Figure 6a, onshore environmental winds (green line; negative values) cause
376 the sea breeze to propagate further inland, and vice versa for offshore winds
377 (positive values). This result regarding offshore flow is consistent with previous
378 studies [e.g. *Arritt, 1993; Finkele, 1998*] which have found that strong offshore flow
379 will reduce the inland penetration of the sea breeze. Also in agreement with our
380 results, laboratory experiments with density currents show that an onshore flow
381 would lead to faster propagation [*Simpson and Britter, 1980*]. However, some
382 studies suggest that sea breeze inland penetration should be retarded, not
383 enhanced, by strong onshore flow due to a reduced temperature gradient between
384 land and sea [*Simpson, 1994; Chiba et al., 1999*]. Our simulations do show that sea
385 breeze fronts with the strongest temperature gradients formed in initially light
386 winds, but they still had only medium values of inland extent (Fig. 7). In three of the
387 143 simulations, the sea breeze stops propagating before the end of the simulation,

388 and in these three cases the winds are initially onshore (not shown). However, in
389 most cases, the onshore winds do not prevent the sea breeze from propagating a far
390 distance inland despite reduced temperature gradients.

391 The next two most important factors contributing to the maximum extent of the
392 sea breeze are the soil saturation fraction and the sea-air temperature difference,
393 which explain about 13%, and 7% of the variance, respectively (blue bars in Fig. 5).
394 Warmer sea surface temperature relative to the air (blue line; values greater than 0
395 in Fig. 6a) leads to slower moving sea breezes that do not extend as far inland. This
396 is due to a reduced air temperature gradient between the land and ocean and is in
397 line with our expectations and understanding of sea breeze circulation
398 thermodynamics. Higher soil moisture also reduces the sea breeze extent (gray line
399 in Fig. 6a). Higher soil moisture reduces the sensible heat flux over land and, as with
400 warmer sea surface temperatures, leads to a reduced gradient in air temperature
401 between the land and over the ocean. These two factors are approximately equally
402 important on average.

403

404 **3.3.2. Sea breeze acceleration**

405 Figure 5 (teal bars) reveals that the initial wind speed is also the most important
406 factor for setting the night-day propagation speed difference. However, for this sea
407 breeze characteristic, the soil saturation fraction is of almost equal importance to
408 the initial wind speed. As with the maximum sea breeze extent, stronger offshore
409 flow and higher soil moisture lead to reduced sea breeze acceleration (green and
410 dark gray lines in Fig. 6b). We hypothesize that low soil moisture can promote rapid

411 cooling of the land surface near and after sunset, thereby inducing a negative
412 sensible heat flux. Winds are relatively calm ahead of the front and stronger behind
413 (on the oceanward side). This leads to stronger cooling of the air behind the sea
414 breeze front and enhances the temperature gradient across the front (not shown),
415 which would increase the propagation speed of the front [*Simpson and Britter,*
416 1980].

417 The initial sea-air temperature difference and the Coriolis effect are of secondary
418 importance for the sea breeze acceleration (teal bars in Fig. 5). Relatively cold sea
419 temperatures lead to greater acceleration of the sea breeze (blue line in Fig. 6b)
420 which is consistent with sea breezes that penetrate further inland (blue line in Fig.
421 6a). A stronger Coriolis effect limits the acceleration of the sea breeze (light gray line
422 in Fig. 6b) due to the turning of the winds by the Coriolis force [*Rotunno, 1983; Yan*
423 *and Anthes, 1987*].

424

425 **3.3.3. Mixed Layer Depth**

426 Different factors are responsible for controlling the variation in the depth of the
427 sea breeze mixed layer than for controlling the sea breeze maximum extent and
428 acceleration. The initial boundary layer height and stable layer strength are the two
429 most important factors for the mixed layer depth (yellow bars in Fig. 5). Initially
430 deep boundary layers capped by weak stable layers promote deeper mixed layers
431 between the sea breeze front and the coast (yellow and pink lines in Fig. 6c).
432 Relatively warm ocean temperatures also promote deeper mixed layers (blue line in
433 Fig. 6c). We note that despite the fact that these mixed layers exist over land, the sea

434 surface temperature plays a bigger role in their depth than the land surface
435 characteristics since this air mass is largely advected from over the ocean to over
436 land. Ahead of the sea breeze front, the mixed layer depth is also strongly controlled
437 by the soil saturation, but not the sea surface temperature (not shown).

438 The other factors do not contribute to a high percentage of the variance of the
439 sea breeze characteristics that were analyzed here. This fact does not imply that
440 these factors have no impact at all. Rather, the factors with a low contribution to
441 variance have a relatively small impact *on average* compared to the other factors
442 that were analyzed. The insignificant factors to the mean may be quite important in
443 certain specific situations, but it is not the intention of this study to understand what
444 those situations are. The intention of the study is to identify the factors that have the
445 largest impacts on average and to understand the average response of the sea
446 breeze characteristics to those factors.

447

448 **4. Aerosol Response**

449 **4.1. Overview**

450 The impact of the eleven factors on the properties of the aerosol spatial
451 distribution in the vicinity of the sea breeze front and coast was also investigated.
452 Since a few simulations did produce clouds which reduced aerosol concentrations,
453 we chose to analyze the tracer field as a proxy for the aerosol concentration, or
454 other air pollutants that do not serve as CCN.

455 First, Figure 8 shows four examples of the sea breeze circulation at 1800 LT the
456 and change in tracer concentration between 0600 (sunrise) and 1800 LT. Land is on

457 the left of the figure, and ocean is on the right. These four examples were chosen to
458 illustrate the impacts of wind speed and soil moisture on the simulations. The sea
459 breeze front location is clearly identifiable in all cases as the place where there is a
460 sudden upward component in the wind vectors. In the right-hand column of Figure
461 8, the sea breeze circulation has a clear inflow branch near the surface and a clear
462 return flow above about 1km. Both of these example simulations were initialized
463 with offshore winds. In the left-hand column, simulations with initially onshore
464 winds are shown, and it is seen that while the sea breeze penetration inland is much
465 greater, the return flow is much weaker. Nonetheless, all four examples show
466 similar structures in the tracer perturbation field. Ahead of the sea breeze front,
467 positive perturbations overlay negative perturbations due to the daytime mixing of
468 the boundary layer and the fact that the simulations were initialized with an
469 exponentially decreasing profile of tracer concentration. As the sea breeze front
470 impinges on this air, the positive perturbation plume is vented out of the boundary
471 layer oceanward in the return flow of the sea breeze circulation. This structure is
472 similar to that seen in sea breeze simulations by *Lu and Turco* [1994] and *Verma et*
473 *al.* [2006]. The edge, or head of this vented air mass is clearly seen by the sharp
474 horizontal gradient of aerosol perturbation marked by the pink stars in Figure 8. It
475 is objectively identified as the most oceanward point with at least a 10 mg^{-1} tracer
476 perturbation. In addition, some of these vented tracers may be advected further
477 upwards by the vertical motions occurring right at the sea breeze front. However,
478 since the convection at the sea breeze front is dry in these simulations, the vertical
479 motions are not particularly strong, and most of this plume is advected horizontally.

480 On the oceanward side of the sea breeze front, tracer perturbations at and near
481 the surface are almost universally negative. Further aloft, we also see widespread
482 areas of negative aerosol perturbations. These maximize at or slightly below the
483 level of the vented head, and seem to be associated with slightly subsiding air that is
484 originating over the ocean and may become incorporated in the sea breeze
485 circulation inflow. The edge of this subsiding ocean air plume is marked with pink
486 crosses in Figure 8 and will be called the “clean plume head”. It is objectively
487 identified as the most landward point along the minimum closed negative
488 perturbation contour (most landward point that is distinguishable from the
489 negative perturbations due to boundary layer mixing). We now use the statistical
490 framework described above to understand which factors most control and influence
491 the properties of the spatial distribution of the tracer. Specifically, we look at the
492 mean surface concentration between the coast and the sea breeze front, the
493 maximum height of a 1% positive aerosol perturbation, and the relative positions of
494 the vented and clean plume heads. Each of these output properties are now
495 discussed in more detail in the following sub-sections.

496

497 **4.2 Sensitivity Analysis**

498 **4.2.1 Average Surface Concentration**

499 The average surface concentration of the tracers between the coast and the sea
500 breeze front was analyzed every three hours starting at 1200 LT. As with the sea
501 breeze characteristics, a statistical emulator of these model responses (one
502 emulator at each time output) was constructed and validated (not shown), and

503 variance-based sensitivity analysis was used to determine the percentage of
504 variance in the tracer concentration attributable to each individual factor.

505 The blue bars in Figure 9 show the percentage of variance of the average surface
506 tracer concentration explained by each of the eleven factors. Only the results for
507 1800 LT are shown; all other times showed qualitatively similar results. The initial
508 boundary layer height, sea-air temperature difference, and initial stable layer
509 strength all contribute 20% or more to the variance in the average surface
510 concentration, and combined explain 91% of the variance. Even at 2400 LT, these
511 factors together explain 84% of the variance (not shown). These are the same three
512 factors that contributed the most variance to the maximum boundary layer height in
513 Figure 5. Furthermore, the average response of the surface tracer concentration to
514 each of these factors (Fig. 10a) mirrors the average response of the boundary layer
515 depth (Fig. 6c), but the trends each have opposite signs. A scatter plot of the mean
516 surface tracer concentration between the coast and the front at 1800 LT and the
517 maximum boundary layer height for the same region confirms the close relationship
518 (Fig. 11). Namely, as would be expected, deep boundary layers lead to more mixing
519 and a reduction of the surface tracer concentration. The color and size of the points
520 in the figure indicate the sea-air temperature difference and initial stable layer
521 height, respectively. Qualitatively, the pattern of color and size is consistent with the
522 statistical results.

523 These results suggest that boundary layer mixing is the most important control
524 on surface tracer concentration behind the sea breeze front. Transport of tracers
525 from locations other than the marine boundary layer, such as the recirculation of

526 vented tracers associated with the sea breeze circulation, are relatively minor in
527 magnitude. The inland extent of a sea breeze and accompanying tracer
528 concentrations will also be important in determining its impact on the local air
529 quality. As such, factors that determine the sea breeze extent and speed such as the
530 initial wind speed and soil saturation (Fig. 5) will also be important for determining
531 local tracer and aerosol concentrations.

532

533 **4.2.2 Maximum Perturbation Height**

534 The orange bars in Figure 9 indicate that only one factor contributes more than
535 10% to the variance of the maximum height of a 1% tracer perturbation, namely,
536 soil saturation. It accounts for 45% of the variance. The stable layer depth and
537 strength combined contribute another 17% of the variance, but each on its own
538 contributes less than 10%. Moister soil leads to smaller perturbation heights (Fig.
539 10b), but the effect becomes negligible at about 0.4 soil saturation fraction. We
540 hypothesize that there are two reasons for the dominance of the soil saturation. Dry
541 soil will promote sensible rather than latent heat fluxes, and thus cause more
542 heating of the near surface air. First, this additional heating helps to deepen the
543 boundary layer ahead of the sea breeze front (not shown), the region which, as
544 discussed above, is the main source of the positive tracer perturbations. Second,
545 warmer near surface air that enters the frontal updraft will be more buoyant, rise to
546 higher heights, and transport high tracer concentrations to those higher heights.

547

548 **4.2.3 Tracer Plume Overlap**

549 Finally, we analyze the relative positions of the clean and vented plume heads.
550 This metric gives an indication of the extent to which the two plumes are
551 interacting, or will interact and mix in the future. It also indicates, to some degree,
552 the likelihood that the clean plume will mix/has mixed with the inflow air. The
553 green bars in Figure 9 show that the wind speed and the soil saturation fraction
554 contribute more or less equally to the variance of this output metric, and combined
555 explain about 50% of this variance. The other factors and/or interactions among the
556 factors explain the other 50%. Moister soil leads to less overlap in the plumes,
557 whereas neutral to weak offshore winds most favor large overlap (Fig. 10c). The
558 four example simulations in Figure 8 were intentionally chosen to demonstrate the
559 importance of these two factors. As mentioned before, the left and right columns
560 show simulations with initially onshore and offshore winds, respectively. In each
561 column, the winds have approximately the same magnitude. Similarly, the top and
562 bottom rows show simulations with similar moderate and low values of the soil
563 saturation fraction, respectively. Of course, all of the other factors vary amongst
564 these four simulations, and so will also contribute to differences in these sea breeze
565 circulations and tracer perturbation fields. Nonetheless, they do demonstrate that
566 low soil moisture tends to lead to deeper boundary layers ahead of the front, and
567 deeper, more pronounced vented plumes that allow the clean plumes to undercut
568 them more easily. As for the wind factor, while all simulations have a well-defined
569 inflow, only the simulations with background offshore flow can efficiently vent the
570 tracers back toward the ocean and override clean plumes.
571

572 **5. Conclusions**

573 In this study, our goal was to identify the most important meteorological and
574 geophysical factors that contribute to variability in sea breeze circulations and
575 aerosol spatial distribution. Our results have applications and implications for
576 numerical weather prediction, air quality, and remote sensing in coastal zones.
577 Although previous studies have identified numerous factors that contribute to sea
578 breeze and aerosol spatial distribution, this is the first study to do so in a way that
579 evaluates numerous factors simultaneously using advanced statistical methods
580 which allowed us to compare the relative importance of the factors. To do so, we ran
581 a large perturbed parameter ensemble of simulations with a cloud-resolving model
582 and interactive land-surface model. Of the factors tested, the initial wind speed had
583 the largest impact on the maximum sea breeze extent, followed by the soil moisture
584 content and the sea-air temperature difference. Onshore flow was not found to
585 retard the sea breeze propagation distance as has been suggested by some previous
586 studies [*Simpson, 1994; Chiba et al., 1999*], but rather consistently led to sea breezes
587 that propagated the furthest distances inland. The soil moisture content was
588 especially important for controlling how much the sea breeze front accelerated
589 between the day and night.

590 We also assessed the relative importance of the same factors for the
591 redistribution of a tracer field that was representative of pollutant concentrations
592 within the coastal zone. Behind the sea breeze front, the surface tracer
593 concentrations were strongly linked to the same factors that controlled mixed-layer
594 depth. This result demonstrates that over land behind the sea breeze front, ocean

595 characteristics are more important than land characteristics for determining the
596 degree of vertical mixing and that vented pollutants were not efficiently recirculated
597 into the sea breeze inflow air. The maximum height of the vented pollutants was
598 most influenced by the soil moisture. We also examined the degree to which the
599 vented pollutants had the potential to mix with cleaner ocean air that was being
600 drawn into the sea breeze inflow. Wind speed and again soil moisture were found to
601 be the two most important factors for controlling this interaction.

602 When considering ways to improve numerical weather prediction, this study
603 serves as a guide for potential avenues of improvement of sea breezes and aerosol
604 redistribution forecasts. While large-scale winds are already well simulated in
605 forecast models, better representation of sea surface temperatures, especially in
606 coastal zones where coarse sea surface temperature analysis products may not
607 appropriately capture local conditions [Lombardo *et al.*, 2016], may lead to
608 improvements in forecasts of aerosol redistribution. While the importance of sea
609 surface temperature has long been recognized, this is the first study to show that it
610 is one of the *leading* causes of uncertainty. Of the factors tested, soil moisture was
611 found to be the most important overall for aerosol redistribution, yet it also may be
612 the most uncertain in current models. It is frequently not well represented in
613 models [Lahoz and De Lannoy, 2014] and therefore likely contributes substantially
614 to real uncertainty in forecasts of aerosol and pollutant transport. While not
615 discussed here, soil moisture will also have a large influence on the amount of dust
616 lofted from the surface in desert regions [Fécan *et al.*, 1998]. This study indicates
617 that more frequent and improved measurements of soil moisture and ocean/land

618 surface properties are needed to reduce the uncertainty in the prediction of sea
619 breeze dynamics and aerosol redistribution.

620 These results regarding tracer concentrations as a proxy for aerosol
621 concentrations apply to our idealized case of a sea breeze without moist convection.
622 Of course, clouds will also have an impact on local air quality conditions here. A
623 follow-up study will address this more complicated scenario.

624

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638

639 **Appendix A**

640 Here we describe the sea breeze identification algorithm. First, we create a
641 “strong” sea breeze mask using the surface potential temperature and cross-coast
642 wind speed averaged in the along-coast direction every 30 minutes. The criteria are
643 that the sea breeze does not exist over the ocean or before sunrise, that the potential
644 temperature gradient is less than 0.1 K m^{-1} , that the wind is inland-directed, and
645 that the wind speed gradient is negative and greater in magnitude than a quarter of
646 the maximum negative wind speed gradient found throughout the entire simulation.
647 In many simulations, these criteria alone are sufficient to identify a good sea breeze
648 mask. However, in complex cases, these criteria are insufficient.

649 Figure A1 demonstrates the procedure for a particularly challenging case.
650 Figure A1a shows the cross-coast wind speed. The sea breeze is clearly visible and
651 exists from the coastline to the edge of the domain. Strong gradients in the wind
652 speed also exist ahead of the front due to gravity wave activity. The strong mask is
653 shown in Figure A1b. The strong mask identifies many points that do not
654 correspond to the sea breeze, it is not continuous in time and space, and it does not
655 start at the coast line.

656 Thus, as a second step, we also create a “weak” sea breeze mask. It uses the same
657 criteria as the strong mask, except that points with a wind speed gradient greater in
658 magnitude than one twentieth (rather than one quarter) of the maximum negative
659 wind speed gradient are included and the inland-directed wind requirement is
660 removed. This weak mask is shown in Figure A1c. It contains far too many points far
661 from the sea breeze, but has the advantage of fully including the sea breeze.

662 Using the weak sea breeze mask, we first pad the region and fill small holes
663 (Figure A1d). Then MATLAB's 'bwconncomp' function is used to identify connected
664 groups of points. Points are considered connected according to Figure A1e where
665 grid boxes labeled 1 are considered neighbors of the central box. The connected
666 region that corresponds to the sea breeze is identified as the one containing the
667 greatest number of points from the strong sea breeze mask (Fig. A1f; the "starting
668 region").

669 For the case in Figure A1, the starting region still contains far too many points
670 that are not near to the sea breeze. These points appear as branches from the "true"
671 sea breeze location. These branches are systematically removed (Figure A1g-h).
672 Finally, remaining points in the starting region that extend further inland than the
673 maximum extent of the sea breeze as determined from the strong sea breeze mask
674 at each output time are also eliminated (Figure A1i).

675 From this final set of points, the sea breeze location is determined. Starting at the
676 first output time with an identified sea breeze, its location is identified as the point
677 with the minimum (most negative) value of the second spatial derivative of the wind
678 speed. Restrictions on the propagation speed are applied for subsequent times. This
679 procedure for identifying the sea breeze location at each time is repeated until the
680 end of the sea breeze is reached.

681

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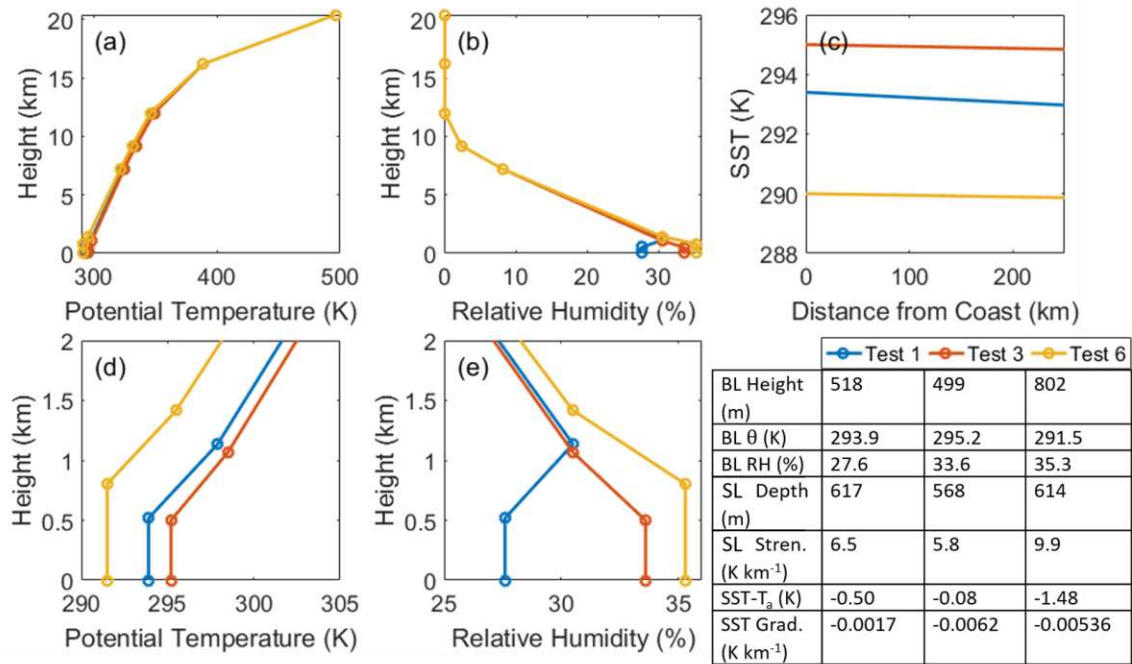
879 **Tables**

880 Table 1. A list of the factors used in this study, the ranges selected, and their
 881 descriptions.

Factor	Range	Description
Atmosphere Factors		
Stable Layer Strength	1–15 K km ⁻¹	Potential temperature lapse rate of the air layer immediately above the boundary layer.
Stable Layer Depth	100–1000 m	Depth of the air layer immediately above the boundary layer.
BL Potential Temperature	285–300 K	Constant with height in the boundary layer.
BL Relative Humidity	20–50%	Constant with height in the boundary layer. We recognize that a well-mixed boundary layer does not have constant relative humidity with height; however, this method ensured that we never accidentally began a simulation with supersaturated conditions. The boundary layer mixing quickly set up a realistic moisture profile after the simulations started.
BL Height	100–1000 m	Distance from the surface to the boundary layer top.
Wind Speed	-5–5 m s ⁻¹	Winds were perpendicular to the coastline. Both the speed and direction were constant with height throughout the depth of the troposphere. Wind shear has also been shown to impact sea breeze circulations [Drobinski <i>et al.</i> , 2011] but was not tested here.
Geophysical Factors		
SST-T _a	-10–10 K	Sea surface temperature (SST) minus the lowest level air temperature (T _a). The factor ranges were chosen such that the SST was never below freezing.
SST gradient	-0.02–0.02 K km ⁻¹	The gradient was applied beginning at the coast such that the SST obtained from the SST-T _a difference was valid at the coast. The ranges for both SST factors is based on the Reynolds SST Analysis [Reynolds <i>et al.</i> , 2007].
T _l -T _a	0–10K	Land surface temperature (T _l) minus the lowest level air temperature.
Soil Moisture	0.1–0.9	Specified as a soil saturation fraction.
Coriolis	0–45°	The Coriolis force was turned on in all simulations and was varied by changing the specified latitude. However, the chosen latitude did not impact the solar zenith angle or the incoming shortwave radiation. See text for more details.

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883 **Figures**

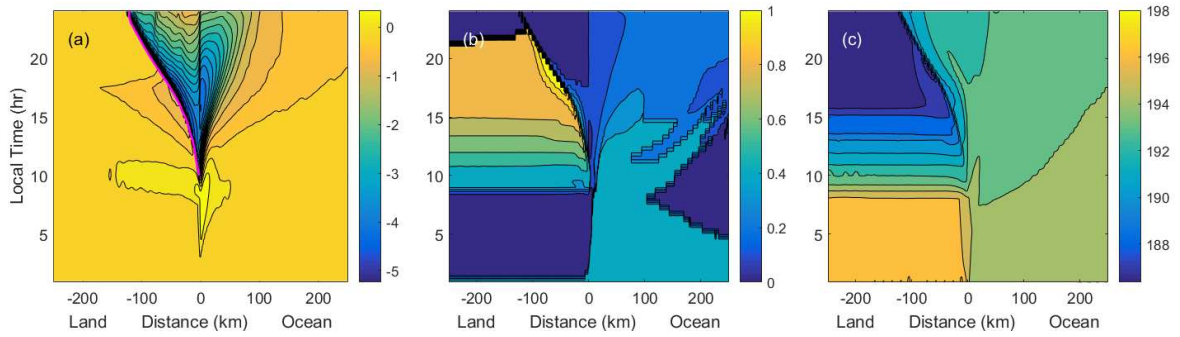


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885 Figure 1. Example initial conditions from Tests 1, 3, and 6. a) Potential temperature
 886 profiles, b) relative humidity profiles, and c) sea surface temperature as a function
 887 of distance from the coast. d) and e) are similar to a) and b), respectively, but show
 888 only the lowest 2km of the atmosphere. The table shows the values of the relevant
 889 factors.

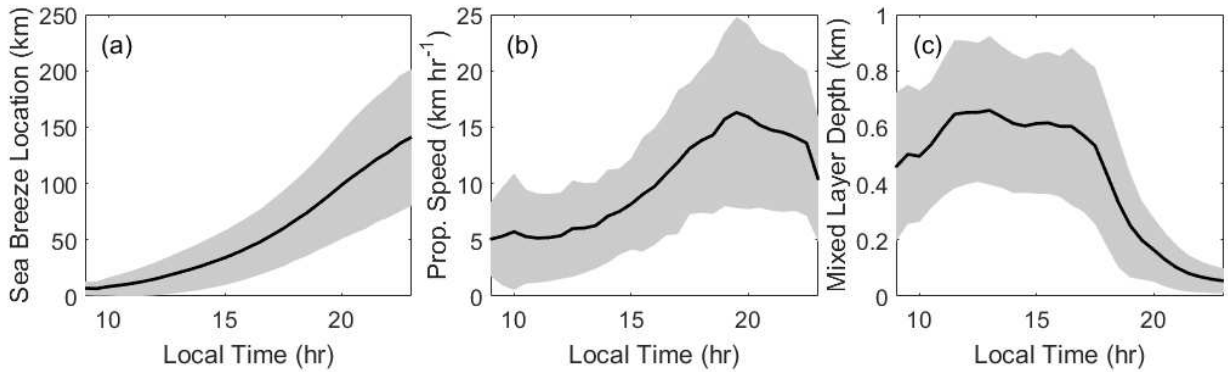
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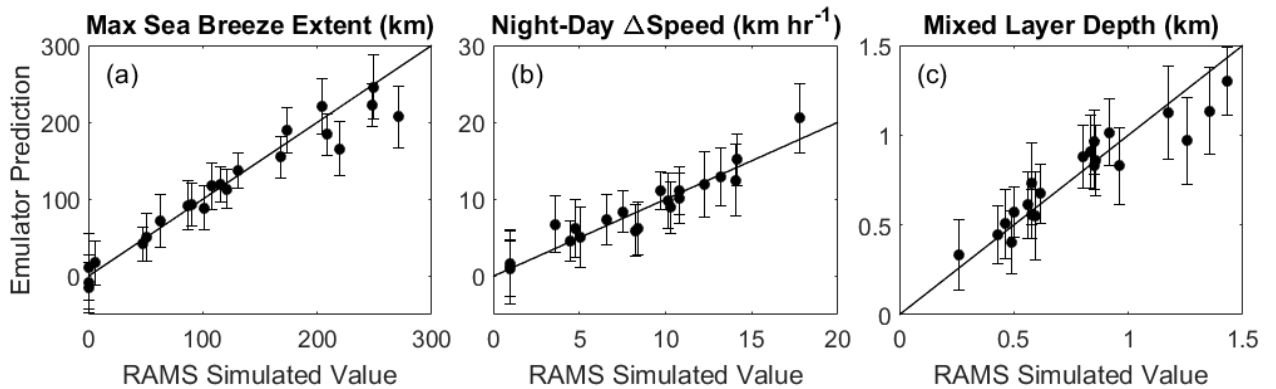
893 Figure 2. Example evolution of the sea breeze from Test 1. Shaded contours show (a)
894 wind speed (m s^{-1}) perpendicular to the coast, (b) surface-based mixed layer depth
895 (km), and (c) tracer surface concentration (mg kg^{-1}). The pink line shows the
896 location of the objectively identified sea breeze.



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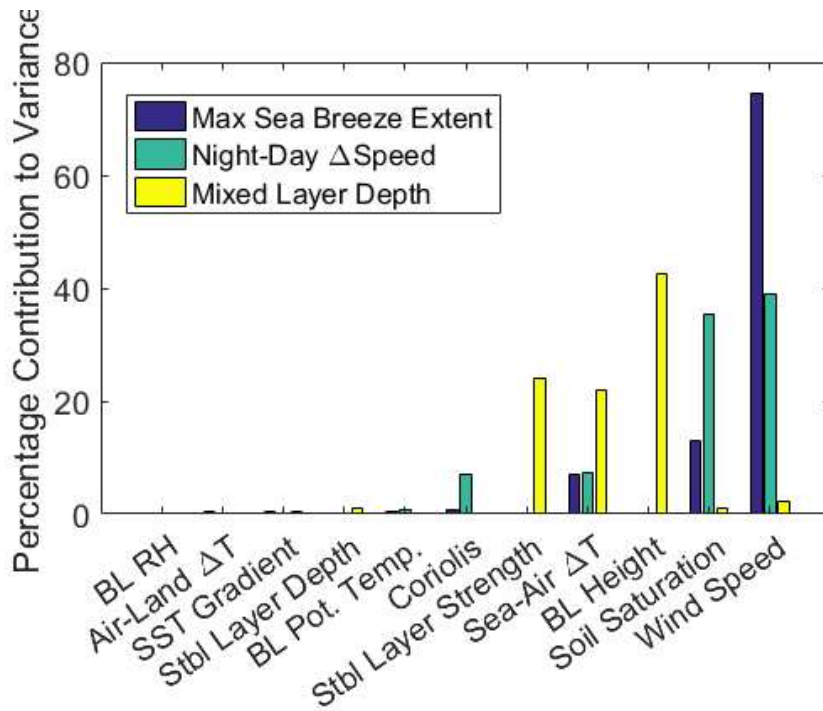
898 Figure 3. Mean and +/- one standard deviation of the (a) location of the sea breeze
 899 front (km inland), (b) the propagation speed (m/s), and (c) the surface-based mixed
 900 layer depth behind the sea breeze front from all 143 simulations.

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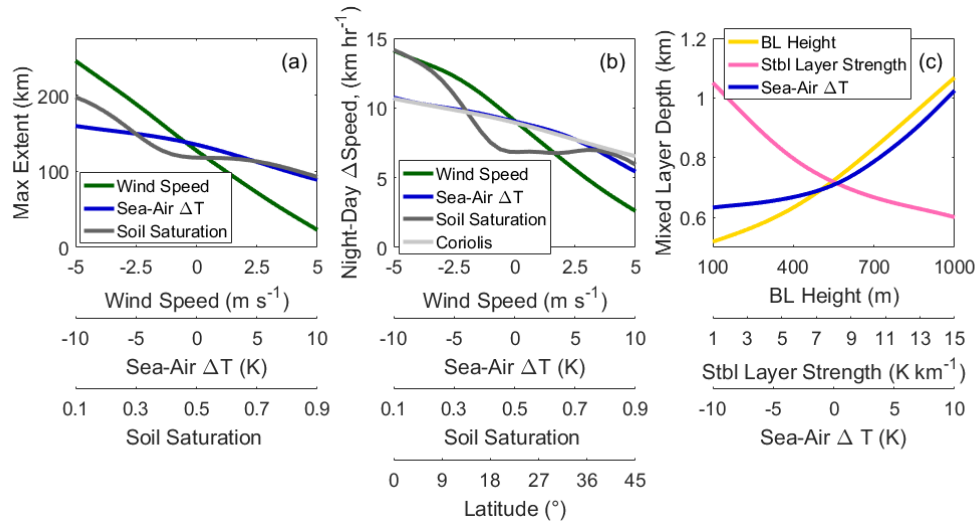
903 Figure 4. Validation of the emulator for (a) maximum sea breeze extent, (b)
 904 difference in nighttime and daytime propagation speed, and (c) surface-based mixed
 905 layer depth over land behind the sea breeze front. The x-axis shows the values
 906 predicted by the RAMS simulations, and the y-axis shows the values predicted by
 907 the emulator, with 95% confidence bounds. The solid line is the 1-to-1 line which
 908 indicates where the emulator and RAMS predict the same value.



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910 Figure 5. Percentage contribution to variance for the maximum sea breeze extent
 911 (navy bars), nighttime minus daytime propagation speed (teal bars), and mixed
 912 layer depth (yellow bars) by each of the eleven factors.

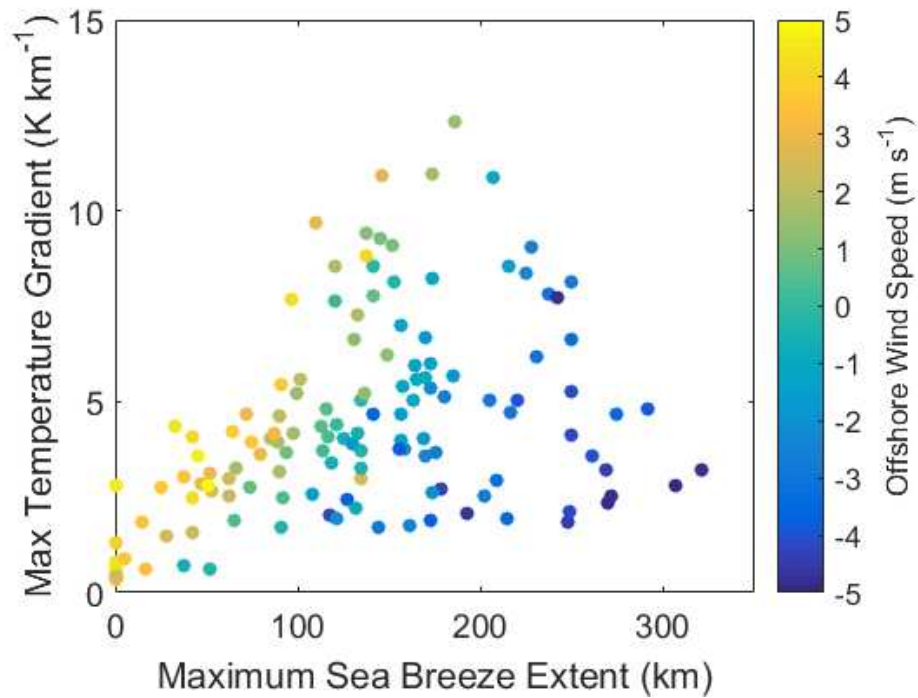
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915 Figure 6. Mean response of the (a) maximum sea breeze extent (km), (b) nighttime
 916 minus daytime propagation speed, and (c) surface-based mixed layer depth behind
 917 the sea breeze front to the factors that contribute 5% or more to the output variance
 918 in each case. Each line corresponds to a different x-axis.

919



920

921 Figure 7. Scatter plot of the maximum sea breeze extent (km) and the time and
 922 domain maximum surface temperature gradient (K km^{-1}). Points have been colored
 923 according to the initial cross-coast wind speed (m s^{-1}). Positive values indicate
 924 offshore winds and negative values indicate onshore winds.

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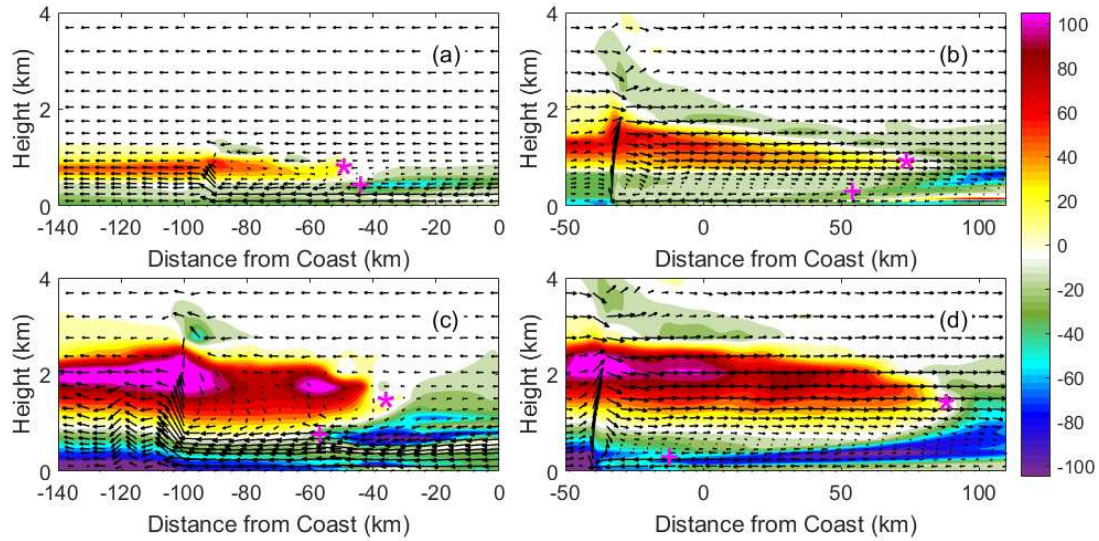
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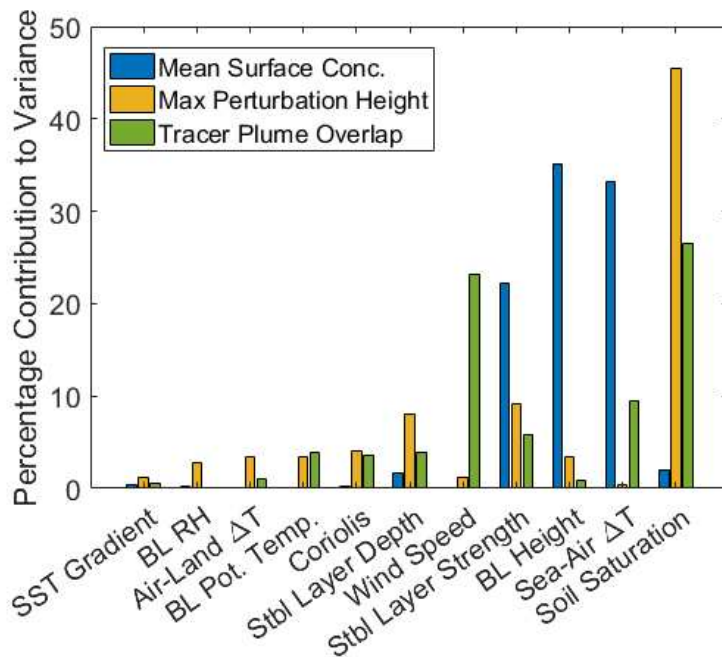
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935 Figure 8. Examples from four simulations of the tracer perturbation field (mg^{-1})
 936 (1800 LT minus 0600 LT), and the cross-coast wind circulation. The simulations are
 937 chosen to demonstrate the impacts of the initial wind speed and soil moisture.
 938 Specifically, (a) low soil moisture and onshore wind, (b) low soil moisture and
 939 offshore wind, (c) moderate soil moisture and onshore wind, (d) moderate soil
 940 moisture and offshore wind. Pink stars show the locations of the vented plume head,
 941 and pink crosses show the locations of the clean plume head.



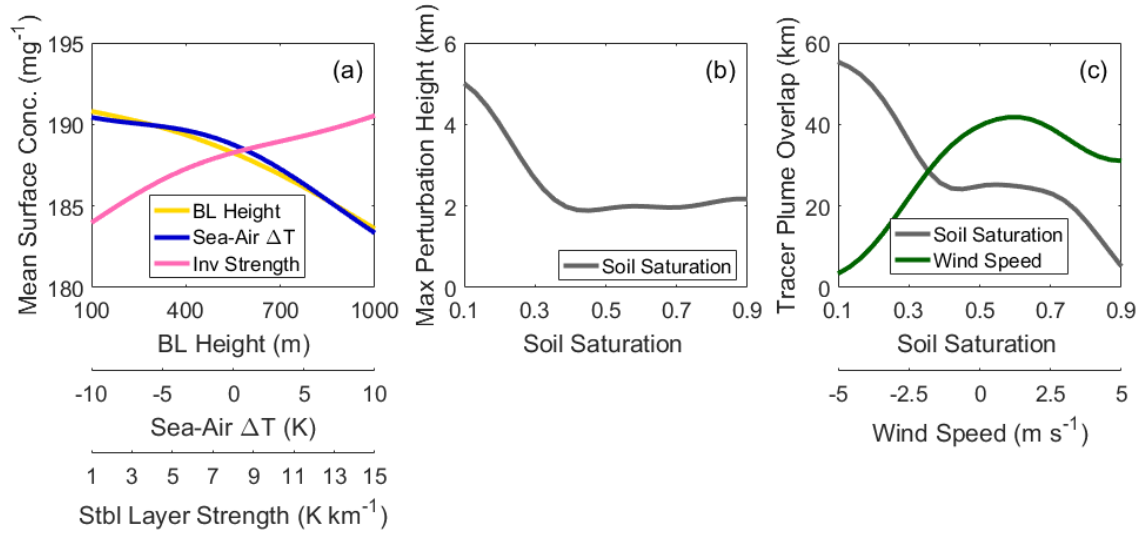
942

943 Figure 9. Like Figure 5, but for the mean surface tracer concentration between the
 944 coast and the sea breeze front at 1800 LT (blue bars), maximum height of a 1%
 945 positive perturbation in tracer concentration (orange bars), and the overlap
 946 distance of the clean and vented plumes (green bars). See the text for more details.

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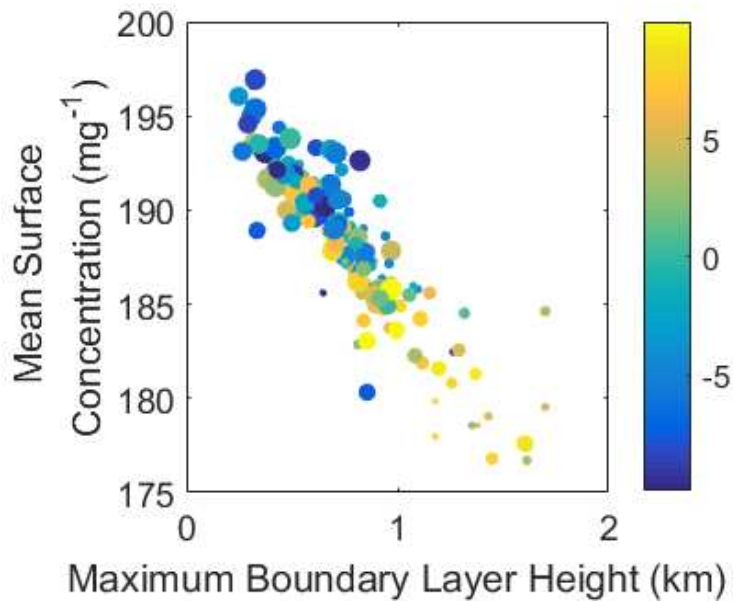


950

951 Figure 10. Like Figure 6, but showing the mean response of factors for each of the

952 three aerosol tracer-related model outputs that contribute 10% or more to the

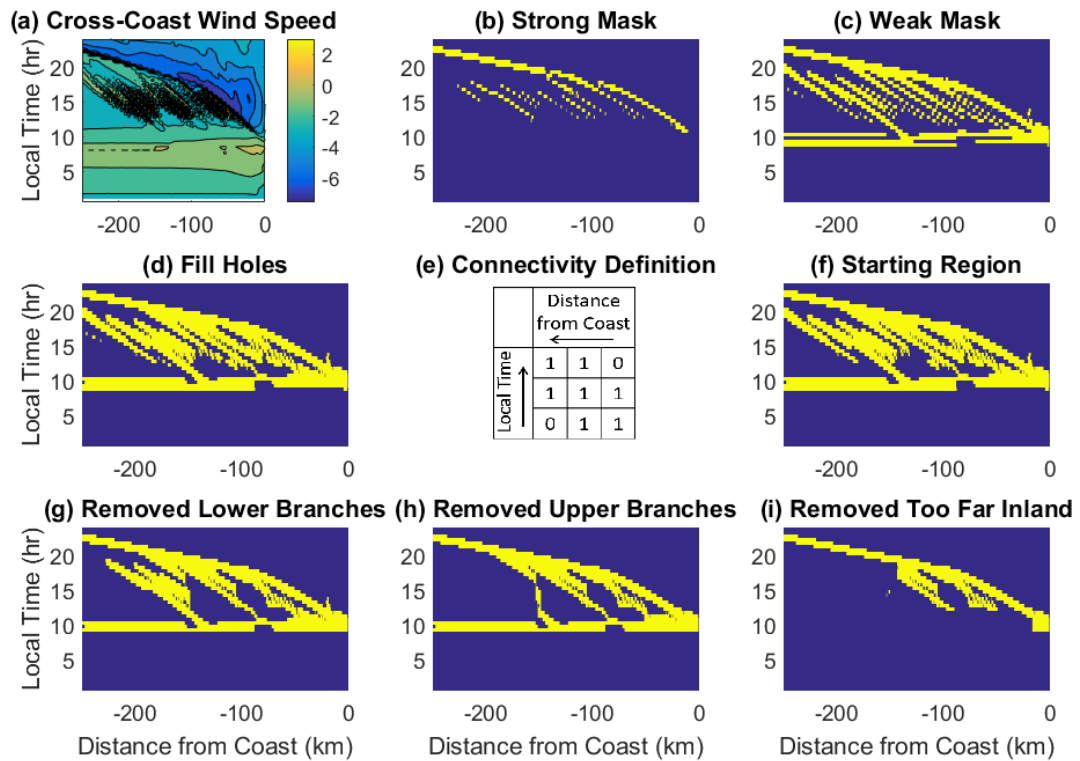
953 model response.



954

955 Figure 11. Scatterplot of the average surface tracer concentration at 1800 LT and
956 maximum boundary layer height between the coast and the sea breeze front from all
957 143 simulations. Colors indicate the sea-air temperature difference (K), and size
958 indicates the initial stable layer strength. Large (small) sizes correspond to strong
959 (weak) stable layers.

960



961

962 Figure A1. A demonstration of part of the sea breeze identification algorithm for one
 963 sea breeze simulation. (a) shows the cross-coast wind speed as a function of time
 964 and distance inland from the coast. (b-d, f-i) show potential sea breeze locations in
 965 yellow after each step of the algorithm. Details about each step are found in
 966 Appendix A. (e) shows the definition of connectivity.