



1 **High accuracy calculation and data quality evaluation of** 2 **ship emissions based on the sniffer method**

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7 **Abstract.** More attention has been paid to the air pollution caused by ship emissions; hence the
8 establishment of accurate emission inventories is an important means to assess the impact on the
9 environment and human beings. The emission factor is an important parameter in the process of
10 compiling the ship emission inventory, yet there is some uncertainty in its estimation based on the sniffer
11 method. In this study, taking the calculation of SO₂ emission factors as an example and aiming at the
12 selection of gas measurement values using the sniffer method, the concept of standard deviation of peak
13 density was proposed to determine the optimal integral interval length of the measured values of SO₂ and
14 CO₂. Then, the improved Manhattan distance was used to characterize the position of the peak points in
15 the SO₂ and CO₂ average series. Using the dynamic time warping algorithm, the corresponding
16 relationship of the peak points in the average series of the measured gases was determined, and the global
17 optimal peak points were selected from it. To evaluate the credibility of calculated emission factors, 16
18 evaluation indexes that reflect the characteristics of the measured data were selected. The confidence
19 interval of 95% of each evaluation index was calculated using self-development sampling of the
20 measured data, and the evaluation result of the evaluation index for the quality of the measured data was
21 obtained. Combined with the data quality label, the indexes with high correct rate were screened. Finally,
22 the evaluation scores were determined according to these selected indexes. We collected a total of 148
23 sets of "SO₂+CO₂" measurement data between 2019 and 2021 using the unmanned aerial vehicle sniffing
24 monitoring system in the Waigaoqiao Port area of Shanghai, China for verification using the method
25 proposed in this study. The results show that for this data set, 12 s is the most suitable integral length,
26 with which the algorithm can automatically calculate the emission factor. The screening results of the
27 global optimal peak points of 129 groups of data are consistent with those of artificial screening, with a
28 correct rate of 87.16%. The accuracy of the combined evaluation of sample entropy (SO₂), information
29 entropy (SO₂), skewness (CO₂) and quartile spacing (SO₂) is 71%. Previous calculation of the emission



factor of ships mainly focused on different conditions such as time, region, fuel, engine, ship type, and navigation status. Our in-depth study proposes a high accuracy ship emission factors calculation method and an evaluation of the quality of the measurement data that reduces uncertainty in the current sniffer technique monitoring ship emission research.

1 Introduction

In the past decade, the development of the global shipping industry has accelerated (UNCTAD, 2021), resulting in increasingly serious emission problems (Chen et al., 2019). Gases and particles emitted by ships will not only pollute the natural environment, but also have an impact on human health (Liu et al., 2016). SO_2 causes frequent acid rain damage to the environment (Matthias et al., 2010) such as the erosion caused to 50% and 30% of the forests in Germany and Poland and Switzerland, respectively (Mohajan et al., 2018). Fine particulate matter ($\text{PM}_{2.5}$) can cause lung cancer and other heart and lung diseases, and results in 2.2 million to 3.3 million deaths worldwide each year (Sofiev et al., 2018). In 2015, a total of 20.1×10^6 tons of NO_x , 11.5×10^6 tons of SO_x , and 1.54×10^6 tons of PM were emitted by global shipping operations (Sofiev et al., 2018). In 2017, EU shipping emissions generated 2.6×10^6 tons of SO_2 and 7.7×10^6 tons of NO_2 (Jonson et al., 2020).

Accurate ship emission inventory is not only the baseline data for analyzing the law of ship emissions, but also the scientific basis for controlling and optimizing supervision measures in relevant management areas (Zhang et al., 2017; Zhang et al., 2017). The calculation of ship emission inventory is carried out using two approaches: top-down and bottom-up. The top-down method is based on the fuel consumption of the ship without considering its specific location, and is suitable for the calculation of the long-term source list on the global scale. Kesgin et al. (2001) used the top-down method to calculate the emissions of CO, CO_2 , $\text{PM}_{2.5}$ from ships in the Turkish Strait. Corbett et al. (1997) studied the global emission inventory using ship fuel. The bottom-up method directly estimates emissions based on the motion state and attributes of the ship, which is more accurate than the top-down method. In recent years, due to the rapid development of the Automatic Identification System (AIS), it is more convenient to obtain the real-time operation status of ships, hence this method is widely used in the research of emission inventory. Papaefthimiou et al. (2016) used a bottom-up approach based on port ship activity to calculate the NO_x , SO_2 , $\text{PM}_{2.5}$ emitted by international cruise ships in 18 ports in Greece. Tichavska et al. (2015) obtained



58 ship activity data through the AIS and studied the monthly relationship between ship emissions and vessel
59 type in Las Palmas Port.

60 Parameter information such as ship speed and position, main engine power, auxiliary power, and
61 emission factors are needed when establishing an emission list. Among them, the static and dynamic
62 information of the ship can be obtained directly using AIS data and other channels, whereas the emission
63 factor can only be determined by measurement, thus the accuracy of the measurement directly determines
64 the accuracy of the emission list (Ekmekçioğlu et al., 2020; Yang et al., 2021; Toscano et al., 2021).

65 There are two ways to measure emission factors: fuel- and power-based. The former can be calculated
66 by measuring the concentration of CO₂ and other pollutants, while the latter needs to obtain real-time
67 data of mainframe power, auxiliary power, and operation mode. The two measurements can be converted
68 to each other when the ship fuel consumption rate is known (Zhang et al., 2016). Sniffer technique is one
69 of the methods based on the fuel emission factor measurement, which can quickly and accurately
70 calculate the ship plume. Balzani Lööv et al. (2014) used the sniffer technique among others to compare
71 the measures of the emission factor and fuel oil sulfur content of ships in the port of Rotterdam. The
72 mobile sniffer technique was the most convenient and accurate, with an average random error of 6% for
73 SO₂ emission factors. Beecken et al. (2014) used a small aircraft carrying sniffer equipment to monitor
74 exhaust emissions from 158 ships in the Baltic Sea and North Sea. The average emission factor of SO₂
75 was $18.8 \pm 6.5 \text{ kg}_{\text{fuel}}^{-1}$, and approximately 85% of the monitored ships met the sulfur content limit set
76 by the International Maritime Organization. Many studies have shown that the emission factor and its
77 accuracy is an important parameter in the compilation of ship emission inventory (Moreno-Gutiérrez et
78 al., 2015; Zhang et al., 2017; Ekmekçioğlu et al., 2020). Therefore, many emission factors measurements
79 have been proposed to obtain accurate results. These experiments focused more on measuring and
80 obtaining emission factors under different conditions such as time, region, fuel, engine, ship type, and
81 navigation status (Sinha et al., 2003; Cooper, 2003; Burgard and Bria, 2016; Peng et al., 2016; Betha et
82 al., 2017; Liu et al., 2018; Bai et al., 2020). However, there is still a lack of in-depth research on how to
83 accurately calculate the emission factor from measurement data and how to evaluate the quality of the
84 measured data.

85 Taking SO₂ as an example, the principle of the sniffer technique is based on the 85% and 87% stability
86 of the carbon content in ship fuel. The concentration ratio of CO₂ to SO₂ generated by fuel combustion
87 is equal to the molar ratio of carbon to sulfur in the fuel and will not change due to tail gas dilution, thus



88 the measurement of CO₂ and SO₂ concentration can be used to calculate the emission factor (Huang et
89 al., 2021). However, various uncertain factors in the calculation process cause nonnegligible interference
90 to the emission factor, which mainly exists in three aspects: first, because the response time of different
91 gas sensors varies, it is difficult to select the measured value of gas at the same time as the calculated
92 emission factor. Therefore, the general method is to select the gas measurement values for a period for
93 the cumulative calculation to reduce the error caused by the response time of different gas sensors that
94 cannot be synchronized. Zhou et al. (2020) proposed to regard the accumulation process as an integral,
95 and then divide the result by the time interval, so as to convert the gas measurement into an average value
96 to find a method that selects the global optimal peak point of the gas average value. The problem of
97 selecting the appropriate integral interval is selecting the global peak point in the average set of measured
98 data. However, the time interval of the integral interval mainly depends on experience. Second, based on
99 the first problem, the selection of the global optimal peak point directly determines the accuracy of the
100 emission factor calculation. However, multiple peaks of SO₂ and CO₂ will appear in gas measurements
101 over a period. Therefore, there is a lack of in-depth research on how to establish a matching relationship
102 between the peak points to determine the global optimal peaks of SO₂ and CO₂. Third, various
103 environmental and equipment factors in the process of ship exhaust gas measurement will interfere with
104 the gas measurement value, hence there is no objective evaluation method for the gas measurement value
105 at present.

106 This study makes an in-depth study and analysis of the above three problems. Aiming at the first problem,
107 the concept of peak density standard deviation is proposed to measure the ability of an integral interval
108 to represent the changing data. The larger the value of the standard deviation of peak density, the more
109 obvious the changes of the data processed by the corresponding integral interval, the clearer the peak
110 trend, and the more accurate the selection of the global optimal peak point. Aiming at the second problem,
111 to select the optimal peak point from many peak points, it is necessary to establish a matching relationship
112 between the average series of the two gases and judge the rationality of all the matching relations. The
113 dynamic time warping (DTW) algorithm was proposed by Itakura (Itakura, 1975), and its function is to
114 measure the similarity of two time series. Dmytrów et al. (2021) recently used the DTW algorithm to
115 evaluate the similarity between energy commodity prices and the daily cases time series for the
116 coronavirus disease (COVID-19). Li et al. (2020) used the DTW algorithm to compare the corresponding
117 relationship between ship trajectory time series, which improved the performance of navigation trajectory



modeling. Applying the DTW algorithm to the screening of peak points can obtain the similarity between CO₂ and SO₂ sequences and the matching relationship between the average sequences of their peak points. Further, combining the criteria for selecting the optimal peak points proposed by Zhou et al. (2019) can select the appropriate gas measurement value for the calculation of emission factors. Aiming at the third problem, 16 evaluation indexes that reflect the data quality are put forward, in which the evaluation index for a single gas measurement value is divided into two cases to use the SO₂ and CO₂ measurement values for evaluation, respectively. The 95% confidence interval of the evaluation indexes are calculated by self-developing sampling for a number of measured data, and the evaluation results of these indexes for the quality of the measured data are given accordingly. Combined with the quality label of the measured data, the correct rate of the index for data quality evaluation can be obtained, and the evaluation indexes with higher accuracy can be selected to form a set for joint evaluation, so as to further improve the accuracy of the gas measurement data evaluation. Finally, using the method proposed in this study, the ship exhaust data measured in Shanghai Waigaoqiao Port are tested, and it is verified that this method can find the appropriate global optimal peak point with high accuracy and then calculate the emission factor, using indexes to jointly evaluate the quality of the measured data.

2 Theory

2.1 Method of calculating ship emission factors

The sniffer method is based on three assumptions: first, the carbon content in different ship fuels is approximately 87% similar. Second, the combustion of carbon and sulfur in ship fuel produces almost all CO₂ and SO₂, while the rest of sulfur and carbon oxides account for only a small part, which can thus be ignored. Third, when the tail gas generated by marine fuel combustion is diluted in the air, the ratio of CO₂ to SO₂ does not change (Hu et al., 2018). Accordingly, the SO₂ emission factor can be calculated by measuring the gas concentration of SO₂ and CO₂ over a period and accumulating the ratio respectively. The formula is (Beecken et al., 2014):

$$EF_{SO_2} [g \text{ kg}_{fuel}^{-1}] = \frac{m(SO_2)}{m(fuel)} = \frac{M(SO_2) \cdot \sum[SO_{2,ppb}]}{M(C)/0.87 \cdot \sum[CO_{2,ppm}]} = 4.64 \frac{\sum[SO_{2,ppb}]}{\sum[CO_{2,ppm}]} \quad (1)$$

where $m(\cdot)$ is the mass, $M(C)$ is the relative atomic mass of carbon, $M(SO_2)$ is the relative molecular mass of sulfur dioxide, and $\sum[\cdot]$ is the cumulative summation of the concentration of the gas to be measured over time.



146 Considering that the sensor cannot achieve complete synchronization, the method of accumulating the
 147 measured values over a period can be adopted instead of using one measured value, that is, the calculation
 148 of the emission factor can be more stable by integrating the measured values of gas over a period. In this
 149 study, we calculate the SO₂ emission factor by converting gas measurements into average values, as
 150 shown in Eq. (2) (Zhou et al., 2020):

$$151 \quad EF_{SO_2} [g \text{ kg}_{fuel}^{-1}] = 4.64 \frac{\int (SO_{2,peak} - SO_{2,bkg}) dt [ppb] / t}{\int (CO_{2,peak} - CO_{2,bkg}) dt [ppm] / t} = 4.64 \frac{AVG(SO_{2,peak}) - AVG(SO_{2,bkg})}{AVG(CO_{2,peak}) - AVG(CO_{2,bkg})} \quad (2)$$

152 where $SO_{2,peak}$ is the peak of SO₂ in the measured data, $SO_{2,bkg}$ is the background value of SO₂ in the
 153 measured data, t is the length of the integral interval, $\int(\cdot)dt$ is the integral calculation function of the
 154 integral interval of t seconds, and $AVG(\cdot)$ is the function of calculating the average measured value in t
 155 seconds.

156 Using the above transformation, the problem of selecting the integral interval of gas using the sniffer
 157 technique is selecting the integral interval and peak point. The empirical value of 10 s was used by Zhou
 158 et al. (2020) in the integration interval, and then by observing and analyzing the changing trend of the
 159 peak point in the average series, the appropriate global optimal peak point was selected for the calculation
 160 of emission factors. Through the above methods, more accurate results can be calculated. However, the
 161 length of the selected integral interval belongs to empirical value, which lacks theoretical demonstration.
 162 In addition, when there are many peak points in a period, there is also uncertainty about how to pair SO₂
 163 and CO₂.

164 2.2 Dynamic time warping algorithm

165 In order to eliminate the inconsistency of response time between SO₂ and CO₂ sensors, it is necessary to
 166 find the matching relationship between the peak points on the average sequence of SO₂ and CO₂, so that
 167 the global optimal peaks with corresponding relationship can be screened. According to the distance
 168 relationship between peak points, this study uses the DTW algorithm to establish the matching
 169 relationship between the SO₂ and CO₂ peak points. The purpose of the DTW algorithm is to find the
 170 difference between each data point in the target and standard time series, calculate the minimum value
 171 after the difference accumulation, and determine the corresponding path, which is used to match the peak
 172 points of SO₂ and CO₂ in this study. The target time series is marked as $X = (x_1, x_2, \dots, x_n)$. The standard
 173 time series is written as $Y = (y_1, y_2, \dots, y_m)$. In this study, we correspond to the results of peak point



174 extraction from the SO₂ and CO₂ average series. f represents the distance between the points on the
 175 target time series and its corresponding standard time series in an unbiased ideal state:

$$176 \quad d(i, j) = f(x_i, y_j) \quad (3)$$

177 The distance matrix D is obtained by calculating the distance between the data points and their
 178 corresponding points in X and Y :

$$179 \quad D_{ij} = d(i, j) \quad (4)$$

180 The shortest distance is to use the cost matrix D_{cost} iteration to calculate the dynamic programming path
 181 distance between the target and the standard sequences, and the shortest distance path represents all the
 182 matching relations of the data points on the two sequences.

$$183 \quad D_{cost}(i, j) = D(i, j) + \min(D_{cost}(i-1), D_{cost}(j-1), D_{cost}(i-1, j-1)) \quad (5)$$

184 The path corresponding to the shortest distance matrix between the CO₂ and SO₂ peak points is obtained
 185 by the DTW algorithm, that is, the matching relationship between the peak points in the SO₂ and CO₂
 186 average sequence is obtained, which can correct the deviation sequence.

187 3 Method

188 The high accuracy calculation of emission factors needs to select the measured values of stable air flow
 189 over a period and eliminate the influence of various uncertain factors as much as possible. In this study,
 190 we first determine the selection method of the optimal integral interval length. Then, use the DTW
 191 algorithm to find the matching relationship between the peak points on the CO₂ and SO₂ average series,
 192 and select the global optimal peak points. Finally, a quality evaluation method of ship exhaust
 193 measurement data is proposed, which is used to evaluate the reliability of the measurement results. The
 194 specific process is divided into the following four steps:

195 1. Selection of integral interval length and extraction of peak points. The concept of standard
 196 deviation of peak density is put forward to analyze the distribution law and changing trend of peak points
 197 in the measured value sequence, the larger the value of standard deviation of peak density is, the longer
 198 the corresponding integral interval can make the calculation of emission factors more stable. The
 199 measured value is converted to the average value of the length of the integral interval, and all the peak
 200 points in the average sequence are extracted;

201 2. DTW-based matching. The DTW algorithm based on the improved Manhattan distance is used



202 to correct the average sequence and obtain the matching relationship between SO₂ and CO₂ peak points;
203 3. Filtering matching relationships. The matching relationship between the peak points in some
204 measured data is established, and all the matching relations are taken as samples for k-means mean
205 clustering. If they can be stably divided into two categories, it shows that the dividing line between the
206 two categories can distinguish between normal and abnormal changes, thus the threshold of concentration
207 change is found. Combined with the time span threshold, the results from step 2 are screened and the
208 abnormal matching results are eliminated. The matching result containing the maximum average value
209 of SO₂ is found among the reserved matching results, and the matching result containing the maximum
210 average value of CO₂ is selected as the global optimal peak point from all the matching results found;
211 4. Evaluation of measurement data quality. Sixteen evaluation indexes, which can characterize
212 the data quality are proposed. For several measurement data obtained, the 95% confidence interval of
213 each index is calculated by self-expansion sampling. If the index value is in the confidence interval, it is
214 marked as 1, otherwise 0. Combined with the quality label of the measured data, some indexes with
215 strong representation ability are selected from the 16 indexes to form a set of indexes for joint evaluation.
216 The distance between the index value of the measured data and overall mean of the central position of
217 the confidence interval is calculated, and the ratio of the distance to the unilateral length of the confidence
218 interval is obtained (a ratio greater than 1 is reassigned to 1). In joint evaluation, if the calculated ratio of
219 all indexes is 1, the quality of the measured data is judged to be poor; otherwise, the average value of all
220 ratios less than 1 is calculated, and the closer the mean is to 0, the better the quality of the measured data
221 is.
222 In Section 3.1, the principle and method of selecting the length of integral interval are introduced in detail,
223 and the definition of peak point is explained. Section 3.2 introduces the use of the DTW algorithm to
224 match peak points so as to correct the average sequence of SO₂ and CO₂. At the same time, a distance
225 calculation method based on the Manhattan distance is proposed, which can represent the distance
226 relationship between the peak points in the average sequence. The calculation method of the threshold
227 used to eliminate abnormal matching relations is described in detail in Section 3.3. Section 3.4 describes
228 the specific method of selecting indexes from the 16 evaluation indexes to form an index set for joint
229 evaluation.



230 3.1 Selection of integral interval length and extraction of peak points

231 When sniffer equipment is used to monitor the ship exhaust, because the response time of SO₂ and CO₂
232 sensors cannot be completely synchronized, there is a deviation between the time series of CO₂ and SO₂
233 measurements. Using the appropriate integral interval length (set to t) to convert the measured value per
234 second into the average value within t seconds can reduce the deviation between time series to a certain
235 extent.

236 However, setting t often adopts an empirical value, which is not supported by theoretical basis generating
237 great uncertainty. If the selected t value is too small, there will be too many small peaks in the overall
238 measurement data set, or a peak composed of multiple data points, which causes great difficulties in the
239 selection of peak values, resulting in great instability in the calculation of emission factors. On the other
240 hand, if the selected t value is too large, the fluctuation of the whole data set is relatively smooth, which
241 cannot show a representative peak trend, which will hinder the selection of the peak value and have a
242 great impact on the calculation of emission factors.

243 This study proposes a method to determine the optimal integral interval from the point of view of data
244 mining, to reduce the uncertainty of artificial selection of empirical values. To select a suitable integral
245 interval for preprocessing, it is necessary to analyze multiple alternative intervals, because the peak points
246 need to be composed of at least three data points, and very large intervals will excessively smooth the
247 data change trend. Therefore, we only need to find the corresponding relationship between the data
248 change trend and interval, thus the selection range of the integral interval length is from 3 s to 30 s. The
249 sliding window algorithm is used to traverse the measured values, with the window size representing the
250 length of the alternative integral interval; the window moves one point at a time, and the ratio of the peak
251 points of each window to the total data points of the window is calculated. The ratio is the peak density
252 of the window, and the peak density standard deviation of the length of the alternative integral interval
253 is calculated to reflect its changing trend in the measured value. Comparing the peak density standard
254 deviation of each alternative integral interval length, the larger the value, the more the length of the
255 integral interval can reflect the fluctuation of the peak density in the measured value. The specific steps
256 of this method are as follows:

- 257 1. Assuming that there are n measurements in a complete measurement process, the sliding
258 window algorithm is used to traverse all the measurements. The window size is the length of
259 the selected integral interval, and the window moves one measured value each time;



260 2. If a measurement point is larger than the left and right adjacent measurement points, the point
 261 is defined as the peak point. The number of peak points in each window is calculated, and the
 262 peak density of the window is calculated following Eq. (6).

$$263 \quad \text{density}(j) = \frac{\text{count}_{\text{peak}(j)}}{\text{count}_{\text{data}(j)}} \quad (6)$$

264 where $\text{density}(j)$ represents the peak density of the j window, $\text{count}_{\text{peak}(j)}$ represents the
 265 number of peak points of the j window, and $\text{count}_{\text{data}(j)}$ represents the total number of
 266 measurement points of the j window;

267 3. The peak density standard deviation of all windows is calculated during this period of
 268 measurement;

$$269 \quad s = \sqrt{\frac{\sum_{j=1}^n (\text{density}(j) - \text{average density})^2}{n-1}} \quad (7)$$

270 4. If there are N segments of complete measurement process, steps 1-3 are performed to get a
 271 total of N peak density standard deviations, and the mean is calculated;

272 5. The alternative integral interval length of 3–30 s is used to perform steps 1–4 respectively, and
 273 the maximum integral interval length is the optimal integral interval length.

274 Using the optimal integral interval length, the measured sequence of SO_2 and CO_2 is transformed into
 275 the average sequence of SO_2 and CO_2 respectively according to Eq. (2), and all the peak points in the
 276 sequence are extracted for subsequent matching.

277 3.2 Matching based on DTW

278 The concentration of SO_2 in the ship plume is generally 0–10 ppm. The concentration of CO_2 and SO_2
 279 are not in the same order of magnitude of 300–10000 ppm. For these to match using the DTW algorithm,
 280 the average sequences of SO_2 and CO_2 need to be normalized by 0–1 to obtain new SO_2 and CO_2
 281 sequences (marked Q and C):

$$282 \quad Q = \left\{ \frac{\text{SO}_2 \text{ data}(i) - \text{SO}_2 \text{ data}(\min)}{\text{SO}_2 \text{ data}(\max) - \text{SO}_2 \text{ data}(\min)} \right\} \quad i = 1, 2, \dots, n \quad (8)$$

$$283 \quad C = \left\{ \frac{\text{CO}_2 \text{ data}(i) - \text{CO}_2 \text{ data}(\min)}{\text{CO}_2 \text{ data}(\max) - \text{CO}_2 \text{ data}(\min)} \right\} \quad j = 1, 2, \dots, n \quad (9)$$

284 The DTW algorithm calculates the similarity based on the Euclidean distance matrix between two
 285 sequences. In the calculation of the Euclidean distance, only one-dimensional numerical value is
 286 considered, whereas the selection of the global optimal peak point needs to consider not only the relative
 287 size of the concentration, and the time span (the response time deviation of different sensors is usually a
 288 few seconds). The matching between two points with a large time span belongs to abnormal matching,
 289 so it is necessary to use two-dimensional the relative position relationship to represent the distance
 290 between two points. The Manhattan distance considers the values on the two axes, which is more suitable



for the selection of the global optimal peak point than the Euclidean distance. Because the average value has been normalized, the time span needs to be converted to a value between 0 and 1, so it is replaced by the ratio of the time span to the total sequence length:

$$d(Q_i, C_j) = \frac{|i-j|}{n} + |y_i - y_j| \quad (10)$$

In the Manhattan distance calculated following Eq. (10), the proportion of $|y_i - y_j|$ is too large, thus we add a compensation coefficient to balance the size of the two dimensions:

$$d(Q_i, C_j) = \frac{|i-j|}{n} * 9 + |y_i - y_j| \quad (11)$$

Through the improved Manhattan distance, a distance matrix of $k * m$ is constructed (the number of SO₂ and CO₂ peak points is k and m, respectively), which is marked as A, in which the point (i, j) represents the distance $d(Q_i, C_j)$ between the i point of Q and the j point of C. The smaller the $d(Q_i, C_j)$ value, the higher the similarity between Q_i and C_j . Finding a warping path in the matrix A starts from the (0,0) point of the matrix to the end of the (k, m) point, and the superposition produces the smallest distance. The warping path is mainly constrained by the following three aspects: monotonicity, continuity, and boundary conditions.

1. The monotonicity constraint means that the warping path can only extend in the prescribed direction. For a point (a, b) on the path and the next point (a', b') on the path, it must satisfy $0 \leq (a' - a)$ and $0 \leq (b' - b)$;
2. The constraint of continuity means that any point in sequence Q and sequence C can be mapped in a warping path, which can only be aligned adjacent to each other and not matched across points. For a point (a, b) and the next point (a', b') on the path, it must satisfy $(a' - a) \leq 1$ and $(b' - b) \leq 1$;
3. The constraint of the boundary condition means that the first and last point on the warping path must be (0,0) and (k, m) .

Starting from (0,0), each point in the sequence Q and C is matched one by one, and the distance is accumulated. When the final cumulative distance is reached (k, m) , the result is the final distance measure of the sequence Q and C, that is, the similarity between Q and C. Recursion can be performed following Eq. (12):

$$\psi(i, j) = d(Q_i, C_j) + \min \begin{cases} \psi(i, j-1) \\ \psi(i-1, j-1) \\ \psi(i-1, j) \end{cases} \quad (12)$$

Each point on the warping path corresponds to a SO₂ and CO₂ peak points, with a matching relationship between the two points. However, some of the peak points extracted from the average series are due to



small fluctuations caused by the interference of external environmental factors during the measurement, which will affect the direction of the warping path when participating in the match. Therefore, the matching results are not all reasonable, and this is what needs to be selected.

3.3 Filter matching relationship

The points of the warping path found by the DTW algorithm in the distance matrix do not have a reasonable matching relationship. Zhou et al. (2019) previously proposed several criteria to be followed when selecting the global optimal peak point: one is to eliminate the sharp changes of the peak point, because these abnormal changes are caused by the uncertainty of the sensor, the monitored gas and its content in the atmosphere will affect the selection of the global optimal peak point; the other is to eliminate the peak point with a time span of more than 20 s.

In a completely ideal case, the average sequence of SO_2 and CO_2 should be in a state of complete synchronization. When the monitoring equipment slowly approaches the plume of the ship, the average value of SO_2 and CO_2 will increase, but when it is far away from the plume, it will be in a decreasing trend. Because the ideal state will not be disturbed by external environmental factors or the sensor itself, at any time, the average difference between SO_2 and CO_2 will remain stable and will not change greatly. However, in the actual measurement, the complex external environment may make the average difference at different time points different, hence it cannot be used as the global optimal peak point. Therefore, it is necessary to find a threshold that can distinguish between normal and abnormal changes, and eliminate the matching results with a large difference in average. In this study, the K-means clustering algorithm is used to cluster the difference of the normalized mean of all matching results (marked as D) and obtain the threshold to distinguish between normal and abnormal changes. The specific process is as follows:

1. The number of initial cluster centers k is 2, that is, the sample set is divided into two categories, normal and abnormal changes;
2. Two data points in D are randomly selected as the initial cluster centers of the two clusters;
3. The similarity between each sample point and the two cluster centers is calculated, and the sample points are divided into the clusters corresponding to the cluster centers with the greatest similarity;
4. The cluster center of each cluster is recalculated based on the samples in the existing cluster;
5. Iteration through steps 3 and 4 is performed until the center of the cluster no longer changes.

After multiple k-means clustering of D, if D can be stably divided into two categories, then the threshold has been found. If the normalized difference of SO_2 and CO_2 in the matching result is greater than the



threshold, it shows that the matching result belongs to abnormal change and should be eliminated.
 According to the above two conditions, the reasonable matching results are screened out, and those
 containing the maximum average value of SO_2 are retained, while the matching results containing the
 maximum average value of CO_2 are selected as the global optimal peak point from all the matching
 results found.

3.4 Evaluation of measurement data quality

Using the above methods, the automatic calculation of emission factors can be realized. However, there
 is no suitable method to evaluate the quality of the measured data. Therefore, this study proposes a
 method to evaluate the quality of the measured data, according to the index calculation results of the
 measured data. In this study, 16 evaluation indexes are proposed, which are sample entropy, information
 entropy, third quartile, standard deviation, skewness, standard deviation of peak density, permutation
 entropy, fuzzy entropy, approximate entropy, mutual information, first quartile, kurtosis, DTW shortest
 distance, quartile spacing, coefficient of variation, and ratio of the number of peak points. Among them,
 the shortest distance of DTW, the ratio of the number of peak points, and mutual information are obtained
 by calculating SO_2 and CO_2 measurement data. The rest of the evaluation indexes can be obtained only
 by calculating SO_2 or CO_2 . To ensure the accuracy of the evaluation results, for these indexes, we need
 to use SO_2 and CO_2 measurement data, and select the set with higher accuracy to calculate the index. The
 role of each evaluation index is shown in Table 1.

Table 1: Sixteen evaluation indexes and their roles in evaluating data quality.

| Evaluation index name | Role |
|------------------------------------|--|
| Sample entropy | |
| Information entropy | Evaluating the random degree of the sequence can be |
| Permutation entropy | used to study whether the complexity of the measured |
| Fuzzy entropy | sequence is related to the selection of peak points. |
| Approximate entropy | |
| DTW shortest distance | Measure the relationship between multiple sequences. |
| Mutual information | |
| Ratio of the number of peak points | Measure the relationship between the difference in the |



| | |
|---|--|
| | number of peak points in a series and the results of global optimal peak point screening. |
| Standard deviation of peak density | Reflect the aggregation trend and data change trend of peak points in the series. |
| First quartile | |
| Third quartile | Reflect the distribution law of measured values. |
| Quartile spacing | |
| Skewness | Measure the asymmetry of the sequence distribution. |
| Kurtosis | Measure the steepness of the sequence distribution. |
| Standard deviation | Measure the degree of dispersion of the sequence as a |
| Coefficient of variation | whole. |

371

372 The uncertainty of the evaluation index can be quantified using the numerical method based on self-
 373 expanding sampling, so as to determine its confidence interval (Wu et al., 2020; Zhong et al., 2007).
 374 Therefore, through 10000 self-developing sampling of the existing measured data and calculating the
 375 average value of each sampling, a set composed of several mean values can be obtained, according to
 376 which the confidence interval of the evaluation index can be obtained. If the index value is in the 95%
 377 confidence interval corresponding to the index, it determines the high-quality of the measured data, which
 378 is marked as 1. If the index value is outside the 95% confidence interval, the measured data is judged as
 379 low-quality data by the index, which is marked as 0. At the same time, when the quality of the measured
 380 data is labeled, the peak trend is obvious, and the high synchronization of the SO₂ and CO₂ average series
 381 is considered as high-quality data, and the quality label is 1; if the two series have large differences and
 382 drastic changes occur frequently, they are considered as low-quality data, and the quality label is 0.
 383 Combined with the evaluation results of indexes and quality labels, the evaluation accuracy of each index
 384 is calculated, and a certain number of indexes with high accuracy are selected to form an index set to
 385 jointly evaluate the data quality. The distance between the index value of the measured data and overall
 386 mean of the central position of the confidence interval is calculated, and the ratio to the unilateral length
 387 of the confidence interval is obtained. The closer the ratio is to 0, the better the quality of the measured
 388 data. On the contrary, the closer to 1 means the worse the quality of the measured data. When the



numerator in the ratio is greater than the denominator, the ratio is greater than 1, and the index value is not in the 95% confidence interval. Therefore, the result with a ratio greater than 1 is also reassigned to 1. In joint evaluation, if the calculated ratio of all indexes is 1, the quality of the measured data is judged to be poor, otherwise the mean value of all ratios less than 1 is closer to 0, indicating a better quality of the measured data.

4 Experiment

4.1 Data

Our research team designed and developed a sniffer system using an unmanned aerial vehicle (UAV) in the "Shanghai Free Trade Zone ship exhaust Monitoring" (MISEE) project. Field tests have demonstrated that it has the advantages of high monitoring accuracy and convenience (Zhou et al., 2019; Zhou et al., 2020). In this study, this system is used to collect SO₂ and CO₂ data of ship emissions. The monitoring site is located at Waigaoqiao Port in Shanghai, which is only 20 km from the city center. Exhaust gas measurement data (SO₂+CO₂) of 148 ships were collected between 2019 and 2021. Six groups of measurement data are defined to show the rationality and accuracy of the integral interval length selection, peak point matching and measurement data quality evaluation method. The six groups of data are 2019-9-27C, 2019-10-17C, 2021-1-13B, 2021-3-10A, 2021-8-18C, and 2021-9-3A. The date in the number is the date on which the measured data is collected in the field, and the letter indicates the group of data collected on that date. Among them, the data quality of 2021-1-13B and 2021-3-10A is better, with a strong synchronization between the two sequences, while the quality of other measured data is poor, reflecting the peak trend that SO₂ and CO₂ sequences cannot keep synchronization.

4.2 Selection of integral interval length

The result of calculating the optimal integral interval length of 148 groups of measurement data using the method discussed in 3.1 is shown in Figure 1. The standard deviation of the peak density corresponding to 12 s is the maximum, that is, 12 s is the optimal integral interval length. Therefore, the measured value per second is replaced with the average of 12 s, and the average sequence is obtained.

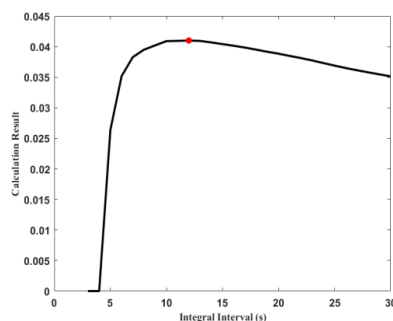
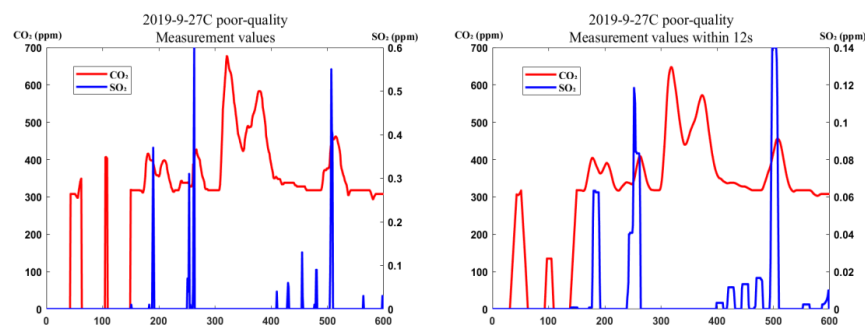


Figure 1. The 3–30 s integral interval length of the peak density standard deviation of the calculated results. The red point is the result of the calculation corresponding to the length of the 12 s integral interval, taking the maximum value.

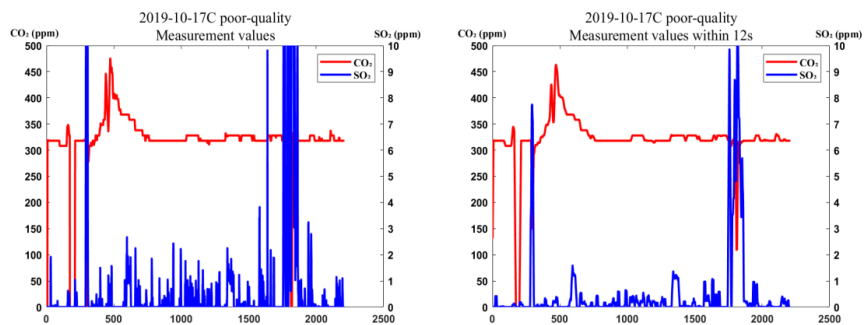
There are differences in the quality of measurement data. High-quality measurement data have a clear peak trend, low-quality measurement data are mixed with small fluctuations, and the peak trend is not obvious. In order to verify the effect of using 12 s as the integral interval, the six groups of measurement data in Figure 2 are taken as an example, which are the measurement data numbered 2019-9-27C, 2019-10-17C, 2021-1-13B, 2021-3-10A, 2021-8-18C, and 2021-9-3A, the abscissa represents the time point, and the interval between the two points, or sampling rate, is 1 s. In addition, the data quality is indicated in the chart title, in which 2021-1-13B and 2021-3-10A are high-quality data, 2019-9-27C, 2019-10-17C, 2021-8-18C, and 2021-9-3A are low-quality data, the left side is the original measurement sequence, and the right side is the average sequence processed with the 12 s integral interval. The changing trends of SO₂ and CO₂ in 2021-1-13B and 2021-3-10A measurement data are basically synchronized. When SO₂ reaches the peak point, CO₂ will also reach the peak point in the subsequent time. The peak points at 175 formed by small fluctuations, then 210 time points in 2021-1-13B measurement data are integrated into a larger peak trend after being converted into an average series. In the 2021-3-10A measurement data, there was a sharp mutation at the 150–165, 190–210, and 300–320 time points of the SO₂ sequence, which changed to a moderate upward and downward trend after processing. At the same time, the platform values at 130, 165, 210, and 265 time points were also converted into peak points that could establish a matching relationship. There are many abrupt changes in the SO₂ sequence of 2019-9-27C measurement data, in which the peak trend at the 260 time point becomes more obvious after being replaced by the average, which can be selected as the global optimal peak. There is no obvious synchronous change in the SO₂ and CO₂ average series in 2019-10-17C, 2021-8-18C, and 2021-9-3A



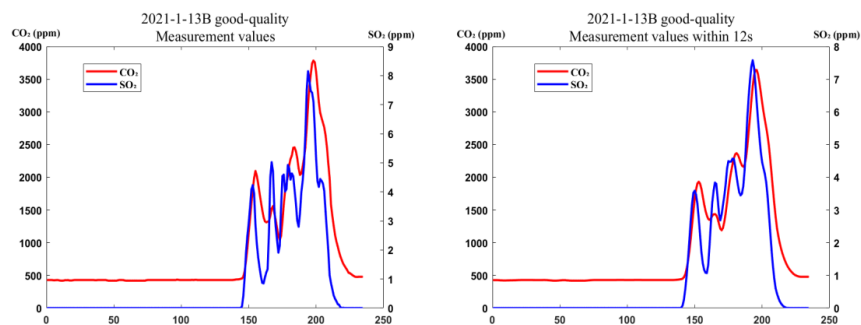
438 measurement data. The average 2019-10-17C sequence can smooth small fluctuations to some extent,
 439 and it can also transform the steep peak trend formed by drastic changes in 1750–1950 time points into
 440 a relatively gentle trend. The SO_2 sequence of 2021-8-18C only has two peak trends at 400, 475 time
 441 points, but because these two peak trends are abrupt, which are converted to average values and flattened
 442 into platform values, and there is almost no synchronization between the two sequences, it is impossible
 443 for this group of low-quality measurement data to select the global optimal peak points. Although 2021-
 444 9-3A has undergone a drastic change, the frequency of the change is not high compared with 2019-10-
 445 17C, hence the effect of the average sequence is more obvious. There are many platform values in the
 446 original CO_2 measurement series, such as those in the 0–45 and 52–90 time points. The average sequence
 447 converts all these platform values into non-platform values, which makes the overall change trend clearer.



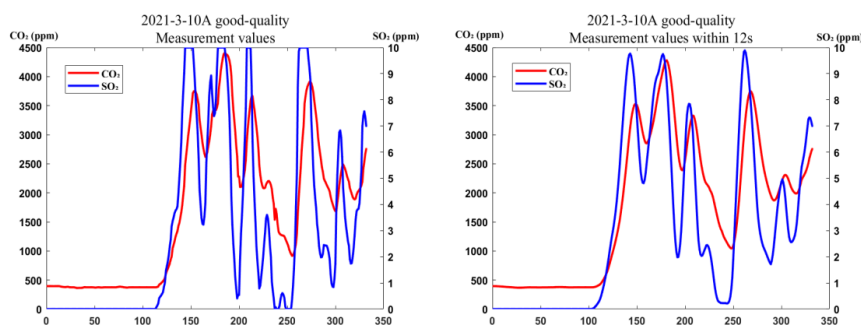
(a)



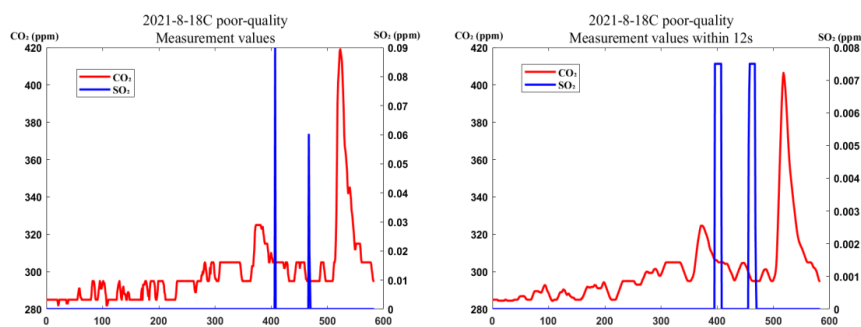
(b)



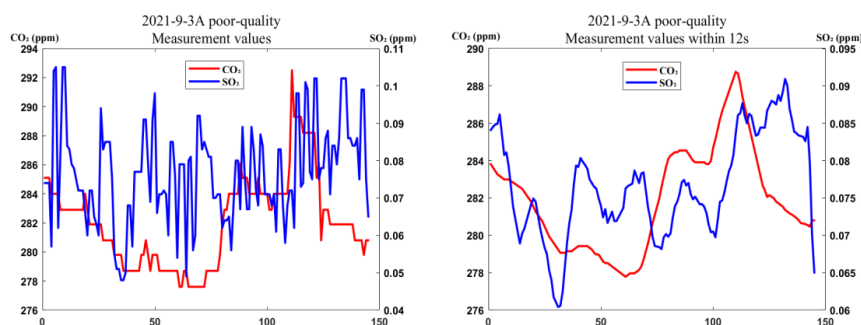
(c)



(d)



(e)



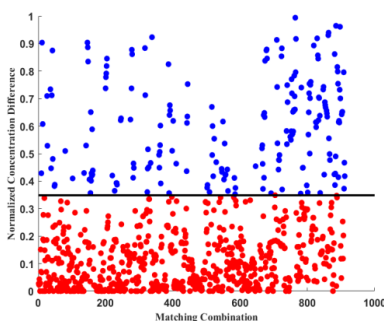
(f)

Figure 2. Groups of measurement data of SO₂ and CO₂. (a) 2019-9-27C; (b) 2019-10-17C; (c) 2021-1-13B; (d) 2021-3-10A; (e) 2021-8-18C; and (f) 2021-9-3A. The time and quality of data measurement are marked in the title. On the left is the unprocessed sequence of measurements, and on the right is the average sequence processed with the length of the 12s integral interval.

4.3 Matching of peak points and screening of global optimal peak points

After the measured value series is converted into an average series, and the peak points of SO₂ and CO₂ are extracted, the corrected time series is transformed into a matching relationship between the peak points of the two average series, and the corresponding peak point of each peak point in another series is found. The DTW algorithm based on the improved Manhattan distance is used to match the peak points of SO₂ and CO₂.

After the peak point matching is complete, the matching results with a time span of more than 20 s and drastic changes need to be eliminated. To find the threshold to distinguish between normal and abnormal changes, calculations are needed. For this reason, we use 148 sets of measurement data for DTW matching, obtain 911 matching results, calculate the difference between the normalized results of SO₂ and CO₂ in each matching result, and then use the K-means clustering algorithm for the 911 differences. The clustering result is shown in Figure 3, the result of multiple clustering is stable, and the threshold is 0.3485. Therefore, after the DTW matching for the peak points of a group of measured data, traversing all the matching results, if the normalized difference between SO₂ and CO₂ is more than 0.3485 or the time span is more than 20 s, cannot be regarded as the global optimal peak point and needs to be eliminated. The matching result containing the maximum average value of SO₂ is found among the reserved matching results, and the matching result containing the maximum average value of CO₂ is selected as the global optimal peak point from all the matching results found.



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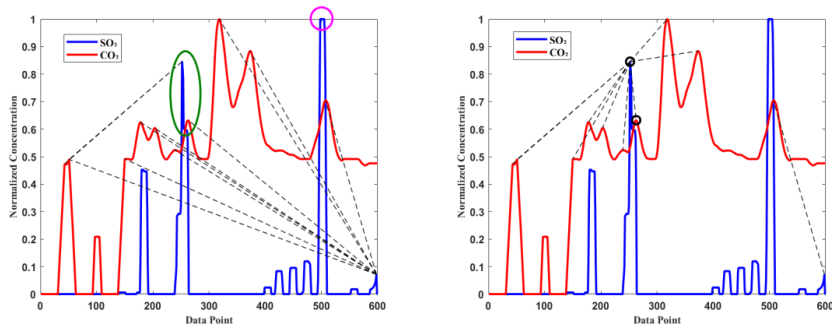
471 **Figure 3. K-means clustering of 911 normalized differences. The red mark point refers to the normalized**
 472 **difference of the normal change, the blue mark point refers to the normalized difference of the abnormal**
 473 **change, and the black line is the threshold to distinguish normal from abnormal changes.**

474 The results of peak point matching show that the improved Manhattan distance can consider the
 475 important time span and concentration difference. Figure 4 shows the results of three groups of
 476 measurement data (2019-9-27C, 2021-1-13B, and 2021-3-10A) screening peak points using Euclidean
 477 distance and improved Manhattan distance in the DTW algorithm. The Abscissa represents the time point,
 478 and the interval between the two points, or sampling rate, is 1 s. The reasonable global optimal peak point
 479 (in the green circle) cannot be found by using the Euclidean distance in 2019-9-27C and 2021-3-10A.
 480 The quality of 2019-9-27C is poor, the variation trend of SO₂ and CO₂ average series is different, and
 481 the platform value cannot be used as peak point at the 500 time point. The quality of 2021-3-10A data is
 482 good, but the matching relationship between SO₂ and CO₂ peak point of synchronous change at the 145,
 483 165, and 260 time points are not established, and the normalized concentration of SO₂ in the selected
 484 global optimal peak point is lower than that of the 260 time point. The reason is that the Euclidean
 485 distance only uses the concentration difference to represent the distance of the peak point, and the
 486 matching will be given priority when there are other peak points with similar concentration near a peak.
 487 The constraint of the warping path leads to the possibility that it can no longer match the later more
 488 suitable peak points. The improved Manhattan distance can ensure that the peak points are matched
 489 preferentially with similar time span and concentration. The 2019-9-27C and 2021-3-10A groups
 490 successfully establish a correct matching relationship between the above peak points when matching
 491 using the improved Manhattan distance. As a result, the appropriate global optimal peak point is found.
 492 The SO₂ and CO₂ of the 2021-1-13B measurement data show a trend of almost synchronous change with
 493 a peak, hence both the Euclidean distance and the improved Manhattan distance give the appropriate



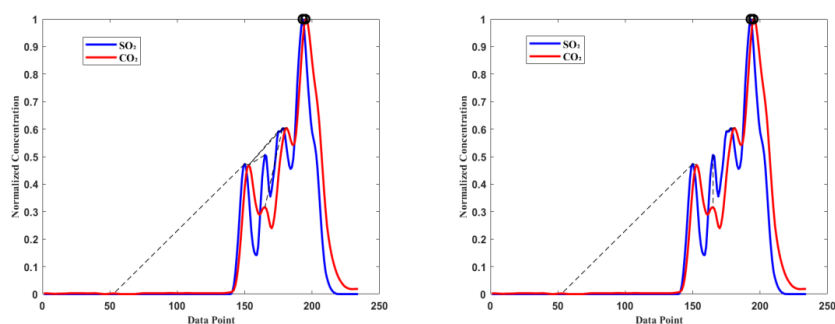
494 global optimal peak. However, the Euclidean distance does not establish a matching relationship between
 495 the peak points of this group at the 170 time point, whereas the improved Manhattan distance achieves
 496 this.

497 Figure 5 shows three groups of measurements with typical problems (2019-10-17C, 2021-8-18C, 2021-
 498 9-3A). There is almost no synchronous change interval between the two time-series of the 2019-10-17C
 499 measurement data, and the peak trend is not clear. When using the screening algorithm, some peak points
 500 with matching relationship are still retained after the time span is more than 20 s and the concentration
 501 difference is more than 0.3485, but these matching results cannot be used as global optimal peak points.
 502 The SO₂ measurement data in 2021-8-18C have two platform-like data (data points in the pink circle),
 503 and there is no peak point of SO₂, so the global optimal peak point cannot be selected. There are 20 peak
 504 points in the SO₂ sequence in 2021-9-3A and only two peak points in the CO₂ sequence. Due to the large
 505 difference between the number of peak points, the warping path is easy to shift to the boundary of the
 506 distance matrix, and the global optimal peak point (the peak point in the green circle) cannot establish a
 507 matching relationship. For 2019-10-17C, the screening algorithm gives the global optimal peak point,
 508 but the result is obviously not a suitable global optimal peak point, which is contrary to the subjective
 509 judgment. For 2021-8-18C, the screening algorithm does not recognize a global optimal peak point,
 510 which is consistent with the subjective judgment. For 2021-9-3A, the screening algorithm also recognizes
 511 no global optimal peak point, but it is contrary to the subjective judgment.



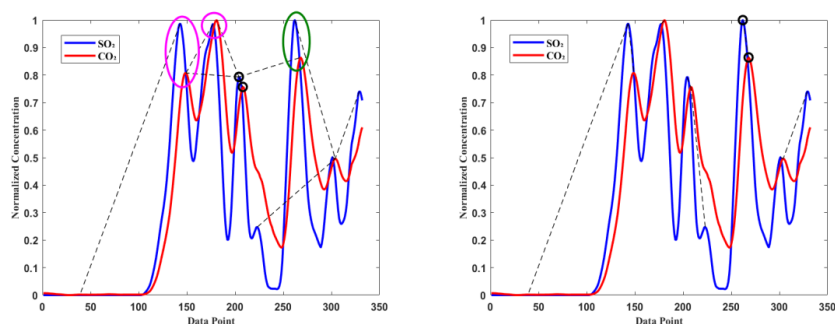
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(a)



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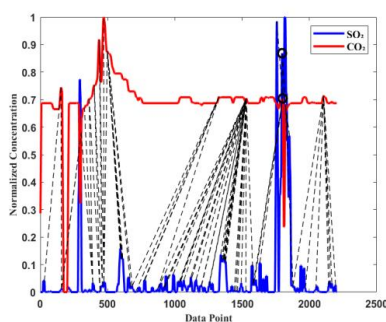
(b)



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(c)

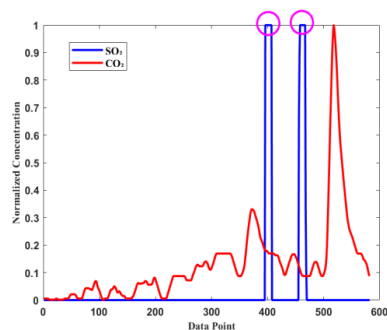
515 **Figure 4.** Four groups of measurement data of SO_2 and CO_2 . (a) 2019-9-27C; (b) 2021-1-13B; and (c) 2021-3-
 516 10A. The left panels are the global optimal peak point screening result using the Euclidean distance, while the
 517 right are the global optimal peak point screening using the improved Manhattan distance. The black line is
 518 the matching relationship between the two points, the small black circle is the global optimal peak point given
 519 by the screening algorithm, the pink circle is the peak points that cannot be regarded as the global optimal
 520 peak points, and the green circle is the appropriate global optimal peak points.



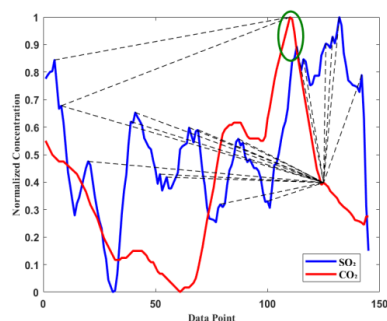
521

522

(a)



(b)



(c)

Figure 5. Three groups of SO₂ and CO₂ measurement data. (a) 2019-10-17C, (b) 2021-8-18C, and (c) 2021-9-3A. Abscissa is the point of time, and the interval between the two points, or sampling rate, is 1 s. The black line shows that there is a matching relationship between the two connected peak points, the pink circle is the peak points that cannot be regarded as the global optimal peak points, the green circle is the appropriate global optimal peak points, and the small black circle is the global optimal peak point given by the screening algorithm.

Of the 148 groups of measurement data screened, 101 groups, in which the artificial screening results are consistent with the algorithm screening, demonstrate the global optimal peak points. Among the remaining data, 19 groups of measurement data show inconsistent results, while 28 groups have poor quality that neither screening could find the global optimal peak points. Regardless of whether the global optimal peak point exists or not, the result of the algorithm is defined as correct when the results of the subjective and algorithm screenings are the same, in this case the correct rate of the screening algorithm is 87.16%. The results of the screening algorithm are consistent with the subjective screening results, but the global optimal peak points are not found, or the large deviation of time series leads to no reasonable



retention of peaks in the screening matching relationship. For this measurement data, the algorithm can identify and provide the reason. There are mainly two cases of inconsistent measurement data, one is that the data can artificially screen the global optimal peak, yet the algorithm does not give the optimal result or directly determines that there is no suitable global optimal peak, the other is that there is no global optimal peak point in the data, and the result given by the algorithm is only a group of peak points where the concentration difference and time span do not exceed the threshold. The first case usually occurs in the measurement data with a large gap in the number of peak points in the average sequence of SO₂ and CO₂. When forming a distance matrix, this difference will cause one side of the row or column of the matrix to be much larger than the other. Limited by the directional constraints of the DTW algorithm, there is no other choice for the warping path to reach the matrix boundary, but can only extend vertically or horizontally along the boundary. Therefore, the appropriate global optimal peak point will not be selected by the warping path. The second situation is more common. Multiple screening conditions are defined in the screening matching relationship, and the matching relations that do not meet the conditions will be eliminated. Although the remaining matching relations meet the conditions, they may not necessarily be the optimal peak points. This situation will occur when the algorithm selects the final value from the reserved peak value.

Table 2: Algorithm screening for groups of measurement data. "Consistent (found)" means that the result given by the algorithm is the same as that of artificial selection and can find the global optimal peak point. "Consistent (not found)" means that the two results are consistent and neither of them has found the global optimal peak point. "Inconsistent" refers to the difference between the two results. "Correct rate" refers to the ratio of the 148 groups of measurement data to the 148 groups of data with "Consistent (found)" and "Consistent (not found)" measurement data.

| Consistent (found) | Consistent (not found) | Inconsistent | Correct rate |
|--------------------|------------------------|--------------|--------------|
| 129 | 28 | 19 | 87.16% |

4.4 Verification of data quality evaluation method

In Section 3.4, 16 indexes are proposed to evaluate the quality of the measured data. The 95% confidence interval of the evaluation index is calculated by 10000 self-development sampling of the collected data, and the results are shown in Table 3.

Table 3: Self-development sampling times of 16 evaluation indexes and the upper and lower bounds of the 95% confidence interval.



| Evaluation index | Self-development sampling times | Lower bound of 95% confidence interval | Upper bound of 95% confidence interval |
|--|------------------------------------|---|---|
| Sample entropy (SO ₂) | 10000 | 0.082153984 | 0.150936086 |
| Information entropy (SO ₂) | 10000 | 3.245317702 | 3.721704023 |
| Third quartile (SO ₂) | 10000 | 0.203210727 | 0.280760482 |
| Standard deviation (SO ₂) | 10000 | 0.211572244 | 0.22958644 |
| Skewness (CO ₂) | 10000 | 1.027746851 | 1.471870163 |
| Standard deviation of peak density (CO ₂) | 10000 | 0.040255915 | 0.045275922 |
| Permutation entropy (SO ₂) | 10000 | 0.694783281 | 0.752033377 |
| Fuzzy entropy (CO ₂) | 10000 | 0.179056426 | 0.216571182 |
| Approximate entropy (CO ₂) | 10000 | 0.140398491 | 0.167099422 |
| Mutual information | 10000 | 0.588883766 | 0.647985481 |
| First quartile (SO ₂) | 10000 | 0.042864083 | 0.089750709 |
| Kurtosis (CO ₂) | 10000 | 5.435791486 | 7.228334146 |
| DTW shortest distance | 10000 | 14.44706187 | 26.07445393 |
| Quartile spacing (SO ₂) | 10000 | 0.152163801 | 0.207432999 |
| Coefficient of variation (SO ₂) | 10000 | 1.651178674 | 1.980617162 |
| Ratio of the number of peak points | 10000 | 1.996089804 | 6.083568681 |

565 The results of the 16 evaluation indexes for 148 groups of measurement data are shown in Table 4. Some
 566 indexes are selected to form the index set. Skewness (CO₂) and information entropy (SO₂) with the
 567 highest accuracy of index evaluation are taken as the elements in the initial subset. After comparing the
 568 accuracy of adding other indexes, it is found that when the elements in the index set are skewness (CO₂),
 569 information entropy (SO₂), sample entropy (SO₂), and quartile spacing (SO₂), the joint evaluation can
 570 achieve relatively good results, with a correct rate of up to 70.95%. When the index continues to increase,
 571 the correct rate decreases, indicating that these indexes can only represent part of the characteristics of
 572 the measured data and have high coupling. Therefore, these four indexes are selected for joint evaluation.
 573 The six groups of measurements in Figure 6 have all been defined. This section uses the quality
 574 evaluation method to evaluate the quality and verify the rationality of the six groups of data. The groups



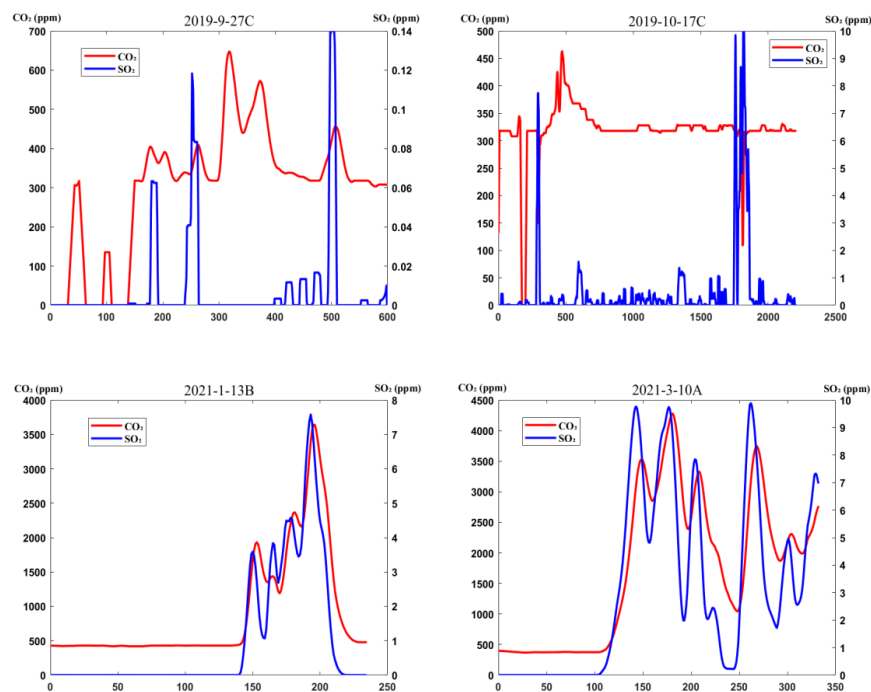
2019-9-27C, 2021-1-13B, and 2021-3-10A are the measurements that can screen out the global optimal peak points, but the SO₂ and CO₂ series in 2019-9-27C do not have a synchronous trend, and only the two series have the same peak trend at 2019-9-27C, thus even if they can be used as global optimal peak points, the ratio of the four evaluation indexes is 1, and the joint evaluation result is poor quality. There are four peak trends in 2021-1-13B, where SO₂ and CO₂ change almost synchronously. The peak trend at the 200 time point is very clear and higher than other peaks, which belongs to the appropriate global optimal peak point, and the result of joint evaluation of indexes is very close to 0. The peak trend in 2021-3-10A is slightly more than that of 2021-1-13B, although altogether is basically synchronous; the peak trend at 145, 160, 260 time points can be observed, while between the global optimal peak point is the priority to select the maximum value of the average SO₂. Finally, the peak point at the 260 time point is selected as the global optimal peak point, and the joint evaluation result of the index is higher than that of 2021-1-13B. The SO₂ average sequence of 2019-10-17C has frequent small fluctuations and abrupt changes over time, and there is no obvious synchronous peak trend, while the SO₂ sequence of 2021-8-18C has platform values only at 400, 480 time points, thus it cannot be used as the global optimal peak point. The average series of SO₂ and CO₂ in 2021-9-3A show a synchronous change trend at 90–110 time points, hence SO₂ fluctuates greatly relative to CO₂. Although the peak point at the 110 time point can be selected as the global optimal peak, and the result of joint evaluation of the index remains 1. To summarize, the results of the quality evaluation methods for poor and good quality data are in line with expectations.

Table 4: Sixteen indexes for the evaluation of 148 groups of measurement data statistics.

| Index | Number of correct evaluation results | Number of wrong evaluation results | Correct rate |
|---|--------------------------------------|------------------------------------|--------------|
| Sample entropy (SO ₂) | 86 | 62 | 58.11% |
| Information entropy (SO ₂) | 90 | 58 | 60.81% |
| Third quartile (SO ₂) | 87 | 61 | 58.78% |
| Standard deviation (SO ₂) | 86 | 62 | 58.11% |
| Skewness (CO ₂) | 91 | 57 | 61.49% |
| Standard deviation of peak density (CO ₂) | 82 | 66 | 55.41% |



| | | | |
|---|----|----|--------|
| Permutation entropy (SO ₂) | 81 | 67 | 54.73% |
| Fuzzy entropy (CO ₂) | 82 | 66 | 55.41% |
| Approximate entropy (CO ₂) | 87 | 61 | 58.78% |
| Mutual information | 76 | 72 | 51.35% |
| First quartile (SO ₂) | 82 | 66 | 55.41% |
| Kurtosis (CO ₂) | 85 | 63 | 57.43% |
| DTW shortest distance | 73 | 75 | 49.32% |
| Quartile spacing (SO ₂) | 88 | 60 | 59.46% |
| Coefficient of variation (SO ₂) | 87 | 61 | 58.78% |
| Ratio of the number of peak points | 74 | 74 | 50.00% |



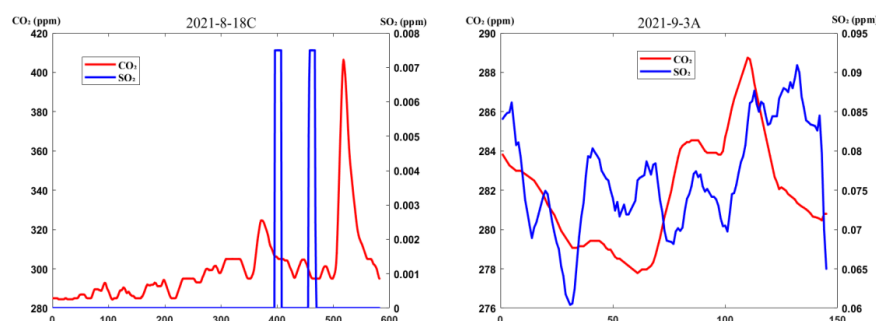


Figure 6. Evaluation of the quality of the six groups of SO₂ and CO₂ measurement data. The Abscissa is the time point, and the interval between the two points, or sampling rate, is 1s.

Table 5: Algorithm screening of six groups of measurement data (2019-9-27C, 2019-10-17C, 2021-1-13B, 2021-3-10A, 2021-8-18C, and 2021-9-3A). The specific values and evaluation results of information entropy (SO₂), sample entropy (SO₂), skewness (CO₂), quartile spacing (SO₂) and the results of joint evaluation of the four indexes.

| Data ID | Algorithm | Information entropy | | Sample entropy | | Skewness | | Quartile spacing | | Result of joint evaluation |
|-------------|-----------|---------------------|------|----------------|--------|----------|------|------------------|--------|----------------------------|
| | | Value | EVAL | Value | EVAL | Value | EVAL | Value | EVAL | |
| 2019-9-27C | √ | 1.7112 | 1 | 0.0307 | 1 | -0.6145 | 1 | 0.0060 | 1 | 1 |
| 2019-10-17C | × | 2.6154 | 1 | 0.0353 | 1 | -3.8664 | 1 | 0.0240 | 1 | 1 |
| 2021-1-13B | √ | 2.6865 | 1 | 0.0272 | 1 | 1.6976 | 1 | 0.1801 | 0.0116 | 0.0116 |
| 2021-3-10A | √ | 5.1502 | 1 | 0.1061 | 0.3050 | 0.2466 | 1 | 0.5737 | 1 | 0.3050 |
| 2021-8-18C | √ | 0.3047 | 1 | 0.0076 | 1 | 3.1325 | 1 | 0 | 1 | 1 |
| 2021-9-3A | × | 5.8638 | 1 | 0.7894 | 1 | 0.4692 | 1 | 0.3711 | 1 | 1 |

"×" indicates that the screening algorithm is inconsistent with subjective judgment

5 Conclusion

The emission factor is an important parameter for compiling ship emission inventory. Various studies have measured emission factors under different conditions. However, there is little attention and research on improving the accuracy, confidence, and automation of the calculation methods. In this study, we propose a high accuracy calculation of ship emission factors and an evaluation of the



quality of measurement data based on the sniffer method. Altogether, we optimize the calculation process, select the appropriate integral interval length to convert the original measurement data into an average value to make the calculation results more stable, and put forward the concept of peak density standard deviation selection for the optimal integral interval length, which reduces the uncertainty caused by the use of empirical values. The average sequence is extracted to find all the peak points, and the matching relationship with the measured series of SO₂ and CO₂ is found by using the DTW algorithm based on the improved Manhattan distance. The unreasonable matching results are eliminated according to the concentration change and time span thresholds analyzed. The maximum concentration of SO₂ and CO₂ in the remaining matching relationship is the global optimal peak point. In order to evaluate the quality of the measured data objectively, 16 evaluation indexes, which can reflect the characteristics of the measured data are selected, and the 95% confidence interval of each index is calculated by self-expanding sampling of the measured data, and combined with the quality label of the measured data. Several indexes with high accuracy of data quality evaluation are selected to jointly evaluate the measured data, further optimizing the accuracy of the evaluation.

We used 148 groups of sniffer measurements collected between 2019 and 2021 to test the rationality of the above methods. When the length of the integral interval is 12 s, the standard deviation of peak density reaches the maximum. Compared with the change trend of several groups of data before and after preprocessing, the peak trend of the data set after preprocessing is more obvious, and most of the nonsignificant trends in the series are smoothed out. Comparing the artificial and algorithm screening results of the global optimal peak points of 148 groups of measured data, 129 groups have the same results, with a correct rate of 87.16%. After 10000 times of self-development sampling, the 16 evaluation indexes all reached the 95% confidence interval. When using four evaluation indexes: information entropy (SO₂), sample entropy (SO₂), quartile spacing (SO₂), and skewness (CO₂), 70.95% of the data quality labels are consistent with the joint evaluation results of the evaluation index set. When using these four indexes to quantify data quality, it is consistent with expectations, which verifies that the data quality evaluation method is feasible.

The emission factor calculation and measurement data quality evaluation methods proposed in this study can reduce the uncertainty in the current sniffer technique monitoring ship emission research, objectively evaluate the measurement data quality, and provide data support for the accurate establishment of an emission inventory. Future work is needed to further analyze the characteristics of the measured data so



as to improve the global optimal peak point screening algorithm. At the same time, it is also necessary to find other evaluation indexes that can reflect the characteristics of the measured data to reduce the coupling in the evaluation index set, improve the accuracy of the joint evaluation index set and quantification of the quality of the data.

Data availability

Please address requests for data sets and materials to Fan Zhou (fanzhou_cv@163.com).

Author contribution

LZ analyzed the experimental data and authored the article. FZ designed the study and provided constructive comments on this research.

Competing interests

The authors declare that they have no conflict of interest.

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