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Evaluation of Data-Driven and Process-Based Real-Time Flow Forecasting Techniques for Informing Operation of Surface Water Abstraction

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Abstract: This paper presents an approach to managing surface water abstraction utilizing real-time flow forecasting and control techniques. To evaluate the effectiveness of alternative data-driven and process-based methods, flow forecasts at a case study site (River Dove, UK) using (1) a probability-distributed rainfall-runoff model (PDM), (2) PDM coupled with an autoregressive integrated moving average (ARIMA) error predictor, and (3) a long short-term memory (LSTM) neural network are integrated into a water resources management model coupled with genetic algorithm optimization to simulate and compare water abstractions, reservoir storage, downstream river flows, and pumping energy costs. When compared to historical data, results show that both PDM plus ARIMA and LSTM forecasts led to improved water abstraction operations, i.e., increased water abstraction volumes during dry periods while maintaining river environmental flows, as well as reduced pumping costs. Cost savings were found to be sensitive to the accuracy of the forecasting technique only within specific flow ranges. This study demonstrates the water resource benefits of real-time flow forecasting in supporting flexible water pumping schedules and further discusses the benefits of alternative modeling approaches in the specific context of controlling water abstraction. **DOI: 10.1061/(ASCE)WR.1943-5452.0001397.** *This work is made available under the terms of the Creative Commons Attribution 4.0 International license, https://creativecommons.org/licenses/by/4.0/.*

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Introduction

Ensuring the resilience and security of water supplies will be one of the most significant challenges facing water utilities worldwide given the potential impacts of climate change and population growth (Cosgrove and Loucks 2015). Surface waters are important sources of drinking water supply, and in many catchments, abstractions from these sources are governed by environmental regulations with specific minimum so-called hands-off ecological river flows (Boddy et al. 2019). Current climate predictions suggest significant reductions in seasonal river flows in many regions (including the UK) over the next 40 years (IPCC 2014), making it increasingly difficult to maintain a balance between water supply and protection of the aquatic environment. The development of new water resource options (e.g., impoundments) is costly, so there is a need to develop techniques for maximizing the potential and resilience of existing water resource assets without compromising environmental regulations. Real-time data sets have been found to be increasingly valuable in many water management contexts to aid adaptive water management and to secure environmental flows in river basins (Ellison et al. 2019). However, surface water abstraction operations are not commonly supported by real-time data and river flow forecasts and as such operational (i.e., hourly to daily) abstraction decisions are frequently made conservatively to avoid breach of regulatory license conditions. As a result, many opportunities to sustainably abstract more water may be missed (Asfaw et al. 2016). Some studies have shown that the use of real-time data and river flow forecasts can provide better understanding of water availability in rivers and, hence, help make informed water abstraction decisions. For instance, Asfaw (2018) showed that the use of river flow forecasts in water abstraction management can help inform adaptive reservoir management policies that maintain appropriate balance between water supply and the environment. Ellison et al. (2019) also showed that real-time weather and flow data could be utilized to increase the capacity of stakeholders in agricultural catchments to make informed decisions to improve agricultural productions while considering environmental requirements, particularly in dry periods.

Another major challenge for water utilities is to supply clean water at minimum capital and operational cost. Approximately, 75% of operational costs of drinking water supply systems are attributed to energy use, and most of this energy is used for pumping water during abstraction, treatment, and distribution processes (Abkenar et al. 2015). One opportunity for reducing operational costs is by optimizing water pumping schedules by shifting operations to low electricity tariff periods. A genetic algorithm (GA) is a type of evolutionary optimization algorithm that has been increasingly used for this purpose. For instance, De Wrachien et al. (2017) used a GA to develop a framework for optimizing pump operations in complex water networks. Abkenar et al. (2015) evaluated

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GA using discrete and continuous methods for optimizing pump operations of water distribution systems. Moradi-Jalal et al. (2004) used a GA to develop a model for the optimal design and operation of water distribution networks. Fecarotta et al. (2018) used an optimization algorithm for optimal pump scheduling of urban drainage station under variable flow conditions. However, all of the aforementioned studies focused on optimizing operations within water distribution networks and drainage systems within which flows are well defined (e.g., with hydrodynamic models), and to date little focus has been given to problems associated with raw surface water abstraction systems (in which water availability is influenced by rainfall, hydrological processes, and local environmental regulations). Optimization of pump operations during surface water abstraction requires a detailed understanding of catchment hydrological processes and coordination of pump operations and anticipated costs with water availability in real time, hence the need for integration with real-time river flow forecasting models. Any such methodologies must also consider the resilience of water resource assets, site-specific operational rules, and environmental regulations (e.g., minimum flow requirements).

While hydrological modeling is commonly used in water resources management studies and system optimization, most studies in the literature focus on integrating long-term flow predictions and water resources management models for water resources planning and optimization of reservoir operational policy (e.g., Quinn et al. 2018; Canuto et al. 2019; Giuliani et al. 2019; Dong et al. 2020) over yearly or larger timescales. For example, Quinn et al. (2018) integrated synthetic streamflows (generated using Cholesky decomposition of resampled historical monthly flows) with a multireservoir optimization model to explore how changes in monsoonal dynamics and human pressures affected multireservoir operating policies for flood protection, hydropower, and agricultural water supply in the Red River basin in Vietnam over a period of 100 years using a monthly time step. Giuliani et al. (2019) integrated river flow forecasts (improved using states of global climate indexes such as Southern and North Atlantic Oscillations captured via a multivariate extreme learning machine method) and a reservoir optimization framework to assess the implications of improved flow forecasts on the reservoir operations of Lake Como in northern Italy over a period of 15 years and using a daily time step. Dong et al. (2020) coupled a hydrological model and a reservoir management scheme to study the implications of reservoir operating policies on the hydrologic regime of the Poyang Lake Basin in China over a period of 20 years and using a daily time step. Most of these studies used daily or monthly time resolutions of climate inputs and flow predictions and focused on studying long-term implications (over a period of 15 years or longer) of potential changes in climate and human pressures on water resources, with the aim of identifying robust operation policies and adaptive water resources management plans. To the best of the authors knowledge, optimization-based approaches have yet to be applied to abstraction management operations and control at subdaily temporal scales utilizing real-time data and models.

Different methods exist for real-time river flow forecasting; they can be broadly classified into process-based models and data-driven models. Process-based models simulate river flows of a catchment using physical or semiphysical equations that take account of various processes of the hydrologic cycle, while data-driven models can learn relationships between variables and relate inputs to outputs without a detailed understanding of the physical processes (Noori and Kalin 2016; Yaseen et al. 2016). An example of a process-based model is the probability-distributed rainfall-runoff model (PDM) (Moore 2007). Real-time flow forecasting in the PDM can be enhanced by complementing the model with forecast updating methods such as error prediction, which allows for the incorporation of information from the most recent flow observations. The PDM model has been widely used for real-time flow forecasting in various catchments across the world (e.g., Cabus 2008; Pechlivanidis et al. 2010; Liu et al. 2015). While process-based models can be efficient in forecasting river flows, their calibration is sometimes difficult due to the large, broad ranges, and complex interactions of model parameters. An alternative data-based method for river flow forecasting is artificial neural networks (ANNs) (Noori and Kalin 2016; Yaseen et al. 2016). A recent ANN method that has been used for river flow forecasting is the long short-term memory (LSTM) network (e.g., Le et al. 2019; Sudriani et al. 2019; Hu et al. 2020). An advantage of LSTM over other methods is its ability to learn long-term temporal dependencies in data, this has shown to provide accurate river flow forecasts. Hu et al. (2020) showed that the performance of a LSTM model in forecasting peak flows of small river catchments was better than other data-driven methods, such as support vector regression and multilayer perceptron. Couta et al. (2019) showed that the performance of LSTM was better than the performance of a process-based model (generalized watershed loading model) in forecasting river flows of the Jinghe catchment in China.

Both process- and data-driven modeling types can be prone to problems such as overfitting (i.e., adding unnecessary complexity) and underfitting (i.e., missing necessary details), which degrade a model's ability to explain or forecast data (Höge et al. 2018). For instance, including unnecessary physical equations or parameters in process-based models or adding unnecessary terms in data-driven models to improve model calibration can result in overfitting, meaning that the model can suffer from high flexibility and poor parameter identifiability with predictions exhibiting a large variance. In overfitting, the model will adapt itself too closely to training (within sample) data by fitting to noise (i.e., small training error). This reduces the model's ability to generalize to test (out-of-sample) data (i.e., large test error) (Hastie et al. 2008; Höge et al. 2018). In such cases, the model is likely to be unable to accurately predict flow patterns that are not well represented in the training data but are within the plausible ranges of natural variability. More incoming data (containing new information) can help reduce the risk of overfitting and ensure that the model has an appropriate predictive capability (Höge et al. 2018). On the other hand, in underfitting or oversimple models, the models can exhibit high bias between predictions and data and will also produce poor generalizations (Hastie et al. 2008; Höge et al. 2018). Ideally, therefore, models should be developed by trading off variance against bias in such a way that minimizes test error, and they should be evaluated based on performance which is related to the models' application (Jakeman et al. 2006).

Current applications and hence testing and evaluation of real-time river flow models mainly focus on flood forecasting and management (e.g., Seo et al. 2009; Rogelis and Werner 2018); little focus has been given to how such techniques could be used to support surface water abstraction management decisions. For this reason, studies of flow forecasting techniques often focus on the performance of various methods in predicting the arrival and magnitude of peak flows. However, real-time surface water abstraction decisions generally require flow forecasting capabilities which primarily focus on flow conditions ranging between minimum environmental flows and water abstraction capacity (Vaze et al. 2011).

The aim of this paper is to develop a novel technique for real-time surface water abstraction operation and to evaluate effectiveness when using different data-driven and process-based real-time flow forecasting models. This evaluation is conducted by testing the approach at a case study site (River Dove catchment, UK) during the period 2017–2018 (which includes a significant period of dry weather). The paper examines how the performance of the flow forecasting technique used influences the outputs of the surface water abstraction system with associated implications for operational decision-making. Flow forecasts from three different models are used and compared in this study; these inclue (1) PDM, (2) PDM coupled with an autoregressive integrated moving average (ARIMA) error predictor, and (3) LSTM.

The paper is organized as follows. The section "Methods" provides background on the case study catchment and describes the structure of the surface water abstraction technique and its different components. The section "Results" presents the results of the historical analysis conducted at the case study site. The implications of the developed methodology for water resource management are discussed in the section "Discussion." Finally, the section "Conclusion" presents the study's conclusions and discusses future work.

Methods

A retrospective analysis of the period 2017–2018 at the case study site was conducted where the optimal hourly pumping (i.e., water abstraction) schedule for each day within this period was sought. The resulting simulations of water abstraction volumes, reservoir storage levels, flows downstream of the abstraction point, and energy costs using flow forecasts from the three studied methods were compared with the corresponding historical observations of abstractions, reservoir storage levels, downstream river levels, and energy costs to investigate the implications for water resources management and the effectiveness of the approach and models used.

Study Area

The Dove catchment, located in the UK midlands, was used as a case study site for this study. The catchment drains an area of approximately 1,020 km^2 and includes Churnet, Tean, Manifold, and Hamps subcatchments. Its elevations range between 550 and 50 m above sea level from its source to its confluence. The River Dove is 72 km long and flows generally south to its confluence with River Trent. The catchment is predominantly rural, and pasture is the main agricultural use (Environment Agency 2014). An environment agency flow gauging station (Marston on Dove) is located at the outlet of the catchment. Water from River Dove is abstracted at a site downstream of the flow gauging station and stored in pumped storage reservoirs for water supply purposes. Pumps at the site are of fixed speed (i.e., they operate at a defined flow rate that is set to either on or off).

Fig. 1 shows the study area and locations of the flow gauging station and abstraction site. Composite radar rainfall data at temporal and spatial resolution of 5 min and 1 km^2 for the catchment during the period 2004–2018 were obtained from the UK Met Office (2003) and daily potential evaporation data were obtained from the UK Met Office's MORCES system (Hough and Jones 1997). Flow measurements at 15 min at the outlet of the catchment were obtained from UK Environment Agency for the same period (a total of 490,560 data points). These measurements were used for model calibration and validation. For all modeling approaches, the data set was split into 70% and 30% for calibration and validation, respectively (resulting in 343,392 points for calibration and 147,168 points for validation).

Model Structure

The surface water abstraction technique in this study is developed by integrating flow forecasting models with a water resources management model coupled with GA. Three alternate flow forecasting methods (described in the following sections) were configured and tested for predicting river flows of the Dove catchment at the abstraction site with a lead time of 24 h using flow observations, rainfall, and potential evapotranspiration (PET) observations up to the forecast origin over the full period of analysis (October 1, 2017–September 30, 2018). This lead time is used because it is the same as the catchment response time (lag time between the centroid of rainfall event and peak discharge in the catchment), so rainfall forecasts are not required to make flow predictions at the abstraction site. The 24-h forecasted flows from each method are then incorporated into the water resources management model, which represents the onsite catchment abstraction system in terms of conveyance infrastructure, abstraction license conditions, reservoir storage, water demand, and energy use plus associated costs. The water resources management model is coupled with a GA optimization that searches for the optimal pump schedule for the given 24-h period based on electricity tariff and site operational constraints (i.e., pump schedule that meets all operational constraints at the minimum cost). Fig. 2 shows a schematic of the methodology, and the following sections explain each component in detail.

Probability Distributed Rainfall-Runoff Model

The PDM (Moore 2007) is tested as a process-based model in this study for river flow forecasting. PDM is a conceptual rainfall-runoff model that transforms rainfall and PET data into river flows at the outlet of a catchment. The model uses a probability density function to characterize the variability of soil-moisture capacity in the catchment. Rainfall in the model is partitioned into direct runoff, groundwater recharge, and soil-moisture storage. Direct runoff is routed through a surface storage component that uses two linear reservoir cascades (O'Connor 1982) to calculate surface runoff. Groundwater recharge is routed through a subsurface storage component that uses a nonlinear storage model (Horton Izzard equation) (Dooge 1973) to calculate base flow. Total river basin flow then is calculated as the sum of surface runoff and base flow.

To drive the PDM model to simulate river flows, composite radar rainfall data between 2004 and 2018 with spatial and temporal resolutions of 1 km^2 and 5 min, respectively, along with PET data, from the UK Met Office, are used. The first year is used as a warm-up period for the model, and the remaining period was split into two parts, with 2005–2013 used for calibration and 2014–2018 used for model validation. To calibrate the model, a Markov chain Monte Carlo technique called DiffeRential Evolution Adaptive Metropolis (DREAM) (Vrugt 2016) is used to estimate the posterior probability distributions of model parameters and their optimal values. Further details of this method can be found in Asfaw et al. (2016).

Probability-Distributed Rainfall-Runoff Model with Error Predictor

The PDM in this study is also complemented by a forecast updating method based on an error prediction (Moore 2007). A feature of errors from conceptual rainfall-runoff models is that they tend to persist, forming a sequence of positive errors (overestimation) or negative errors (underestimation). This structure in the error sequence can be analyzed, and an error predictor can be developed for the prediction of future errors between simulated and observed flows. Predicted errors are then added to predictions of the deterministic rainfall-runoff model to provide an updated flow forecast. One of the most commonly used error predictors is the

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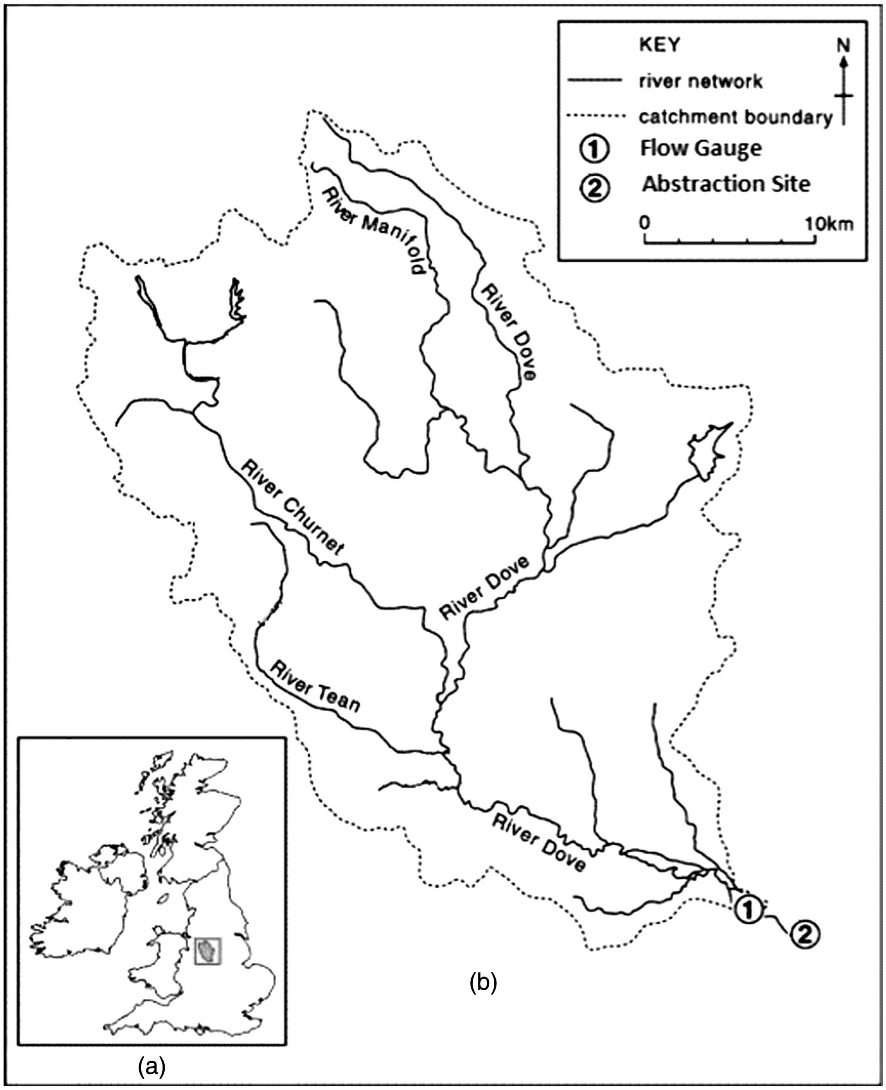


Fig. 1. Location of Dove catchment, Marston flow gauging station, and abstraction site. [Reprinted from Geomorphology, Vol. 47 (1), J.M. Goodson, A.M. Gurnell, P.G. Angold, and I.P. Morrissey, "Riparian seed banks along the lower River Dove, UK: their structure and ecological implications," pp. 45–60, © 2002, with permission from Elsevier.]

autoregressive integrated moving average (ARIMA) given in the following form [Eq. (1)]:

$$\varepsilon_t = c + \emptyset_1\varepsilon_{dt-1} + \emptyset_2\varepsilon_{dt-2} + \cdots + \emptyset_p\varepsilon_{dt-p} + \theta_1 a_{t-1} + \theta_2 a_{t-2} + \cdots + \theta_q a_{t-q} + a_t \quad (1)$$

where c is constant; $\varepsilon_{t-1}, \varepsilon_{t-2}, \ldots$ are the past errors between simulated and observed flow values; $a_{t-1}, a_{t-2}, \ldots$ are the past residual errors from a moving average model; $\emptyset$ and θ are coefficients; p is the number of autoregressive terms; d is the degree of differencing; and q is the order of moving average. The last three parameters are used for fitting the ARIMA model and usually denoted by ARIMA(p, q, d).

A third-order autoregressive model with one degree differencing and dependence on three past model errors (3,1,3) was found to be an appropriate choice for real-time flow forecasting of the Dove catchment with a lead time of 24 h (Moore 2007).

Artificial Neural Network

A data-driven methodology is also used in this study to forecast flows of River Dove, namely, the LSTM neural network. Generally, ANNs are able to identify relationships from a given pattern and hence relate input and output variables in a complex system. They consist of interconnected neurons that are organized based on a particular arrangement (Noori and Kalin 2016). For instance, a feedforward network has links connecting neurons from the input layer, through to one or more hidden layers, to an output layer (Dawson and Wilby 2001). Each link is assigned with a weight that represents the relative strength of corresponding neurons to predict the input-output relationships (Govindaraju and Ramachandra 2000). Another arrangement is that of recurrent neural networks (RNNs), which have a chainlike structure of repeating modules that are used as memory cells to store important information from previous processing steps (Le et al. 2019). Unlike feedforward networks, RNNs use feedback loops to feed information back from outputs to inputs of a previous layer (Kumar et al. 2004). This recursive structure allows RNNs to handle temporal dependencies between observations. One limitation of RNNs is their limited ability to learn long-term temporal dependencies due to the gradient vanishing problem over the long term (Kim et al. 2018). LSTM is a class of RNNs developed by Hochreiter and Schmidhuber (1997) to overcome the gradient problem in RNNs using memory

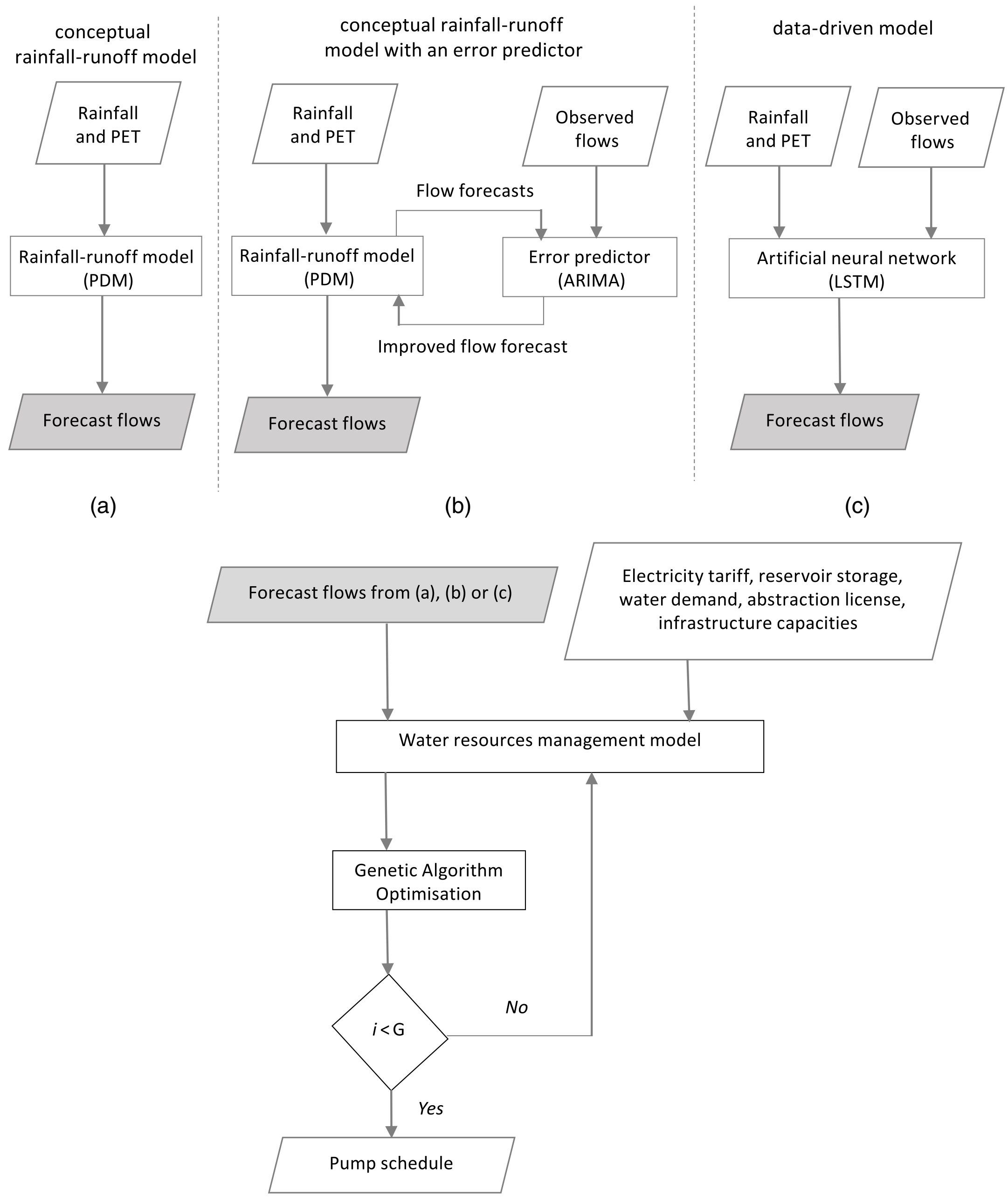


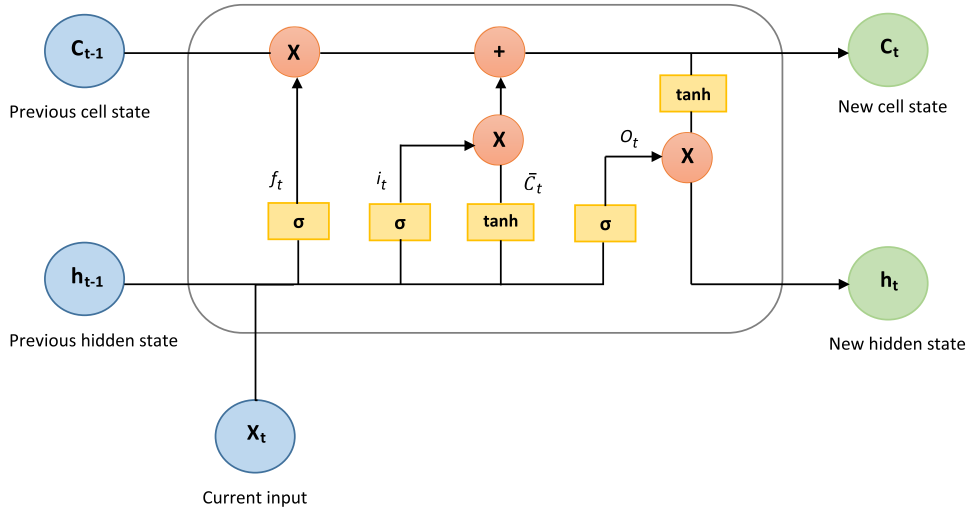
Fig. 2. Schematic diagram showing components of developed methodology for optimizing water abstractions and pumping operations based on forecasted river flows from process-based and data-driven models. G = total number of generations used in genetic algorithm; and i = iteration number.

cells and gates to regulate flows into and out of memory cells. Fig. 3 shows a typical LSTM network unit (Olah 2015). This structure of LSTM makes it possible to learn long-term dependencies in data for prolonged periods of time (Le et al. 2019). Further details about the architecture of LSTM networks and underlying equations can be found in Hochreiter and Schmidhuber (1997) and Le et al. (2019). Recent examples of the use of LSTM in hydrological applications can be found in Le et al. (2019), Sudriani et al. (2019), and Hu et al. (2020).

The LSTM neural network in this study consisted of three layers. The first two layers contained 50 neurons each, followed by an output layer. The LSTM network was trained using rainfall, PET, and flow data of the Dove catchment during the period 2005–2013. Development, training, and validation of the LSTM model was conducted using Keras [Python (version 3.7.3) deep learning library] (Chollet 2015). Training of the network focused on minimizing a loss function by updating weights: the loss function used in this study is the mean square error, and the adaptive moment optimization algorithm (ADAM) is used to minimize the loss. A batch size of 30 and 1,000 epochs was found to give the best performance for forecasting flows in the Dove catchment with a lead time of 24 h.

Flow Forecast Model Validation

Fig. 4 shows a sample of simulated and observed flows of River Dove at the Marston gauging station during the validation period for three different forecasting models: (1) PDM, (2) PDM and ARIMA, and (3) LSTM. Fig. 5 shows the corresponding empirical cumulative distribution function (ECDF) of the residuals between



$$f_t = \sigma(W_f[h_{t-1}, X_t] + b_f)$$
$$i_t = \sigma(W_i[h_{t-1}, X_t] + b_i)$$
$$\bar{C}_t = tanh(W_c[h_{t-1}, X_t] + b_n)$$
$$C_t = C_{t-1} f_t + \bar{C}_t i_t$$
$$O_t = \sigma(W_o[h_{t-1}, X_t] + b_o)$$
$$h_t = O_t tanh(C_t)$$

Where W and b are weights and bias vectors respectively for forget gate (f), input gate (i), candidate ($\bar{C}$), and output gate (O).

Fig. 3. LSTM neural network unit. [Adapted from Olah (2015).]

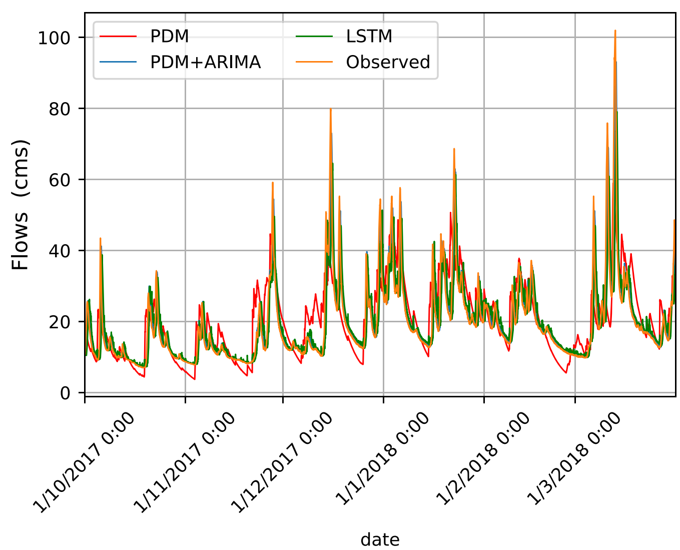


Fig. 4. Simulated flows of River Dove at Marston gauging station during validation period from PDM, PDM and ARIMA, and LSTM models compared to corresponding observed flows at 15-min time step.

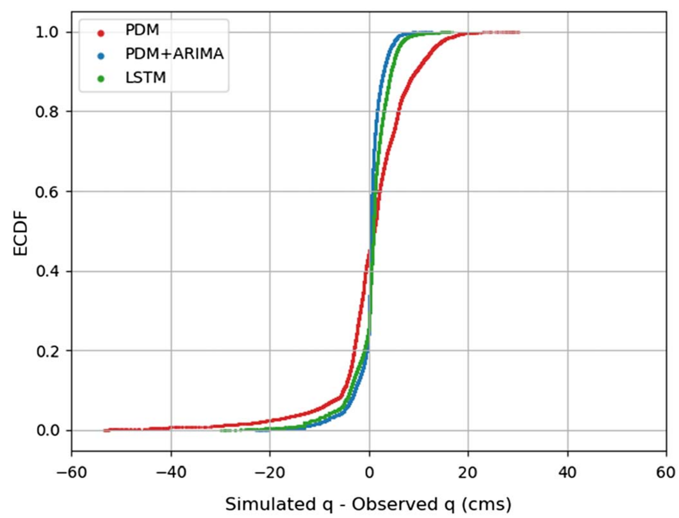


Fig. 5. Empirical cumulative distribution function (ECDF) of difference between simulated and observed flows (residuals) of River Dove during validation period.

simulated and observed flows from the three models. These results suggest that variation between simulated and observed flows is greater in the PDM-only model compared to variations for the PDM coupled with ARIMA and LSTM models. Nash Sutcliffe efficiency (NSE) values for the PDM plus ARIMA model and the LSTM model during the validation period (2014–2018) (i.e., out-of-sample data) were greater than 0.90, suggesting a good performance of these models when representing flows in the Dove at the outlet of the catchment (Moriasi et al. 2007). A similar performance was reported by Fan et al. (2020) and Kratzert et al. (2018) showing that ANN models can provide comparable results to conceptual rainfall-runoff models in forecasting river flows. On the other hand, the NSE value for the PDM only model during validation period (2014–2018) was 0.65. This demonstrates the significant improvements in the performance of PDM when the model is coupled with ARIMA. Similar results were reported by Liu et al. (2015), which showed that when NSE values are relatively low (e.g., NSE $\leq$ 0.65), there is sufficient room for ARIMA to update flow forecasts and improve performance. To further check the model performance on unseen data, a k-fold cross validation with $k = 4$ (9 years for calibration and 3 years for validation) is used to evaluate the capabilities of the three forecasting models in reproducing flows at the outlet of the catchment. The values of the NSE coefficient for all folds using PDM coupled with ARIMA and LSTM ranged from 0.84–0.92 and 0.82–0.91 during calibration and validation, respectively. On the other hand, the NSE coefficient for the PDM-only model ranged from 0.66–0.72 and 0.62–0.66 during calibration and validation, respectively. The NSE values during validation showed patterns similar to those of the NSE values during calibration for all three forecasting models. These results suggest the ability of both PDM coupled with ARIMA and LSTM models to predict out-of-sample data satisfactorily, and hence that the models are not overfitted.

It is worth mentioning that all models in this study underestimated some peak flows. However, in this study, the predictions of service flows (the range between minimum environmental flow and the maximum capacity of the abstraction pumping infrastructure) are of greater significance because the focus of this study is to inform water abstraction management decisions. Further evaluation of the different techniques in the context of abstraction systems therefore requires coupling of the forecasting methods to a water resources management model such that the performance in terms of cost savings and resource efficiency can be quantified over the full analysis period.

Water Resources Management Model

Forecasted flows from each of the forecasting models are incorporated into a water resources management model coupled with GA optimization. The water resources management model uses an hourly on/off pump schedule for each 24-h period, generated by the GA (see the following section), to calculate water abstraction volume, and the model then subsequently calculates resulting corresponding reservoir storage levels, residual river flows to the downstream of the abstraction point, energy requirements, and associated costs. This is calculated based on an hourly time step with resulting outputs aggregated over each 24-h period. For a time step (t) of each 24-h period, water available for abstraction (A_t) is calculated based on forecasted flow at time t (Q_t) and regulatory minimum flow requirement ($Q_{\min}$) [Eq. (2)]

$$A_t = \begin{cases} 0 & Q_t \leq Q_{\min} \\ Q_t - Q_{\min} & Q_t > Q_{\min} \end{cases} \tag{2}$$

Abstraction of water from the river (S_t) is then constrained by an intake capacity (C_{Intake}) and reservoir capacity ($C_{\text{Reservoir}}$) [Eq. (3)]

$$S_t = \min(A_t, C_{\text{Intake}}, C_{\text{Reservoir}} - R_{t-1}) \tag{3}$$

where R_{t-1} is reservoir storage at the previous time step; and $C_{\text{Reservoir}} - R_{t-1}$ is the free volume present in the reservoir. Then volume in the storage reservoir at each time step (R_t) is calculated using Eq. (4), where D_t is water demand at time t

$$R_t = R_{t-1} + S_t - D_t \tag{4}$$

The energy required for pumping water into the reservoir (E_t) is calculated using Eq. (5)

$$E_t = (\rho S_t g H)/\delta \tag{5}$$

where ρ = water density; g = gravitational acceleration constant; H = head (fixed based on site data); and δ = pump efficiency. The cost of pumping water at each time step (Z_t) is calculated by multiplying E_t by the corresponding electricity tariff (P_t) [Eq. (6)]

$$Z_t = E_t \times P_t \tag{6}$$

The daily volume of water abstracted is then calculated by summing all water abstraction volumes during the 24-h lead time [Eq. (7)]

$$S = \sum_{t=1}^{24} S_t \tag{7}$$

Similarly, the daily energy cost for pumping water is calculated using Eq. (8)

$$Z = \sum_{t=1}^{24} Z_t \tag{8}$$

Reservoir storage is calculated at each time step based on historical water demand data, water abstraction from the river, and operational constraints. Water abstraction from the river is constrained by intake capacity [250 Million Litres/day (Ml/day)] and total storage capacity (19,845 m^3).

The study used historical water demand and electricity tariff data during the 2017–2018 period as provided by the water utility. The electricity tariff can vary on an hourly basis, with times between 16:00 and 19:00 generally being most expensive. The implementation of this methodology is therefore dependent on knowledge of the electricity tariff and anticipated water demand over the forecast lead time. In the UK such anticipated price tariff information is supplied to industrial users in advance (Watson and Rai 2013). Water utilities also commonly utilize water demand models to predict usage over similar periods (Romano and Kapelan 2014).

The water resources management model is coupled with GA optimization, which involves searching for the optimal pump schedule (from a solution space of 2^{24} possible pump schedules) using an objective function to minimize energy plus GA penalty costs (see subsequent discussion) within the 24-h period (Z_{mod}) while also considering the site operational constraints and water resource requirements.

Genetic Algorithm for Optimizing Pump Operations

A GA is an evolutionary optimization method that has been used by many different researchers (Abkenar et al. 2015; Wang et al. 2009; De Wrachien et al. 2017) for optimizing water pump operations. A feature of evolutionary optimization methods is that they are able to find optimal solutions from a large solution space by evaluating a relatively small group of potential solutions (Abkenar et al. 2015). This is most likely because these methods use stochastic operators, such as crossover and mutation, that are less likely restrict searches to a local optimum compared to traditional optimization methods, which depend on the existence and continuity of the derivative of a loss function (Simpson et al. 1994).

In GAs, a random group of solutions is first created to form the initial population. In this case, each candidate solution is a 24-bit binary string (chromosome) with ones and zeros corresponding to hourly pump on and off conditions, respectively. The GA is used to determine a single pump schedule over 24 h, so the solution space consists of 2^{24} possible solutions.

Under the initial generation, a GA randomly selects two solutions (parents), and each iteration applies crossover and mutation processes to generate new solutions with modified chromosomes (children). A group of best solutions (children) is then selected from a current generation to form a subsequent generation. Repeating these processes over a given number of generations, the GA moves toward an optimal solution (i.e., pump schedule that meets all operational constraints at minimum cost). In this model, the GA used probabilities for crossover and mutation of 0.65 and 0.15, respectively. With a population size of 2,000 pump schedules, the GA would stop when 400 generations were produced without a significant increase in fitness or after reaching a total of 800 generations. Approximately, optimal solutions were converged to in under 50 generations (see convergence plot in the Supplemental Materials, which demonstrates the performance of the GA over its run time). The final pumping schedule reported by the GA in this application is the best pumping schedule found during the optimization process.

The optimization algorithm in this study has different operational water resource targets for the winter and summer seasons. During winter (October 1–April 1), the algorithm attempts to fill the reservoir up to 95% of its total capacity (according to the current water abstraction protocol of the water utility) by the end of the season. This is done by calculating the change in reservoir storage during the 24-h period (ΔR) and comparing it to a daily target of increase in reservoir storage (μ) estimated based on the need to fill the reservoir up to 95% of its capacity by April 1. A penalty value (u) is added to the daily cost of pumping (Z) for solutions that result in ΔR being less than μ [Eq. (9)]

$$Z_{mod} = \begin{cases} Z + u & \Delta R < \mu \\ Z & \text{otherwise} \end{cases} \tag{9}$$

The GA is set to minimize the total daily cost, including any penalties (Z_{mod}), so the use of the penalty value will reduce the chances that the method will select a solution that violates the daily filling target ($\Delta R > \mu$). The value of u is directly proportional to the difference between $\bar{R}$ and μ. This ensures that the GA will always prioritize solutions that increase reservoir storage volumes during this period.

During summer (April 1–September 30), the algorithm attempts to maintain storage levels above a predefined reservoir control curve while also matching abstraction to daily water demand. The reservoir control curve defines the storage volumes that must be maintained to ensure a reliable water supply to meet water demand and that are predefined by the water utility. Penalty values are added to the cost of solutions that violate any of these requirements during the summer period and, hence, reduce the chances of selection by the GA [Eq. (10)]

$$Z_{mod} = \begin{cases} Z + u_r + u_d & R_t < R_{\text{control}} \text{ or DS} < 1 \\ Z & \text{otherwise} \end{cases} \tag{10}$$

where R_{control} is the corresponding reservoir storage volume based on the reservoir operational control curve; DS is water demand satisfaction calculated by dividing the estimated amount of supplied water by the actual water demand; u_r is a penalty value added when the reservoir level falls below the control curve; and u_d is a penalty value added when DS < 1. If the summer targets are met, no penalty values are added (u_r and u_d are both equal to zero). The value of u_r increases linearly as the difference between R_t and R_{control} increases, and the value of u_d increases linearly as the DS value decreases. This ensures that the GA will prioritize solutions that are closer to meeting summer resource targets (i.e., solutions that result in the highest reservoir storage levels and water demand satisfaction).

Results

Fig. 6(a) shows simulations of daily water abstractions from River Dove for the analysis period based on the results of the GA informed by flow forecasts using (1) PDM, (2) PDM coupled with ARIMA, and (3) the LSTM model compared with historical water abstraction volumes, and Fig. 6(b) shows the corresponding missed water volumes (i.e., difference between simulated and observed water abstractions) based on the three forecasting methods. Generally, simulated water abstraction volumes were found to be approximately at intake capacity during October–November. Then water volumes slightly dropped until May, possibly due to more expensive electricity rates, which resulted in turning off pumps more frequently to avoid high costs. During the period from June to September, water abstraction volumes fluctuated owing to reduced river water availability above the specified minimum environmental flows.

Simulated water abstractions resulting from the three flow forecasting methods were generally greater than observed abstractions during the period October–May. Occasionally, observed water abstractions were greater than simulated abstractions, which might be because the GA suggested turning off pumps during high tariff periods, thereby resulting in relatively less water abstraction from the river. Simulation results suggest that on average 25 Ml/day of additional water would have been abstracted during the period October–May if any of the three flow forecasting methods had been used based on the difference between observed and GA-simulated abstraction values. During the summer period (June–September), underestimation of flows by the PDM-only approach resulted in

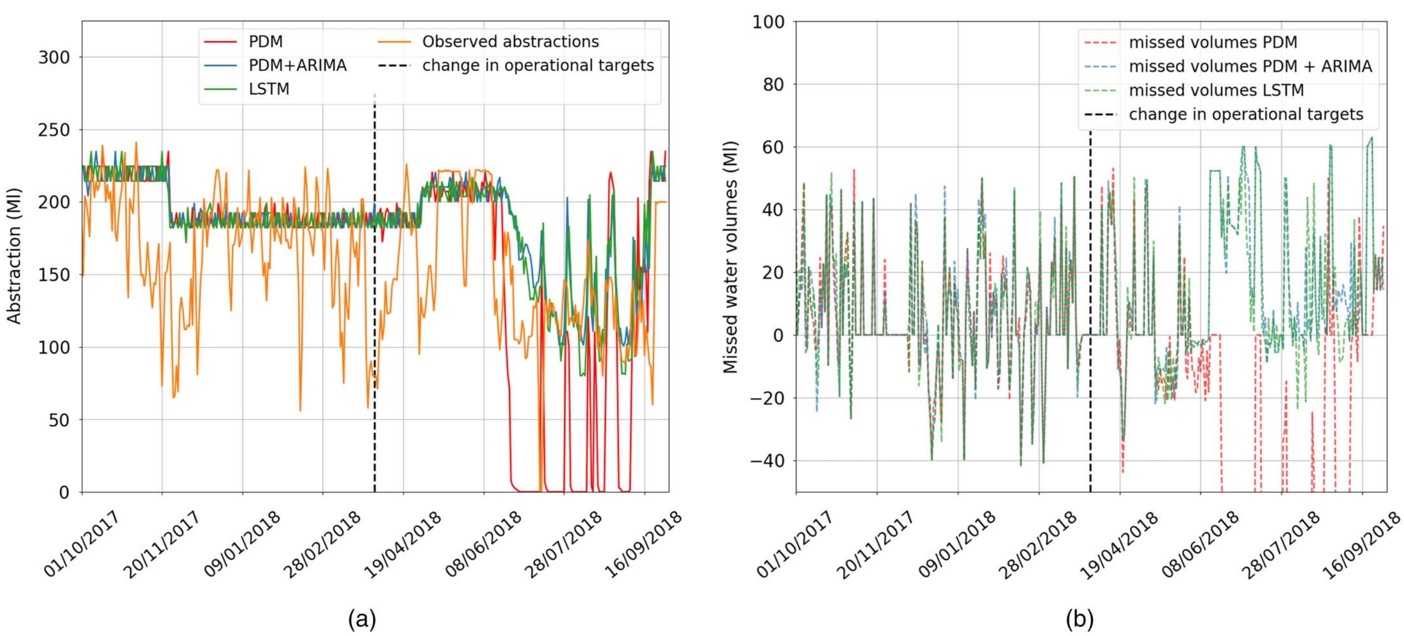


Fig. 6. (a) Simulated daily water abstraction resulting from optimization algorithm using PDM, PDM coupled with ARIMA, and LSTM models compared to actual abstractions from River Dove; and (b) corresponding missed water volumes (i.e., difference between simulated and observed) during historical period 2017–2018. Change in water resources operational targets occurs on April 1.

the optimization algorithm suggesting no abstractions most of the time, likely because of the need to satisfy the minimum river flow requirement. More accurate flow forecasts by both PDM coupled with ARIMA and by LSTM models allowed additional water volumes (on average 25 Ml/day) to be abstracted during the June–September period without breaching minimum flow regulations when compared to historical values. Intermittent periods of higher abstraction proposed by these simulations during the dry summer periods suggest that the method successfully identifies opportunities for increased abstraction during short periods of higher river flow.

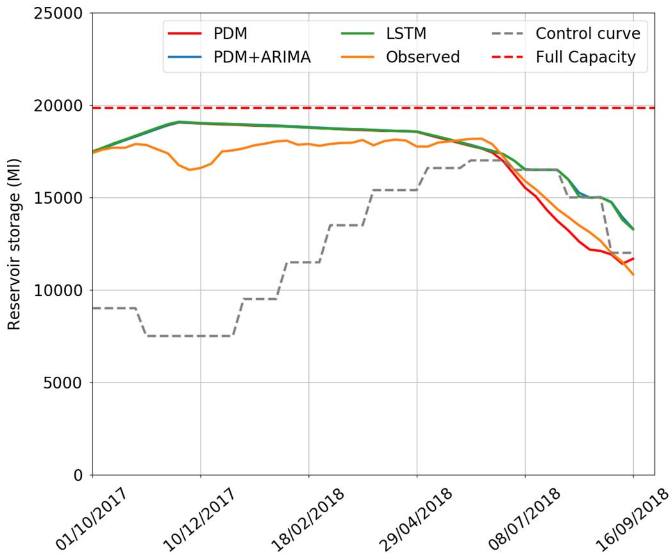
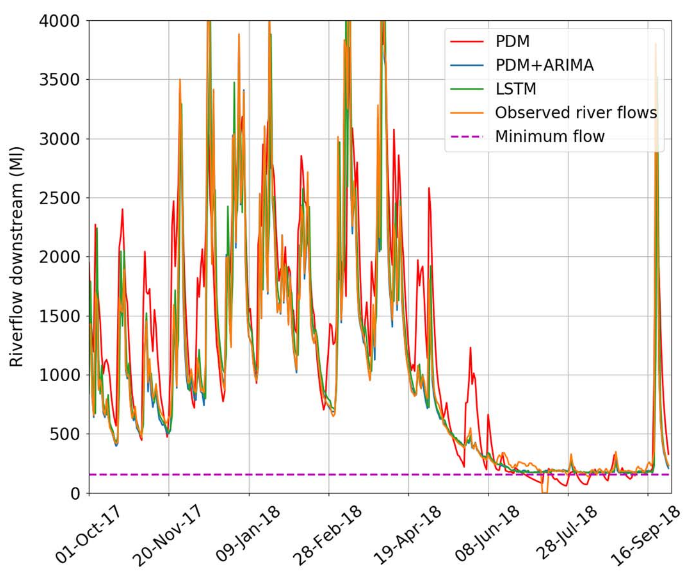


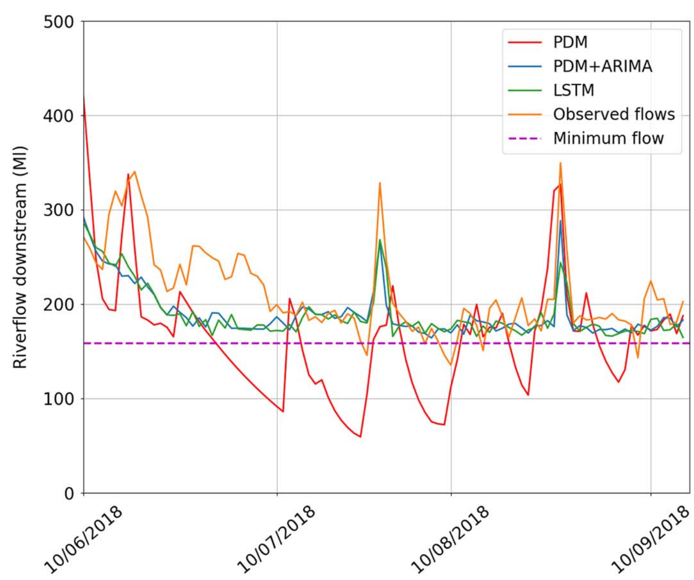
Fig. 7. Simulated reservoir storage levels from optimization algorithm using PDM, PDM coupled with ARIMA, and LSTM models compared to actual storage levels and operational curve during period 2017–2018.

Fig. 7 shows a comparison of simulated reservoir storage levels resulting from running the model with flow forecasts from PDM, PDM coupled with ARIMA, and LSTM models together with historical reservoir storage levels and the operational control curve. Simulation results from the three flow forecasting techniques suggest that the reservoir could have been filled with 600 Ml (equivalent to 3% of its total capacity) of additional water by the start of summer if any flow forecasting scheme had been used. During summer, rapid declines in reservoir storage levels, which cause levels to fall below the control curve, could have been avoided using flow forecasts of PDM coupled with ARIMA or LSTM models. On the other hand, underestimation of flows during the low-flow periods by the PDM-only model resulted in insufficient abstraction and, hence, reservoir levels dropping below the control curve.

Fig. 8(a) shows a comparison of simulated flows in River Dove downstream of the abstraction point resulting from running the optimization algorithm using flow forecasts of the three different techniques—PDM, PDM coupled with ARIMA, and LSTM—together with observed historical flows downstream of the abstraction point and regulatory minimum flow requirement of 159 Ml/day. The figure suggests insignificant differences in the performance of GA during winter for the three flow forecasting methods. However, the accuracy of flow forecasts has a significant impact on the performance of the GA during the low-flow period between June and September [Fig. 8(b)]. During this period, underestimation of low flows by the PDM-only model resulted in simulated river flows downstream of the abstraction point falling below the minimum flow requirement. However, more accurate forecasts by the PDM coupled with ARIMA and LSTM models resulted in simulated river flows being below the actual flows (due to increased abstractions) but above the minimum flow requirement, suggesting additional water (2,500 Ml) could have been abstracted during the low-flow period without breach of environmental license conditions. The analysis shows that opportunities to sustainably abstract more water during the low-flow period have been missed approximately 75% of the time.



(a)



(b)

Fig. 8. Simulated flows of River Dove downstream of abstraction point resulting from optimization algorithm using flow forecast from PDM, PDM coupled with ARIMA, and LSTM models compared with actual observations (a) during historical period October 2017–September 2018; and (b) during low-flow period (June–September).

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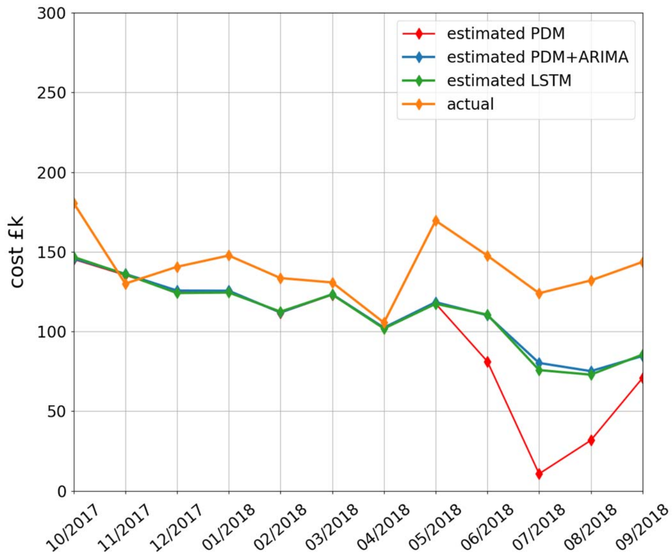

Fig. 9. Monthly estimated pumping costs (GBP £ ,000) resulting from optimization algorithm using flow forecast from PDM, PDM coupled with ARIMA, and LSTM models compared with actual costs during historical period October 2017–September 2018.

Fig. 9 shows estimated (modeled) pumping costs resulting from implementing the optimization algorithm using flow forecasts of PDM, PDM coupled with ARIMA, and LSTM models compared to actual historical energy costs. This figure suggests a possible cost savings of approximately £0.35 million for this site per annum if flow forecasts from PDM coupled with ARIMA or LSTM models were used in the optimization algorithm. This is due to the optimization algorithm's successfully avoiding pumping during high electricity tariff periods where operational constraints at the site allowed this. The figure also shows that during summer the cost savings per month were higher, suggesting that the optimization algorithm led to higher savings when balancing all water resource requirements (i.e., water demand, reservoir storage, and minimum river flow requirements) while also considering energy costs. Hence, more accurate flow predictions (using PDM coupled with ARIMA or LSTM models) during dry/summer periods allowed improved coordination of pump operations (and energy use) with water availability in real time, compared to both historical performance and the decisions made by the GA based on flow forecasts of PDM only. Inaccurate flow forecasts from the PDM-only model resulted in lower energy costs because of decisions by the optimization algorithm to switch off pumps due to insufficient predicted water in the river for abstraction. This further highlights the importance of including periods of low flow in hydrological model calibration/training and validation data sets when applied in the context of informing water abstraction operations.

Discussion

Though it should be noted that day-to-day operational abstraction decisions may be influenced by a greater range of factors than can fully be accounted for in the proposed approach, when compared to historical records simulation results based on flow forecasts from PDM coupled with ARIMA and LSTM models suggest that the developed technique for surface water abstraction has the potential to increase water abstraction volumes (on average 25 Ml/day of additional water) without compromising environmental licenses and significantly reducing operational costs at the case study site (≈ 20% per annum). Simulation results suggested that opportunities to abstract more water, especially during dry periods such as the one in 2018, can have significant impacts in terms of raising reservoir levels and avoiding the need to trigger drought management actions. Such opportunities to abstract more water sustainably by taking better advantage of short periods of increased river flows and increased reservoir levels can help maintain the supply–demand balance during droughts and, hence, contribute to improving resilience against such events. This in turn increases the potential of existing water supply systems and also reduces the need for future investments associated with developing new water resources (estimated at £1 million/Ml/day of water in the UK) (OFWAT 2015).

Simulation results showed comparable performance of the GA during winter (October–April) for all three flow forecasting methods, suggesting that the algorithm is less sensitive to the accuracy of flow forecasts during wetter seasons. This is because there always tends to be sufficient water in the river during winter to meet both demand and environmental requirements, so the optimization becomes less sensitive to the accuracy of the flow forecast. Setting the appropriate abstraction schedule during this period mainly constitutes a balance between storage targets and pumping costs. Results at the case study site demonstrate some energy cost savings (10%) from the proposed method when compared to observed data as well as minor differences in stored water levels. However, during the dry season (May–September), the GA methodology based on the PDM-only flow forecast failed to abstract sufficient water to maintain storage levels owing to less accurate predictions of flows compared to the other two forecast models (PDM coupled with ARIMA and LSTM model). This highlights that the performance of a flow forecasting technique has a significant impact on decisions made by the optimization algorithm during low-flow periods and, hence, operational pumping costs. During this period, the available flow in the river becomes a more relevant constraint, meaning the performance of the methodology is sensitive to the accuracy of the flow forecast. Overestimation of flows when river levels are close to the minimum flow requirement can result in the GA's suggesting abstraction of water while in reality there is no water available for abstraction. Similarly, underestimation of flows can result in the GA's suggesting small abstractions when in fact water is available and could be used to offset water demand or fill reservoirs. Cost savings and increases to abstraction volumes are also more significant in summer/dry periods due to the GA's ability to more effectively balance storage, cost, and environmental targets than traditional techniques, for example, by taking better advantage of short periods of increased river flow forecasts by the PDM and ARIMA or ANN methods.

When considering the relative merits of different modeling approaches, the work highlights the value of considering the end-use application within any evaluation, rather than simply considering the accuracy of predictions in isolation. That is, the value of the model should be considered in light of its ability to answer the *question of interest to the user*, as discussed in Minsky (1965). For example, within this study, all the hydrological models underestimated peak flows. This might be because climatic inputs in this study are averaged over the catchment, so rainfall and evaporation data used in the hydrological models might have contained bias that propagated into streamflow forecasts. This could possibly be addressed by increasing complexity, such as through the use of bias-correction methods (e.g., quantile mapping or generalized linear models) to reduce bias (Zhang et al. 2015).

However, as previously discussed, during high flows water abstraction operations and resulting cost efficiencies at the site are largely insensitive to the accuracy of flow forecasts (as a result of the pump's capacity being lower than the water available in the river). During the summer/dry months, the PDM and ARIMA or LSTM methods were observed to have a similar accuracy ($NSE \geq 0.90$) and demonstrated a predictive capability sufficient for modeling purposes to inform water abstraction decision-making during the analysis period and preserve environmental flows. Only slight differences were observed in the performance of the GA based on the PDM coupled with ARIMA and LSTM flow forecasting models (e.g., predictions of annual energy costs within 0.30%). This may be attributed to (1) the availability of considerable amounts of informative data for this catchment (i.e., including periods of low flows); and (2) a lack of significant changes to the hydrological system during the period covered by the forecast model.

Hence, when considering the relative merits of data-driven versus process-based models in the context of water resources management, the usefulness of the model should not be merely measured by its methodological correctness and accuracy but should also consider the degree to which it can help water managers and decision makers (Solomathine and Ostfeld 2008) and potential transferability to alternate catchments. The water resources application sought in this study is concerned with the estimation of total volumes of water at the outlet of the catchment, with service flows (the range between the minimum river flow requirement and the capacity of the abstraction site) being of particular interest. Hence, detailed understanding of hydrological processes (as provided by process-based models) are not strictly required. Within this catchment, results indicate that the data-driven model (LSTM) is able to capture service flows and deliver predictive performance that is equal to the performance of the process-based model (PDM coupled with ARIMA), and only slight differences in the performance of the GA based on the two flow forecasting techniques are observed. This demonstrates the capabilities of data-driven models in this context and the potential value of such models in informing operational decision-making concerning water abstraction. However, within this study, sufficient data were available for a detailed calibration and validation (including over low-flow periods). A potential risk in both process-based and data-driven models in catchments where data is limited is that they converge to a model that is apparently true based on the limited available data but that may not be able to constrain predictions to a plausible range (Höge et al. 2018). Further investigations in scenarios with more limited data sets are required to ensure the robustness of these methods against future uncertainties and to check the predictive capabilities of PDM plus ARIMA and LSTM in more data-scarce environments. A validation of the applicability of the LSTM model compared to process-based models in a wider variety of catchments is also required (i.e., transferability of the LSTM model to other catchments).

Another factor that can influence the model selection process is the computational time required for model calibration. The calibration of process-based models is sometimes more challenging due to complex interactions between parameters. Coupling a process-based rainfall-runoff model with an error prediction method to update flow forecasts increases the number of parameters requiring calibration and, hence, significantly increases computational times. For example, calibrating the PDM coupled with ARIMA using the calibration data set (2005–2013) can take up to 1 day using a standard PC. The LSTM model tends to require shorter computational times for calibration (up to 8 h). Model comparison in this context could be further extended by generating multiple working hypotheses of each modeling type with varying complexities (Khatami et al. 2019) and evaluating models based on model selection criteria that aim to find the model of optimal complexity (optimal trade-off between goodness of fit and model complexity) for a given modeling goal (Höge et al. 2018).

It should also be noted that the optimization algorithm in this study is developed based on a catchment with a time of concentration of approximately 24 h. Implementing the optimization algorithm on catchments with different times of concentrations may require different configurations of the flow forecasting schemes, water demand and energy price information, and the adjustment of forecast lead time and duration of pump schedule accordingly. There is further potential to develop systems for pump schedule optimization based on longer lead times via the incorporation of radar rainfall predictions; however, more work is needed to understand how increased uncertainties associated with rainfall forecasts could be accounted for in such methods (Nguyen and Bae 2019; Tian et al. 2019).

One limitation of this study is that time encoding of the pump schedule is simplified as 24-bit binary string with all site pumps able to be turned on and off sharply at the start of each hour. In more complex operations, a more practical encoding of the pump schedule may be required that would allow for a flexible start and end of each site pump's duty cycle. Moreover, the investigation in this study is limited to fixed speed pumps. The incorporation of variable-speed pumps into the problem will require adjusting the solution array to include information about the rotational speed of pumps. The technique described here can be further developed via the use of continuous encoding methods that use pairs of genes to indicate the start and end of each pump's duty cycle (Abkenar et al. 2015; Wang et al. 2009), or genes in the solution array could include fractional numbers between the minimum speed ratio of each pump and 1 (fully on) instead of binary on and off conditions. However, these options are likely to considerably increase the size of the solution space together with convergence times (Abkenar et al. 2015). This study could also be extended by expanding the search space to explore time-adapting schedules (i.e., different pumping schedules through the year) and, hence, assess how seasonally varying schedules impact water resource operations.

In this study, water resources management is considered based on a fixed environmental flow. New reforms in surface water abstraction management may introduce more robust environmental flow designations, including interannual variation in environmental flows to improve the balance between ecological requirements and water demand (DEFRA 2019). Some studies (e.g., Hough et al. 2019) have shown that varying environmental flows throughout the year can improve ecological function while also increasing the overall volume of water available for use. Hence, the use of such optimization algorithms in light of such designations may further improve the resilience of water supply systems.

The developed optimization algorithm could also be linked to water quality models that are able to forecast short-term fluctuations of pollutant loads in surface water (e.g., Asfaw et al. 2018). This could enable coordination of pump operations with water availability and water quality in real time while also considering energy costs, hence providing a more comprehensive tool for infrastructure operators to manage surface water abstractions. It is also anticipated that such methodologies will be of increasing relevance under more flexible electricity systems (i.e., more decentralized energy generations, renewable energy, and electricity storage) with a larger variability in energy availability and corresponding periods of surplus, low-cost energy supplies.

Future work may also extend the approach to enable optimization of pumping and water release operations in multireservoir systems. This can include a multiobjective optimization algorithms coupled with real-time models and environmental data to help inform coordinated multipurpose operations of reservoir systems that consider various factors, such as flood control, water supply, and environmental requirements, along with energy costs. Most current studies in the literature pertaining to the optimization of operations of multireservoir systems focus on restoring flows for downstream ecosystems (e.g., Mao et al. 2016) or maximizing the potential of hydropower generation (e.g., Anand et al. 2018; Ahmadianfar et al. 2019).

Conclusion

This work compared the ability of different real-time flow forecasting techniques to improve subdaily raw water abstraction operations. A novel technique for surface water abstraction was developed for this purpose by integrating river flow forecasting, a water resources management model, and a genetic optimization algorithm. Using the developed algorithm, a retrospective analysis for the study period (2017–2018) was conducted comparing historical water abstractions, reservoir storage levels, river flows downstream of the abstraction point, and energy costs with simulations based on river flow forecasts from three different forecasting methods. The methods for flow forecasting in this study included process-based models (PDM rainfall-runoff model only and PDM rainfall-runoff model coupled with ARIMA) and a data-driven (LSTM) model. Comparison of results from the three forecasting techniques suggested that the performance of flow forecasting has significant impacts on the decisions made by the water abstraction model during low-flow periods where water availability is a key constraint. PDM coupled with ARIMA and LSTM models showed comparable accuracy in forecasting river flows at the outlet of the catchment, which was significantly better than the performance of PDM only. Simulation results showed that the GA-based technique has the potential to significantly increase water abstraction volumes and reduce operational energy costs without compromising environmental licenses at similar sites, in particular by taking advantage of short-term periods of elevated river flow. This suggests the benefits of utilizing real-time flow forecasting and flexible water pumping schedules to maximize the value of existing surface water resources, and in some cases this may reduce the need for significant investment to increase the resilience of supply. The study also suggested that real-time data-driven models can have a predictive performance similar to that of process-based models in this context, illustrating their potential value in informing operational decision-making concerning water abstraction. Live operational testing of the modeling-led abstraction methods at a range of sites is required to fully validate the approach and robustly quantify the potential of the technique to increase supply resilience and lower energy costs.

Data Availability Statement

Some or all data, models, or code generated or used during the study are proprietary or confidential in nature and may be provided only with restrictions (e.g., anonymized data). Please contact the corresponding author for further details.

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Supplemental Materials

Fig. S1 is available online in the ASCE Library (www.ascelibrary.org).

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