

1 Regulatory Implications of Integrated Real-Time Control

2 Technology under Environmental Uncertainty

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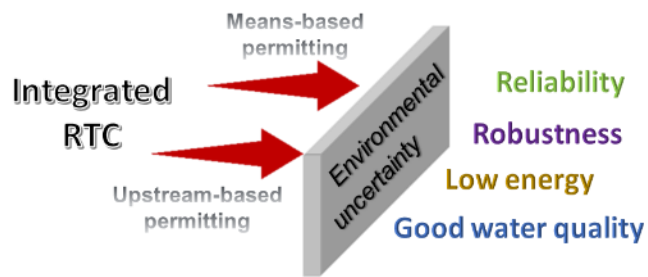
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7 **Abstract**

8 Integrated real-time control (RTC) of urban wastewater systems, which can
9 automatically adjust system operation to environmental changes, has been found in
10 previous studies as a cost-effective strategy to strike a balance between good surface
11 water quality and low greenhouse gas emissions. However, its regulatory implications
12 have not been examined. To investigate the effective regulation of wastewater systems
13 with this technology, two permitting approaches are developed and assessed in this
14 work - upstream-based permitting (i.e. environmental outcomes as a function of
15 upstream conditions) and means-based permitting (i.e. prescription of an optimal RTC
16 strategy). An analytical framework is proposed for permit development and
17 assessment using a diverse set of high performing integrated RTC strategies and
18 environmental scenarios (rainfall, river flow rate and water quality). Results from a case
19 study show that by applying means-based permitting, the best achievable, locally
20 suitable environmental outcomes (subject to 10% deviation) are obtained in over 80%
21 of testing scenarios (or all testing scenarios if 19% of performance deviation is allowed)
22 regardless of the uncertain upstream conditions. Upstream-based permitting is less
23 effective as it is difficult to set reasonable performance targets for a highly complex
24 and stochastic environment.

25 **TOC**



26

27 1. Introduction

28 In the quest for a sustainable future, critical infrastructures such as urban wastewater
 29 systems (UWWSs, i.e. sewers and wastewater treatment plants (WWTPs)) need to
 30 concurrently achieve good environmental water quality, low greenhouse gas (GHG)
 31 emissions and efficient resource (e.g. chemicals, energy) consumption¹⁻⁴. It is
 32 common to find 'dumb' WWTPs with fixed operation throughout the year under great
 33 variation of system inputs (e.g. wastewater inflow rate can increase by six times when
 34 it rains⁵) and the receiving waterbody (e.g. the 95%ile river flow rate can be tens to
 35 hundreds of times the 5%ile^{6,7}). This inevitably leads to overtreatment of wastewater
 36 in some occasions yielding excessive GHG emissions and resource usage and under-
 37 treatment in some other occasions not fulfilling the demand of the recipient. To address
 38 this, the operation of WWTPs needs to be both flexible and responsive and a promising
 39 approach to this is to 'smarten' system operation by employing integrated real-time
 40 control (RTC)⁸⁻¹². This technology can be used to adjust system operation
 41 automatically in real-time (seconds to hours) based on the monitoring of environmental
 42 and system changes so that more intensive wastewater treatment is applied under less
 43 favorable conditions and vice versa. It can be jointly used with *local* or *global* RTC in
 44 WWTP whereby actions in one process unit are determined by measurements in the
 45 same or other unit(s) within the WWTP rather than by conditions in the sewer and/or
 46 the receiving waterbody as in *integrated* RTC¹¹. Our previous modelling study⁹ has
 47 shown that by coordinated and optimal (fixed) operation of an activated sludge WWTP
 48 with the sewer, 8% of energy cost can be saved than the baseline operation; an

49 additional 7% of energy consumption can be reduced without violating the
50 environmental water quality standards by decreasing air flow rate in the WWTP when
51 wastewater load from the sewer is low and river flow is high. As more intensive
52 wastewater treatment is applied under heavy rainfall or low river flow, the application
53 of integrated RTC can also mitigate spikes of pollutant concentration in the recipient
54 (e.g. caused by combined sewer overflows (CSOs)). Compared to other flexible
55 operational approaches with longer response time steps (i.e. seasonal/monthly/daily
56 aeration), integrated RTC entails reduced cost, lower environmental risk (mitigated
57 pollution spikes) and higher resilience (timely intervention against adverse situations)⁹.
58 Successful implementations of integrated RTC have been reported in the
59 Netherland^{13,14}, Denmark^{15,16}, Germany¹⁷ and other countries^{18,19} as a novel and cost-
60 effective solution to deliver a better water environment. However, they mainly focus on
61 improving effluent quality by exploiting the storage/treatment capacity of UWWs or
62 on reducing CSOs to more sensitive recipients. Few (if any) of the current practices
63 monitor and utilize the temporal variability of the environmental assimilation capacity.

64 A key barrier to the adoption of the recipient responsive integrated RTC is the
65 potential conflict with the traditional permitting policy on wastewater effluent discharges.
66 As with other new technologies, the diffusion of this form of integrated RTC is
67 influenced by various factors such as technical maturity (e.g. reliability and robustness
68 of equipment)⁸ and applicability (e.g. compatibility with existing infrastructure)¹¹,
69 operational/managerial requirements¹¹, financial investments²⁰, social acceptance¹¹
70 and regulatory risks (compliance of existing policies)^{20,21}. The technological barrier can
71 be overcome as the recipient responsive integrated RTC uses similar instruments
72 (sensors, controllers and actuators) and control algorithms to those of current RTC
73 practices¹¹. Moreover, rapid technology development is ongoing as evidenced by the
74 increased reliability of *in situ* nutrient sensors²², improved data interpretation by
75 multivariate calibration of sensors²³ and application of advanced data analytics²⁴, and

76 enhanced remote data transmission across systems empowered by the Internet of
77 Things (IoT)¹⁹. The establishment of an RTC system involves considerable investment
78 and commitment, yet it is still a cost-effective strategy compared to the traditional
79 capital-intensive scheme, e.g. \$100 million sewer expansion was avoided by installing
80 \$6 million RTC system in South Bend, USA²⁵. Further, this technology can open up
81 more opportunities by the enriched insights on system performance. Field trial and
82 demonstration of the technology shall provide more confident information on its cost
83 and benefits and boost its social acceptance. Yet as the goal of system control moves
84 towards direct, overall environmental performance, greater fluctuations in effluent
85 water quality are likely to occur in accordance with the changing environment. This is
86 not detrimental to the recipient as relaxed treatment is only allowed under high
87 environmental assimilation capacity, but it increases risk of violating the fixed
88 numerical permit. In the conventional regulatory framework, WWTP effluent discharge
89 permit is developed based on annual (flow rate and water quality) statistics of effluent
90 and upstream river for achieving a predefined downstream river water quality. As such,
91 only one aspect of environmental impacts (i.e. water quality) is considered; moreover,
92 the regulation mainly focuses on WWTP effluent while other pollution sources such as
93 CSOs that jointly determine the environmental water quality are weakly controlled.
94 Therefore, the traditional permitting approach is not suitable for the regulation of the
95 recipient responsive integrated RTC and a different permitting approach is needed to
96 ensure that this technology is operated to its full potential, i.e. the optimal and
97 coordinated operation of sewer and WWTP is applied and multiple environmental
98 outcomes are delivered in a balanced manner.

99 A fit-for-purpose permitting policy should be environmentally protective,
100 technically achievable, and robust under uncertainty. Despite the environmental and
101 economic benefits of the recipient responsive integrated RTC being comprehensively
102 analyzed and demonstrated in previous studies, there is a limit to its capability like any

103 other technologies. For example, although integrated RTC aims at direct
104 environmental outcomes, the actual achievable results are determined by many factors
105 especially the upstream river water quality and flow rate (affecting dilution ratio of
106 wastewater effluent) which are highly dynamic and stochastic^{20,26,27}. Hence, it is
107 essential to firstly understand the potential of this integrated RTC in a changing and
108 uncertain environment so that rational regulatory targets can be set. Integrated
109 modelling of UWS and the receiving river^{8,28,29} is a useful tool to simulate the
110 interactions between the environment and the UWS. It has been employed for the
111 evaluation of integrated RTC in previous studies, however, only single sets of input
112 data were used which are insufficient to represent the stochastic nature of the
113 environment. As such, comprehensive integrated system simulations fed by large
114 environmental input datasets need to be conducted to support the permitting studies.

115 Built on the evidence base provided by comprehensive system simulations, a new
116 permitting approach can be explored. Due to the strong influence of natural stochastic
117 processes and upstream wastewater discharges on downstream environmental water
118 quality, it would be unfair to wastewater service providers (WWSPs) if the traditional
119 outcome focused regulatory approach is applied to set fixed permit limits on the final
120 environmental outcomes. Upstream-based permitting²⁰, a variation of the conventional
121 approach by setting different downstream environmental targets for different upstream
122 conditions, is a more reasonable option. As such, the influence from upstream river to
123 downstream performance can be recognized in the appraisal of the effectiveness of
124 wastewater treatment. Yet no studies have been reported on the operationalization of
125 this regulatory concept; also, its viability for the oversight of this integrated RTC
126 depends on whether the best achievable outcomes can be reliably estimated for
127 various background conditions. Means-based permitting is another regulatory
128 approach which mandates the installation and/or operation of a technology (i.e. mean)
129 instead of the end state (i.e. outcome)^{29,30}. Previous studies suggested this approach

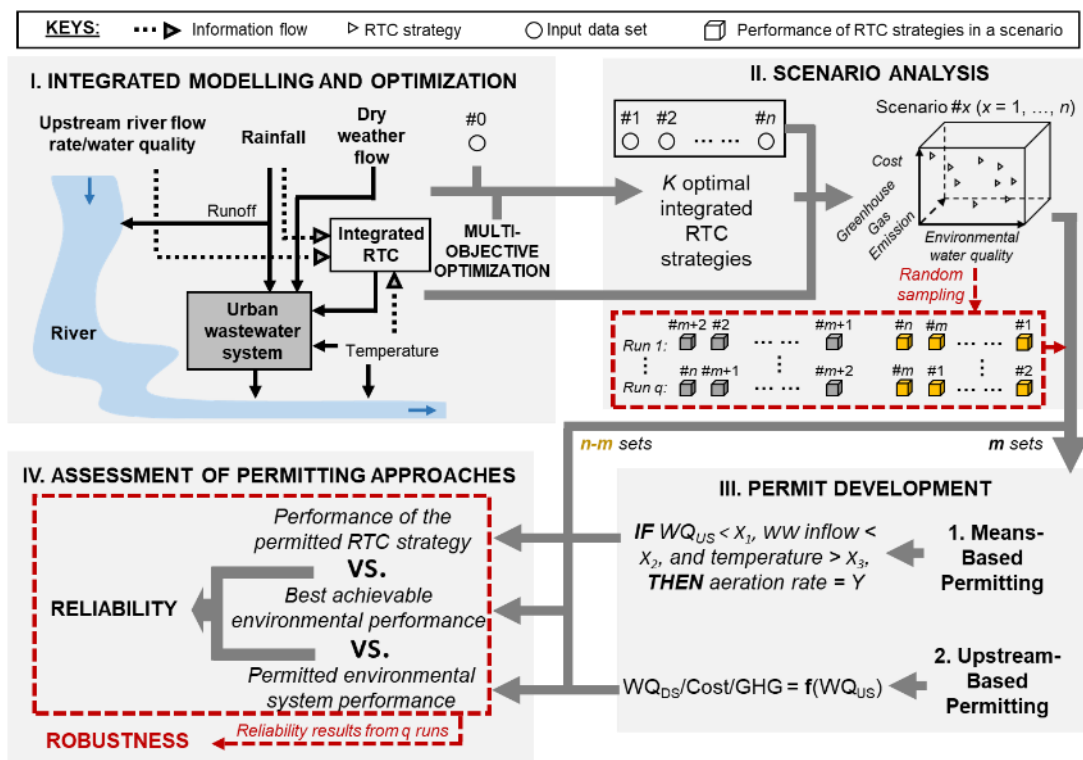
130 being especially effective in promoting best practices where the desirable final
131 outcomes cannot be practically monitored or quantified without deep uncertainty^{29,31}.
132 For example, the prescription of the integrated operational plan of an UWWWS has been
133 found to be effective in regulating the overall system discharges, i.e. CSOs (weakly
134 and ineffectively monitored) and WWTP effluent. This regulatory option seems
135 promising for the implementation of the recipient responsive integrated RTC as this
136 control technology is built on the integrated operation of UWWWSs and it is difficult to
137 prescribe target on downstream river water quality as mentioned earlier. Nevertheless,
138 its applicability remains to be explored, i.e. if there exists at least one RTC strategy for
139 an UWWWS that produces superior, desirable performance under most environmental
140 situations.

141 To fill the research gaps discussed above, this study investigates the viable form(s)
142 of permitting for effective regulation of the operation of the recipient responsive
143 integrated RTC in UWWWSs under stochastic environmental changes. The performance
144 of two representative and promising approaches, i.e. upstream-based and means-
145 based permitting, are examined in achieving satisfactory and balanced overall
146 environmental benefits under various conditions. To provide a sound basis for the
147 permitting studies, the best performing RTC strategies are developed based on
148 integrated UWWWS modelling and multi-objective optimization and are assessed by a
149 range of environmental scenarios for uncertainty analysis. By applying to a case study,
150 the reliability and robustness of the two permitting approaches are evaluated and
151 discussed.

152 **2. Methodology**

153 An analytical framework is established for the development and appraisal of the two
154 proposed permitting approaches as presented in Figure 1. Numerical simulation and
155 multi-objective optimization and scenario analysis are firstly conducted in parts I and II

156 respectively to generate the optimal integrated RTC strategies and their performance
 157 under various environmental conditions. Based on (part of) the generated performance
 158 database, permits by the two different regulatory approaches are developed in part III.
 159 The rest of the performance RTC datasets are employed to assess reliability of the
 160 permitting approaches in the final part; the variation in reliability (i.e. robustness) if
 161 different databases are used for permit development/assessment is also evaluated, as
 162 highlighted by the red dashed lines. Details of the four parts are described as follows.



163
 164 Figure 1. Analytical framework for the development and appraisal of means-based and
 165 upstream-based permitting approaches

166 2.1 Integrated UWWS Modelling and Optimization

167 Integrated UWWS modelling is employed for detailed simulation of the hydraulic and
 168 biochemical processes in the collection, transportation and treatment of combined
 169 sewerage (i.e. rainfall runoff and domestic wastewater) in an UWWS and assimilation
 170 of wastewater discharged to the receiving water^{8,28,29}. The sewer, WWTP and river are
 171 represented individually by different mathematical models and connected by converter
 172 models for synchronous simulation³². The software platform SIMBA^{32,33} is employed

173 for integrated modelling in this study, though other platforms can also be used such as
174 WEST^{14,34}, SYNOPSIS⁸ and CITY DRAIN³⁵ as reported in literature. The control
175 system is incorporated in the modelling and is appraised by dynamic simulations. As
176 the catchment, UWWS and river are represented in an integrated manner, direct
177 assessment can be made on the various impacts of the operation of an UWWS.

178 The control framework, i.e. which variables are monitored for the control of which
179 operational variable(s) (an example is provided in the following paragraph), and
180 performance objectives are defined by decision-makers according to local needs.
181 Optimization of RTC strategies is then conducted to quantify the variables in the control
182 scheme towards maximizing the performance results. As a good RTC scheme needs
183 to be built on a good operational scheme, the settings of fixed system operation in the
184 UWWS are optimized together with the control scheme. Non-dominated Sorting
185 Genetic Algorithm–II (NSGA-II) ³⁶, a popular evolutionary algorithm for multi-objective
186 optimization, is employed in this study. By mimicking the natural selection and
187 evolution process, NSGA-II starts with a population of candidate RTC strategies, which
188 continuously evolves in each generation towards achieving better optimization
189 objective values. The optimal RTC strategies are then assessed for their performance
190 under different environmental scenarios (part II) to support permit development (part
191 III) and appraisal (part IV) as described in Sections 2.2 to 2.4, respectively.

192 Figure 1 illustrates the framework using the control scheme employed for the case
193 study in Section 3, where the upstream river water quality, wastewater inflow and
194 temperature are monitored in real-time to guide the operation of aeration rate in the
195 UWWS, as illustrated by the dashed arrows in part I (i.e. ‘information flow’). ‘If-Then’
196 rules are used as the control algorithm, where control actions are defined in the
197 consequence (i.e. ‘Then’) statement corresponding to criteria in the conditional (i.e. ‘If’)
198 statement^{8,9}. The formulation of the control rules is illustrated in part III of Figure 1.
199 Based on a one-year simulation (in general, permit is developed and assessed on a

200 yearly basis in practice) with input dataset #0, values of the monitoring and/or control
201 variables (i.e. X_1 , X_2 and X_3 , and Y , which refer to the threshold value for poor/good
202 river water quality, low/high wastewater inflow rate, low/high temperature, and aeration
203 tier value in the case study respectively) and fixed operational settings are optimized
204 to improve environmental water quality and reduce GHG emissions and operational
205 cost (i.e. the performance objectives, which correspond to the three axis of the figure
206 in part II). As more than one goal is pursued, k ($k>1$) optimal RTC strategies are
207 produced which either delivers superior result in certain objective(s) or balanced
208 results on all objectives. No strategy is dominated or outperforms the others in all
209 objectives³⁶.

210 **2.2 Scenario Analysis**

211 As shown in part II of Figure 1, the k optimal strategies are appraised under n scenarios
212 with different input datasets (river flow rate and water quality and rainfall) to analyze
213 their performance under an uncertain environment. As detailed (time intervals in
214 minutes) environmental monitoring data especially on water quality parameters is of
215 limited availability, random sampling is employed to generate a sufficient number of
216 input datasets. This is achieved by mixing and matching data collected at different
217 places or years, i.e. a one-year time series data is randomly selected from all available
218 ones of each input variable to combine them into a single dataset. For example, n
219 ($1 \leq n \leq 500$) input datasets can be generated by random sampling if there are 5, 10 and
220 10 time series data for three input variables respectively. Driven by human activities,
221 dry weather flow (DWF) to the WWTP usually shows recurring daily patterns
222 insignificantly influenced by environmental changes^{5,8}, hence the same diurnal
223 patterns are applied to the flow rate/water quality of DWF in all simulations.

224 The first m scenario analyses (i.e. datasets #1 to # m in Figure 1) provide the
225 training data for deriving permits (illustrated by the arrow pointing from part II to part
226 III) and the other $n-m$ scenarios for testing the reliability (i.e. the arrow from part II to

227 part IV). Random sampling is conducted to select different datasets for permit
228 development/assessment, which is repeated for q times by the cross-validation
229 technique³⁷ as illustrated by the red dashed box in part II of Figure 1. As such, the
230 robustness of the permitting approaches against the selection of input datasets can be
231 assessed as presented in Section 2.4.

232 **2.3 Permit Development**

233 To develop the permits, the k RTC strategies are firstly ranked in all m scenarios as
234 the best strategy in one scenario may not yield superior outcomes in another. In each
235 scenario, the best performance results are used to develop upstream-based permitting
236 and the corresponding RTC strategy is recorded for the derivation of means-based
237 permitting. As multiple strategies will be non-dominated in cases with multiple
238 objectives, criteria are defined to select a single, most desirable RTC strategy in each
239 scenario to facilitate permit development. The criteria can be maximization of system
240 performance in one objective (i.e. one aspect of performance is valued more than
241 others) or a converted single objective by assigning weights to different objectives,
242 and/or meeting predefined limits on certain/all performance objective(s). The definition
243 of the criteria depends not only on the preferences of stakeholders but also on the
244 potential of the existing infrastructures which can be estimated from the scenario
245 analyses.

246 Among the p ($1 \leq p \leq \min(k, m)$) high performing RTC strategies selected from the
247 m simulations, the one that appears in the largest number of scenarios is the most
248 promising solution and is chosen as the means-based permit. For upstream-based
249 permitting, the performance of the selected RTC strategy is recorded against the
250 corresponding upstream condition in each scenario and a regression analysis is then
251 conducted between the upstream data and performance results of the m scenarios.
252 Based on the fitted function, the (50% or 95%) prediction interval³⁸ is prescribed as the
253 upstream-based permit, i.e. the upper and lower limits of expected system

254 performance (e.g. downstream river water quality, energy cost and GHG emissions as
255 represented by 'WQ_{DS}', 'Cost' and 'GHG' in part III of Figure 1) for any given upstream
256 environmental condition (e.g. upstream river water quality as represented by 'WQ_{US}' in
257 Figure 1).

258 **2.4 Appraisal of Permitting Approaches**

259 Reliability is assessed by comparing the best achievable outcomes among the k
260 strategies in each testing scenario with the performances of the permitted RTC
261 strategy for means-based permitting or with the permitted performances for upstream-
262 based permitting. Reliability of means-based permitting is defined as the percentage
263 of scenarios where the permitted RTC strategy provides the best performance or worse
264 but of acceptable level of deviation in performance. Reliability of upstream-based
265 permitting is measured by the percentage of scenarios where the best achievable
266 performance value falls within the prescribed permit range. q random runs are made,
267 and the average and range of the reliability values show the robustness of the
268 permitting approaches.

269 **3. Case study**

270 **3.1 Study Site and Its Assessment**

271 The proposed permitting approaches are appraised using a well-studied semi-
272 hypothetical case, which consists of seven urban sub-catchments, a combined sewer
273 system adapted from a literature standard³⁹, an activated sludge WWTP based on the
274 Norwich (UK) treatment work, and a hypothetical river^{8,9,28,40}. Detailed description of
275 the case study site and its modelling are presented in Section S1 of the supporting
276 information.

277 Total (unionized and ionized) ammonia is the pollutant of particular concern,
278 although processes related to other water quality parameters such as BOD₅,
279 suspended solids and DO are also simulated. The total ammonia concentration, in
280 90%ile and 99%ile values as regulated by the EU Water Framework Directive
281 (WFD)^{41,42}, is assessed at a river reach one kilometer downstream of the discharge of
282 WWTP effluent. There is limited chemical usage in the operation of the studied UWWS,
283 thus energy consumption is used to represent operational cost in this study. As energy
284 consumption is also a reasonable indicator of GHG emissions^{4,43}, energy cost is used
285 to indicate both GHG emissions and operational cost in this work. As such, the control
286 schemes are optimized against three objectives in this study, which are the 90%ile and
287 99%ile total ammonia concentration in the river (hereafter referred to as '90%ile AMM'
288 and '99%ile AMM'), and the energy cost entailed in the operation of the UWWS
289 (calculation method provided in Section S2).

290 **3.2 Operational and Control Schemes**

291 Following our previous study on integrated RTC⁹, the control scheme is formulated in
292 the 'If-Then' rules (provided in Section S4) as illustrated below.

293 *"IF upstream river total ammonia concentration ≥ 0.1 mg/L, wastewater inflow rate \leq
294 $41,250$ m³/d and temperature ≥ 15 °C, THEN aeration rate = Y_1 m³/h.*

295 *(ELSEIF ... THEN ...)*

296 *ELSEIF upstream total ammonia concentration < 0.1 mg/L, wastewater inflow rate \leq
297 $41,250$ m³/d and temperature < 15 °C, THEN aeration rate = Y_8 m³/h"*

298 WWTP inflow rate is monitored for system control as increased inflow (e.g. under
299 wet weather) means higher load to be treated which usually compromises the
300 treatment efficiency if no enhanced effort is applied. Temperature is also monitored as
301 it has a strong influence on the biological treatment efficiency. River water quality is

302 used to represent upstream condition due to its direct impact on downstream water
303 quality. River flow rate is not used for guiding integrated RTC in this study, however,
304 its influence is examined and discussed as described in Sections 3.3 and 4.5. Based
305 on a preliminary assessment, the threshold values in the antecedent, conditional
306 statement are determined as in the example above to classify good/not-so-good
307 upstream river water quality, dry/wet weather, and winter/non-winter period. Although
308 there are eight possible combinations of the states of the three variables in the
309 conditional statement, two aeration tiers (i.e. Y) are used in this study. This can
310 improve the efficiency of the optimization of the tier values with limited compromise in
311 reliability as suggested by a preliminary analysis presented in Section S3. The time
312 step for the control is 15 min. The two aeration tier values as well as key operational
313 settings in the UWWS are optimized by NSGA-II to minimize the downstream total
314 ammonia concentration and energy consumption based on a one-year simulation.
315 Details of the optimized operational and control variables and their feasible value
316 ranges are presented in Section S5.

317 **3.3 Input Datasets and Parameter Settings**

318 A one-year input data set from a monitoring site in the Midlands, UK, is employed for
319 operational and control optimization. For the uncertainty analysis, 100 ($n = 100$) input
320 datasets are generated by random sampling of 40, 40 and 6 one-year 15 min increment
321 time series of rainfall, river water quality and river flow rate, respectively, collected from
322 different sites and years (2008-2018) in the UK⁴⁴. The six river flow rate data series
323 have the same pattern but at different scales, as they are based on a single one-year
324 time series (i.e. the same one for control optimization) but multiplied by different
325 coefficients (i.e. scaled up or down) so that the ratios between average river flow rate
326 and wastewater discharge rate are 1.5, 3, 4.5, 6, 7.5 and 15, respectively. Thereby,
327 the impact of dramatic variations in river flow rate, which is not impossible especially
328 under climate change, can be simulated and assessed. River water quality has much

329 smaller fluctuations than river flow rate as represented in annual statistical parameters.
330 As such, the 40 different river water quality data series are scaled so that their median
331 values are similar to that of the input dataset used for control optimization (0.1 NH₃-N
332 mg/L). 80 ($m = 80$) of the 100 scenarios are used to develop permits whilst the other
333 20 scenarios for testing the reliability of the permitting approaches. 200 ($q = 200$)
334 random runs are conducted for the robustness analysis.

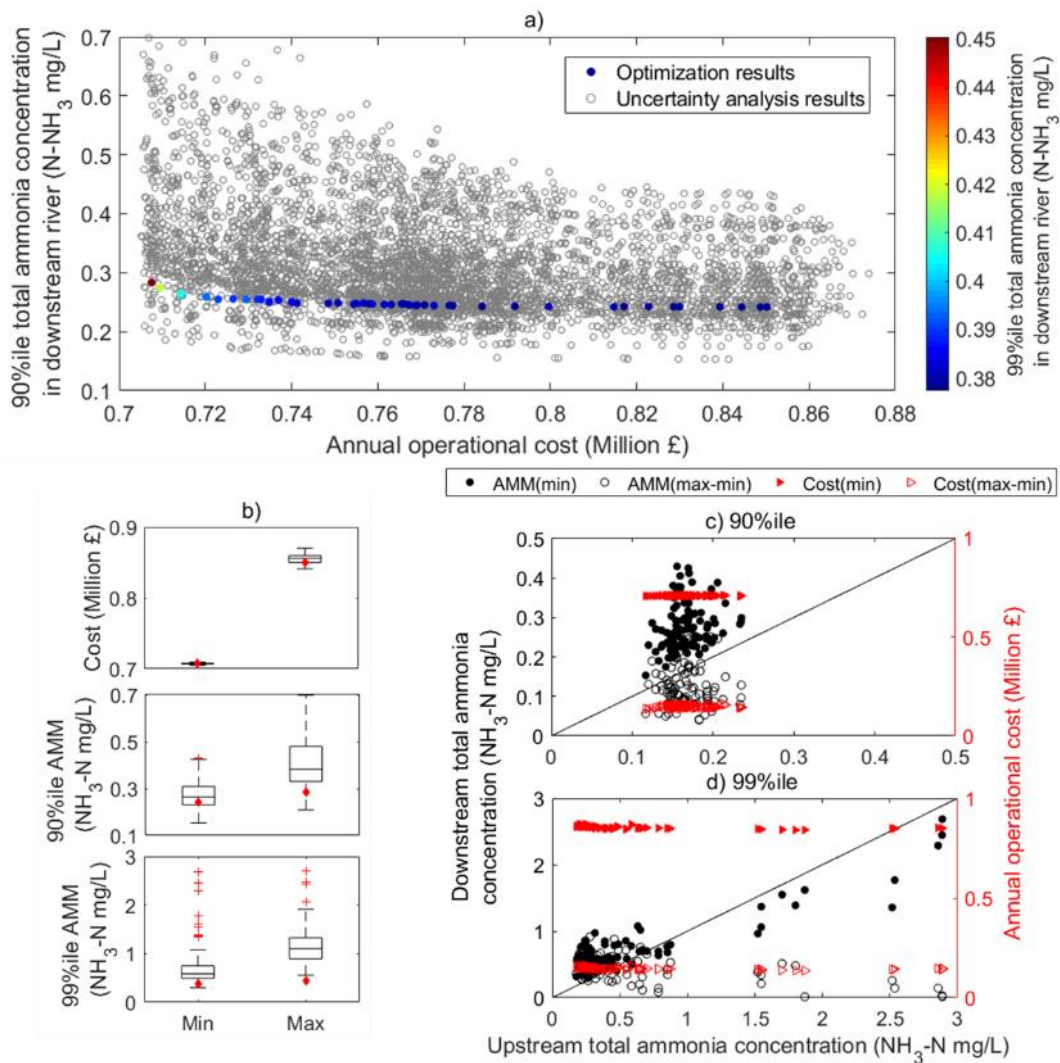
335 **4. Results and Discussion**

336 The integrated RTC strategies developed by the multi-objective optimization algorithm
337 are analyzed in Section 4.1, which provide insights on the relationships between the
338 performance objectives and a basis for setting reasonable regulatory targets embodied
339 in the two permitting approaches as presented in Section 4.2. The development
340 processes and reliability of means-based permitting and upstream-based permitting
341 are described in Sections 4.3 and 4.4 respectively. The evaluation of the robustness
342 of the two permitting approaches is presented in Section 4.5. Discussion on the
343 comparison of the two approaches and the implications for real-life implementation is
344 provided in Section 4.6.

345 **4.1 Performance of Integrated RTC Strategies**

346 49 ($k = 49$) integrated RTC strategies are found to be non-dominated in the multi-
347 objective optimization. They all comply with the legislative constraints on total ammonia
348 concentration but still show diverse performances as presented by the colored dots in
349 Figure 2a ('Optimization results'). A clear trade-off can be seen between operational
350 cost and 90%ile AMM as the pollutant concentration becomes higher when cost
351 decreases, i.e. higher cost is required to achieve better environmental water quality.
352 The color of the dots represents 99%ile AMM and transits from blue to red with
353 increasing 90%ile AMM, suggesting the positive correlation between 90%ile AMM and

354 99%ile AMM. The relationships (trade-off or positive correlation) between the three
 355 objectives are unchanged under different environmental scenarios. This is because
 356 their correlation coefficients r between cost and 90%ile AMM, cost and 99%ile AMM,
 357 and 90%ile AMM and 99%ile AMM lie within [-0.76, -0.88], [-0.49, -0.89], and [0.53,
 358 0.98], respectively in the 100 scenarios for uncertainty analysis.



359

360 Figure 2 a) The optimal integrated RTC solutions (colored dots) and their performance under
 361 uncertainty analysis (grey dots); b) boxplots of the minimum or maximum values of the three
 362 objectives in the uncertainty analysis; and c) and d) minimum (filled marks) or range (unfilled
 363 marks) of downstream total ammonia (black dots, 90%ile AMM in c) and 99%ile AMM in d) or
 364 cost (red triangles) against the upstream water quality in the uncertainty analysis

365 The performances of the control schemes can vary greatly in different scenarios. This
 366 can be suggested from Figure 2a where the results of the 49 RTC strategies in the 100
 367 scenarios are presented in grey circles (i.e. 'Uncertainty analysis results'). Results of

368 99%ile AMM are not shown so that the 'optimization results' can be clearly seen. Figure
369 2a shows the wide value range in 90%ile AMM compared to that of the 'optimization
370 results'. To quantify the variation, non-dominated sorting is conducted to select non-
371 dominated optimal strategies in each scenario and the performance boundaries (i.e.
372 minimum and maximum values) of the optimal strategies are summarized by boxplots
373 in Figure 2b. Each boxplot is based on 100 minimum/maximum results in one
374 performance objective. The maximum and minimum values, the 25%ile and 75%ile
375 and 50%ile values of each 100 values are presented by the upper and lower whiskers,
376 the lower and upper bounds of box and the black line within the box, respectively. The
377 environmental standard limits for 90%ile AMM (0.3 NH₃-N mg/L) and 99%ile AMM (0.7
378 NH₃-N mg/L) cannot be met even by the best performing RTC strategies in many
379 scenarios. This clearly shows the significance of natural background dynamics in
380 affecting environmental quality compliance.

381 Compared to the 'optimization results' marked as red diamonds in Figure 2b, the
382 minimum and maximum operational cost of the optimal RTC strategies vary within [-
383 0.3%, 0.3%] and [-1.1%, 2.3%], respectively. This corresponds to the results presented
384 in Figures 2c and 2d, where the minimum (red filled triangles) and range (red unfilled
385 triangles) of operational cost show minor change with the upstream water quality.
386 Moreover, the variation in the cost of single RTC strategies in the uncertainty analysis
387 is between -5.2% and 5.3% (not presented in figures). This shows that energy
388 consumption is, at the face value, insignificantly affected by environmental changes
389 especially in comparison with the fluctuation in downstream river water quality as
390 presented later in this section. However, the level of fluctuation is comparable to that
391 of the savings this technology can bring, e.g. 7% of energy saving as mentioned in the
392 introduction section. This suggests the obvious impact of the dynamic environment on
393 the energy consumption, however its proportion to the total amount is low as a

394 considerable amount of energy input is necessary for the running of the treatment
395 process even under the optimal way of operation.

396 By contrast, the variations in the minimum and maximum total ammonia
397 concentrations are much bigger, which are between [-37%, 78%] and [-26%, 147%]
398 for 90%ile AMM and [-20%, 612%] and [23%, 499%] for 99%ile AMM. The great
399 variations in 99%ile AMM are largely caused by the change in upstream conditions as
400 the correlation coefficients between the upstream 99%ile AMM and the minimum and
401 the range in downstream 99%ile AMM are 0.92 and -0.53, respectively. The minimum
402 downstream 99%ile AMM is close to the upstream 99%ile AMM value, as can be seen
403 in Figure 2d where the black filled dots are located near the black line ($y = x$) especially
404 at higher upstream concentration values. The correlation between the upstream and
405 minimum downstream 90%ile AMM is weak ($r = 0.23$, presented as black dots in Figure
406 2c). Moreover, the difference in 90%ile AMM by various RTC strategies can be
407 comparable to that of the upstream 90%ile AMM. This indicates the strong influence
408 of the operational and control scheme of UWWs on 90% AMM (but not on 99% AMM).

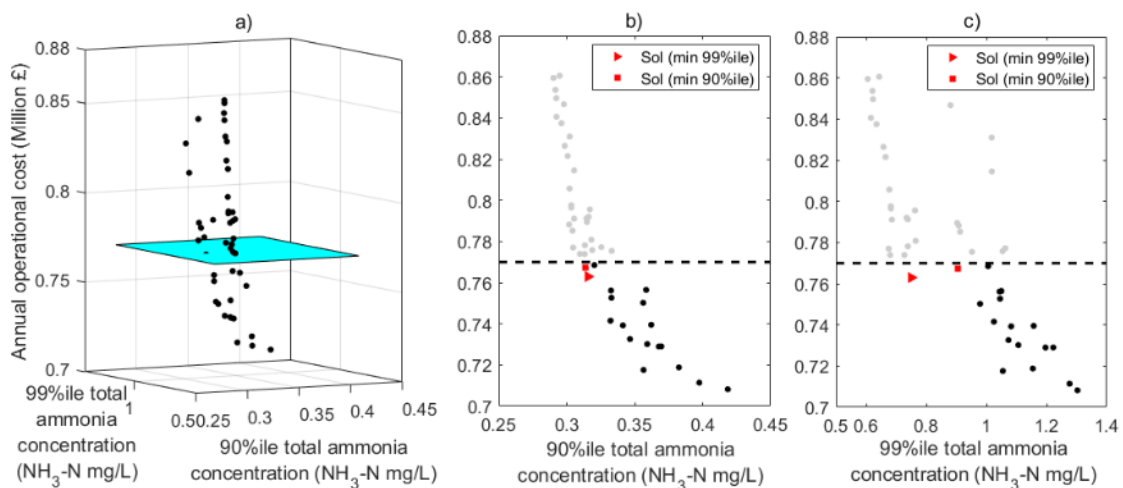
409 **4.2 Selection of Optimal RTC Strategies for Permitting**

410 Due to the high sensitivity of downstream water quality to upstream changes as shown
411 in Section 4.1, it is impossible to apply the traditional outcome-based permitting
412 approach and set fixed limits on all performance outcomes. This highlights the
413 significance of the permitting studies in this work.

414 As the operational cost of an RTC scheme is subject to minor change under
415 different environmental scenarios, a threshold limit of cost can be set by stakeholders
416 to restrict system performance in this aspect. £0.77 million is used in this work which
417 is approximately the average of the median values of the two boxplots in the first
418 subplot of Figure 2b. Among the RTC strategies that yield lower operational cost than
419 the threshold, the one that produces the highest environmental water quality is

420 selected for permitting. As such, the RTC strategy that can provide the best and
421 balanced environmental outcomes that suits the local needs can be identified and used.
422 Note that other screening criteria can be used as long as one RTC strategy can be
423 selected in each scenario.

424 The screening process is illustrated in Figure 3 using results from one scenario.
425 The performances of the optimal RTC strategies are plotted against the three
426 objectives in Figure 3a and against the pair of objectives between cost and 90%ile
427 AMM/99%ile AMM in Figures 3b/3c. Strategies below the blue surface in Figure 3a
428 (the threshold for operational cost), which correspond to the dots below the dashed
429 lines in Figures 3b and 3c, are assessed further for their environmental water quality.
430 The strategy presented in the red triangle ('Sol (min 99%ile)') yields the lowest 99%ile
431 AMM, however, its 90%ile AMM is slightly higher than the strategy shown as the red
432 square ('Sol (min 90%ile)'). This highlights that a conflict can exist between the two
433 statistical parameters on total ammonia concentration, despite their strong correlation
434 in general. As the difference between 90%ile AMM is much smaller than that of 99%ile
435 AMM, as observed in this scenario run (Figures 3b and 3c) and others, 99%ile AMM
436 is used as the key criteria for the selection of RTC strategy for permitting. As such,
437 permits are developed based on strategies that can provide the best overall
438 environmental water quality whilst satisfying the restriction on operational cost.

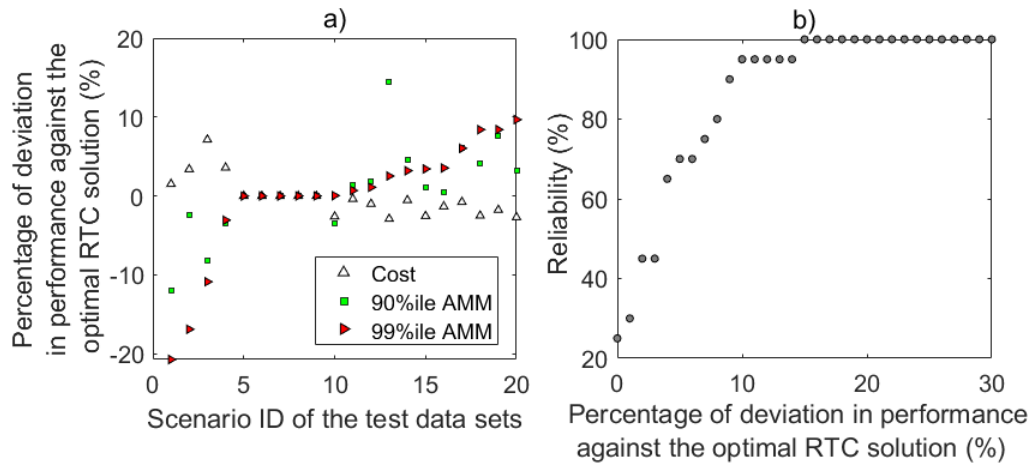


440 Figure 3 Illustration of the selection of desirable, optimal RTC strategy for permitting

441 **4.3 Means-Based Permitting and Its Reliability**

442 14 RTC strategies are selected in the 80 scenarios for permit development, which
443 show superior results in 17, 14, 13, 9, 7, 6, 4, 4, 1, 1, 1, 1, 1 and 1 scenarios,
444 respectively. The settings of the 14 RTC strategies are provided in Section S6. The
445 top two high performing RTC strategies have very similar features compared with
446 others, e.g. overflow thresholds are relatively high and storm tank emptying rates are
447 low. As such, the storage capacity in the UWWS is fully utilized reducing overflow spills;
448 also the storm tank is emptied at a low rate to reduce the hydraulic shock to the
449 treatment process. The second top strategy has a larger low tier aeration rate, hence
450 is prone to exceed the limit on energy cost. As strategy No. 14 performs the best in the
451 largest number of scenarios, it is the most desirable RTC strategy and its control
452 rules/settings are prescribed as the permit for this case study.

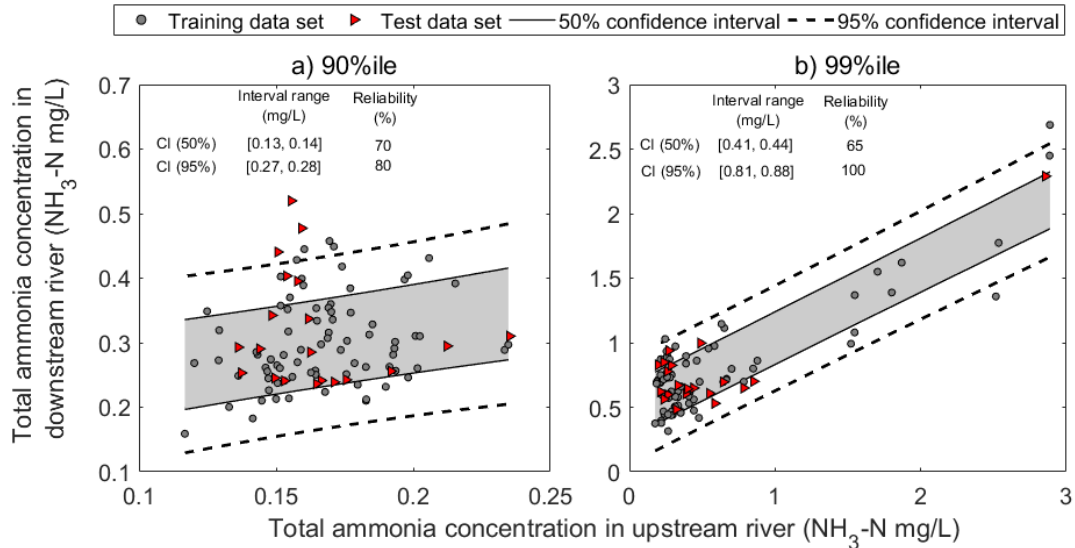
453 The performance of the permitted RTC strategy is compared to the best
454 performances in the 20 testing scenarios identified according to the same criteria
455 described in Section 4.2. The percentages of deviation in cost, 90%ile AMM and
456 99%ile AMM are plotted in Figure 4a in white diamonds, green squares and red
457 triangles, respectively. It can be seen that the permitted strategy is the best solution in
458 five testing scenarios where the three symbols overlap at y value of zero; in scenario
459 No. 10, its 99%ile AMM is slightly higher (0.05%) than the optimal solution but the cost
460 and 90%ile AMM are both lower. Based on the performance results in Figure 4a, the
461 reliability of means-based permitting can be derived, which is dependent on the
462 acceptable level of deviation in system performance as shown in Figure 4b. For
463 example, the reliability is 25% (i.e. $\frac{5}{20} \times 100$) if no deviation is allowed. The reliability
464 becomes 30%, 70%, 75%, 80%, 90%, 95% or 100% if 1%, 5%, 7%, 8%, 9%, 10% or
465 15% of performance deviation (only higher values, i.e. worse performances, are
466 accounted as deviation) are acceptable respectively.



467
 468 Figure 4 a) Comparison of the performance of the permitted RTC strategy against the best
 469 performing strategies in the testing scenarios; and b) reliability of the means-based permitting
 470 approach

471 **4.4 Upstream-Based Permitting and Its Reliability**

472 As river water quality is the only upstream condition factor incorporated in the control
 473 algorithm, downstream performance is prescribed as a function of upstream water
 474 quality. For each testing scenario, the best achievable, desirable downstream 90%ile
 475 or 99%ile total ammonia concentration is presented against the upstream river quality
 476 value by a grey dot in Figures 5a or 5b. As the data points suggest a linear correlation,
 477 they are fitted to linear functions and the 50% (solid lines with grey colored fillings) or
 478 95% (dashed lines) confidence interval (CI) of the fitted functions is set as the
 479 upstream-based permit. The top and bottom lines of the 50% or 95% CI are almost
 480 parallel to each other as can be seen from the summary of interval ranges at different
 481 upstream water quality (i.e. the 'Interval range' column marked in Figure 5). The higher
 482 the level of confidence, the wider the value range for the permit. For example, if 90%ile
 483 AMM at upstream is 0.15 NH₃-N mg/L, the permit for the downstream 90%ile AMM is
 484 [0.22, 0.36] NH₃-N mg/L if using the 50% CI or [0.16, 0.42] NH₃-N mg/L if the 95% CI
 485 is employed. As environmental changes have limited impacts on operational cost of
 486 the UWWWS, £0.77 million is set as the permit for any upstream conditions but a minor
 487 range of deviation (e.g. 5% as suggest in Section 4.1) can be allowed.



488

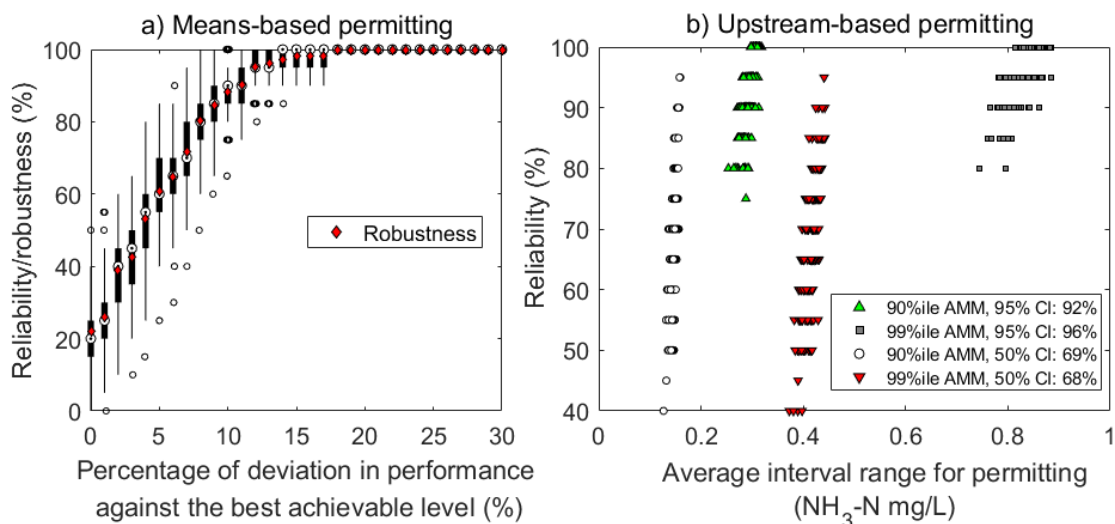
489 Figure 5 Development of upstream-based permits (50% or 95% confidence intervals) based
 490 on training datasets (grey dots) and reliability analysis based on the testing datasets (red
 491 triangles)

492 The permits are compared against the best performance results in the 20 testing
 493 scenarios (red triangles in Figure 5) to assess the reliability of the upstream-based
 494 permitting approach. Results on the reliability are marked in Figure 5, which is derived
 495 by counting the percentage of red triangle data points that fall within the CIs; those that
 496 are below the CIs are not considered to be desirable as higher river quality is likely to
 497 yield higher GHGs. The reliability of the permit on 90%ile AMM is 70% if the 50% CI is
 498 used, which increases to 80% if the 95% CI is permitted. The reliability of the permit
 499 on 99%ile AMM is 65% or 100% if the 50% or 95% CI is used. As the permit on
 500 operational cost is a requirement rather than a prediction, it is not considered in the
 501 assessment of the reliability of upstream-based permitting. However, the necessity of
 502 incorporating cost limit in the permit is discussed in Section 4.5.

503 4.5 Robustness of the Permitting Approaches

504 Figure 6 shows the change in the reliability of the two permitting approaches in the 200
 505 random runs, based on which the robustness (average reliability) values can be
 506 obtained as marked in red diamonds in Figure 6a and in the legend of Figure 6b. Each
 507 boxplot in Figure 6a is based on 200 reliability values by the random runs. The

508 reliability of means-based permitting can vary as great as 50% for low levels of
 509 performance deviation. The average reliability is 22%, 53%, 85%, 97% or 100% if 0%,
 510 5%, 10%, 15% or 19% of performance deviation is allowed respectively, which are
 511 slightly lower than those obtained in Section 4.3 (i.e. 25%, 65%, 90%, 95% and 100%,
 512 respectively). The reliability of upstream-based permitting is also sensitive to the use
 513 of datasets, especially if the 50% CI is employed for permitting. The reliability range
 514 between [75%, 100%], [80%, 100%], [40%, 95%], and [40%, 95%] for 90%ile AMM&95%
 515 CI, 99%ile AMM&95% CI, 90%ile AMM&50% CI, and 99%ile AMM&50% CI,
 516 respectively. Their average reliability values are 92%, 96%, 69% and 68% respectively,
 517 which are close to the reliability results obtained in Section 4.4 (i.e. 80%, 100%, 70%
 518 and 65% respectively).

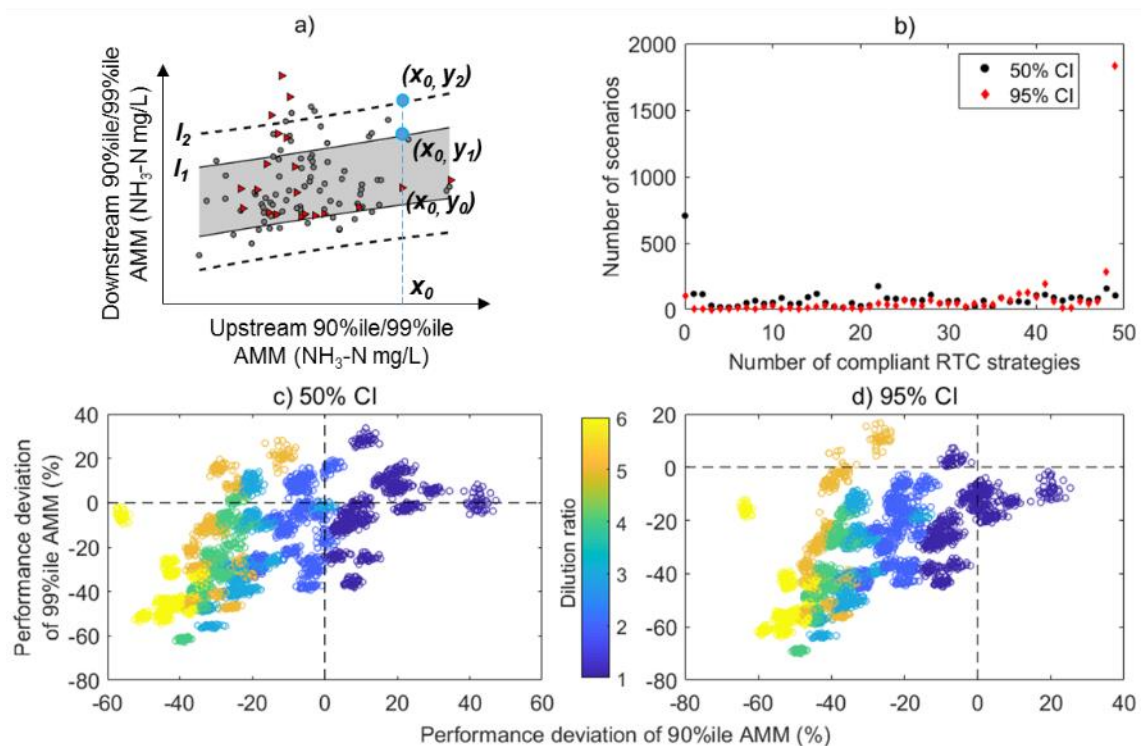


519

520 Figure 6 Robustness of the permitting approaches based on the reliability results from 200
 521 random runs

522 Despite the high reliability values displayed in Figure 6b (especially those related to
 523 the 50% CI), the value range of an upstream-based permit is quite wide (i.e. large x
 524 value in Figure 6b) rendering the environmental protectiveness of this permitting
 525 approach in doubt. As such, the best achievable, desirable performances in each
 526 testing scenario are compared with the upper permit values (i.e. the less stringent
 527 boundaries) for deeper understanding of the upstream-based permitting. Figure 7a
 528 illustrates how the calculation is made using the red triangle with coordinate values of

529 x_0 and y_0 , which represents the best performing RTC strategy in one testing scenario.
 530 Comparisons are made between y_0 and y_1 or y_2 (i.e. the upper permit values based on
 531 the 50% or 95% CI), and the results of $\frac{y_0 - y_1}{y_1} \times 100$ and $\frac{y_0 - y_2}{y_2} \times 100$ are presented in
 532 Figures 7c and 7d, respectively. The x values are the results on 90%ile AMM and the
 533 y values are those on 99%ile AMM. The dot color represents the dilution ratio in that
 534 scenario. There are 4000 (20x200) data points in Figures 7c and 7d although they are
 535 based on maximally 100 scenarios. This is because the confidence intervals change
 536 when different scenarios are selected for permit development, i.e. y_1 and y_2 would vary
 537 in different random runs resulted from the change in I_1 and I_2 in the example in Figure
 538 7a.



539

540 Figure 7 a) Illustration of the calculation of performance deviation in c) and d); b) number
 541 of RTC strategies that comply with upstream-based permits on both 90%ile and 99%ile
 542 AMM in the 4000 testing cases; c) and d) performance deviation of the best achievable
 543 results against the upper upstream-based permit values based on 50% CI (c) and 95% CI
 544 (d) in all testing cases

545 Results in Figure 7d are lower than but similar to (e.g. the distribution of the data points,
 546 color pattern) those in Figure 7c, which can be expected as the upper line of the 95%
 547 CI is above and almost parallel to that of the 50% CI as shown in Figure 7a. The

548 performance deviation in 90%ile and 99%ile AMM lie between [-58%, 47%] and [-63%,
549 34%] respectively against the 50% CI based permit and [-65%, 25%] and [-70%, 17%]
550 respectively against the 95% CI based permit. A high, positive deviation value indicates
551 the permit is too strict and is not technically achievable or can only be met using
552 operational schemes that emit more GHG emissions than desired, while a high,
553 negative deviation value suggests the permit is too relaxed which poses an
554 environmental threat.

555 To illustrate the real-life implications of the upstream-based permitting from
556 another perspective, the RTC strategies (out of the 49 high performing RTC strategies)
557 that comply with both 90%ile and 99%ile AMM permit limits in each of the 4000 testing
558 cases are identified and the results are summarized in Figure 7b. The black dot or red
559 diamond at $x = 0$ show that the permit (base on 50% or 95% CI) is not technically
560 achievable in 705 or 100 testing cases (i.e. $y = 705$ or 100). On the other hand, all the
561 49 RTC strategies can meet the permit in 105 or 1831 testing cases (i.e. the y value of
562 the black dot/red diamond is 105 or 1831 at $x = 49$); yet many RTC strategies do not
563 meet the constraint on operational cost as shown in Figure 3 and Section 4.2. This
564 clearly shows that overly high GHG emissions are possible if they are not regulated in
565 the upstream-based permitting.

566 A clear color pattern is exhibited horizontally in Figures 7c and 7d, i.e. higher
567 performance deviation in 90%ile AMM (not 99%ile AMM) at lower dilution ratio (the dot
568 color is dark blue at larger x value). This shows that 90%ile AMM is strongly influenced
569 by the river flow rate and the permit limit on 90%ile AMM tends to be overly tight with
570 lower dilution ratio and vice versa. This suggests the potential to improve the proposed
571 upstream-based permitting by prescribing different permits for different levels of
572 upstream river flow rate. However, the environmental outcomes become highly
573 uncertain under low river flow rate, as can be seen from the wide distribution of dark
574 blue points in Figures 7b and 7c. As such, the limitation in the upstream-based

575 permitting is evident for low river flow conditions, where effective and reasonable
576 regulation is mostly needed. As such, the upstream-based permitting may not be
577 beneficial to both the WWSPs and the regulators/environment.

578 **4.6 Smart Permitting for Integrated RTC**

579 The purpose of applying the integrated RTC technology is to deliver the best
580 achievable, balanced environmental outcomes against the highly uncertain natural
581 dynamics. Yet as in a recipient responsive integrated RTC scheme the operation of an
582 UWWS varies with environmental changes, it seems uncertain whether this smart
583 technology can be reasonably regulated. In other words, is it possible to tell if an
584 integrated RTC system is running to its full potential and not misused or improperly
585 operated? This study provides a sound evidence for answering this question based on
586 computational experiments which enable the appraisal of the technology represented
587 by a variety of high performing strategies under a wide range of environmental
588 scenarios. Two potential permitting approaches (upstream-based permitting and
589 means-based permitting), suggested from the literature but not yet investigated, are
590 examined in this study on their reliability and robustness for the regulation of the
591 recipient responsive integrated RTC.

592 Results demonstrate that it is not reasonable to apply the traditional outcome-
593 based permitting and prescribe permit limits on downstream river water quality as it is
594 strongly influenced by the upstream conditions (especially 99%ile AMM). It is beyond
595 the capability of the integrated RTC technology (and even any other technologies) to
596 achieve a predefined downstream environmental target under any conditions. UWWS
597 discharges are found to be a significant factor in influencing 90%ile AMM; moreover,
598 a linear function can be reasonably established between the upstream and
599 downstream 90%ile AMM based on the optimal and desirable integrated RTC
600 strategies. As such, upstream-based permitting seems to be promising for the

601 regulation of UWWs applying recipient responsive integrated RTC. However, results
602 show that 90%ile AMM is also influenced by the dilution capacity of the environment
603 and the upstream-based permit based on input datasets covering all flow regimes
604 tends to be too relaxed to be environmental protective if the river flow rate is high and
605 too strict to be technically achievable under low river flow conditions. This approach
606 can be improved by setting different permits for different flow regimes, however its
607 performance under low dilution ratio conditions is likely to be unsatisfactory and needs
608 to be addressed in future studies.

609 The means-based permitting, which prescribes the control scheme and settings
610 to be followed, is an unconventional regulatory approach especially for the wastewater
611 industry. However, this work suggests that it is actually a viable and more reasonable
612 approach for the regulation of integrated RTC than the traditional outcome focused
613 approach. Although the permitted RTC strategy is not likely to provide exactly the best
614 achievable results in all/most situations, the performance is still satisfactory. In the
615 case study of this work, the reliability can be over 80% if 10% of performance deviation
616 from the best achievable outcomes is allowed.

617 The upstream-based permitting provides more flexibility in system operation
618 (favorable to WWSPs) and less managerial burden to the regulators. For example, for
619 means-based permitting, there is a need to validate the accuracy of the integrated
620 UWWs model and the representativeness of the input datasets in permit development
621 and to carefully audit for the review of permit compliance. However, it is difficult to
622 predict the best achievable river water quality under the stochastic river dynamics. As
623 such, the upstream-based permitting is likely to pose a high risk to both the WWSPs
624 and the environment. By contrast, the uncertainty in the performance of the integrated
625 RTC technology is much lower. We found that the comparative performance of
626 different RTC strategies is subject to minor changes at different environmental
627 conditions, which is key to the reliable and robust performance of the means-based

628 permitting. By applying the proposed framework of permit development, a control
629 scheme that balances the different (even conflicting) environmental objectives and suit
630 the local needs can be identified and permitted. For practical implementation of the
631 means-based permitting, the prescribed control settings may be allowed to vary within
632 a limited range as proposed by prior studies²⁹, which needs to be carefully examined
633 and specified in the permit.

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643 **Supporting Information**

644 Definition of the case study site; formulation of operational cost; preliminary
645 assessment on the number of aeration tiers; If-Then control rules for the case study;
646 value ranges for operational variables; and settings of high performing control
647 strategies.

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