

1 **Puncture Failure Size Probability Distribution for CO₂ Pipelines¹**

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9

10 **Abstract**

11 The safe operation of pressurised CO₂ pipelines is key to the success of Carbon Capture
12 and Storage as a viable means for tackling global warming. As such, the prediction of
13 their puncture size in the event of pipeline failure and how it compares with that of
14 hydrocarbon pipelines are fundamentally important questions that must be resolved for
15 the subsequent pipe risk assessment and mitigation planning. The above requires the
16 use of sufficient failure statistics to derive the corresponding puncture size probability
17 distribution. Nevertheless, this presents a significant challenge for CO₂ pipelines given
18 their relatively small number currently in operation. In order to address such a challenge,
19 this paper presents the development and application of a robust statistical analytical

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20 technique for the confident prediction of the puncture failure size probability
21 distribution for CO₂ pipelines in the absence of sufficient failure statistics. The above
22 involves fitting statistical distributions to the historical puncture size failure data using
23 the Maximum Likelihood Estimator (MLE). The minimum acceptable sample size
24 sufficient for acquiring a reliable MLE is determined by calculating the mean squared
25 error of the MLE as a function of the data sample size. To improve the estimation
26 confidence given the scarcity of historical failure data, the bootstrapping method is
27 employed to obtain the 95% confidence interval of the MLE. The application of the
28 above technique to pressurised CO₂ and hydrocarbon pipelines indicates that as
29 compared to the latter, CO₂ pipelines are most likely to experience smaller puncture
30 size failures (e.g. ≤ 50 mm), thus resulting in smaller magnitude but more prolonged
31 releases. This directly impacts the preventive and emergency response planning
32 required especially in the case of buried CO₂ pipelines where small leaks can remain
33 undetected for long periods.

34

35 **Keywords:** Carbon Capture and Storage (CCS), CO₂ pipelines, High-pressure pipeline
36 safety, Pipeline failure probability distribution

37

38 **1. Introduction**

39 The intensive use of fossil fuels has resulted in excessive CO₂ emissions worldwide,
40 leading to global warming. Carbon Capture and Storage (CCS), involving the capture

41 of CO₂ from fossil fuel power plants and industrial operations such as cement and steel
42 making for the subsequent long-term geological storage, is widely recognised as a key
43 player in addressing the above issue. According to the Global CCS Institute (GCCSI,
44 2020), the amount of captured CO₂ needed for the energy sector to achieve net zero
45 emission will increase significantly by hundred-fold in the next three decades, reaching
46 around 5.6 Gt in 2050.

47

48 An essential part of the CCS chain involves the large-scale transportation of the
49 captured CO₂ to the storage site. High-pressure pipelines are widely considered or
50 already being employed as the most practical and economical transport option
51 (Mahgerefteh et al., 2012). In Norway, for example, Sleipner and Snøhvit projects each
52 inject ca. 1 million tonnes of CO₂ per year into saline aquifers (GCCSI, 2021; Ringrose,
53 2018) employing sub-sea pipelines. Several CCS projects are being developed
54 connecting onshore capture facilities to offshore geological storage locations. These
55 include Northern Lights (Norway), Porthos and Athos (Netherlands), ERVIA (Ireland)
56 and ACORN (UK). Many plan to commence operation well before 2030, operating at
57 the order of 1 million tonnes of captured CO₂ per year (Moe et al., 2020) using high-
58 pressure (80 to 110 bar) pipelines with diameters typically ranging from 100 to 600 mm.
59 Taking advantage of the economies of scale, many CCS projects comprise industrial
60 clusters, connecting several major emission sources using common pipeline
61 transportation network and storage infrastructures. Major examples in the UK include

62 Humber Zero, Net Zero Teesside and HyNet (GCCSI, 2021).

63

64 Given the above, the global demand for high-pressure CO₂ pipelines is expected to
65 increase substantially, with estimates ranging from 95,000 to 500,000 km in length by
66 2050 (IEA, 2010).

67

68 In the case of densely populated areas, such as most regions in Europe, pipeline routing
69 through or near densely populated areas may become inevitable (Cosham and Eiber,
70 2008; Koornneef et al., 2010; Vitali et al., 2022). This poses a risk in the event of an
71 accidental release. At CO₂ concentration of 10% v/v, an exposed individual would lapse
72 into unconsciousness in 1 min. At above 20% v/v, the gas is instantaneously fatal
73 (Pohanish and Greene, 1996). The ability of CO₂ to collect in depressions in the land,
74 in basements and in other low-lying areas such as valleys near the pipeline route,
75 presents a significant hazard if leaks continue undetected (Barrie et al., 2004).
76 Hydrocarbons such as natural gas will eventually ignite or explode in such areas if, and
77 when, conditions are right, but CO₂ can remain undetected for a very long time
78 (Mahgerefteh et al., 2008). Additionally, the captured CO₂ will be usually mixed with
79 potentially toxic impurities such as H₂S at low concentrations (ca. 50 ppm; Jensen et
80 al., 2014) whose natural dispersion might be impeded by the dense CO₂ vapour layer
81 close to the ground, further increasing the hazard.

82

83 There are several other hazards associated with the accidental release of CO₂. It can act
84 as an ignition source for nearby combustible materials due to friction induced static
85 discharge. In 1953, such an incident resulted in 29 fatalities (Barrie et al., 2004). CO₂
86 also reacts with water to form carbonic acid leading to the corrosion of carbon steel
87 pipelines (Nesic, 2012). Supercritical CO₂, widely considered to be the most
88 economical state for pipeline transportation is a powerful solvent giving possible toxic
89 contamination and sealing problems (Connolly and Cusco, 2007).

90

91 The accidental release of CO₂ following a pipeline puncture and the subsequent Joule
92 Thomson expansion cooling may result in the pipe wall temperature dropping below its
93 ductile to brittle transition temperature, giving rise to the risk of the initial puncture
94 transforming into a running brittle fracture (Mahgerefteh and Atti, 2006).

95

96 If the CO₂ temperature drops below its triple point (-56.6 °C at 0.518 MPa; Angus et
97 al., 1973) during its rapid expansion, for example during emergency depressurisation,
98 the resulting solid CO₂ may cause vent valve blockage. Finally, the unusually high
99 saturation pressure of CO₂ reduces the pipeline's resistance to long running ductile
100 fractures (Aursand et al., 2013).

101

102 Given the above hazards, along with the extensive projected use of CO₂ pipelines as
103 part of the CCS chain, it is clear the risks associated with their operation must be

104 reliably predicted in order to implement appropriate mitigation steps to reduce such
105 risks to as low as reasonably practicable.

106

107 An important part of the risk assessment process for pressurised pipelines involves
108 calculating the probability of loss of containment events. Such information is in turn
109 employed to estimate the individual and societal risk levels (Goodfellow et al., 2012)
110 forming the basis for appropriate control and emergency mitigation planning.

111

112 To this end, many studies (see for example Duncan and Wang, 2014; EGIG, 2018;
113 Lyons et al., 2020) have focused on collecting pipeline failure statistics and estimating
114 the corresponding frequencies for given failure modes such leak, puncture, or Full Bore
115 Rupture (FBR). Among these modes, the through-wall punctures, formed often as a
116 result of corrosion or external interference, are found to be by far the most frequent
117 (Lydell, 2000). Given that the puncture size directly affects the failure consequences
118 and hence the subsequent determination of the appropriate control and mitigation
119 measures, a reliable technique for estimating the puncture size failure frequency must
120 be established. The efficacy of such techniques (see for example Duncan and Wang,
121 2014) is largely dependent on ensuring that a ‘sufficiently’ large number of real incident
122 data points are available to be representative. This is however problematic in the case
123 of CO₂ pipelines given their relatively low number. As of 2021, there were only ca.
124 8000 km of CO₂ pipelines; almost entirely for enhanced oil recovery and mostly located

125 in the United States (IEA, 2021). This compares with over 4.6 million km of pressurised
126 hydrocarbon pipelines crossing the globe (CIA, 2021).

127

128 Accordingly, given the above, it is imperative that i) a sufficiently large sample size is
129 taken to determine the generic puncture frequency and ii) a rigorous methodology is
130 employed to determine the corresponding puncture size probability distribution.
131 Another important issue to address is how such a probability distribution for CO₂
132 pipelines compares to that of hydrocarbon pipelines.

133

134 Several methodologies to determine the generic puncture frequency for CO₂ pipelines
135 have been reported in the open literature; the most popular being those based on using
136 natural gas pipelines data as a proxy. CO₂ and natural gas pipelines are similar in their
137 construction materials, fabrication techniques and failure mechanisms (Barrie et al.,
138 2005; Duncan and Wang, 2014).

139

140 To obtain the puncture size probability distribution, a histogram using existing pipeline
141 failure data is constructed by first segmenting the entire range of puncture sizes into a
142 series of intervals (bins) and then counting how many values fall into each bin. Duncan
143 and Wang (2014) employed the above technique to approximate the puncture diameter
144 occurrence probability distribution for CO₂ pipelines using the incident data from the
145 Pipeline and Hazardous Material Safety Administration (PHMSA) database. In their

146 study, puncture diameters ranging between 0 and 380 mm were divided into 6 bins. The
147 analysis showed that the most prevailing puncture diameters were between 50 to 100
148 mm, whereas medium-sized punctures (150 to 200 mm) had the lowest probability of
149 occurrence.

150

151 The resulting histogram can be parameterised and extended to a smooth probability
152 distribution function. The validity of such functions is largely dependent on the size of
153 the sample employed to derive the underlying histograms. Despite their usefulness,
154 methods to reliably handle ‘small’ samples sizes are not well established.

155

156 Given the above limitation, in most risk assessment studies for pressurised pipelines,
157 the puncture size is usually assumed to be a discrete variable as opposed to continuous
158 variable as is the case in reality. In many of these studies only a limited number of
159 representative puncture sizes are used to cover the whole size spectrum and as a result
160 the predicted failure risk levels can only present rough estimations, rendering the
161 subsequent strategies for risk mitigation uncertain.

162

163 Medina et al. (2012), for example used only two representative puncture sizes of 10 and
164 40 mm and FBR to calculate the expected cost of pipeline failure consequences for a
165 risk-based optimisation of emergency shut down valve spacing for on-shore pipelines.

166 Rusin and Stolecka (2015) on the other hand, used the same approach to calculate the

167 frequency of the various failure modes for CO₂ pipelines for optimising inline
168 emergency isolation valve spacing. The through-wall failure was simply assumed to be
169 either puncture or rupture with the ratio of puncture/rupture occurrence probability taken
170 as 9:1.

171

172 Considering the above limitations, this paper presents the development of a statistical
173 analytical technique for determining reliable puncture failure size probability
174 distribution for pressurised CO₂ pipelines using available historical failure data. The
175 above involves a) using the Maximum Likelihood Estimator (MLE) to fit statistical
176 distribution functions to historical failure data for estimating the unknown fitting
177 parameters that characterise these statistical distribution functions, and b) performing a
178 Monte Carlo simulation test to assess the quality (statistical significance) of the MLE
179 based on the data sample size. When the MLE 'quality' is low, a bootstrapping method,
180 which can artificially inflate the sample size, is employed to calculate the MLE
181 confidence intervals.

182

183 The paper proceeds as follows. Section 2 commences with a brief introduction, filtering
184 and processing of the pipelines failure historical data used for this study, followed by
185 the description of the methodology employed to obtain a credible probability
186 distribution of the puncture size. In Section 3, the 'quality' of MLE is first evaluated
187 based on Monte Carlo simulation tests involving calculating the corresponding mean

188 squared error of the MLE. Next, puncture size probability distributions derived from
189 the filtered and processed historical failure data alongside the recommended fitting
190 parameters for CO₂ pipelines are presented and compared against those for natural gas
191 and crude oil pipelines. Conclusions and suggestions for future work are presented in
192 Section 4.

193

194 **2. Methodology**

195 **2.1 Data review**

196 Several bodies collecting and publishing the failure statistics for CO₂ and hydrocarbon
197 pipelines exist (see for example Concawe, 2011; EGIG, 2018; PHMSA, 2020), but few
198 provide detailed information on the size of through-wall puncture. This study adopts
199 the Pipeline and Hazardous Material Safety Administration (PHMSA) database where
200 such information is available. The puncture size, assumed to be oval, is expressed in
201 terms of Equivalent Puncture Diameter (EPD) given by Koch (2008):

202

$$202 \quad \text{EPD} = 1.55 \frac{A^{0.625}}{P^{0.25}} \quad (1)$$

203

204 where A and P are respectively the oval puncture cross-section area and perimeter
205 calculated based on the circumferential and longitudinal lengths of the puncture
206 recorded in the database.

207

208 The PHMSA database holds data on the loss of containment incidents for federal and
209 state-regulated CO₂ and hydrocarbon pipelines operating in the US since 1970s. Whilst
210 the focus is on CO₂ pipelines, this study also examines natural gas and crude oil
211 pipelines punctures size failure probability distributions for comparison purposes as
212 compared to those for CO₂ pipelines.

213

214 In much of the databases spanning over 50 years, the records are of varying quality and
215 level of detail for the various incidents. So, it is necessary to review and filter such data
216 before use. The PHMSA updates its reporting criteria for pipeline incidents every 10 to
217 20 years for the past 5 decades. This study employs the data since 2010, when the
218 reporting criteria were last updated. The raw data are publicly available from the
219 PHMSA database (PHMSA, 2020). From 2010 to present, 6495 loss of containment
220 incidents have been recorded but not all are relevant for this study for the following
221 reasons.

222

223 First, a large proportion of the loss of containment incidents are reported for leaks from
224 pipeline auxiliary equipment (e.g. relief valves, compressors, connectors) rather than
225 those from the pipeline itself. Second, the puncture size information is reported for
226 selected incidents only. Taking account of the above limitations leads to a remaining
227 total of 1906 useful EPD data points employed in the current work.

228

229 **2.2 Statistical distribution models**

230 The probability distribution of a continuous variable is often expressed as the
231 Cumulative Distribution Function (CDF). In this study, we employ the Weibull and
232 lognormal distributions as the potential statistical functions to represent the CDF of the
233 puncture size. Both functions are widely used in reliability engineering for the
234 assessment of pipeline failures (see for example Chaplin, 2015; Goodfellow et al.,
235 2012). Other possible distributions such as the gamma and exponential distributions
236 have been used to a much lesser extent and hence are not considered here. The CDF of
237 the Weibull distribution takes the form:

238

$$F(x; \alpha, \beta) = 1 - e^{-\left(\frac{x}{\alpha}\right)^\beta} \quad x \geq 0 \quad (2)$$

239

240 where α and β are respectively the scale and shape parameters of the Weibull
241 distribution. x and F respectively represent the random variable and CDF.

242

243 The CDF of the lognormal distribution is given by:

244

$$F(x; \mu, \sigma) = \frac{1}{2} \operatorname{erfc} \left(-\frac{\ln x - \mu}{\sigma\sqrt{2}} \right) \quad (3)$$

245

246 where μ and σ are respectively the mean and standard deviation of the variable, x .
247 erfc , on the other hand, refers to the complementary error function which is defined as:

248

$$\operatorname{erfc}(x) = -\frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt \quad (4)$$

249

250 Typical examples of Weibull and lognormal CDFs are respectively shown in Figures 1

251 and 2.

252

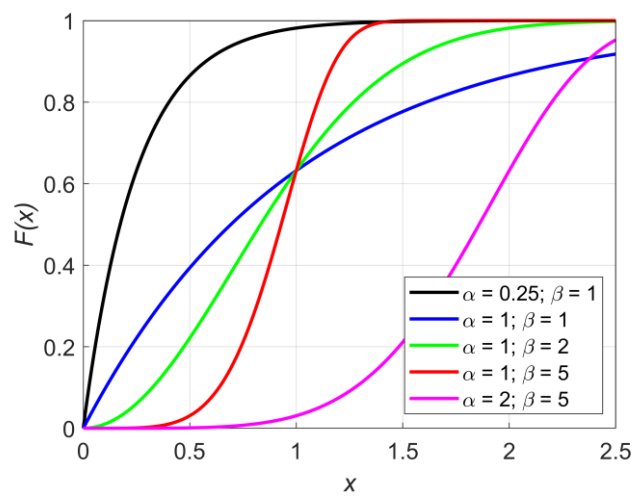


Figure 1. Typical examples of Weibull CDF showing the variation of the CDF against the random variable.

253

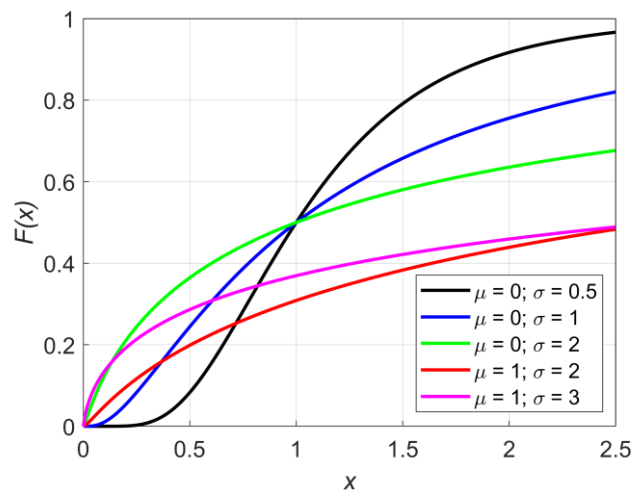


Figure 2. Typical examples of lognormal CDF showing the variation of the CDF against the random variable.

254

255 **2.3 Distribution fitting**

256 The selected puncture size sample data from the PHMSA database (PHMSA, 2020)
257 described in Section 2.1 are fitted to both Weibull and lognormal distributions described
258 in Section 2.2 to acquire the fitting parameters. The Maximum Likelihood Estimator
259 (MLE) is used for this purpose to best characterise the probability distribution of the
260 sample data. The MLE is a widely adopted method for estimating the parameters of an
261 assumed probability distribution for a given set of observed data, by finding the
262 parameter values that will most likely generate the observed data. Mathematically, the
263 MLE can be defined as:

264

$$\hat{\theta} \stackrel{\text{def}}{=} \underset{\theta}{\operatorname{argmax}} L(\theta; X) \quad (5)$$

265

266 where θ is the unknown true parameter characterising the assumed probability
267 distribution and $\hat{\theta}$ refers to the MLE of θ . X denotes the data sample that contains
268 n observations (x_1, x_2, \dots, x_n) of the data population. L , on the other hand, is called
269 the likelihood function which calculates the product of the probability densities of each
270 value in X and is mathematically expressed as:

271

$$L(\theta; X) = \prod_{i=1}^n f(x_i; \theta) \quad (6)$$

272

273 In essence, the process of maximum likelihood estimation is to find the estimator that
274 maximises the likelihood function, Eq. (6).

275

276 According to Ginos (2009), the MLE is among the most dependable statistical
277 estimators for parameter estimation. Some appealing features of the MLE include it
278 being consistent, efficient and asymptotically normal (Long and Freese, 2006).
279 However, these properties have been only proven to hold as the number of data being
280 used in the estimation process approaches infinity (Ji, 2020). This is an issue in the case
281 of CO₂ pipeline failures, where relatively small sample sizes are available thus limiting
282 the applicability of MLE for the present study. Given this, whether the sample size can
283 suffice for a high-quality MLE needs to be determined.

284

285 Eliason (1993) suggested that a sample size of more than 60 is usually large enough for
286 estimating no more than 5 parameters using MLE. Long and Freese (2006) on the other
287 hand, suggested that it is risky to use MLE with sample sizes smaller than 100, while
288 sample sizes over 500 seem adequate. However, most of the literature dealing with
289 MLE do not provide specific sample size guidelines. In general, there are no rules of
290 thumb, and the appropriate sizes heavily depend on the question at hand.

291

292 In this study, to determine the appropriate sample size, the quality of MLE is assessed
293 by examining the mean squared error which is the averaged square difference between
294 the estimated and the actual values (Ryan, 2007). The use of mean squared error is very
295 common in the study of MLE (see for example Ginos, 2009; Nielsen, 2011), and it is
296 considered an excellent general-purpose error metric for numerical predictions (Neill
297 and Hashemi, 2018). Mathematically, the mean squared error of the MLE, $\hat{\theta}$ to an
298 unknown parameter, θ is defined as the addition of the variance and bias squared:

299

$$\text{MSE}(\hat{\theta}) = \text{Variance}(\hat{\theta}) + \text{Bias}^2(\hat{\theta}, \theta) \quad (7)$$

300

301 where MSE denotes the mean squared error and the variance and bias are respectively
302 given by:

303

$$\text{Variance}(\hat{\theta}) = E \left[(\hat{\theta} - E[\hat{\theta}])^2 \right] \quad (8)$$

304

$$\text{Bias}(\hat{\theta}, \theta) = E[\hat{\theta}] - \theta \quad (9)$$

305

306 where E denotes the expected value.

307

308 In the present study, we perform Monte Carlo simulation tests to investigate the quality
309 of MLE based on computing the mean squared errors for different sample sizes. The

310 tests involve, i) determining the Weibull and lognormal distribution parameters and
311 sample sizes being tested; ii) for a given sample size, N , calculating the corresponding
312 MLE using N data randomly sampled from the Weibull and lognormal distributions
313 determined in step i); iii) repeating step ii) for a sufficiently large number of times
314 (typically over 1,000 times) and computing the corresponding mean squared error.

315

316 **2.4 Determination of probability distribution**

317 Following the above Monte Carlo simulation tests, the sample size sufficing for a high-
318 quality Maximum Likelihood Estimator (MLE) is obtained. For sufficiently large
319 samples, the resulting high-quality MLE can be used with confidence to characterise
320 the probability distribution of the puncture size. However, given that two distribution
321 models (i.e. Weibull and lognormal) are employed in this work, the one-sample
322 Kolmogorov-Smirnov (K-S) goodness-of-fit test (Kolmogorov, 1933) involving
323 comparing the sample data with the predictions of both models is further employed to
324 determine which model provides a statistically better fit representing the sample
325 population. The test process involves, i) specifying a null hypothesis; ii) computing the
326 K-S statistic and critical value at a chosen significance level and iii) accepting the null
327 hypothesis if the K-S statistic is smaller than the critical value or rejecting the null
328 hypothesis if otherwise.

329

330 The K-S statistic is computed based on quantifying the greatest vertical distance

331 between the empirical CDF (the sample data) and the CDF of the reference distribution,
332 that is (Conover, 1999):

333

$$D = \sup_x |F_n(x) - F(x)| \quad (10)$$

334

335 where D denotes the K-S statistic. \sup stands for supremum which means the
336 greatest. $F_n(x)$, on the other hand, is the empirical CDF for n ordered sample data
337 points $(x_1 < x_2 < \dots < x_n)$, which is a step function jumping up by $1/n$ at each of the n
338 data points.

339

340 The critical value, on the other hand, is usually determined using a K-S test critical
341 value table, which can be easily obtained from several literature, such as Massey Jr
342 (1951). In particular, for $n \geq 40$, the critical value is computed based on a specific
343 equation depending on the chosen significance level. In the current study, a significance
344 level of 0.01 is chosen for the K-S test and the corresponding equation for calculating
345 the critical value is given by:

346

$$\text{Critical value} = \frac{1.63}{\sqrt{n}} \quad (11)$$

347

348 To deal with the small sample sizes, the bootstrapping method, which can artificially
349 inflate the sample size by random sampling with replacement is employed to calculate

350 the MLE confidence interval. The methodology was first introduced by Efron (1979)
351 for making inferences from data without making strong distributional assumptions, and
352 was later employed by many authors for enhancing the confidence in using MLE for
353 small samples (see for example Tsagkanos, 2008; Wei and Li, 2019). Unlike the case
354 for sufficiently large samples where a single value of the MLE is acquired, the
355 bootstrapping process produces a range of values where the MLE is expected to lie. It
356 should be noted that for small samples which may not be statistically representative of
357 the population being considered, the aforementioned K-S test cannot accurately reflect
358 the goodness-of-fit between the model predictions and the data. Given this, the
359 probability distributions derived based on either Weibull or lognormal models are
360 considered statistically valid for the purpose of this study if the bootstrapping method
361 is employed.

362

363 The bootstrapping process comprises the following steps. First, the bootstrap samples
364 are generated. This involves resampling the original data sample with replacement to
365 create a resampled dataset (also known as a bootstrap sample) that have the same size
366 as the original sample. Second, the MLE of each bootstrap sample is computed based
367 on Eqs. (5) and (6). Third, the above first and second steps are repeated for a sufficiently
368 large number of times to obtain a distribution for the possible values of the MLE. Fourth,
369 the MLE confidence interval is calculated based on the distribution obtained from the
370 third step. Several options including the normal approximation method, percentile

371 method, bias-corrected method etc. can be adopted to calculate the MLE confidence
372 interval. In this study, the percentile method, which is considered suitable for small
373 samples (Wei and Li, 2019), is employed. The MLE confidence interval based on the
374 percentile method can be given as follows (Jung et al., 2019):

375

$$[\hat{\theta}_{\text{lower limit}}, \hat{\theta}_{\text{upper limit}}] = [\hat{\theta}_j, \hat{\theta}_k] \quad (12)$$

376

377 where j and k respectively refer to the j th and k th quantiles of the collection of
378 the possible MLE values ordered from lowest to highest. Here, j and k are
379 respectively:

380

$$j = \frac{s}{2} \times B \quad (13)$$

381

$$k = \left(1 - \frac{s}{2}\right) \times B \quad (14)$$

382

383 where s is the level of significance and B is the number of bootstrap samples
384 generated in the bootstrapping process.

385

386 **3. Results and discussion**

387 **3.1 Monte Carlo simulation setup**

388 In this section, four tests following the Monte Carlo simulation steps described in

389 Section 2.3 are performed. Based on investigating several assumed distributions, tests
390 1 to 4 respectively examine the MLE quality as a function of sample size for Weibull
391 scale parameter, Weibull shape parameter, lognormal mean, and lognormal standard
392 deviation. Each test examines three pairs of parameters varying the value of the tested
393 parameter whereas fixing that of the non-tested parameter. The corresponding
394 parameter values for tests 1 to 4 are given in Table 1. The investigated values are
395 selected based on the fact that small pipeline punctures are far more frequent than large
396 ruptures (Lydell, 2000).

397

398 For each pair of examined parameter values, the mean squared error of the MLE is
399 calculated for a wide range of sample sizes, $N = 10, 20, \dots, 100, 200, \dots, 500$. The
400 following details how the Monte Carlo simulation steps described in Section 2.3 are
401 implemented for a given N .

402

403 First, N data are randomly selected from the distribution characterised by the
404 examined value pair using a random value generator. Second, using the selected N
405 data, the MLE to the examined parameter is computed based on Eqs. (5) and (6). Third,
406 in order to accurately approximate the mean squared error of the examined MLE,
407 10,000 MLEs to the examined parameters are generated by repeating the above steps.
408 The mean squared error of these MLEs is then computed based on Eq. (7).

409

410 The above process is executed for each investigated sample size. The resulting mean
 411 squared errors are then plotted against the corresponding N . As such, a figure showing
 412 the variation of the MLE mean squared error as a function of the sample size is obtained.
 413

Table 1. Summary of the Weibull and lognormal distribution parameter values examined in the four Monte Carlo simulation tests for investigating the quality of MLE based on the sample size.

Test no.	Tested parameter	Non-tested parameter
1	Weibull scale parameter, $\alpha=1, 1.5, 2$	Weibull shape parameter, $\beta=2$
2	Weibull shape parameter, $\beta=1.5, 2, 2.5$	Weibull scale parameter, $\alpha=1$
3	Lognormal mean, $\mu=0, 0.5, 1$	Lognormal standard deviation, $\sigma=1$
4	Lognormal standard deviation, $\sigma=1, 1.5, 2$	Lognormal mean, $\mu= 0.25$

414

415 3.2 Monte Carlo simulation results

416 Figure 3 presents the simulation results for tests 1 to 4 described in Table 1, respectively
 417 showing the variations of the MLE mean squared error as a function of the sample size,
 418 N for the Weibull scale parameter, Weibull shape parameter, lognormal mean, and
 419 lognormal standard deviation. Figure 4 on the other hand shows the same results plotted
 420 in logarithmic scale to aid visualisation.

421

422 As may be observed from both Figures 3 and 4, three distinct regions describing the

423 behaviour of the mean squared error variation with sample size may be identified.

424 Initially, when the sample size is smaller than ca. 100, the mean squared error drops

425 significantly indicating that the MLE quality is highly sensitive to the sample size and

426 therefore the MLE should be used with caution in this region. At sample sizes between

427 100 to 200, the rate of decrease in mean squared error slows down, indicating that using

428 samples with more than 100 data points will substantially improve the MLE quality. In

429 the third region where the sample size surpasses 200, the rate of decrease in mean

430 squared error further slows down, meaning that further increasing the sample size

431 provides limited improvement in the MLE quality.

432

433 The above indicates that the minimum acceptable sample size sufficing for acquiring a

434 reliable MLE is at least 100 while with ideally more than 200 data points, sufficiently

435 reliable statistical representation of the puncture size data population may be obtained.

436

437 Figure 4 provides a closer look at the mean square error for large sample sizes. Here,

438 for all tested parameters, the mean squared error drops almost linearly when the sample

439 size is increased from 100 to 200, suggesting minimal marginal increase in the MLE

440 quality. When the sample size exceeds 200, the mean squared error tend to converge

441 between the 0.001 to 0.01 range, again indicating that further increasing the sample size

442 provides limited improvement in the MLE quality. This further strengthens the
 443 conclusion drawn from Figure 3 that 100 is the minimum acceptable sample size
 444 sufficing for acquiring a reliable MLE while more than 200 is ideal.
 445

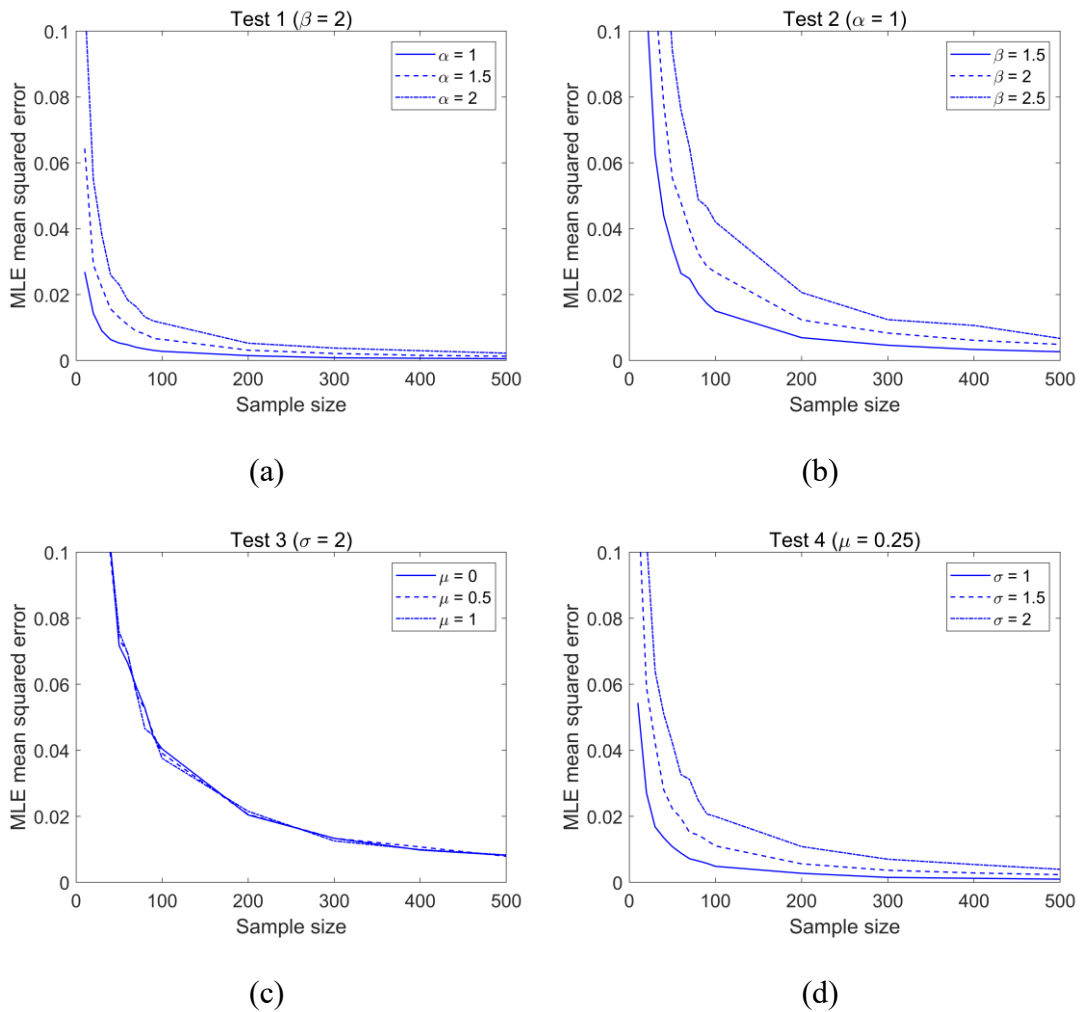


Figure 3. Simulation results for tests 1 to 4 described in Table 1 showing the variations of the MLE mean squared error as a function of the sample size, N for the Weibull scale parameter (a), Weibull shape parameter (b), lognormal mean (c), and lognormal standard deviation (d).

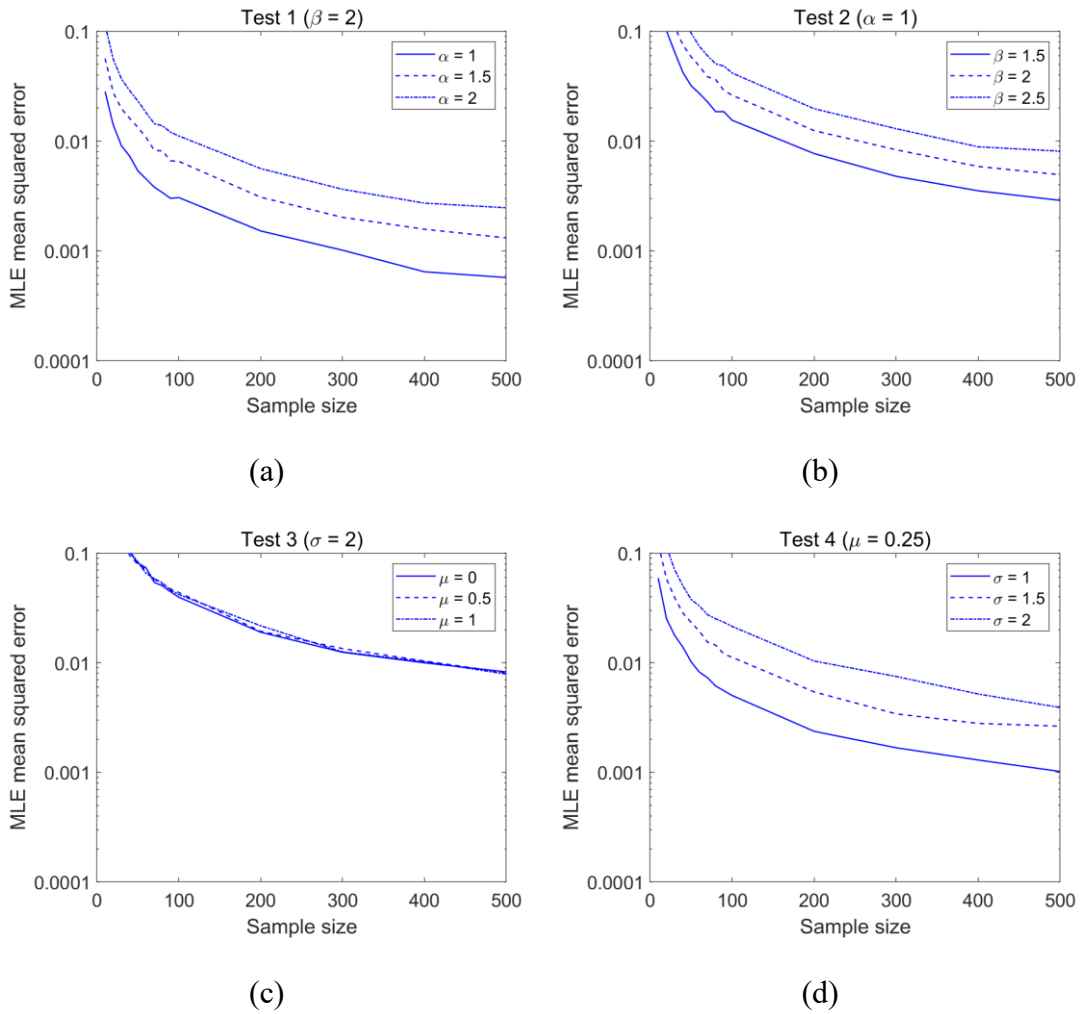


Figure 4. Simulation results for tests 1 to 4 presented in Table 1 showing the logarithmic variations of the MLE mean squared error as a function of the sample size, N for the Weibull scale parameter (a), Weibull shape parameter (b), lognormal mean (c), and lognormal standard deviation (d).

447

448 3.3 Probability distribution results

449 The following section presents the application of the methodology presented in Section
 450 2 to obtain the probability distribution of the equivalent puncture diameter data from
 451 the PHMSA database (PHMSA, 2020). Here, 1456 data points (see Section 2.1) are

452 divided into three pipeline inventories, covering natural gas, crude oil and CO₂. The
 453 corresponding data counts, and parameter estimation methods determined based on the
 454 results of the Monte Carlo simulation tests (see Section 3.2) are summarised in Table 2.
 455

Table 2. Failure counts summary from the PHMSA database and parameter estimation methods employed for deriving the probability distributions of the equivalent puncture diameter for natural gas, crude oil and CO₂ pipelines.

Pipe fluid	Failure count	Parameter estimation method
Natural gas	1072	MLE with K-S test
Crude oil	816	MLE with K-S test
CO ₂	18	MLE with bootstrapping

456
 457 As can be observed from Table 2, the failure counts for both natural gas and crude oil
 458 pipelines exceed the minimum acceptable sample size (i.e. 100) for acquiring a reliable
 459 MLE, as concluded in Section 3.2. As a result, their puncture size probability
 460 distribution parameters can be estimated confidently using MLE and therefore a further
 461 bootstrapping step is not necessary. For CO₂ pipelines on the other hand, the
 462 corresponding failure count of 18 is far less than the 100 threshold and therefore the
 463 bootstrapping technique is employed to enhance the MLE confidence.

464

465 **3.3.1 Natural gas pipelines**

466 Figure 5 presents the comparison of the variation of the cumulative failure probability

467 versus equivalent puncture diameter for the field data against the predictions by the
468 Weibull and lognormal Cumulative Distribution Functions (CDFs) for natural gas
469 pipelines. The parameters for the Weibull and lognormal CDFs and the corresponding
470 K-S test results including the null hypotheses, K-S test statistics and critical values are
471 summarised in Table 3. The critical value used for accepting or rejecting the null
472 hypothesis in the K-S test (see Section 2.4) is calculated using Eq. (11).
473

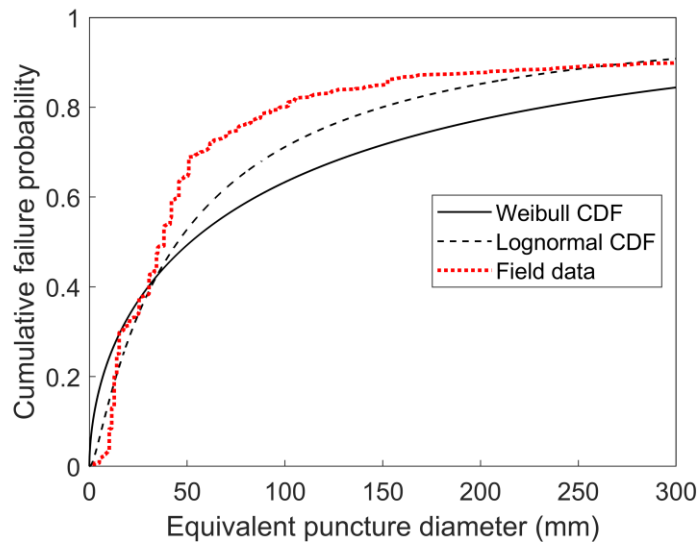


Figure 5. Comparison of the variation of the cumulative failure probability versus equivalent puncture diameter for the field data (data points) against the predictions by the Weibull (solid line) and lognormal (dashed line) CDFs for natural gas pipelines.

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Table 3. Summary of the parameters of the predicted Weibull and lognormal CDFs and the corresponding K-S test results including the null hypotheses, K-S test statistics and critical values for natural gas pipelines.

Distribution	Parameter	Value
Weibull	Scale parameter, α	99.475
	Shape parameter, β	0.562
	Null hypothesis	“The data are from a Weibull distribution.”
	K-S test statistic	0.213
	Critical value	0.053
Lognormal	Mean, μ	3.812
	Standard deviation, σ	1.422
	Null hypothesis	“The data are from a lognormal distribution.”
	K-S test statistic	0.173
	Critical value	0.053

477

478 The K-S test results in Table 3 show that the K-S statistics for both Weibull and
479 lognormal CDFs are greater than their critical values, meaning the null hypotheses are
480 rejected (see Section 2.4). This indicates that both CDFs are not statistically good fits
481 to the field data. However, visually, the lognormal CDF appears to be a better fit overall
482 as it more closely mirrors the recorded data throughout. The lognormal CDF can hence
483 be recommended to represent the probability distribution of the equivalent puncture
484 diameter for natural gas pipelines, with the lognormal mean and standard deviation

485 respectively being 3.812 and 1.422.

486

487 As can be observed from the recommended lognormal CDF in Figure 5, as the
488 equivalent puncture diameter increases, the rate of increase in the cumulative failure
489 probability generally slows down. The steepest rise is observed when the equivalent
490 puncture diameter increases from 0 to ca. 100 mm, meaning that relatively smaller
491 punctures have a higher probability of occurrence for natural gas pipeline failures as
492 compared to catastrophic ruptures. Specifically, around 70% of such failures are in the
493 form of punctures smaller than 100 mm. On the other hand, punctures smaller than 50
494 mm account for ca. 45% of the failures while ruptures which have an equivalent
495 puncture diameter equal to or over 150 mm, only accounts for 20%.

496

497 **3.3.2 Crude oil pipelines**

498 Figure 6 shows the comparison of the variation of the cumulative failure probability
499 versus equivalent puncture diameter for the field data against the predictions by Weibull
500 and lognormal CDFs for crude oil pipelines. The parameters of the Weibull and
501 lognormal CDFs and the corresponding K-S test results including the null hypotheses,
502 K-S test statistics and critical values are summarised in Table 4. The critical value used
503 for accepting or rejecting the null hypothesis in the K-S test (see Section 2.4) is
504 calculated using Eq. (11).

505

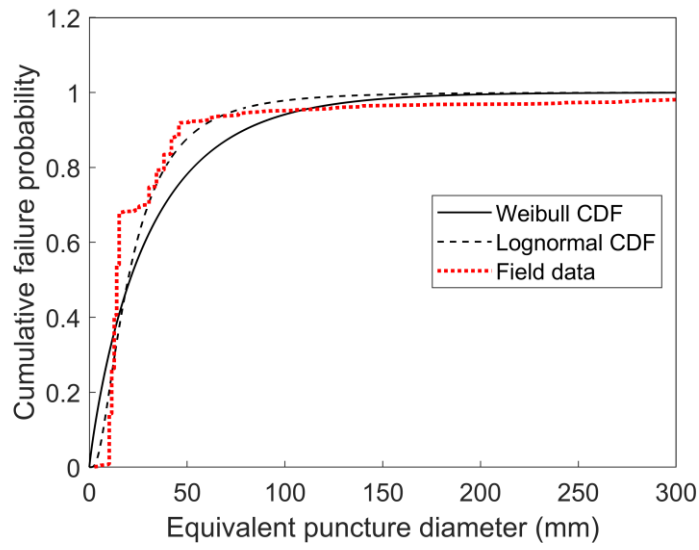


Figure 6. Comparison of the variation of the cumulative failure probability versus equivalent puncture diameter for the field data (data points) against the predictions by Weibull (solid line) and lognormal (dashed line) CDFs for crude oil pipelines.

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Table 4. Summary of the parameters of the predicted Weibull and lognormal CDFs and the corresponding K-S test results including the null hypotheses, K-S test statistics and critical values for crude oil pipelines.

Distribution	Parameter	Value
Weibull	Scale parameter, α	0.11831.259
	Shape parameter, β	0.897
	Null hypothesis	“The data are from a Weibull distribution.”
	K-S test statistic	0.284
	Critical value	0.073
Lognormal	Mean, μ	2.984
	Standard deviation, σ	0.801
	Null hypothesis	“The data are from a lognormal distribution.”
	K-S test statistic	0.065
	Critical value	0.073

517

518 As can be seen from Figure 6, in general both Weibull and lognormal data show good
519 agreement with the field data. However, the K-S test results in Table 4 suggest
520 differently. The K-S statistic for the test of Weibull distribution is greater than the
521 critical value while that for the test of lognormal distribution is otherwise smaller. This
522 means that the null hypothesis for Weibull distribution is rejected while that for
523 lognormal distribution can be accepted. The above indicates that the data are more
524 likely to be drawn from the lognormal CDF. Visually, the lognormal CDF more closely

525 follows the field data covering the most prevalent pipeline failures (equivalent puncture
526 diameter < 100 mm, accounting for ca. 90% of the failures), whence best represents the
527 probability distribution of the equivalent puncture diameter for crude oil pipelines, with
528 the lognormal mean and standard deviation respectively being 2.984 and 0.801.

529

530 Comparing to the recommended CDF for natural gas pipelines (see Figure 5), it is
531 obvious that the equivalent puncture diameter is more concentrated at smaller values
532 (< 100 mm) in the corresponding CDF for crude oil pipelines, indicating that small
533 punctures are more frequent in crude oil pipelines. This may be attributed to the fact
534 that in the PHMSA database records, more natural gas pipeline failures are initiated by
535 mechanisms (e.g. excavations and natural forces) that are more likely to result in
536 catastrophic failures.

537

538 **3.3.3 CO₂ pipelines**

539 In the case of CO₂ pipelines, only 18 equivalent puncture diameter data (see Table 2)
540 are available; far less than the 100 sample size threshold required for obtaining a
541 reliable Maximum Likelihood Estimator (MLE) (see Section 3.2). The bootstrapping
542 method described in Section 2.4 is therefore employed to calculate the MLE confidence
543 interval. To specify, the bootstrapping process which involves creating resampled
544 datasets that have the same size as the original one, is first implemented to generate a
545 number of bootstrap samples for CO₂ pipelines, each containing 18 equivalent puncture

546 diameter data points. The resampling is performed with replacement and thus the
547 resulting bootstrap samples may or may not be identical to the original dataset. To
548 ensure that a sufficiently large number of the possible bootstrap samples are accounted
549 for, 20,000 iterations of the resampling of the original dataset are carried out,
550 corresponding to 20,000 bootstrap samples. Once all the bootstrap samples are obtained,
551 the data points for each bootstrap sample are fitted to both Weibull and lognormal
552 distributions following the distribution fitting process based on Eqs. (5) and (6). The
553 resulting 20,000 MLEs are then segmented into 50 equi-distance bins by their values to
554 generate a distribution of the possible values of the MLE. Using the distribution, the
555 corresponding confidence interval can then be calculated based on Eq. (12). The chosen
556 level of significance, α for obtaining the confidence interval (see Eqs. (13) and (14))
557 is 0.05, corresponding to 95% confidence.

558

559 Figure 7 demonstrates an example bootstrapping result for the MLE of the lognormal
560 mean, μ . As may be observed, the possible values of MLE are normally distributed,
561 varying from ca. 2.5 to 3.5. The arithmetic mean of the MLE (i.e. the mean of the
562 resulting normal distribution) is 2.927. The lower and upper bounds of the 95%
563 confidence interval covering the majority of the possible values are respectively 2.659
564 and 3.227. Similar distribution of the MLE is also observed for the Weibull scale &
565 shape parameters and the lognormal standard deviation. The corresponding arithmetic
566 means and 95% confidence intervals of the MLEs for these investigated parameters are

567 summarised in Table 5.

568

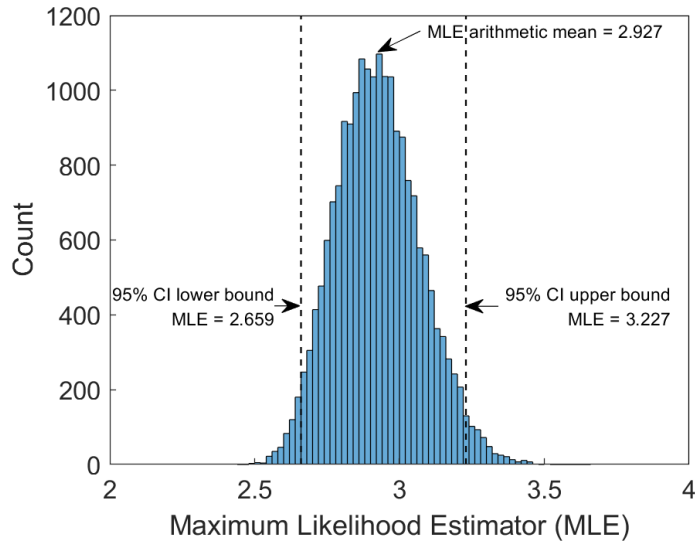


Figure 7. The bootstrapping result for the lognormal mean, μ , showing the Confidence Interval (CI) and arithmetic mean of the MLE.

569

Table 5. Summary of the arithmetic means and 95% confidence intervals (dashed lines) of the MLEs for the Weibull scale & shape parameters and the lognormal mean & standard deviation.

Distribution	Parameter	95% confidence interval	Arithmetic mean
Weibull	Scale parameter, α	[17.808, 36.976]	26.217
	Shape parameter, β	[1.171, 2.247]	1.559
Lognormal	Mean, μ	[2.659, 3.227]	2.927
	Standard deviation, σ	[0.354, 0.791]	0.593

570

571 The confidence intervals summarised in Table 5 essentially represent the tolerable

572 uncertainties in the prediction of the MLE. As such, any CDF characterised by the MLE
573 in these intervals can be used with confidence to represent the probability distribution
574 of the equivalent puncture diameter for CO₂ pipelines. Figure 8 presents the resulting
575 Weibull and lognormal CDF ranges derived from these intervals showing the variation
576 of the cumulative failure probability versus equivalent puncture diameter for CO₂
577 pipelines. The lower and upper bounds of the ranges are noted in the figure. The
578 corresponding recommended CDFs for natural gas and crude oil pipelines respectively
579 obtained in Sections 3.2.1 and 3.2.2 are also presented for comparison purposes.

580

581 As discussed in Section 2.4, given that the sample size involved in deriving the above
582 results is small, the K-S test cannot accurately reflect the goodness-of-fit between the
583 model predictions and the data and hence, both Weibull and lognormal predictions are
584 considered statistically valid for the purpose of this study.

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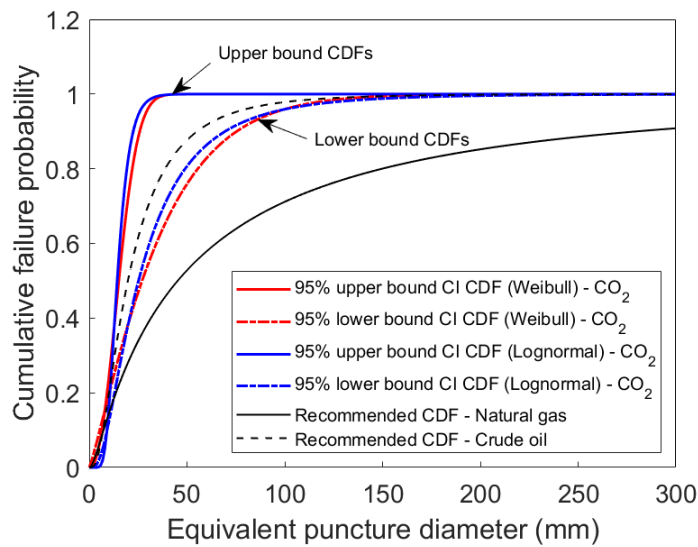


Figure 8. Weibull and lognormal CDF ranges derived from the Confidence Intervals (CIs) summarised in Table 5 showing the variation of the cumulative failure probability versus equivalent puncture diameter for CO₂ pipelines. The corresponding recommended CDFs for natural gas and crude oil pipelines respectively obtained in Sections 3.2.1 and 3.2.2 are also presented for comparison purposes.

589

590 As can be observed from both lower and upper bound CDFs in Figure 8, it is estimated
 591 that punctures smaller than 50 mm account for ca. 80% to 99% of the failures for CO₂
 592 pipelines. In comparison, only ca. 45% of the failures for natural gas pipelines are in
 593 the form of punctures smaller 50 mm. The corresponding number for crude oil pipelines
 594 is ca. 90% which is lower than the upper bound value of the estimated range for CO₂
 595 pipelines. The above suggests that small punctures are generally more common in CO₂
 596 pipelines. This may be attributed to the fact that in the PHMSA database records, a

597 major proportion of the CO₂ pipeline failures are resulted from corrosions which are
598 more likely to initiate small but continuous releases rather than catastrophic ruptures.
599 The presence of even small amounts of water (ca. > 650 ppm; Connell, 2005) as a
600 common impurity in CO₂ pipelines also makes them more prone to corrosion. It should
601 be noted that the above conclusions are drawn based on the data currently held in the
602 PHMSA database. The pipelines from which these data were extracted were mostly
603 constructed before 2010, some even dating back to several decades ago when the pipe
604 construction criteria were different from current ones. While corrosion may remain a
605 major failure cause of future CO₂ pipelines due to the presence of corrosive impurities
606 (e.g. water, H₂S) in the CO₂ stream, other failure mechanisms such as external
607 interference and ground movement etc. which are likely to cause more catastrophic
608 releases should not be ignored. With the expected growing number of deployed CO₂
609 pipelines, failures due to such mechanisms may become increasingly dominant. In
610 addition, the continued improvement in pipeline design standards, as well as cathodic
611 protection techniques will render failures resulting from corrosion and material defects
612 less probable. The above may change the puncture size profile for future CO₂ pipeline
613 failures. Nevertheless, the technique developed here can serve as a powerful tool
614 complimented with the growing wealth of failure data.

615

616 Using Figure 8, decision makers can select from a range of credible CDFs based on
617 their subjective preferences to represent the failure probability distribution of the

618 equivalent puncture diameter for the design or/and risk assessment of CO₂ pipelines.
619 For example, the lower bound CDF can be taken as the worst-case scenario CDF for
620 determining the risks associated with CO₂ pipeline failures, as it represents the highest
621 probability occurrence of larger puncture sizes among the possible CDFs. It should be
622 however noted that although the upper bound CDF is considered statistically valid, in
623 practice, it is more reasonable to use the CDFs closer to the lower bound as they cover
624 a wider range of puncture sizes, providing greater safety margins for quantitative risk
625 assessment.

626

627 **4. Conclusions**

628 The development and application of a statistical analytical technique for determining
629 puncture size probability distribution for pressurised CO₂ pipelines was presented.

630

631 A particularly important feature was addressing the pressing dilemma of the relatively
632 small pool of the recorded historical data available for CO₂ pipelines to ascertain a
633 reasonable prediction of their failure risks in the context of CCS operations and how
634 these are compared against those for hydrocarbon pipelines.

635

636 The methodology involved fitting the Weibull and lognormal distributions to the
637 puncture diameter data obtained from the PHMSA database using the Maximum
638 likelihood Estimator (MLE) method in conjunction with either Kolmogorov-Smirnov

639 (K-S) test if the sample size was deemed sufficiently large, or, bootstrapping if not.
640 Whether the sample size being employed was statistically representative was
641 determined by calculating the corresponding MLE quality using Monte Carlo
642 simulation. Using the above method, the puncture diameter probability distribution,
643 expressed as the Cumulative Distribution Function (CDF) was determined for CO₂
644 pipelines and compared against those for hydrocarbon (natural gas and crude oil)
645 pipelines.

646

647 Remarkably, the results obtained indicated that as compared to the hydrocarbon
648 pipelines, CO₂ pipelines are more likely to experience smaller puncture size failures (at
649 least 80% of the failures being in the form of punctures smaller 50 mm), thus resulting
650 in smaller magnitude but more prolonged releases. This directly impacts the preventive
651 and emergency response planning required especially in the case of buried CO₂
652 pipelines, where small leaks can remain undetected for long periods.

653

654 Furthermore, despite being a continuous highly random variable, in practice, the
655 through-wall puncture size in pressurised pipelines is often taken as a discrete variable
656 meaning that only limited range of representative puncture sizes are selected thus
657 compromising the validity of the subsequent quantitative risk assessment performed.
658 The present study fills this important gap by introducing a method for accurately
659 predicting the puncture size failure probability distribution by treating it as a continuous

660 function.

661

662 In addition to calculating the puncture size profile governing the subsequent risk
663 following pipeline failure, the proposed method can fully capture the randomness of
664 the through-wall puncture size. This provides a reliable prediction of the expected
665 puncture size following pipeline failure, thus enabling a more accurate evaluation of
666 the failure risk. This is particularly important for pipelines where the failure statistics
667 data available are sparse, such as those for CO₂ pipelines.

668

669 It should be noted that, in the present study, the statistical significance of the samples
670 employed to derive the distributions is only assessed based on the sample size. Whether
671 the sample ideally covers, for example, a sufficiently wide range of operating
672 conditions, or the entire range of puncture size is not investigated. Given this, future
673 work should focus on investigating the sample statistical significance based on other
674 sample features, such as the ‘sample quality’.

675

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681

682 **Data availability statement**

683 The raw data used for this research have been made available at
684 doi:10.5522/04/22015280.

685

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