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1 **Data analytics for fuel consumption management in**
2 **maritime transportation: Status and perspectives**

3

4 **Abstract**

5 The shipping industry is associated with approximately three quarters of all world
6 trade. In recent years, the sustainability of shipping has become a public concern, and
7 various emissions control regulations to reduce pollutants and greenhouse gas (GHG)
8 emissions from ships have been proposed and implemented globally. These regulations
9 aim to drive the shipping industry in a low-carbon and low-pollutant direction by
10 motivating it to switch to more efficient fuel types and reduce energy consumption. At
11 the same time, the cyclical downturn of the world economy and high bunker prices
12 make it necessary and urgent for the shipping industry to operate in a more cost-
13 effective way while still satisfying global trade demand. As bunker fuel consumption is
14 the main source of emissions and bunker fuel costs account for a large proportion of
15 operating costs, shipping companies are making unprecedented efforts to optimize ship
16 energy efficiency. It is widely accepted that the key to improving the energy efficiency
17 of ships is the development of accurate models to predict ship fuel consumption rates
18 under different scenarios. In this study, the ship fuel consumption prediction models
19 presented in the literature (including the academic literature and technical reports,
20 which are a typical type of “grey literature”) are reviewed and compared, and models
21 that optimize ship operations based on fuel consumption prediction results are also
22 presented and discussed. Current research challenges and promising research questions
23 on ship performance monitoring and operational optimization are identified.

24

25 **Key words**

26 Maritime transportation, ship fuel consumption prediction, ship performance prediction,
27 ship energy efficiency optimization, ship performance optimization

28 **1. Introduction**

29 **1.1 Background**

30 Seaborne transport is the most energy-efficient mode of transportation, and it forms
31 the backbone of international trade and global supply chains (Christiansen et al., 2004;
32 Kawasaki and Lau, 2020). According to the United Nations Conference on Trade and
33 Development (UNCTAD), more than three fourths of merchandise traded globally by
34 volume is carried by sea (UNCTAD, 2019). As the shipping industry is mainly powered
35 by heavy fuel oil, it also creates a large environmental footprint due to its emissions of
36 greenhouse gases (GHGs) and polluting substances (Cheaitou and Cariou, 2012;
37 Adland et al., 2017; Cheaitou et al. 2020; Gu et al., 2020; Wang et al., 2021). As early
38 as 1973, the International Maritime Organization (IMO) established the Marine
39 Environment Protection Committee (MEPC) to address marine pollution and GHG
40 emissions. In the years since, various global conventions and regulations have been
41 proposed and implemented to reduce shipping emissions (Gholizadeh et al., 2020). The
42 most important is the International Convention for the Prevention of Pollution from
43 Ships (MARPOL) adopted by the IMO (MEPC), which addresses several marine
44 pollution issues, such as oil spills, the transportation of noxious liquids and other
45 harmful substances, sewage, garbage, and ship air pollution (IMO, 2011). In 1997,
46 MARPOL Annex VI introduced regulations to prevent air pollution by limiting the
47 emissions of sulfur oxides (SO_x), nitrous oxides (NO_x), and other ozone-depleting
48 substances from ship exhausts (IMO, 1997). Regulations to reduce GHG emissions
49 (e.g., carbon dioxide (CO₂), methane (CH₄), nitrous oxide (N₂O), and ozone (O₃)) from
50 shipping activities were introduced in an amendment to MARPOL Annex VI in 2011
51 (MEPC, 2011). As a consequence of these regulations, sulphur emission control areas
52 (SECAs) and nitrogen emission control areas (NECAs) have been established across
53 the world, and various ship energy efficiency indicators and monitoring systems for
54 reducing GHG emissions have been proposed (Tseng and Ng, 2020). The IMO has
55 called on shipping companies to reduce their emissions to 50% of their 2008 levels by
56 2050. The major regulations on shipping emissions are summarized in Table 1.

Table 1. Regulations to reduce emissions from shipping

| Regulation | Related documentation | Time of implementation | Organization | Object(s) | Area(s) | Main contents | Notes |
|---|-------------------------|-------------------------------------|--------------|---|---|--|--|
| SECAs | MARPOL Annex VI | 1 Jan 2015 | IMO (MEPC) | All ships sailing in SECAs | Four SECAs: the Baltic Sea, the North Sea, the North American Sea, and the United States Caribbean Sea | The maximum fuel sulphur content cannot exceed 0.1% m/m when sailing in SECAs | None |
| NECAs | MARPOL Annex VI | a) 1 Jan 2016, and b) 1 Jan 2021 | IMO (MEPC) | New ships with marine diesel engines with output of 130 kW or higher and new engines installed in all ships on or after a) 1 Jan 2016, and b) 1 Jan 2021 sailing in NECAs | a) The North American area and the United States Caribbean Sea, and b) the North Sea and the Baltic Sea | NO _x regulations tier III is implemented in NECAs | NO _x regulations tier III requires that engines under 130, between 130 and 1199, and over 1200 propeller revolutions per minute (RPM) should have the total weighted cycle emission limit as 3.4, 2.4, and 2.0 (g/kWh) respectively |
| Global sulfur content limit in fuel | MARPOL Annex VI | 1 Jan 2020 | IMO (MEPC) | All existing ships | Areas outside SECAs | The maximum fuel sulphur content cannot exceed 0.5% m/m | None |
| European Union (EU) Monitoring Reporting and Verification (MRV) | EU regulation 2015/757 | 1 Jan 2018 | EU | All ships with a gross tonnage above 5000 arriving at, within, or departing from ports under the jurisdiction of a Member State of EU | Global shipping lines with either origin or destination at the ports in the Member States of EU | Accurate monitoring, reporting, and verification of CO ₂ emissions from related ships | The fuel consumption and CO ₂ emission data per ship for 2018 and 2019 have already been published |
| IMO data collection system (DCS) | MARPOL Annex VI | 1 Jan 2019 | IMO (MEPC) | All ships with a gross tonnage of 5000 and above | Global | Reporting verified fuel consumption data via their flag states | Ships' names and IMO numbers will be anonymized when publishing |
| Energy efficiency operation index (EEOI) | MEPC.1 /Circ.684 | July 2009 | IMO (MEPC) | All existing ships | Global (voluntary) | Performance improvement by the efforts in operation | Average indicator of the ship/fleet operational efficiency of all types of fuels during a voyage (Operational CO ₂ indicator) |
| Energy efficiency design index (EEDI) | Resolution MEPC.203(62) | Jan 2013 | IMO (MEPC) | New and contracted ships on or after 1 Jan 2013 or delivered on or after 1 July 2015, and existing ships undergone major conversions | Global | Performance improvement of ship hardware | An index indicating the energy efficiency of a ship in terms of g CO ₂ /tonne/nautical mile for a specific ship operational condition (CO ₂ design index) |
| Ship energy efficiency and management plan (SEEMP) | Resolution MEPC.203(62) | Jan 2013 | IMO (MEPC) | All existing ships | Global | Several steps are required: planning, monitoring, self-evaluation, and improvements | Use EEOI as a benchmark |
| Combination measure of EEXI and CII | MEPC 75 virtual session | In progress | IMO (MEPC) | All existing ships | Global | Combination of technical and operational approaches to reduce ships' carbon intensity | EEXI is short for energy efficiency existing ship index, and it is based on EEDI. CII is short for carbon intensity indicator and should be recorded in ships' SEEMP |

59 However, despite the growing number of strict environmental protection
60 regulations implemented by the IMO and individual countries and regions, emissions
61 from shipping continue to increase overall. The main fuel-based pollutants and GHG
62 emissions in the international shipping industry between 2012 and 2017, according to
63 estimates based on a top-down methodology in the fourth IMO GHG study (IMO, 2020),
64 are summarized in Table 2. Although the total cargo loaded only slightly increased from
65 9,195 million tons in 2012 to 10,716 million tons in 2017 (UNCTAD, 2019), there was
66 a significant increase in all types of emissions. The massive amounts of pollutants and
67 GHGs emitted by the shipping industry are having an adverse impact on both human
68 health and the global climate. As air emissions from vessels are proportional to the fuel
69 consumption of the main and auxiliary engines (including boilers), especially in terms
70 of the emissions of CO₂, NO_x, and SO_x (Kontovas, 2014; Adland et al., 2019; Peng et
71 al., 2020; Wu and Wang, 2020), better management of fuel consumption during ship
72 operation could improve the energy efficiency of ships and thus reduce their emissions
73 (Perera and Mo, 2016).

74 **Table 2. International shipping emissions from 2012 to 2017 (IMO, 2020)**

| Emission/Year | 2012 | 2013 | 2014 | 2015 | 2016 | 2017 |
|------------------------------------|----------|----------|----------|----------|----------|----------|
| CO ₂ (million tonnes) | 614.1 | 612.3 | 634.2 | 657.9 | 675.3 | 693.4 |
| CH ₄ (tonnes) | 10,156.8 | 10,120.6 | 10,414.9 | 11,205.9 | 11,745.4 | 12,397.5 |
| N ₂ O (thousand tonnes) | 34,296.5 | 34,270.0 | 35,568.4 | 36,942.3 | 37,957.5 | 39,059.2 |
| SO _x (thousand tonnes) | 8,260.2 | 7,888.9 | 7,825.3 | 8,116.6 | 8,943.3 | 9,252.3 |
| NO _x (thousand tonnes) | 14,927.4 | 14,606.2 | 14,683.6 | 15,357.1 | 15,780.8 | 16,201.9 |
| NM VOC (thousand tonnes) | 596.4 | 592.6 | 603.0 | 633.0 | 653.8 | 675.4 |
| PM (thousand tonnes) | 1,271.2 | 1,237.8 | 1,228.3 | 1,258.3 | 1,352.4 | 1,399.1 |
| BC (thousand tonnes) | 54.4 | 55.8 | 60.1 | 59.9 | 60.7 | 62.2 |

75 Note: NMVOC is the abbreviation for non-methane volatile organic compounds. PM is the abbreviation for particulate matters.
76 BC is the abbreviation for black carbon.

77

78 **1.2 Energy efficiency improvement and emission reduction strategies**

79 In addition to stricter emissions regulations, high bunker prices that cyclically occur
80 and downturns in the shipping market have also pushed the shipping industry to adopt
81 measures to improve energy efficiency and thus to reduce emissions (Beşikçi et al.,
82 2016). Currently, two main solutions are applied to improve ship energy efficiency:
83 technical solutions and operational solutions (Leifsson et al., 2008; Wong et al., 2015;
84 Coraddu et al., 2017; He et al., 2017; Theocharis et al., 2019). Technical solutions
85 include upgrading propellers, optimizing vessel size, and designing the hull shape to
86 reduce vessel resistance; using lightweight materials to reduce vessel weight; selecting
87 efficient power systems and machinery; switching fuel type; using scrubbers;
88 recovering waste heat; and using solar or wind power and shore power (Wan et al. 2018).
89 There are three main categories of operational solutions according to the SEEMP, as
90 listed in Table 3 (IMO, 2009; Ballou, 2013). Common operational measures adopted in

91 the shipping industry include improving on-time arrival consistency using route
 92 optimization tools, reducing routing decision errors, reducing excessive vessel motions
 93 to minimize ship and cargo damage, increasing crew comfort, reducing the ship's
 94 structural maintenance, and routing optimization considering ECAs, as discussed by
 95 Ballou (2013). Given that the high volatility of the shipping market heavily affects
 96 shipping operators' revenues, slow steaming is commonly adopted, and the main effects
 97 of which are classified by Cariou et al. (2019) into three categories: economic
 98 implications, environmental implications, and service-related implications. Such
 99 analysis provides valuable insights of vessel management for both academic research
 100 and the shipping industry.

101 **Table 3. Energy efficiency improving measures recommend by SEEMP**

| Category | Measures |
|----------------------------|---|
| Fuel efficiency operations | <ul style="list-style-type: none"> • Improving voyage planning by e.g., ship route optimization • Weather routing • Just-in-time arrival at ports • Speed optimization, including slow steaming, sailing at optimal speed, and gradual increase in speed when leaving port • Shaft power optimization, including running at constant RPM and usage of electronic engine management systems • Switching fuel type • ... |
| Ship handling optimization | <ul style="list-style-type: none"> • Trim optimization • Ballast optimization • Propeller design and water inflow optimization • Optimized using of rudder and autopilot • Fleet management • Improving cargo handling • ... |
| Maintenance | <ul style="list-style-type: none"> • Hull/propeller maintenance, including hull cleaning, repairing, and painting, and propeller cleaning and polishing • Marine engine maintenance • ... |

102 Nevertheless, it has been pointed out by Wan et al. (2018) that the technical
 103 measures currently available are struggling to steer the shipping industry in an energy-
 104 efficient and low-carbon direction because their application not only requires
 105 engineering innovation but also carries a hefty price tag: the average cost per ton of
 106 CO₂ reduction ranges from US\$50 to \$200, while the emissions trading price in the
 107 United States is US\$5 to \$15 per ton (Eide et al., 2011). In contrast, operational
 108 measures to improve energy efficiency carry much less cost and do not require an initial
 109 investment, and well-designed operational solutions can achieve promising energy
 110 savings (Wan et al., 2018). However, applying effective and efficient operational
 111 solutions is not a trivial task, as various factors can influence the actual fuel
 112 consumption of a ship in practice, which makes it difficult to capture the relationship
 113 between the influencing factors and the fuel consumption rate. As illustrated by Sourtzi
 114 (2019), ship design (e.g., main dimensions, propulsion system, propeller design,

115 hull/steel structure and cargo arrangement), vessel operational performance (e.g.,
116 sailing speed, draft, trim, displacement, hull performance, and drydocking), and
117 environmental conditions (e.g., wind, wave, and current conditions, water and air
118 temperature, and water depth) all influence ship fuel consumption and therefore energy
119 efficiency. Another barrier to implementing operational changes is that the shipping
120 industry itself is reluctant to adopt energy efficiency measures. This is mainly due to a
121 range of issues in the development and implementation of fuel consumption
122 management strategies, namely split incentives in stakeholders, inadequate information
123 and transparency about energy efficiency and incentive structures, information
124 uncertainty, and decisions made for short-term gain (Poulsen, 2011; Mansouri et al.,
125 2015). There is thus an urgent need to propose and promote more effective and
126 applicable ship fuel management measures to reduce fuel consumption and improve
127 energy efficiency. It is widely acknowledged that the basis of such measures is the
128 accurate estimation of the relationship between a ship's fuel consumption and
129 determinants such as mechanical factors, sailing behaviors, and environmental factors
130 using appropriate prediction algorithms before (or during) a voyage (Pedersen and
131 Larsen, 2009; Soner et al., 2018; Meng et al., 2016; Yang et al., 2019b; Farag and Ölçer,
132 2020). The focus of this review is therefore the literature on ship fuel consumption
133 prediction models and fuel management models from the last 13 years (2008 to 2021).
134 Literature from earlier periods is excluded because data-driven models for ship
135 performance monitoring only started to appear in the last 13 years. The limited number
136 of related papers and reports gives us an opportunity to summarize the details of the
137 reviewed literature in lists and to make comprehensive comparisons of fuel
138 consumption prediction models. Promising future research directions are outlined based
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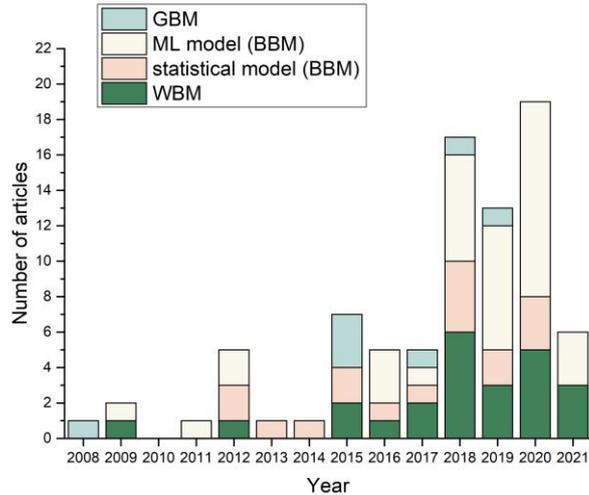
147 **2. Literature review method and structure**

148 Given the focus on fuel consumption prediction models and the fuel management
149 models derived from them, we searched the Scopus, Google Scholar, and Science
150 Citation Index databases using keywords related to fuel consumption prediction and

151 management, such as “ship fuel consumption prediction,” “ship fuel consumption
 152 estimation,” “ship energy efficiency prediction,” “ship energy efficiency estimation,”
 153 “ship fuel efficiency,” “ship fuel management,” and “ship performance monitoring.”
 154 We identified relevant papers in the initial search and then checked the papers and
 155 reports cited by them and that cite them. Considering our main focus on fuel
 156 consumption prediction models, we excluded papers that only propose fuel
 157 management measures and assume that the relationship between fuel consumption and
 158 the various influencing factors (e.g., sailing speed) is deterministic. Finally, we
 159 identified 83 related papers, 53 of which propose fuel consumption prediction models
 160 for ship performance monitoring only (termed ship performance monitoring models)
 161 and 30 of which propose two-stage models for fuel consumption prediction and
 162 management to achieve ship operational optimization (termed ship operational
 163 optimization models). We classify these models into three categories, namely white-
 164 box models (WBM), black-box models (BBMs), and grey-box models (GBMs) based
 165 on Haranen et al. (2016). Descriptions of the three categories and the number of related
 166 papers in each are presented in Table 4. We also analyzed the publishing years of the
 167 83 papers according to the prediction models presented. The statistical models and
 168 machine learning (ML) models in BBMs were considered separately. The results are
 169 shown in Figure 1.

170 Table 4. Description and overview of the prediction models in this review

| Type | Description (Haranen, 2016) | Examples (Yang et al., 2019) | Sub-types | No. of related papers |
|------|--|---|--|-----------------------|
| WBM | A WBM is based on a priori knowledge and physical principles of the vessel power system, and its structure and parameters are all known. | Holtrop-Mennen method (Holtrop, 1977, 1978, 1984; Holtrop and Mennen, 1978, 1982), Kristensen-Lützen method (Kristensen and Lützen, 2012). | None | 24 |
| BBM | A BBM is established using experimental or practical sailing data and is purely data driven. Therefore, no prior knowledge or physics insight is needed when training a BBM. | Statistical models (e.g., multiple linear regression), machine learning models (e.g., artificial neural networks, tree-based models, and support vector machines). | a) BBM based on statistical modeling: statistical models are used for fuel consumption prediction, which focuses on explaining the relationship between fuel consumption and various influencing factors. b) BBM based on ML: machine learning models are used for fuel consumption prediction, which focuses more on accurate prediction results and model generalizability. | a) 17 b) 35 |
| GBM | GBMs are developed based on both the physical properties underlying WBMs and knowledge extracted from experimental or operational data in BBMs. | A WBM is first developed based on hydrodynamic knowledge, then a BBM is used to estimate or adjust some of the coefficients, as in Journée et al. (1987), Meng et al. (2016), and Yang et al. (2019). | None | 7 |



Note: the number of papers in 2021 is not fully counted.

Figure 1. Summary of the reviewed papers by year

Figure 1 indicates that the number of papers on the predication of ship fuel consumption increased after 2014 and especially after 2018. Moreover, as shown in Table 4, about 63% of the papers develop BBMs for ship fuel consumption prediction, whereas more than 40% of the 83 papers use ML model based BBMs to predict fuel consumption. Figure 1 also shows that there has been an increasing trend of using BBMs based on ML for fuel consumption prediction. Between 2017 and 2020, the use of WBM for fuel consumption prediction also showed an upward trend. In contrast, papers using GBMs for fuel consumption prediction are relatively evenly distributed over the 13-year review period.

3. Review of data and prediction models in current literature

3.1 Input data overview

Given the complexity of vessel engine power systems and sea and weather conditions, numerous ship-related internal factors and external environmental factors affect the fuel consumption rate and thus energy efficiency (Adland et al., 2021). We divided the data that serve as the inputs to the fuel consumption prediction models into four categories according to the data source: ship mechanical data, ship operational data, ship maintenance data, and sea and weather conditions. Ship mechanical data include parameters related to static ship dimensions and information about the power system. Ship operational data mainly comprise information on ship voyage and sailing behavior and ship mechanical conditions in operation, such as power system performance, displacement, and hull conditions. Ship maintenance data are mainly related to information on ship dry docking. Sea condition data cover sea water temperature, waves, swells, and currents, and weather condition data mainly cover wind and air pressure.

198 A major data source is the daily noon report prepared by the ship's chief engineer
199 and sent by the ship's master to the shipping company and shore management (Pedersen
200 and Larsen, 2009; Pedersen et al., 2015; Lu et al., 2015; Beşikçi et al., 2016; Meng et
201 al., 2016; Yuan and Nian, 2018; Uyanık et al., 2019; Du et al., 2019; Adland et al., 2020;
202 Işıklı et al., 2020). Although noon reports may differ, the main content is consistent:
203 types of daily fuel consumption, basic voyage information (e.g., voyage number, date
204 and time of report, load condition, and ship position), sailing behavior information (e.g.,
205 average sailing speed and sailing distance since last report, propeller slip, and average
206 engine revolutions per minute), and sea and weather conditions (e.g., wind, current,
207 wave, and swell conditions). However, as noon reports are completed manually, their
208 accuracy cannot be guaranteed. Furthermore, only one record is made per day, which
209 reduces the data quality and quantity (Bocchetti et al., 2013, 2015; Erto et al., 2015;
210 Chaal, 2018; Farag and Ölçer, 2020).

211 For modern ships equipped with onboard sensors, sensor data serve as another
212 important data source (Petursson, 2009; Petersen et al., 2012a, 2012b; Bocchetti et al.,
213 2015; Jeon et al., 2018; Soner et al., 2018; Lepore et al., 2019; Capezza et al., 2019;
214 Man et al., 2020; Farag and Ölçer, 2020; Wang et al., 2016, 2020). To obtain various
215 types of data, different types of sensors should be installed onboard. For example, fuel
216 consumption sensors, global positioning system (GPS) receivers, shaft power testers,
217 wind speed sensors, and water depth sonars are installed on cruise ships to obtain
218 instantaneous data on fuel consumption, ship navigation speed, speed and torque shaft,
219 wind speed, and water depth (Wang et al., 2016). Fuel consumption sensors, GPS
220 receiving devices, and shaft power meters are used in tankers to acquire real-time data
221 on fuel consumption, ship navigation speed, longitude and latitude, and shaft speed and
222 power (Wang et al., 2020).

223 Another widely adopted onboard system is the automatic identification system
224 (AIS), which enables ships to broadcast and receive messages to and from other ships
225 or coastal authorities that are also equipped with the AIS. The AIS provides static
226 information (e.g., ship identity, size, and type), dynamic information (e.g., ship position,
227 sailing speed, heading degree, rate of turn, navigation status, and reporting time stamp),
228 and voyage-related information (e.g., destination, estimated time of arrival, and draught)
229 (Yang et al., 2019a). Onboard sensors and the AIS provide consecutive data streams at
230 a much higher frequency (e.g., every few seconds or minutes) and quality than noon
231 reports. However, the data acquisition costs are much higher.

232 The engine room logbook, which tracks of all a ship's machinery parameters,
233 performance, maintenance, and malfunctions, can provide both static and dynamic

234 mechanical data during ship operation (Uyanik et al., 2020). Ship information is also
 235 provided by online resources (Huang et al., 2018; Man et al., 2020; Linh and Ngoc,
 236 2020; Yan et al., 2020; Li et al., 2018, 2020). For example, static mechanical data and
 237 maintenance records can be found in Lloyd’s Register and the World Shipping Register.
 238 The surrounding sea and weather data can be found on sea and weather forecast
 239 websites, such as National Marine Environmental Forecasting Center (NMEFC),
 240 National Oceanic and Atmospheric Administration (NOAA), Weathernews Inc. (WNI),
 241 Copernicus Marine Environment Monitoring Service (CMEMS), the European Centre
 242 for Medium-Range Weather Forecasts (ECMWF), etc. Detailed features of the four data
 243 categories used in current literature and their sources are shown in Table 5.

244 **Table 5. Features and sources of common data categories**

| Data | Features | Sources |
|--------------------------------|--|--|
| Ship mechanical data | Ship dimension: length, beam, gross tonnage, deadweight, berth number on cruise ships, etc. Power system: engine parameters, design speed, RPM at design speed, etc. | Onboard sensors, noon report, engine room logbook, AIS, etc. |
| Ship operational data | Ship voyage and sailing behavior: speed over ground (SOG), speed through water (STW), sailing time since last dry docking, sailing distance since last record, ship course, type of fuel used, fuel density and temperature, etc. Ship mechanical condition while operating: propeller pitch, rudder angle, main engine load and working hours, engine RPM, stabilizer fin operation time, turbo exhaust temperature, trim angle, draft, displacement, shaft generator, hull and propeller fouling condition, wetted surface area, etc. | Noon report, AIS, engine room logbook, Lloyd’s Register, World Shipping Register, etc. |
| Ship maintenance data | Dry docking data, etc. | Records from shipping company, Lloyd’s Register, World Shipping Register, etc. |
| Sea and weather condition data | Sea conditions: sea depth, sea water temperature and density, direction and value of wave, swell, and current, etc. Weather conditions: direction and value of wind, air density and temperature, etc. | Noon report, onboard sensors, online sea and weather forecast websites, etc. |

245

246 **3.2 General fuel consumption prediction procedure**

247 To obtain accurate vessel fuel consumption prediction results, several key issues
 248 need to be considered (Zheng, 2021). First, the objectives, resources, and requirements
 249 of the ship energy efficiency management project must be clarified. The objectives may
 250 include the prediction target (e.g., ship fuel consumption rate, ship emission status, or
 251 ship energy efficiency indicator) and the prediction accuracy expected. Resources refer
 252 to the available data sources and computational power, if big data are being used.
 253 Requirements are related to the specific application context: who would the users of the
 254 ship fuel consumption prediction model be and what kind of presentation format would
 255 they expect? For example, academic researchers and technicians would expect more
 256 details of the fundamental theory and detailed implementation procedure of a prediction
 257 model, whereas the onboard crew would be more interested in the ease of use of the
 258 graphical user interface of the model and would pay less attention to the theories behind
 259 it. Another aspect of model requirements is the model transparency or explainability,

260 that is, whether the underlying and working processes of the prediction model need to
261 be completely or partially explainable or whether only high prediction accuracy is the
262 goal.

263 Second, the datasets needed to fulfill the objectives identified in the first step should
264 be selected, with consideration of the availability of data sources and shipping domain
265 knowledge. The appropriate data (or features) should then be collected and combined
266 from various datasets and sources. Data quality and quantity should be checked after
267 data collection. Data pre-processing is then conducted, which includes, but is not
268 limited to, data cleaning, feature dimension reduction, data transformation, and dataset
269 splitting for prediction model training, validation, and testing.

270 Third, appropriate prediction models that fulfill the objectives and requirements
271 identified in the first step must be selected, with consideration of the advantages and
272 disadvantages of the different approaches presented in the literature and reports or
273 adopted by the relevant authorities. The different types of vessel fuel consumption
274 prediction models are classified and analyzed in the following sections. Alternatively,
275 novel prediction models can be developed to achieve particular requirements or to
276 improve prediction accuracy, with specific model parameters and hyperparameters
277 determined as necessary. Finally, model performance must be validated, including in
278 practical scenarios.

279

280 **3.3 Review of white-box models (WBMs)**

281 In WBMs, the basic model construction procedure is to calculate the resistances
282 encountered by a ship from different sources based on physics principles and
283 hydrodynamics laws. The total resistance consists of calm water resistance and the
284 additional resistance presented by wind, waves, shallow water, and other external
285 factors. Once the overall resistance condition is modeled, the engine power required to
286 drive the ship at a certain speed and the corresponding fuel consumption rate can be
287 calculated (Haranen et al., 2016). Emissions from ships, including those of various
288 pollutants and GHGs, can then be calculated based on the engine power and fuel
289 consumption results from the WBM. A total of 24 papers on WBMs were reviewed, of
290 which 16 are on ship performance monitoring (listed in Table 6) and 8 are on ship
291 operational optimization (listed in Table 7).

Table 6. Ship performance monitoring via WBM (16 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Journal |
|------------------------------------|---|---|--|---|--|--|
| Jalkanen et al. (2012) | A RoPax ship | Ship operational data from AIS; ship mechanical data from IHS Fairplay | Fuel consumption and ship emissions of pollutants and GHG in the Baltic Sea surrounding the Danish Straits | STEAM2 | The performance is slightly better than STEAM | Atmospheric Chemistry and Physics |
| Goldsworthy and Goldsworthy (2015) | 7125 vessels operating in the whole Australian region | Ship operational data from AIS in the whole Australian region; ship mechanical data from Lloyd's database | Fuel consumption and emissions of pollutants and GHG | A generic model based on ship activities | R ² is 0.9787 for fuel consumption prediction for a bulk carrier for testing | Environmental Modelling & Software |
| Moreno-Gutiérrez et al. (2015) | Ships that passed through the Strait of Gibraltar during 2007 | Ship operational data from dynamic AIS data; ship mechanical data from Lloyd's Register and IHS Fairplay | Fuel consumption, delivered power and the emissions of pollutants and GHG in 2007 | 9 generic inventory methods from papers and reports published in EU and USA | STEAM (Jalkanen et al., 2009) is the most realistic approach to calculate the energy consumption, while Goldsworthy (Goldsworthy and Renilson, 2013) is the most complete method which applies emission factors for total emission calculation | Energy |
| Rakke (2016) | A ship fleet consisting of about 16,000 ships | Ship operational and mechanical data from AIS and a public database | Ship fuel consumption and emissions of pollutants and GHG | Holtrop-Mennen model | The error rate is about 5% for a small number of ships for model testing | Master thesis at Norwegian University of Science and Technology (NTNU) |
| Tillig et al. (2017) | A tanker ship | Ship mechanical and operational data; sea and weather conditions based on simulation | Ship fuel consumption per route | A generic model with resistance prediction using Technical University of Denmark (DTU) method, Holtrop-Mennen method and computational fluid dynamics (CFD); power and RPM prediction using Holtrop-Mennen method | Not applicable | Proceedings of the Institution of Mechanical Engineers, Part M |
| Johansson et al. (2017) | Global ships in 2015 | Ship operational data from AIS; ship mechanical data from IHS Fairplay and classification societies | Global ship fuel consumption and emissions of pollutants and GHG | STEAM3 | The predicted global ship fuel consumption is qualitatively in agreement with those in the third GHG study of IMO and that reported by the International Energy Agency | Atmospheric Environment |
| Orihara and Tsujimoto (2018) | A tanker and a bulk carrier | Ship mechanical and operational data from ship logbook; sea and weather conditions from ship logbook | Ship speed, engine power, and fuel consumption | A physical simulation model | Not applicable | Journal of Marine Science and Technology |
| Tillig et al. (2018) | A RoRo ship and a tanker ship | Ship mechanical and operational data, and sea and weather conditions based on simulation | Ship fuel consumption prediction during design process | Monte Carlo simulation | The error rate is about 12% in very early design phase and less than 4% in very late design phase | Ships and Offshore Structures |
| Simonsen et al. (2018) | Three cruise ships | Ship mechanical and operational data from AIS; | Fuel consumption at sea and in port, respectively | Model proposed in IMO's third GHG emission study | R ² between 0.3 and 0.4 in the test set | Energies |

| | | | | | | |
|------------------------------------|---|---|---|--|--|----------------------------------|
| Huang et al. (2018) | Ships in Ningbo-Zhoushan port | port survey reports/real world data from <i>MS Finnmarken</i> Ship operational and mechanical data from AIS; sea and weather data from online resources | Fuel consumption and emissions of pollutants and GHG | A generic model based on ship activities considering the influences of ocean environment | The relative error rate is within 10% | Transportation Research Part D |
| Merien-Paul et al. (2018) | A bulk carrier | Ship operational data in different sailing statuses and the geo-spatial data | Fuel consumption | A generic model based on bottom-up fuel consumption prediction approach | Not applicable | Transportation Research Part D |
| Goldsworthy and Goldsworthy (2019) | Ships berthing at four ports in Australia in 2016 | Ship operational data from AIS; ship mechanical data from IHS Markit Maritime & Trade | Fuel consumption and emissions of pollutants and GHG from auxiliary engines and boilers | A generic model based on Goldsworthy and Goldsworthy (2015) and Goldsworthy (2017) | Not applicable | Science of the Total Environment |
| Moreno-Gutiérrez et al. (2019) | A Ro-Pax ferry | Ship operational data from noon report; ship mechanical data from IHS | Ship fuel consumption and emissions of pollutants and GHG | 4 existing general methods proposed in papers or by organizations and a newly proposed model combining the 4 existing models | The newly proposed model combines the advantages of the 4 methods and can be applied to different fleets | Science of the Total Environment |
| Tillig and Ringsberg (2019) | A tanker ship | Ship mechanical and operational data | Fuel consumption | A four degree-of-freedom simulation model | Not applicable | Ships and Offshore Structures |
| Medina et al. (2020) | A container ship | Ship operational data; wind data from ERA-5 database | Fuel consumption | A simple analytical model and a semi-empirical formula considering wind conditions | Not applicable | Transportation Research Part D |

Table 7. Ship operational optimization via WBM (8 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Optimization objective(s) | Decision variable(s) | Solution approach(es) | Journal |
|-----------------------------|--------------------------------|--|------------------------------------|--|--|---|---------------------------------|--|--|
| Li et al. (2018) | An oil tanker | Ship operational and mechanical data from experiment; sea and weather data from online resources | Fuel consumption per hour | A white-box simulation model based on Kwon's model | Not applicable | To minimize fuel consumption and maximize route cost reduction over a given route | Sailing speed | The internal penalty function | Ocean Engineering |
| Tillig et al. (2020) | A container ship and a tanker | Ship mechanical data and weather statistics from Monte Carlo simulation | Fuel consumption per hour | A pure white-box model based on Tillig et al. (2017, 2018), Tillig and Ringsberg (2019) | Not applicable | To minimize fuel consumption over a voyage | Sailing speed | Development of a simulation model called ShipCLEAN in Matlab | Transportation Research Part D |
| Wang et al. (2020) | A tanker ship | Ship operational data from onboard sensors; sea and weather data from ECMWF | Fuel consumption per nautical mile | A generic model considering multiple environmental factors | Not applicable | To minimize fuel consumption | Sailing route and sailing speed | Particle swarm optimization (PSO) algorithm | Ocean Engineering |
| Yang et al. (2020) | A tanker ship | Ship operational and mechanical data; sea and weather data from noon report | Fuel consumption per hour | The DTU-SDU (University of Southern Denmark) model | The overall average relative error of all segments on a route is 1.36% | To minimize fuel consumption over a given route | Sailing speed through water | Generic algorithm | Sustainability |
| Li et al. (2020) | A container ship | Ship operational and mechanical data from experiment; sea and weather data from online sources | Fuel consumption per hour | A white-box model based on Kwon's model and the International Towing Tank Conference (ITTC) | Not applicable | To minimize fuel consumption and the ship operating costs over a given route | Sailing speed | Linear approximation (COBYLA) in SciPy | Applied Ocean Research |
| Wang et al. (2021) | A tanker ship | Ship operational data and mechanical data from towing tank tests; sea and weather data from online resources | Fuel consumption per hour | A white-box model based on towing tank tests, ISO reports, and JONSWAP spectrum | Not applicable | To minimize fuel consumption and increase arrival punctuality over a voyage | Ship engine power | A combination of dynamic programming and generic algorithm | Transportation Research Part D |
| Fan et al. (2021) | A cruise ship | Ship operational data, mechanical data, sea and weather conditions from an onboard energy efficiency monitoring system | Fuel consumption per voyage | A generic model considering water velocity based on regression analysis | Not applicable | To minimize total fuel consumption over a voyage | Main engine speed | Dynamic programming algorithm | Proceedings of the Institution of Mechanical Engineers, Part M |
| Tzortzis and Sakalis (2021) | A container ship | Ship operational data, mechanical data, sea and weather conditions from onboard sensors | Fuel consumption | A white-box model based on several current models such as Holtrop (1984), Holtrop and Mennen (1982), ITTC (2021), and MAN (2018), etc. | Not applicable | To minimize total fuel consumption over a voyage | Sailing speed | Dynamic programming algorithm applied on a specific route after segmentation | Ocean Engineering |

296 Most of the WBM in the 24 papers listed in Tables 6 and 7 are based on ship
297 operational data (23 papers) and mechanical data (21 papers), with half also relying on
298 sea and weather data. None consider ship maintenance data (14 papers, especially those
299 in recent years). In addition to fuel consumption prediction, nearly half of the models
300 also predict ship emissions, including pollutants such as SO₂, NO_x, carbon monoxide
301 (CO), PM and GHGs, such as CO₂ (9 papers). Most of the WBM are developed by the
302 authors themselves, although some papers adopt WBM proposed by other
303 organizations, such as the IMO, ITTC, and DTU-SDU, or by other authors. Two studies
304 by Moreno-Gutiérrez et al. (2015 and 2019) compare the advantages and disadvantages
305 of different types of WBM and develop an improved WBM. Twelve of the 24 papers
306 do not discuss the performance of fuel consumption prediction models, whereas in the
307 papers in which model performance is presented, different test scenarios and metrics
308 are used, making direct performance comparisons difficult. Of the 8 papers dealing with
309 ship operational optimization models listed in Table 7, 5 discuss single-objective
310 optimization models that aim to minimize fuel consumption, and the other 3 consider
311 dual-objective optimization models that simultaneously minimize fuel consumption
312 and maximize route cost reduction, minimize ship operational costs, or increase arrival
313 punctuality. Six of the optimization models choose ship sailing speed as the decision
314 variable, and 2 consider ship engine power and main engine speed. A detailed
315 description of the approaches adopted in WBM for ship fuel consumption prediction
316 is given in Appendix B.1.

317 The main advantage of WBM is that they can be applied at the initial stage of ship
318 design and during sea trials, as the model structure and parameters are fully known from
319 a priori knowledge and theoretical insights based on physical and hydrodynamics laws,
320 naval architecture principles, computational fluid dynamics methods, and ship model
321 tests. Furthermore, as WBM are developed based on physics principles, they are
322 transparent and explainable and are thus widely used in the shipping industry. Despite
323 these advantages, there are some clear disadvantages of WBM. First, WBM use
324 various assumptions from model structure to parameter estimation, and their
325 performance is strongly influenced by these assumptions. The ship resistance
326 components are treated separately and their interactions are ignored, which may result
327 in inconsistencies in the WBM developed (Haranen, 2016). As a result, the suitability
328 and generalizability of WBM can be poor (Haranen, 2016; Yang et al., 2019b). Second,
329 as much a priori knowledge about the whole vessel system is needed to calibrate WBM,
330 their development and application may be restricted, because such knowledge may be
331 difficult to comprehend for a non-expert. Third, as WBM are deterministic models,

332 which means that their structure and parameters are given and fixed and thus no
 333 randomness can be included to allow data uncertainty to be modeled, the models cannot
 334 learn from the data. Consequently, it is difficult to improve their performance given that
 335 data accumulate during ship operation. In addition, the deterministic property also
 336 makes WBM's vulnerable to noisy data, which are common in practice.

337

338 3.4 Review of black-box models (BBMs)

339 3.4.1 Review of BBMs based on statistical modelling

340 BBMs based on regression models are a type of classical model widely used in
 341 studies on ship fuel consumption prediction. The main procedure begins with
 342 feature/data acquisition and pre-processing. Then, reasonable assumptions are made,
 343 and suitable regression models are chosen. Next, the model parameters are estimated
 344 using real or simulated ship operational data, and finally, the model's fit and
 345 generalization abilities are validated. One stream of BBMs is based on statistical
 346 modeling for fuel consumption prediction, which mainly aims to identify the
 347 relationship between fuel consumption and sailing speed, as it is widely believed by
 348 researchers and practitioners that ship sailing speed is the most significant determinant
 349 of ship fuel consumption. A ship's fuel consumption rate at sea is usually treated as
 350 proportional to its sailing speed to a power of α . The cubic law, which adopts $\alpha = 3$,
 351 is particularly well known (Ryder and Chappell, 1980; Ronen, 1982, 2011; Wang and
 352 Meng, 2012; Du et al., 2019; Ronen et al., 2020); in practice, however, α can be
 353 smaller or larger than 3 depending on many factors, such as ship type, real sailing speed,
 354 and the surrounding sea and weather conditions (Wang and Meng, 2012).

355 Table 8. Power of speed-fuel consumption in current literature (6 papers/reports)

| Literature | Shipping sector and fleet size | Range of power | Data resources |
|-----------------------------|---|---|---|
| Notteboom and Cariou (2009) | Container ships | 3.3 | Ship operational and mechanical data from Lloyd's Fairplay Database |
| Wang and Meng (2012) | Container ships in a liner shipping network | 2.7 to 3.3 | Ship operational data provided by a global liner shipping company |
| MAN Diesel and Turbo (2018) | Tanker | 3.2 to 3.8 | Not applicable |
| | Bulk carrier | 3.0 to 3.6 | |
| | Container ship | 3.1 to 3.4 | |
| Adland et al. (2018) | Ro-pax | 3.4 to 4.8 | Ship operational data and sea and weather data from noon report; ship maintenance records |
| | 8 crude Oil tankers | 1.452 (laden) to 2.144 (ballast) | |
| Kristensen (2019) | Oil tanker | 1.6 to 4.8 | Ship mechanical data from Clarkson |
| | Bulk carrier | 1.6 to 4.3 | |
| | Container ship | 1.8 to 4.4 | |
| Adland et al. (2020) | 16 crude oil tankers | For Aframax tankers, the elasticity ranges from 0.114 to 3.783; for Suezmax tankers, the elasticity ranges from 0.760 to 3.667 in different speed intervals | Ship operational data and sea and weather data from noon report |

356 Although the cubic law relation between a ship's sailing speed and the fuel
 357 consumption rate is widely adopted, Notteboom and Cariou (2009) conduct a

358 pioneering study using regression analysis on ships' operational and mechanical data
359 extracted from Lloyd's Fairplay Database and estimate an empirical relationship
360 between sailing speed and installed power for container ships. Since then, numerous
361 studies estimate the relationship between ship sailing speed and the corresponding fuel
362 consumption rates for different ship classes under various conditions.

363 Many of the studies listed in Table 8 use ship operational data and mechanical data
364 to calibrate the speed–fuel consumption curves, but most do not explicitly consider the
365 influence of the surrounding sea and weather conditions. Adland et al. (2018, 2020)
366 incorporate various such conditions, such as wind, swell, current, and waves, into their
367 statistical fuel consumption prediction models. Adland et al. (2018) also focus on the
368 impact of periodic hull cleaning and dry docking operations on vessels' energy
369 efficiency and Adland et al. (2020) deeply explore fuel consumption–speed curves, both
370 of which are important but challenging issues in vessel fuel consumption prediction and
371 optimization. More sophisticated models that consider factors in addition to operational
372 and mechanical factors, such as sea and weather conditions and ship maintenance data,
373 are summarized in Table 9. Studies of ship operation optimization based on statistical
374 models are presented in Table 10.

Table 9. Ship performance monitoring via BBMs based on statistical modelling (13 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Journal |
|-----------------------------------|---|---|--|---|--|--|
| Bocchetti et al. (2013) | Twin cruise ships | Ship operational data and sea and weather conditions from onboard data acquisition device | Fuel consumption per voyage | Multiple linear regression (MLR) analysis | Average R^2 is 0.9875 in the training set | Conference proceedings |
| Coraddu et al. (2014) | A RoPax vessel | Ship mechanical and operational data from ship monthly report | Fuel consumption per nautical mile and EEOI | Monte Carlo based simulation | Not applicable | Proceedings of the Institution of Mechanical Engineers, Part M Journal of Ship Research |
| Bochetti et al. (2015) | A cruise ship | Ship maintenance and operational data, and sea and weather conditions from noon report and onboard sensors | Fuel consumption per voyage | MLR analysis | R^2 is at least 0.93 in the training set | Journal of Ship Research |
| Erto et al. (2015) | A cruise ship | Ship maintenance data and operational data, and sea and weather conditions from onboard sensors | Fuel consumption per mile | MLR analysis | R^2 is 0.94 in the training set | Quality and Reliability Engineering International |
| Bialystocki and Konovessis (2016) | A pure car and truck carrier | Ship operational data and sea and weather conditions from noon report | Fuel consumption per day | Polynomial regression | R^2 is 0.7557 in the training set | Journal of Ocean Engineering and Science |
| Jia et al. (2017) | 483 VLCCs | Ship operational data from AIS; mechanical data from Clarksons World Fleet Register | Fuel consumption per voyage, GHG and pollutant emissions per voyage | Bottom-up vessel fuel consumption calculation | Not applicable | Transportation Research Part D |
| Lepore et al. (2018) | A Ro-Pax cruise ship | Ship operational data and sea and weather conditions from onboard multisensory system | Fuel consumption per hour | Multiway partial least-squares (PLS) regression | R^2 is 0.82 in cross validation | Quality and Reliability Engineering International |
| Adland et al. (2018) | 8 crude Oil tankers | Ship operational data and sea and weather conditions from noon report; ship maintenance data provided by a shipping company | Fuel consumption per day | MLR analysis | R^2 ranges from 0.685 to 0.834 in the training set | Journal of Cleaner Production |
| Lepore et al. (2019) | A Ro-Pax cruise ship | Ship operational data and sea and weather data from onboard sensors | Fuel consumption per hour, energy efficiency initiative (EEI), and GHG emissions | Orthogonal least squares-partial least squares method | Not applicable | Quality Engineering |
| Capezza et al. (2019) | Two Ro-Ro Pax ships | Ship operational data and sea and weather conditions from onboard sensors | Fuel consumption per hour | PLS regression | Not applicable | Transportation Research Part D |
| Adland et al. (2020) | 16 oil tankers | Ship operational data and sea and weather conditions from noon report | Fuel consumption per day | Piecewise linear regression | R^2 ranges from 0.739 to 0.885 when dividing the speed values into three endogenous thresholds | Transportation Research Part E |
| Işıklı et al. (2020) | A bulk carrier | Ship operational data and sea and weather conditions from noon report | Fuel consumption per day | Response Surface Methodology | R^2 is 0.8037 in test set | Journal of Cleaner Production |
| Le et al. (2020a) | Five classes of container ships grouped by size | Ship operational data per voyage and mechanical data provided by a Korean shipping company | Fuel consumption rate (ton/TEU/knot) | MLR analysis | MAPE ranges from 11.62% to 20.71% in cross validation | Maritime Policy & Management |

Table 10. Ship operational optimization via BBMs based on statistical modelling (4 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Optimization objective(s) | Decision variable(s) | Solution approach(es) | Journal |
|----------------------|---|---|--------------------------------|---|--|---|--|---|---------------------------------|
| Wang and Meng (2012) | Container ships in a liner shipping network | Ship operational data from a liner shipping company | Fuel consumption per day | Linear regression (LR) | R ² is at least 0.96 in training set | To minimize fuel consumption in the liner shipping network | Sailing speed and the number of ships deployed on each route of a liner shipping network | A novel outer-approximation algorithm | Transportation Research Part E |
| Yao et al. (2012) | Container ships for a single shipping liner service | Ship operational data from a shipping company | Fuel consumption per day | LR | Not applicable | To minimize total bunker fuel related cost for a shipping liner service | Bunkering ports and amounts, and sailing speed | CPLEX | Computers & Operations Research |
| Lee et al. (2018a)* | A container ship | Ship operational data from a liner shipping company and sea and weather data from CMEMS | Fuel consumption per day | An LR model extended from Yao et al. (2012) | Error rate is 7.5% in the test set | To minimize fuel consumption and maximize service level agreement via a decision support system | Sailing speed | PSO algorithm | Computers & Operations Research |
| Lee et al. (2018b) | A container ship | Ship operational data and sea and weather conditions | Fuel consumption per unit time | Polynomial regression | The error is within 0.5% compared with the actual data | To minimize fuel consumption over a voyage | Heading angle and engine RPM | Non-dominated Sorting Genetic Algorithm (NSGA)-II | Ocean Engineering |

Note *: DSS is implemented in the paper

379 All 17 of the papers listed in Tables 9 and 10 use ship operational data at sea, and
380 12 also consider the surrounding sea and weather conditions. Unlike studies on WBMs,
381 most of which consider ship mechanical data, only 3 of these 17 papers use ship
382 mechanical data. In addition, 3 papers consider ship maintenance data regarding dry
383 docking, 2 papers predict ship energy efficiency indicators such as EEOI and EEI, and
384 2 papers predict GHG and pollutant emissions. The consideration of the above-listed
385 factors is thus far rarer in BBM research than in studies on WBMs. Among the statistical
386 models adopted for fuel consumption prediction, linear regression models, including
387 simple linear regression and multiple linear regression, are the most popular, being used
388 in 3 and 6 papers, respectively. Polynomial regression models are used in 2 papers.
389 Piecewise linear regression is also used to allow multiple linear models to be fitted to
390 the data in different ranges of X . In addition, 3 papers use PLS regression. As shown
391 in the tables, most of the papers present model performance metrics (e.g., R^2 , MSE,
392 MAE, and MAPE) for either or both a training set and a test set, which differs from
393 studies of WBMs. A detailed illustration of BBMs based on statistical modeling is given
394 in Appendix B.2. In addition, although most of the papers only consider one specific
395 vessel in developing tailored models for ship fuel consumption prediction, some of the
396 studies consider a fleet containing several (sister) vessels, yielding prediction models
397 that are more sophisticated and practical. For example, Adland et al. (2018) use noon
398 reports of a fleet of 8 identical Aframax-size crude oil tankers, and those of a fleet of
399 10 Aframax product tankers and 6 Suezmax vessels (Adland et al., 2020) to identify the
400 relationships between various influencing factors and vessel fuel consumption
401 conditions. Le et al. (2020a) use the voyage records of more than 100 container ships
402 to estimate fuel consumption.

403 Three of the 4 papers developing ship operational optimization models aim to
404 minimize fuel consumption/costs; the fourth constructs a bi-objective function that
405 minimizes fuel consumption and maximizes the service level agreement via a decision
406 support system (DSS), aiming to support decision makers who are not experts in
407 prediction and mathematical modeling and analysis (Lee et al., 2018). However, the
408 decision variables of these 4 papers vary. One paper only considers sailing speed, while
409 two papers consider sailing speed and the ship deployment/bunkering port and amount
410 simultaneously. One paper also considers the heading degree and engine RPM when
411 sailing.

412

413 **3.4.2 Review of BBMs based on machine learning (ML)**

414 Recent years have witnessed a boom in studies that develop BBMs based on ML

415 for fuel performance monitoring, driven by the accessibility of massive amounts of data
416 on ship energy efficiency, especially from onboard sensors, and increases in
417 computational power. Similar to the procedure for developing BBMs based on
418 statistical modeling, practical ship operational data should be collected and pre-
419 processed, as data quality and quantity play major roles in all types of ML models.
420 Suitable ML models are then chosen and developed based on the requirements, and the
421 input data are then further pre-processed if necessary. Hyperparameters should be tuned
422 based on the training and validation sets to improve the model's generalization ability.
423 Finally, model performance is validated using the test set. Compared with statistical
424 models, ML models are more suitable for dealing with high-dimensional data, and thus
425 can incorporate a wider range of input features. However, their black-box nature
426 decreases their interpretability compared with statistical modeling approaches. We
427 summarize ship performance monitoring models and ship operational optimization
428 models adopting BBMs based on ML in Tables 11 and 12.

Table 11. Ship performance monitoring via BBMs based on ML (20 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Journal |
|----------------------------|--------------------------------|--|---|--|--|--|
| Pedersen and Larsen (2009) | A tanker ship | Ship operational data and sea and weather conditions from noon report | Fuel consumption per hour | ANNs | The error rate is about 7% in test set | Conference proceedings |
| Petersen et al. (2012a) | A ferry ship | Ship operational data and sea and weather conditions from onboard sensors | Fuel consumption per hour | ANNs | The root mean square error (RMSE) is 47.2 in the test set | Ship Technology Research |
| Petersen et al. (2012b) | A ferry ship | Ship operational data and sea and weather conditions from onboard sensors | Fuel consumption per hour | ANNs and Gaussian processes (GPs) | The RMSE for ANNs and GPs is 47.2 and 51.4, respectively in the test set | Journal of Marine Science and Technology |
| Wang et al. (2018) | A ship fleet of COSCO | Ship mechanical and operational data, and sea and weather conditions derived from the software of a shipping company | Fuel consumption per hour | LASSO regression | The mean absolute error (MAE) is 4.9 in test set | Transportation Research Part D |
| Soner et al. (2018) | A ferry ship | Ship operational data and sea and weather conditions from onboard sensors | Fuel consumption per hour | Tree-based models including bagging, random forest (RF), and bootstrap ANNs | The RMSE for bagging, random forest, and bootstrap is 45.2, 43.5, and 41.3, respectively in test set | Ocean Engineering |
| Jeon et al. (2018) | A bulk carrier | Ship operational data and sea and weather conditions from onboard sensors | Main engine fuel consumption per day | ANNs | Median R^2 is 0.9383 of tangent Sigmoid ANNs in test set | Journal of Mechanical Science and Technology |
| Yuan and Nian (2018) | An oil tanker | Ship operational data and sea and weather conditions from noon report | Fuel consumption per hour | GPs | The RMSE is 0.4418 in validation set | Conference paper |
| Gkerekos et al. (2018) | A reefer vessel | Ship operational data and sea and weather data from noon report | Fuel consumption per sailing distance | 5 machine learning models: decision tree (DT), RF, support vector regressor (SVR), shallow and deep neural networks | R^2 ranges from 0.7 to 0.9 in k-folding | Conference proceedings |
| Gkerekos et al. (2019) | A bulk carrier | Ship operational data and sea and weather data from noon reports; automated data logging & monitoring (ADLM) systems | Fuel consumption per day | 12 machine learning models: linear regression, LASSO, Ridge, elastic net, DT, RF, k-nearest neighbors (KNN), support vector machine (SVM), extra tree model, boosting model, bagging model, ANNs | When data from noon report is used, R^2 of the models ranges from 0.7011 to 0.9146 in test set; when data from ASLM systems are used, R^2 ranges from 0.7269 to 0.9729 in test set | Ocean Engineering |
| Soner et al. (2019) | A ferry ship | Ship operational data and sea and weather conditions from onboard sensors | Sailing speed through water and fuel consumption per hour | Ridge regression and LASSO regression | The RMSE in ridge and LASSO regression models is 48.7 L/h and 44.6 L/h, respectively, in the test set | Journal of Marine Science and Technology |
| Sourtzi (2019) | A passenger ship | Ship operational data and sea and weather data from electronic voyage reports extracted from the MRV software | Fuel consumption per hour | A multi-layer feed-forward neural network model | The mean absolute percentage error (MAPE) is 2.16% in the test set | Master thesis at the University of Piraeus |
| Panapakidis | A passenger | Ship operational data and sea and weather | Ship fuel | Long short-term memory | The MAPE of three case studies ranges from 2.177 | Electronics |

| | | | | | | |
|-----------------------------------|---|--|---|---|---|---|
| et al. (2020) | ship | conditions from voyage report | consumption per hour | (LSTM) and Elman neural network (ENN) | to 2.506 | |
| Peng et al. (2020) | 8019 ship records at the Jingtang Port | Ship arrival time, handling volume and goods, berth, type of trade et al. at Jingtang Port | Ship fuel consumption at port | 5 machine learning models: gradient boosting regression (GBR), RF, BP neural network, liner regression and KNN | R ² of the 5 models ranges from 0.46 to 0.91 in test set | Journal of Cleaner Production |
| Man et al. (2020) | Five ferries | Ship operational data from onboard sensors, ship log and AIS; sea and weather data from online sources and government department | Fuel consumption per journey | Multi-layer perceptron (MLP) and self-organizing map (SOM) | Average relative error is 140% in MLP and 110% in SOM in the test set | Applied Sciences |
| Farag and Olcer (2020) | A tanker ship | Ship operational data and sea and weather data from onboard sensors and weather hindcast information | Total energy consumed, total voyage fuel consumption, total CO ₂ emissions, and average propulsion power | A combined ANN and MLR | The error rate is 0.43% in test set | Ocean Engineering |
| Uyanık et al. (2020) | A container ship | Ship operational data and sea and weather data from noon reports, engine logbook, and sensors | Fuel consumption per day | 14 machine learning models: Ada boost, Bayesian ridge, DT, elastic net, GBR, hist gradient boosting, kernel ridge, KNN, LASSO regression, MLR, MLP, RF, ridge regression, SVM | R ² ranges from 0.96502 to 0.99999 in validation set | Transportation Research Part D |
| Le et al. (2020b) | Five classes of container ships grouped by size | Ship operational data per voyage and mechanical data provided by a Korean shipping company | Fuel consumption per sailing distance | ANNs | MAPE ranges from 7.4 to 16.8 | Maritime Policy & Management |
| Karagiannidis and Themelis (2021) | A container ship | Ship operational data and sea and weather conditions from onboard measuring device | Fuel consumption per day | ANNs with feature engineering | RMSE ranges from 0.64 to 3.42 in test set | Ocean Engineering |
| Kim et al. (2021) | A container ship | Ship operational data and sea and weather data from an onboard alarm monitoring and control system | Fuel consumption per sailing distance | ANNs and MLR | R ² ranges from 0.8 to 0.9936 in test set | Journal of Marine Science and Engineering |
| Zhu et al. (2021) | A passenger ship | Ship operational data and sea and weather data from onboard sensors | Fuel consumption per sailing time | MLR, SVR, ANNs | ANN has the best performance, followed by LR and SVR | Journal of Marine Science and Engineering |

Table 12. Ship operational optimization via BBMs based on ML (15 papers)

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Optimization objective(s) | Decision variable(s) | Solution approach(es) | Journal |
|----------------------------|--------------------------------|---|---|---|--|--|--|---|--|
| Petersen (2011) | A domestic ferry | Ship operational data and sea and weather data from onboard sensors | Fuel consumption per hour | 4 machine learning models: ANNs, GPs, Gaussian mixture model (GMM), time-delay networks | The RMSE of the models is about 50 L/h in test set | To minimize fuel consumption | Trim | Enumeration | Master thesis in DTU |
| Beşikçi et al. (2016)* | An oil tanker | Ship operational data and sea and weather data from noon report | Fuel consumption per hour | ANNs | R^2 is 0.759 in test set | To minimize fuel consumption | Sailing speed, RPM, trim, wind and sea effects | Developing a decision support system | Computers & Operations Research |
| Rudzki and Tarelko (2016)* | A tall ship | Ship operational, mechanical, and maintenance data, and sea and weather data from sea trials | Sailing speed and fuel consumption per hour | ANNs | The mean squared error (MSE) is 0.0813 in training set | To propose a two-objective optimization problem regarding fuel consumption and speed | Propeller pitch and engine rotation speed | Weighted-sum method considering two objectives | Ocean Engineering |
| Wang et al. (2016) | A cruise ship | Ship operational data and sea and weather data from onboard sensors | Wind speed, water depth, and fuel consumption per meter | Wavelet neural network | Not applicable | To minimize fuel consumption | Main engine speed | A dynamic optimization method proposed by the authors | Transportation Research Part D |
| Farag (2017)* | An oil tanker | Ship operational data and sea and weather data from the ship's automatic monitoring system, AIS, and weather hindcast information | Fuel consumption | ANNs and MLR analysis | Model accuracy is 97.45% in test set | To maximize ship energy efficiency | Sailing speed and heading angle | Development of a DSS by Excel and Matlab | Mater thesis at World Maritime University |
| Chaal (2018)* | A tanker ship | Ship operational data and sea and weather data from onboard sensors and software | Fuel consumption per hour | DT, AdaBoost DT, KNN and ANNs | R^2 ranges from 0.74 to 0.96 in test set | To minimize fuel consumption | Trim, trim and route | Generic algorithm | Master thesis at World Maritime University |
| Du et al. (2019) | Two container ships | Ship operational data and sea and weather data from noon report | Fuel consumption per day | ANNs | The RMSE ranges from 8.23 to 10.25 in test set | To minimize fuel consumption | Sailing speed, trim, speed and trim | Enumeration and dynamic programming | Transportation Research Part B |
| Zheng et al. (2019) | A cruise ship | Ship operational data from AIS | Fuel consumption per hour | ANNs | Model accuracy is more than 0.9 in test set | To minimize fuel consumption over a voyage | Sailing speed | Four improved PSO algorithms | Journal of Cleaner Production |
| Sun et al. (2019) | A bulk carrier | Ship operational data and sea and weather data from onboard sensors | Sailing speed and fuel consumption | ANNs | The MSE is 0.911×10^{-7} in the training set | To minimize EEOI | Engine revolution | Genetic algorithm | Journal of Marine Science and Engineering |
| Zhang et al. (2019) | A general cargo ship | Ship operational data from AIS and sea and weather | EEOI | ANNs | R^2 is about 0.96 in validation set | To optimize ship energy efficiency | Route | Ant colony algorithm | Ocean Engineering |

| | | | | | | | | | |
|-----------------------------|--------------------|---|---|--|--|---|-----------------|---|---|
| Tarelko and Rudzki (2020)* | A tall ship | data from NMEFC Ship operational data and sea and weather data from noon report | Fuel consumption per hour and sailing speed | ANNs | The error rate between 0.8% and 2.8% in test set | To minimize fuel consumption and maximize sailing speed | Sailing speed | MATLAB optimization toolbox | Neural Computing and Applications |
| Gkerekos and Lazakis (2020) | A crude oil tanker | Ship operational data from noon report, sea and weather data from CMEMS | Fuel consumption per hour | ANNs | R ² is 0.894 in the test set | To minimize fuel consumption | Sailing route | Modified Dijkstra's algorithm | Ocean Engineering |
| Linh and Ngoc (2020) | A liner ship | Ship operational data from a shipping company; sea and weather data from online resources | Fuel consumption of a route | Deep ANNs with 10 hidden layers | The MAPE is 5.89% in test set | To minimize fuel cost | Route | Asymmetric traveling salesman problem algorithm | The Asian Journal of Shipping and Logistics |
| Yan et al. (2020) | A dry bulk ship | Ship operational data and sea and weather data from noon report and EMCWF | Fuel consumption per hour | RF | The MAPE is 7.91% in test set | To minimize fuel consumption over a voyage | Sailing speed | CPLEX | Transportation Research Part E |
| Tran (2020) | A bulk ship | Ship operational data and sea and weather data from noon report | Fuel consumption per voyage | A fuzzy c-means clustering method (unsupervised) | Not applicable | To optimize ship energy efficiency | Loading of ship | A fuzzy analytical hierarchy process (AHP) method | Ocean Engineering |

432 Note *: DSS is implemented in the paper

433 Tables 11 and 12 show that 34 of the 35 papers leverage ship operational data to
434 predict ship fuel consumption during sailing, and the other uses ships' trading and
435 berthing information at port to predict in-port fuel consumption. Most of the papers
436 consider sea and weather conditions in ship performance monitoring (31 papers).
437 However, only 2 papers utilize ship mechanical data for fuel consumption prediction
438 and only 1 uses maintenance data. Unlike WBMs, which are widely used to predict ship
439 emissions as well as fuel consumption, ML models are seldom used to predict emissions
440 (only 1 paper does so). Artificial neural networks (ANNs), including back propagation
441 neural networks, multi-layer perceptron (MLP), and wavelet neural networks, are the
442 most popular ML models, being used in 29 of the 35 studies. Linear regression models,
443 including ordinary least squares (OLS), as well as regularized linear regression models,
444 such as least absolute shrinkage and selection operator (LASSO) regression, ridge
445 regression, and elastic net regression, are the next most popular, followed by tree-based
446 models such as the decision tree (DT), random forest (RF), Adaboost DT, and gradient
447 boosting DT models. Support vector machine (SVM) and k-nearest neighbor (KNN)
448 ML models are also popular. All these models are supervised ML models, where the
449 data label, i.e., the fuel consumption rate, is used in model training. Some unsupervised
450 ML models are also used, such as self-organizing maps (SOM) (Man et al., 2020), the
451 Gaussian mixture model (GMM) (Petersen, 2011), and fuzzy c-means clustering (Tran,
452 2020) models. In addition, although onboard sensors are widely used to collect nearly
453 real-time ship sea trial data, no more than 10% of the 35 papers use deep learning
454 models to achieve more accurately predict fuel consumption (3 papers).

455 Most of the papers developing BBMs for ship fuel consumption listed in Tables 11
456 and 12 present model performances for unseen data (e.g., on test and validation sets or
457 in k-fold cross validation). This differs from WBMs, where one third of the papers do
458 not give metrics for model performance in training, validation, or test sets, and also
459 differs slightly from BBMs based on statistical modeling, where many papers only
460 present model fitting performances for the training set. This is because WBMs are based
461 on a priori knowledge and physical insights into a system with known structure and
462 parameters to disclose the theoretical basis underlying various influencing factors and
463 the prediction target. In contrast, BBMs based on ML more strongly emphasize the
464 bias–variance tradeoff to achieve better model generalization ability. The mean squared
465 error of a prediction model can be decomposed into two components: a bias component
466 and a variance component. When model complexity increases, the variance tends to
467 increase, and the squared bias tends to decrease. However, if the model is too complex,
468 it will adapt too much to the training data and will not generalize well to unseen data

469 (i.e., it will have large test errors). In contrast, if the model is not complex enough, it
470 will underfit the training data and have large bias, again leading to poor generalization
471 ability. Therefore, one of the goals of BBMs based on ML is accurate prediction of new
472 and unseen data based on statistical patterns in a training set.

473 To explore the underlying of the models for ship fuel consumption prediction using
474 ML-based BBMs, we briefly present the basic ideas underlying them and their pros and
475 cons in Appendix B.3. For more comprehensive discussion and analysis of these models,
476 readers are referred to Hastie et al. (2014) and Friedman et al. (2001).

477 Some papers compare the performance of different ML models using the same data
478 set. For example, Petersen et al. (2012a, 2012b) and Soner et al. (2018, 2019) use ship
479 operational data and the surrounding sea and weather data from the onboard sensors of
480 a domestic ferry. Based on model validation results, it is concluded that bootstrap tree-
481 based model is the most suitable model for fuel consumption prediction using this
482 dataset (Soner et al., 2018), followed by RF and LASSO regression (Soner et al., 2018,
483 2019). GPs have the worst performance on the test set among all the ML models,
484 possibly because they eschew the Gaussian assumption. In addition, Gkerekos et al.
485 compares 5 ML models (2018) and, in another study, 12 ML models (2019), and Uyanık
486 et al. (2020) compares 14 ML models for fuel consumption prediction. Gkerekos et al.
487 (2018) shows that RF and SVR perform better than DT and ANNs with different
488 structures, including deep neural networks. Uyanık et al. (2020) concludes that linear
489 regression-based models, including Bayesian ridge, kernel ridge, multiple linear, and
490 ridge models, perform better than all the ML models, including other types of linear
491 regression models, tree-based models, KNN, and ANNs. Gkerekos et al. (2019) also
492 compares the model performance using datasets from manually filled noon reports and
493 onboard automated data logging & monitoring (ADLM) systems. The results show that
494 model performance evaluated using the coefficient of determination (R^2) can be
495 significantly improved if sensor data are used. In addition, SVM with a radial basis
496 function (RBF) as the kernel has the best performance when using training data
497 constructed from noon reports, and the extra trees model performs best when using
498 training data constructed from ADLM systems.

499 Of the 15 papers developing two-stage models for ship operational optimization, 9
500 papers aim to minimize fuel consumption or fuel costs and 4 aim to optimize ship
501 energy efficiency. Two papers aim to minimize fuel consumption while maximizing
502 sailing speed. These 15 papers also consider other decision variables than sailing speed,
503 such as trim settings, sailing route, loading of ships, and engine performance indicators.
504 Five papers implement DSSs to better assist the decision makers.

505 Compared with WBMs, BBMs, whether based on statistical modeling or ML, have
506 better fitting ability for training data and the highest prediction accuracy for unseen data.
507 BBMs based on ML usually have better generalization ability than BBMs based on
508 statistical modeling (Petersen et al., 2012b). Another advantage of BBMs over WBMs
509 is that no a priori knowledge regarding the vessel physics is required, as BBMs are
510 purely data-driven. In addition, because the model is calibrated and the parameters are
511 estimated using experimental or operational data, BBMs can learn from real situations
512 better as data accumulate, and in theory, their generalization performance and ability to
513 handle noisy data should improve. According to the Vapnik–Chevronenkis (VC)
514 dimension, a larger training dataset size should improve machine learning model
515 performance by reducing overfitting (Juda and Le, 2019). However, noise and errors in
516 the data from ships’ noon reports and onboard sensors are likely to limit the
517 improvement of model performance as data accumulate.

518 However, BBMs also have several disadvantages. As BBMs are purely data-driven,
519 a large quantity of high-quality data is needed for model construction, and thus the data
520 quantity and quality have substantial effects on model performance. Therefore, BBMs
521 cannot to be used in the vessel design and initial sea trial stages, where data availability
522 is limited. It should be noted from Tables 9 through 12 that the sample size of ship data
523 used to construct BBMs based on statistical modeling and ML in the literature is usually
524 small, as most studies consider only one or two vessels of the same type. The available
525 data tend to be especially limited for models using noon reports.

526 Another main drawback of BBMs is their poor interpretability: the models are
527 usually complex and difficult to intuitively explain. As they are trained in a purely data-
528 driven way, they are not informed by basic vessel physical knowledge, and thus experts
529 in the shipping industry have difficulty accepting them. The complex structure of ML
530 models, combined with the large number of estimation parameters, endows them with
531 a strong ability to learn the training data, including specific details and noise. However,
532 this can weaken their generalization ability. For example, Friedman et al. (2001) states
533 that ANNs, which learn a large number of weights, tend to overfit the data at the global
534 minimum. Therefore, to improve model performance, regularization techniques should
535 be adopted, such as the early stopping rule, validation sets, and weight decay. However,
536 it is not trivial to find a balance between overfitting and model complexity, especially
537 when the data contain noise, which will generate counterintuitive prediction results in
538 the ML models. For example, if we increase the input sailing speed while keeping all
539 other input variables fixed, we expect the predicted fuel consumption to increase;
540 however, ML models may predict the opposite. Shipping experts may be highly

541 resistant to ship fuel consumption prediction models that violate the concepts of domain
542 knowledge and data science in such a serious way.

543 One last point concerns how the BBMs developed for ship fuel consumption
544 prediction in the reviewed literature solve the common challenges in regression analysis,
545 especially endogeneity and correlations. As both ship sailing speed and engine power
546 (and thus fuel consumption) are set based on the surrounding sea and weather
547 conditions together with other external factors, the problem of endogeneity in these
548 studies is inevitable. Similarly, sailing speed and the surrounding sea and weather
549 conditions are correlated: for example, the captain must slow down in bad weather for
550 safety reasons. Both problems are seldom addressed by the BBMs based on statistical
551 modeling in the reviewed literature. The only study that addresses the endogeneity
552 problem is that by Adland et al. (2020), who proposes a novel framework to estimate
553 the elasticity (including speed intervals) of the speed–consumption relationship to
554 partially address the problem of endogeneity, which enables better exploitation of the
555 explanatory variables and better explanation of the speed–consumption relationship.
556 This initial but meaningful step toward solving more advanced challenges in vessel
557 energy management and green shipping has significance for follow-up research.
558 Regarding multicollinearity between features, it is reported in Le et al. (2020b) that a
559 pairwise correlation between two independent variables indicates a potential
560 multicollinearity problem, whereas further examination of tolerance and the variance
561 inflation factor (VIF) does not yield any multicollinearity concerns. In addition, the
562 authors claim that as their research focuses on fuel consumption prediction rather than
563 identification of the factors affecting fuel consumption and their detailed effects, the
564 problem of multicollinearity can be safely ignored. In addition, Lepore et al. (2019) and
565 Capezza et al. (2019) develop PLS models to reduce multicollinearity by reducing the
566 predictors to a smaller set of uncorrelated components and performing least squares
567 regression on these components.

568 Endogeneity is seldom considered in the studies proposing BBMs based on ML,
569 except for Du et al. (2019), in which the endogeneity of engine RPM, which depends
570 on variables outside the engine, such as sailing speed, draft, trim, and sea and weather
571 conditions, is considered in variable selection. In BBMs based on ML, correlations
572 between features can be reduced by pre-processing data and adopting suitable ML
573 models for fuel consumption prediction. The use of correlation analysis to identify and
574 delete features that are highly correlated with each other, known as feature selection, is
575 common before developing ML models: it can be found in Lee et al. (2018), Farag and
576 Ölçer (2020), Karagiannidis and Themelis (2021), and Kim et al. (2021), where domain

577 knowledge is used for feature selection; in Wijaya et al. (2020), where principal
578 component analysis (PCA) is used; and in Kim et al. (2021), where LASSO is used.
579 Moreover, some ML models can inherently overcome the problem of correlations
580 between features. A typical example is ensemble tree-based models (e.g., random forest
581 and gradient boosting decision tree), which are used in Soner et al. (2018), Chaal (2018),
582 Gkerekos et al. (2019), Uyanik et al. (2020), Yan et al. (2020), Peng et al. (2020), and
583 are resistant to collinearity for two reasons. First, only a random subset of features is
584 used to construct each tree, and thus, it is likely that only one of a group of correlated
585 features will be selected per tree. Second, if two or more highly correlated features are
586 selected to construct the same tree, no explicit preference for one over the other(s) will
587 be imposed when selecting the next leaf-splitting step, as the features can be regarded
588 as interchangeable with respect to leaf impurity reduction. Another typical example is
589 regularized linear regression models such as ridge regression and LASSO regression,
590 where some features are retained while others are discarded by setting their coefficients
591 to zero. Specifically, size constraints are imposed on the coefficients in ridge regression
592 using L2 regularization (Gkerekos et al., 2019, Soner et al., 2019, Uyanik et al., 2020)
593 and in LASSO using L1 regularization (Petersen et al., 2012, Gkerekos et al., 2019,
594 Soner et al., 2019, Uyanik et al., 2020).

595

596 **3.5 Review of grey-box models (GBMs)**

597 There are two types of GBMs in the literature. In the first type, namely sequential
598 GBMs, two or more models are developed in a series, including at least one WBM and
599 one BBM, and then the WBM(s) and BBM(s) are combined to form a single GBM. For
600 example, a BBM can be developed to process the raw data and the initial prediction
601 results are then fed into a WBM, or vice versa (Leifesson et al., 2008, Coraddu et al.,
602 2017). The other type is parallel GBMs. In one such case, a WBM is first established
603 based on theoretical principles and vessel physical laws, and then the unknown
604 parameters are estimated by BBMs from experimental data (Meng et al., 2016; Yang et
605 al., 2019b). In another case, a priori knowledge (used in WBMs) is integrated into a
606 BBM by introducing model regularization (Caraddu et al., 2017 and 2018). Currently,
607 there are few GBMs for ship fuel consumption prediction. The existing ship
608 performance monitoring models and operational optimization models based on GBMs
609 are summarized in Tables 13 and 14, respectively.

610 **Table 13. Ship performance monitoring via GBMs (4 papers)**

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Prediction model performance | Journal |
|------------------------|-----------------------------------|---|----------------------------------|---|---|--|
| Leifsson et al. (2008) | A container ship | Ship operational and mechanical data; sea and weather data | Fuel consumption per hour | A WBM, a BBM, a sequential GBM, and a parallel GBM | GBMs can slightly improve the performance of WBM; the prediction accuracy of GBM and BBM is similar | Simulation Modelling Practice and Theory |
| Caroddu et al. (2015) | A Panamax chemical/product tanker | Ship operational and mechanical data, and sea and weather data from onboard sensors | Fuel consumption and shaft power | A WBM, a BBM, and a parallel GBM | The WBM performs worse; the GBM can achieve the same performance as the BBM using less historical data | Conference proceedings |
| Meng et al. (2016) | A container ship | Ship operational data and sea and weather data from noon report | Fuel consumption per day | GBMs with parameters estimated by sequential estimation procedure | R ² of the first model is at least 0.928, root mean squared residuals of the second model is no more than 10 in training set | Transportation Research Part B |
| Yang et al. (2019b) | A crude oil tanker | Ship operational and mechanical data, and sea and weather data from noon report | Fuel consumption per day | A generic algorithm-based GBM | R ² is 0.9003 in the training set | Annals of Operations Research |

611
612 **Table 14. Ship operational optimization via GBMs (3 papers)**

| Literature | Shipping sector and fleet size | Data type and resources | Prediction target(s) | Fuel consumption prediction model | Fuel consumption prediction model performance | Optimization objective(s) | Decision variable(s) | Solution approach(es) | Journal |
|-----------------------|--------------------------------|--|--|---|---|------------------------------|----------------------|--|---|
| Caraddu et al. (2017) | A tanker ship | Ship operational data and sea and weather data from onboard sensors | Shaft power, shaft torque, and fuel consumption | A WBM, a BBM, a naive GBM and advanced GBM (denoted by N-GBM and A-GBM) | Best MAPE of N-GBM and A-GBM is 0.79 and 0.92, respectively | To minimize fuel consumption | Trim | Enumeration | Ocean Engineering |
| Lu et al. (2015)* | Two tanker ships | Ship mechanical and operational data, and sea and weather conditions from noon report and NOAA | Ship fuel consumption per tonne of cargo and per nautical mile | A GBM based on modified Kwon's methods | The error rate is 5.12% for one tanker ship and 7.15% for the other tanker ship in test set | To minimize fuel consumption | Route | Setting up grid system on world map and selecting the optimal route manually | Ocean Engineering |
| Coraddu et al. (2018) | A tanker ship | Ship operational data and sea and weather data from onboard sensors | Shaft power, shaft torque, fuel consumption | A WBM, a BBM, a N-GBM, and a A-GBM | The MAPE is within 2% in the test set | To minimize fuel consumption | Trim | Enumeration | Soft Computing for Sustainability Science |

613 Note *: DSS is implemented in the paper

614 Tables 13 and 14 show that all of the papers developing GBMs for fuel consumption
615 prediction use ship operational data and sea and weather data, and most also use ship
616 mechanical data (4 papers). However, ship maintenance data are not used in these
617 models. Regarding the structure of the developed GBMs, 3 papers develop both
618 sequential and parallel GBMs, and most of the others develop parallel GBMs. A more
619 detailed illustration of the GBMs, especially what WBMs and BBMs they contain and
620 how they are combined with each other, is given in Appendix 3.4.

621 An advantage of GBMs is that they can combine WBMs, which are explainable
622 and based on solid physical insights, with BBMs, which have high accuracy.
623 Theoretically, therefore, their performance should be better than that of BBMs and also
624 partially explainable even with fewer historical training data (Yang et al., 2019b). This
625 should largely prevent unreasonable prediction results that contradict domain
626 knowledge, and guarantee prediction accuracy. Unfortunately, these trends are not
627 obvious in current research results in the literature listed in Tables 13 and 14.

628

629 **3.6 Review of technical reports**

630 Technical reports published by the government, academic institutions, and
631 companies on ship fuel consumption make up a body of “grey literature” that provide
632 considerable insights into this area. The GHG studies published by the IMO, including
633 the First, Second, Third, and Fourth IMO GHG Studies published in 2000, 2009, 2014,
634 and 2020, respectively, are the most authoritative technical reports regarding ship fuel
635 consumption and emission analysis. The 4th IMO GHG Study, which is the latest in
636 this series, estimates the consumptions of different types of fuels and the emissions in
637 international voyages from a more macro-scale perspective than most of the academic
638 studies reviewed in this study (IMO, 2020). It adopts both a top-down approach (by
639 leveraging World Energy Statistics, including fuel sales data and emission factors to
640 estimate the total mass of fuel consumption and the corresponding emissions) and a
641 bottom-up approach (by leveraging AIS-transmitted data to describe individual vessels’
642 operational activity). Detailed instructions and formulas to estimate the specific fuel oil
643 consumption and various types of emissions are given in the report. It also makes
644 comparisons between the top-down and bottom-up estimation approaches for ship fuel
645 consumption and emissions, and the bottom-up method is found to estimate absolute
646 values that are consistently higher than those of the top-down method.

647 Apart from the IMO, research institutions and companies around the world also
648 publish technical reports on ship fuel consumption prediction and analysis. For example,
649 researchers from the Technical University of Denmark and University of Southern

650 Denmark propose and analyze methods to predict ship resistance and the corresponding
651 propulsion power (Kristensen and Lützen, 2012). Various types of resistance, such as
652 frictional resistance, incremental resistance, air resistance, steering resistance, and
653 residual resistance, are considered to calculate a ship’s total resistance, and the required
654 effective power is then derived. Researchers from Chalmers University of Technology
655 summarize models and methods for ship energy efficiency management (Tillig et al.,
656 2015). Their report includes the components of a vessel as a whole system, models, and
657 tools to monitor ship energy efficiency (classified into holistic models, subsystem
658 models, and commercial tools and software), and energy-saving measures. The Arctic
659 Climate Change, Economy and Society (ACCESS) adopts a semi empirical–analytical
660 approach to calculate the fuel consumptions of bulk carriers, oil tankers, and LNG
661 carriers under different ice conditions for the past (1960 to 2020) and present (1960 to
662 2020) and predicts them for the future using software called ICEROUTE (ACCESS,
663 2014). MAN Energy Solutions, a leading engine production company, published a
664 report titled “Basic principles of ship propulsion” that clarifies elements of a ship’s
665 structure and propulsion system. The report presents the relationships between ship
666 propulsion power and the influencing factors, such as the speed, environmental
667 regulations, hull, and propeller, for different types of ships (MAN, 2018).

668

669 **4. Future research questions**

670 The development of data-driven ship performance monitoring models and
671 operational optimization models in academic research is relatively new. We hope that
672 we have provided glimpses of its potential to reduce the emissions of pollutants and
673 GHG from international shipping activities and to decrease vessel operating costs for
674 shipping companies.

675 It should be noted that in practice, given the fact that several factors are determined,
676 including but not limited to the cargo intake, the surrounding sea and weather conditions,
677 and the range of speed values given by commercial contracts, ship operators can only
678 have limited degrees of freedom to control their vessels so as to reduce fuel
679 consumption and emissions. The main objective of existing ship fuel consumption
680 prediction models is to provide more accurate estimations of fuel consumption rates
681 under various conditions, such as sailing at various speeds and trim settings under
682 different sea and weather conditions and hull/propeller fouling conditions. Considering
683 the actual performances achieved thus far, we propose four scenarios in which ship
684 operators can consider using fuel consumption prediction models and voyage
685 optimization models.

686 1) If ship maintenance records (e.g., drydocking, hull and proper cleaning) can be
 687 taken into account in the fuel consumption prediction model, fuel consumption rates
 688 under different fouling and degradation conditions can be estimated, which can give
 689 insight into vessel maintenance for ship operators.

690 2) When accurate weather forecasts within a short period can be obtained, dynamic
 691 and stochastic fuel consumption prediction and, subsequently, voyage optimization
 692 (e.g., speed and trim optimization) can be achieved by only considering the sub-voyage
 693 of two to three days ahead while taking into account the preset allowable arrival time
 694 to the end of each sub-voyage. If the sea and weather conditions change or the sub-
 695 voyage is completed, new dynamic and stochastic voyage planning should be made.

696 3) When accurate weather forecasts for a longer period than that needed to complete
 697 the voyage between a certain origin–destination pair can be obtained, given the earliest
 698 and latest allowable arrival times to the destination, speed and/or trim optimization can
 699 be conducted for the whole voyage.

700 4) The ship fuel consumption prediction models developed under different sea and
 701 weather conditions can also shed light on weather routing to enhance maritime safety
 702 while reducing fuel consumption and emissions, as they can predict fuel consumption
 703 rates under various sea and weather conditions in different geographical locations.

704 Based on the above summary and comparison of the three types of models for ship
 705 fuel consumption prediction, namely WBM, BBMs based on statistical modeling/ML,
 706 and GBMs, together with the ship operational optimization models based on the fuel
 707 consumption prediction results, we outline some promising future research questions
 708 from three perspectives: data, prediction models, and management strategies, as listed
 709 in Table 15.

710 Table 15. Outline of future research questions

| Category | Questions |
|-----------------------|--|
| Data | a. How to consider more valid features, e.g., hull and propeller roughness, ship damage, and engine performance degradation in fuel consumption prediction models? |
| Prediction models | a. How to construct GBMs by combining WBMs and BBMs more effectively? |
| | b. How about applying deep learning models for fuel consumption prediction? |
| | c. How to incorporate domain knowledge into BBMs? |
| | d. How to develop a comprehensive fuel consumption prediction model for different types of ships? |
| Management strategies | e. How about comparing the newly proposed ship performance monitoring tools in the papers with the existing tools proposed by organizations (e.g., IMO, ITTC) and analyzing their pros and cons? |
| | f. What are the advantages and disadvantages of various machine learning models for fuel consumption prediction? |
| | a. How to measure and reduce the inaccuracy of the fuel consumption prediction model in the first stage brought to the operational optimization model in the second stage? |
| | b. How to combine the ever-changing sea and weather conditions with ship operational optimization models, especially in a real-time manner? |
| | c. How to consider the fluctuations of fuel prices and freight rates in operational optimization? |
| | d. How about combining the ship performance monitoring models with liner shipping network design, such as fleet deployment, and cargo routing? |
| | e. How to conduct sensitivity analysis based on the prediction results to generate managerial insights? |

711 **4.1 Data**

712 Research questions regarding the data used in fuel consumption prediction models
713 aim to take a wider range of relevant features into account to achieve more accurate
714 prediction results. For example, Adland et al. (2018)'s study of the effects of hull
715 damage, hull and propeller fouling, and engine degradation on fuel consumption relies
716 on both before–after and difference-in-difference estimators. These findings are
717 instructive to ship operators and can serve as key building blocks for the optimization
718 of vessel maintenance intervals. Meanwhile, such conditions can be difficult to observe
719 and evaluate in practice, and thus no studies directly take their impact into consideration.
720 In addition, ship maintenance records, which can be used to improve the overall ship
721 safety level and energy efficiency, are accessible from shipping companies and vessel
722 databases. Therefore, we expect that taking ship maintenance data into account in ship
723 performance monitoring can make fuel consumption prediction more accurate and
724 efficient. Nevertheless, as shown in Section 3, few ship fuel consumption prediction
725 models take the time since last dry docking into consideration (Bocchetti et al., 2015;
726 Erto et al., 2015; Rudzki and Tarelko, 2016; Adland et al., 2018, 2020), and other ship
727 maintenance information, such as hull and propeller cleaning, main engine maintenance,
728 and major overhaul information, is seldom considered.

729

730 **4.2 Prediction models**

731 Research into fuel consumption prediction models aims to improve their
732 performance from three perspectives: improvement of prediction accuracy,
733 development of unified models, and comparison of different models. In addition to
734 incorporating more valid features to improve model accuracy, other strategies, such as
735 developing GBMs that combine WBM and BBMs more effectively and developing
736 deep learning-based prediction models if data quantity allows, are also promising
737 alternatives. In addition, if domain knowledge can be contained in BBMs, such as the
738 monotonicity and convexity of speed-to-fuel consumption prediction, it can not only
739 improve prediction performance but also significantly improve the interpretability and
740 credibility of BBMs.

741 Current BBMs developed for fuel consumption are usually tailored, which means
742 that they are trained using the sailing data of a single ship, and thus their accuracy can
743 only be guaranteed if applied to monitor the performance of that ship. As calibrating
744 fuel consumption prediction models can be a complex and time-consuming process,
745 this tailored property has restricted the generalization of BBMs. This situation could be
746 improved if unified BBMs that can be universally applied were developed.

747 Some ship fuel consumption and emission prediction models are proposed and
748 implemented in practice by organizations, companies, and research institutes, such as
749 those summarized in Section 3.5. In addition, various ship performance monitoring
750 models are developed and validated in academic papers, but few are compared with
751 existing models using uniform datasets and evaluation metrics. Therefore, the pros and
752 cons and the suitable application scenarios of the newly proposed models are not clear,
753 which may inhibit their potential to reduce ship emissions. Another issue is the lack of
754 comparison and systematic analysis of the various ML models used for fuel
755 consumption prediction using different datasets. Tables 11 and 12 show that tree-based
756 models such as RF have superior performance compared with other popular ML models
757 (Gkerekos et al., 2018, 2019). However, in our experience, the tree-based models may
758 not be suitable for direct application to fuel consumption prediction without
759 modification. The main reason is that the output of tree-based models is not continuous
760 when all other features are fixed while the values of one feature, such as sailing speed,
761 change from small to large (Yan et al. 2020). This discontinuous output is totally
762 contradictory to domain knowledge in the shipping industry and is inappropriate as an
763 input into the subsequent operational optimization models.

764

765 **4.3 Management strategies**

766 The first research question associated with ship fuel consumption management
767 strategies is how to reduce the influence of the inaccuracy of fuel consumption
768 prediction models on the subsequent ship operational optimization model. One viable
769 way is to reduce the inaccuracy of the fuel consumption prediction model in the first
770 stage. However, it can be difficult to further improve the prediction accuracy given
771 limited data quality and quantity, and the generalization error cannot be fully eliminated.
772 Therefore, other ways to reduce such adverse influences, especially considering the
773 relationship between the fuel consumption prediction and management models, are
774 worthy of investigation. Another question is how to consider the fluctuation of the
775 factors with uncertainty in the ship operational optimization model, such as the ever-
776 changing sea and weather conditions, fuel prices, and freight rates. In addition, as few
777 studies (one exception being Wang and Meng [2012]) combine data-driven ship fuel
778 consumption prediction models with liner shipping network design, such research
779 questions remain to be investigated. In addition, managerial insights generated from
780 sensitivity analysis based on fuel consumption prediction models developed from
781 experimental or operational data are also worthy of investigation, as they can be a
782 guideline for daily vessel operations.

783 4.4 Some other common challenges in regression models

784 Finally, other common challenges in regression models, such as endogeneity and
785 collinearity, are not adequately considered and addressed in the literature on ship fuel
786 consumption prediction. Vessel propulsion systems are quite complex: various internal
787 and external factors interact and can influence actual fuel consumption, but such factors
788 cannot be fully captured and considered in a single model. In addition, in actual voyages,
789 ship sailing speed and engine power are simultaneously set based on various external
790 factors, such as the sea and weather conditions. Consequently, the problem of
791 endogeneity is inevitable in ship fuel consumption prediction models. Sailing speed,
792 which is regarded as the most important determinant of fuel consumption rates, is
793 influenced by various surrounding factors, especially the sea and weather conditions,
794 and the features considered in fuel consumption prediction models might be highly
795 correlated.

796 Vessel fuel consumption prediction models based on ML rely heavily on feature
797 engineering, which includes valid feature selection, new feature construction, feature
798 washing and encoding, and feature importance identification, and they therefore can be
799 viewed as a pure black box in the prediction step: all related features after processing
800 are input into a certain ML model or an ensemble of homogeneous or heterogeneous
801 ML models, and the result is generated as the output of the prediction model (Friedman
802 et al., 2001). Therefore, the problem of endogeneity is rarely discussed in the context
803 of ML-based prediction models. The problem of feature correlation can also be
804 addressed in the process of feature engineering, especially by feature selection through
805 filter-based (by considering the relevance of each feature and the prediction target),
806 wrapper-based (by considering the influence of each feature on the prediction
807 performance), and embedded methods (conducted by a specific prediction model)
808 (Harrington, 2012).

809 Endogeneity and feature correlation problems can heavily degrade the applicability
810 and performance of BBMs based on statistical modeling. For example, severe
811 multicollinearity increases the variance of the coefficient estimates by making them
812 very sensitive to minor changes in the model. Consequently, the coefficient estimates
813 are unstable and difficult to interpret, and the statistical power of the prediction model
814 is weakened. In addition, one of the most important OLS assumptions is that the errors
815 are uncorrelated with the dependent variables. If this assumption is violated, an OLS
816 model can produce biased and inconsistent parameter estimates, and the hypothesis
817 tests will produce misleading results. How to overcome the problems of
818 multicollinearity and endogeneity in BBMs based on statistical modeling is therefore

819 worthy of further investigation.

820

821 **5. Conclusion**

822 This paper reviews the literature on ship fuel consumption prediction and the ship
823 energy efficiency management and optimization models developed over the past 13
824 years. Major recent emission control regulations and ship energy efficiency indicators
825 are first reviewed. Next, strategies to improve ship energy efficiency recommended by
826 SEEMP and adopted by the shipping industry in practice are discussed. The features
827 and sources of the main datasets, namely ship operational data, mechanical data,
828 maintenance data, and sea and weather data used for ship fuel consumption prediction
829 models, are presented, and the prediction model construction procedure and the related
830 literature published in the past 13 years are reviewed. We divide fuel consumption
831 prediction models in the academic literature into three main categories: white-box
832 models (WBM), black-box models (BBM), and grey-box models (GBM) that
833 combine WBM and BBM. As there are only 84 related papers and reports, we list
834 their details and make a comprehensive comparison of ship performance monitoring
835 models, such as the data required for model calibration, their pros and cons, and their
836 applicable scenarios. We provide a detailed illustration of the approaches developed for
837 the three types of models from various perspectives. Technical reports, a typical type of
838 grey literature published by the government, academic institutions, and companies, are
839 also covered in this review to give a more comprehensive picture of the literature on
840 ship energy consumption management. Finally, current research challenges and
841 promising research questions are outlined.

842 This paper is the first comprehensive review of the literature on ship fuel
843 consumption prediction and management. Accurate fuel consumption prediction is the
844 foundation of improving vessel energy efficiency and thus reducing pollutant and GHG
845 emissions from the shipping industry. It is also a fundamental step toward zero-emission
846 shipping. The content of this review will be of interest to academic scholars, shipping
847 industry practitioners, and maritime policy makers. It can thus help to address one of
848 the most important and urgent contemporary issues faced by the IMO and the whole
849 maritime industry: achieving environmental sustainability in shipping.

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855 **Appendix A. List of acronyms used in the review**

| Abbreviation | Explanation | Abbreviation | Explanation |
|--------------|--|----------------|--|
| ACCESS | Arctic Climate Change, Economy and Society | LSTM | long short-term memory |
| AHP | analytical hierarchy process | MAE | mean absolute error |
| AIS | automatic identification system | MAPE | mean absolute percentage error |
| ANNs | artificial neural networks | MARPOL | The International Convention for the Prevention of Pollution from ship |
| ASLM | automated data logging & monitoring | MEPC | Marine Environment Protection Committee |
| BBM | black-box model | ML | machine learning |
| BC | black carbon | MLP | multi-layer perceptron |
| CFD | computational fluid dynamics | MLR | multiple linear regression |
| CII | carbon intensity indicator | MRV | Monitoring Reporting and Verification |
| CMEMS | Copernicus Marine Environment Monitoring Service | MSE | mean squared error |
| CO | carbon monoxide | NECAs | nitrogen emission control areas |
| DCS | data collection system | NMEFC | National Marine Environmental Forecasting Center |
| DSS | decision support system | NOAA | National Oceanic and Atmospheric Administration |
| DT | decision tree | NSGA | non-dominated sorting genetic algorithm |
| ECMWF | The European Centre for Medium-Range Weather Forecasts | OLS | ordinary least squares |
| EEDI | energy efficiency design index | PCA | principal component analysis |
| EEI | energy efficiency initiative | PLS | partial least-squares |
| EEOI | energy efficiency operation index | PM | particulate matters |
| EEXI | energy efficiency existing ship index | PSO | Particle swarm optimization |
| ENN | Elman neural network | R ² | coefficient of determination |
| EU | European Union | RBF | radial basis function |
| GBM | grey-box model | RF | random forest |
| GBR | gradient boosting regression | RMSE | root mean square error |
| GHG | greenhouse gas | RPM | revolutions per minute |
| GMM | Gaussian mixture model | SECAs | sulphur emission control areas |
| GPS | global positioning system | SEEMP | ship energy efficiency and management plan |
| GPs | Gaussian processes | SOM | self-organizing map |
| IMO | International Maritime Organization | STEAM | ship traffic emission assessment model |
| ITTC | International Towing Tank Conference | SVM | support vector machine |
| KNN | k-nearest neighbors | SVR | support vector regressor |
| LASSO | absolute shrinkage and selection operator | UNCTAD | United Nations Conference on Trade and Development |
| LR | linear regression | WBM | white-box model |
| | | WNI | Weathernews Inc. |

856 **Appendix B. A more detailed illustration of the prediction approaches**

857 **B.1 WBMs**

858 WBMs based on solid physical insights are the most classical and well-studied
859 stream of methods for ship fuel consumption prediction, as their structure is completely
860 known and the parameters are estimated through theoretical methods and towing tank
861 tests. As vessel fuel consumption estimation approaches based on WBMs are complex
862 and are largely based on physical theories, especially in the calculation of resistances
863 from multiple sources, their detailed presentation is outside the scope of this study.
864 Readers are referred to Schneekluth and Bertram (1998) and to Newman (2018) for
865 more information on calm-water resistance estimation, and to Salvesen (1978), Kwon
866 (2008), Panigrahi et al. (2012), and Cai et al. (2014) for a more detailed introduction to
867 added resistance calculation. In this review, we mainly discuss the different types of
868 resistance encountered by a ship when sailing, as shown in Table B.1.

Table B.1. Summary of common resistances encountered by a ship in sailing

| Source of resistance | Description | Influencing factors | Related literature/estimation methods |
|------------------------|--|---|--|
| Total hull resistance | A ship experiences a force acting opposite to its direction of motion as it moves through calm water. | Sailing speed, hull form (draft, beam, length, wetted surface area), and water temperature | The procedures proposed by Holtrop and Mennen (1982), by Kristensen and Lutzen (2012), and by ITTC (2008); The resistance curve from CFD computations, and the results of towing tank tests |
| Wave making resistance | As a ship moves through water, many wave systems are created and interact by adding or reducing each other's effects. | Ship hull shape, seakeeping characteristics of the ship, and sea spectrum | The procedures proposed by Salvesen (1978), by Kwon (2008), by Panigrahi et al. (2012), by ITTC (2014), and by Liu and Papanikolaou (2016) |
| Ocean currents | Ocean currents can be categorized into global and tidal current, and they can either accelerate or retard a ship depending on its direction. It is also the main cause of the difference between speed through water and speed over ground of a sailing ship. | Ship' heading and sailing speed over ground, current velocity and direction | The procedure proposed by Windeck (2013) and Cai et al. (2014) |
| Winds | Winds contribute to the creation of waves and act as a force on the vessel as wind resistance. | Ship's heading and sailing speed over ground, the cross-sectional area of a ship above the waterline, wind velocity and direction | The procedures proposed by Kristensen and Lutzen (2012), Windeck (2013), ITTC (2014); Wind tunnel test and the CFD simulation |
| Ocean waves | Ocean waves are caused by external factors such as wind and storm, which are different from the wave making resistance. They expend a ship's energy by increasing the wetted surface area of the hull, rolling, pitching, and heaving. | Ship' heading and sailing speed over ground, wave velocity and direction | The procedure proposed by ITTC (2014); Seakeeping experiments and simulations, slender-body theory, 3D panel methods, and the CFD simulation |
| Shallow waters | The resistance faced by a ship increases when sailing in shallow water, which is defined by the absolute water depth and the ship's draught, due to several factors: 1) shallow water increases the water flowing speed under the hull and thus increases the viscous resistance on the hull; 2) the faster moving water decreases the pressure under the hull and thus increase the wetted surface area; 3) wave making resistances increases in shallow water. | Water depth, ship hull conditions, and sailing speed | The procedure proposed by Schlichting (1934, 1979); The CFD simulation |
| Hull fouling | Hull fouling of a ship increases surface roughness and thus increases the viscous and friction resistances | Ship hull form and scale, and the hull fouling conditions | The procedure proposed by Foteinos et al. (2017), Oliveira et al. (2018), Song et al. (2020); The CFD simulation and towing tests |

871 After the total resistance faced by a ship is estimated, it is possible to calculate the
872 towing power to move the ship through water given a required sailing speed. The
873 towing power can be calculated as the product of the total resistance and the required
874 speed over water. The required nominal power of the propulsion engine can be
875 determined, and the fuel consumption of the ship can be estimated based on the power
876 requirement in different sailing activity phases (Zis et al., 2020).

877

878 **B.2 BBMs based on statistical modelling**

879 Given n ship operational records, the set of k influencing factors (called
880 predictor variables) is denoted by X , with one influencing factor denoted by x_i , and
881 the observed fuel consumption rate (called the response variable) is denoted by y . The
882 details of BBMs based on statistical modeling are summarized in Table B.2.

Table B.2. Summary of popular BBMs based on statistical modelling in ship fuel consumption monitoring

| Model | Basic ideas | Assumption | General format | Common parameter estimation approach |
|----------------------------------|---|---|--|---|
| Simple linear regression | Study the relationship between the $k = 1$ predictor variable denoted by x and the response variable y in a linear form. | <ul style="list-style-type: none"> The relationship between X and y is linear and additive. The errors are independent, normally distributed with mean zero and a constant variance. | $y = \beta_0 + \beta_1 x + \varepsilon$ | Least squares |
| Multiple linear regression | Study the relationship between the $k, k \geq 2$ predictor variables in set X and the response variable y in a linear form. | <ul style="list-style-type: none"> In multiple linear regression, the predictor variables are independent of each other. The relationship between X and y is linear or curvilinear. The errors are independent, normally distributed with mean zero and a constant variance. The predictor variables are independent of each other. | $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \varepsilon$ | |
| Polynomial regression | The nonlinear relationship between X and y is modelled as an n th degree polynomial in X . | <ul style="list-style-type: none"> The relationship between X and y is linear or curvilinear. The errors are independent, normally distributed with mean zero and a constant variance. The predictor variables are independent of each other. | $y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \dots + \beta_h X^h + \varepsilon$ | Least squares |
| Piecewise linear regression | X is partitioned into intervals with a separate line segment fitted to each interval. | The assumptions of simple linear regression | Suppose there are two breakpoints: x' and x'' . Then $y = \begin{cases} \beta_0' + \beta_1' x, & \text{for } x \leq x', \\ \beta_0'' + \beta_1'' x, & \text{for } x' < x \leq x'', \\ \beta_0''' + \beta_1''' x, & \text{for } x > x''. \end{cases}$ | LOESS (locally estimated scatterplot smoothing) estimation for breakpoints, and least squares for parameter estimation in the simple linear regression in each interval |
| Partial least squares regression | A linear regression model based on principal components regression to deal with the situation where the number of predictor variables is larger than the observations, or when there is multicollinearity among X . | \ | Please refer to 'Algorithm 3.3 <i>Partial Least Squares</i> ' in Section 3.5 of Hastie et al. (2017). | Please refer to Haenlein and Kaplan (2004). |

885 **B.3 BBMs based on ML**

886 Details of the BBMs based on ML techniques are summarized in Table B.3.

887 Table B.3. Summary of popular BBMs based on ML in ship fuel consumption monitoring

| Model | Basic idea | Sub classes used in the related literature | Pros | Cons |
|-------------------|--|--|---|--|
| ANN | A supervised model aims to extract linear combinations of the inputs as derived features, and then model the target as a nonlinear function of these features. | Back propagation neural networks, MLP, wavelet neural networks, deep learning models | <ul style="list-style-type: none"> • Good at modeling nonlinear data with a large number of inputs • A flexible model where several layers of neurons can be contained | <ul style="list-style-type: none"> • A pure black-box model lacking interpretability • Computationally expensive if many layers of neurons are contained • Easy to overfit the data, especially in case of limited data |
| LR | A supervised model assumes that the regression function is linear in the inputs. The inputs multiplied by some constants are added up to get the output. | OLS | <ul style="list-style-type: none"> • Easy to understand and implement • Computationally inexpensive • Able to provide an adequate and interpretable description of how the inputs affect the output • Able to outperform fancier nonlinear models especially with small numbers of training cases | <ul style="list-style-type: none"> • Too strong assumption regarding the linear relationship between the inputs and the output • Easy to be influenced by outliers and noises in data • The prediction ability on unseen data may not be satisfactory |
| Regularized LR | A type of restricted LR model based on shrinkage methods applied to the regression coefficients to reduce variance. | LASSO, ridge regression, elastic net regression | <ul style="list-style-type: none"> • Address the problem of multicollinearity in data when LR is applied • Reduce the problem of overfitting • Relative interpretability can be retained | <ul style="list-style-type: none"> • Weaken the interpretability of an LR model due to feature selection • Complicate the LR model by introducing more hyperparameters |
| Tree-based models | A supervised model successively splits the data into smaller segments until all the target variables are the same or until the dataset can no longer be split. | DT, RF, Adaboost DT, gradient boosting DT | <ul style="list-style-type: none"> • A single tree is easy to understand and interpret, which also allows for visual representation • Little data preprocessing is needed, and can even deal features with missing values • Feature selection happens automatically when a tree grows • Single DTs are easy to be ensemble • Different types of pruning methods can be applied to improve model generalization ability • Kernels can be used to effectively deal with high-dimensional data • Work very well when there is clear margin of | <ul style="list-style-type: none"> • A single DT with high variance is highly like to overfit the data • Lack smoothness in the prediction surface in regression setting |
| SVM/SVR | A supervised model aims to split the data using a decision boundary (hyperplane). The prediction results are regarded to be more | | <ul style="list-style-type: none"> • Kernels can be used to effectively deal with high-dimensional data • Work very well when there is clear margin of | <ul style="list-style-type: none"> • Easy to be influenced by noises in data, especially those causing overlapping • Not suitable for large datasets |

| | | | |
|--------------------------|---|---|---|
| | reliable if the data points are farther from the decision boundary. | separation between classes | |
| KNN | A supervised model aims to find the K most similar (closest) training samples of a certain test sample where the closeness is evaluated by distance (e.g., Euclidean distance, Cosine distance, and Manhattan distance) | <ul style="list-style-type: none"> As only a subset of training points (i.e., support vectors) is used in the decision function, it is memory efficient Very intuitive and easy to implement, as there is no 'training' step to build the model like the other ML models It can immediately adapt when new training data are collected | <ul style="list-style-type: none"> The speed of algorithm declines very fast as the number of samples/features grows Very sensitive to outliers A priori specification of the value of 'K' is needed |
| SOM | An unsupervised model which can be viewed as a constrained version of K-means clustering, in which the prototypes are encouraged to lie in a one- or two-dimensional manifold in the feature space | <ul style="list-style-type: none"> The data can be interpreted and understood to some extent Able to deal with large and complex datasets with a short amount of time | <ul style="list-style-type: none"> Large amount of data is needed to develop meaningful clusters Hard to deal with categorical data |
| GMM | An unsupervised and probabilistic model that assumes all the data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters. A GMM model is implemented by expectation-maximization (EM) algorithm | <ul style="list-style-type: none"> It is one of the fastest algorithms for learning mixed models It is more flexible in terms of cluster covariance allowing for soft classification | <ul style="list-style-type: none"> Might take a long time to run than other similar models such as K-means Based on the assumption of Gaussian distribution of the data points |
| Fuzzy c-means clustering | An unsupervised and soft clustering method where each data point can belong to more than one cluster with the basic idea similar to K-means | <ul style="list-style-type: none"> Allow for soft classification as the data points can belong to more than one cluster with a likelihood To deal with datasets with overlaps better | <ul style="list-style-type: none"> A priori specification of the value of 'c' is needed Sensitive to noises in data Euclidean distance measures can unequally weight underlying factors |

889 **B.4 GBMs**

890 Details of the GBMs developed in current literature are summarized in Table B.4.

891 **Table B.4. A more detailed description of the GBMs proposed in current literature**

| Literature | WBM used | BBM used | How to combine the WBM and BBM | Findings |
|------------------------|---|---|--|---|
| Leifsson et al. (2008) | A generic model based on physical principle | A feed forward ANN model | <ul style="list-style-type: none"> • A serial GBM: a set of input features is first fed into the WBM, and the estimated fuel flow rates and the vessel's speed through water are fed to the BBM to predict the real fuel flow rate and the vessel's speed through water • A parallel GBM: the set of input features to both the WBM and BBM is the same, with the WBM predicting the fuel flow rate and the vessel's speed through water and the BBM modeling the residual of the predicted and actual fuel flow rate and vessel speed | <ul style="list-style-type: none"> • The performance of the serial and parallel GBM is similar • There is a slight improvement of the GBMs developed over the WBM • The performance of the developed GBMs is similar to that of the BBM • The extrapolation ability and the ability to incorporate physical phenomena in model development are illustrated by model simulations |
| Coraddu et al. (2015) | A generic model based on the knowledge of physical processes | Regularized least squares | The a priori knowledge considered in the BWM is included in the BBM using Gaussian kernel in the regularization process | <ul style="list-style-type: none"> • GBM can incorporate the a priori knowledge of a WBM into a BBM while slightly improving the prediction accuracy of the BBM • Less data (about only half) is needed to construct a GBM compared to the BBM with the same performance |
| Lu et al. (2015) | A generic model with still water resistance modelled by Holtrop and Mennen's method and added resistance modelled by a modified Kwon's method | Speed-power curve estimated from ship operational records | The total power transmission efficiency from brake power of the main engine to the final effective power in the WBM is estimated from the speed-power curve calibrated from ship sea trial documents | Apart from the ability to predict ship fuel consumption under various conditions, the proposed GBM can also be used to examine the fouling effects of hull and propeller, and the engine degradation trends |
| Meng et al. (2016) | Two generic models considering various fuel consumption influencing factors such as sailing speed, displacement, wind, and wave | A least squares method and a sequential parameter estimation procedure for parameter estimation of the WBMs | <ul style="list-style-type: none"> • Parameters of the first nonlinear regression model considering speed and displacement are estimated by a linear least-square method • Parameters of the second nonlinear regression model are estimated by a sequential calibration procedure with the trust region algorithm | Besides data quality, the form of the regression model developed for fuel consumption prediction and the optimization algorithm used for coefficient calibration together govern the fitting performance |

| | | | | |
|-----------------------|---|---|---|--|
| Coraddu et al. (2017) | A WBM based on the knowledge of physical underlying processes | developed Regularized least squares, LASSO regression, and RF | <ul style="list-style-type: none"> • A Naive approach (N-GBM): the output of the WBM is used as a new feature of the BBM • An advanced approach (A-GBM): the regularization process in the BBM is changed to include some a priori information | <ul style="list-style-type: none"> • Both the N-GBM and A-GBM improve the BBM just by few percentages regarding model accuracy • WBM can help GBM to obtain higher accuracy with respect to BBM by using much less data • An onboard trim optimization method is proposed based on the fuel consumption prediction results of the GBMs • GBM can combine the high prediction accuracy of BBM while reducing the amount of data required and the total computation time for training the model by adding WBM components |
| Coraddu et al. (2018) | A WBM based on the knowledge of physical processes | Regularized least squares, LASSO regression, and RF | <ul style="list-style-type: none"> • An N-GBM: the output of the WBM is used as a new feature of the BBM • An A-GBM: the regularization process in the BBM is changed to include some a priori information | <ul style="list-style-type: none"> • The developed GA-based GBM can make full use of the collected data and estimate all parameters together in one-time run • The developed GA-based GBM can provide accurate fuel consumption estimation for all weather directions • The output of WBM is always among the seven most important features for the GBMs |
| Yang et al. (2019) | A procedure based on basic principles of ship propulsion | A generic model to estimate the unknown parameters of the WBM | Fuel consumption is first modelled considering wind and waves factors in a WBM. The problem of parameter estimation of the developed WBM is formulated as a least squares minimization model and solved by a generic algorithm based on real operational data. The developed model is called GA-based GBM | |

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