Mapping of heavy metal pollution in river water at daily time-scale using spatio-temporal fusion of MODIS-Aqua and Landsat satellite imageries

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Abstract

For river water quality monitoring at 30m×1-day spatio-temporal scales, a spatial and temporal adaptive reflectance fusion model (STARFM) is developed for estimating turbidity (T_u), total suspended solid (TSS), and six heavy metals (HV) of iron, zinc, copper, chromium, lead and cadmium, by blending the Moderate-Resolution Imaging Spectroradiometer (MODIS) and Landsat (L_s) spectral bands. A combination of regression analysis and genetic algorithm (GA) techniques are applied to develop spectral relationships between T_u - L_s , TSS- T_u , and each HV-TSS. The STARFM algorithm and all the developed relationship models are evaluated satisfactorily by various performance evaluation measures to develop heavy metal pollution index-based vulnerability maps at 1-km resolution in the Brahmani River in eastern India. The Monte-Carlo simulation based analysis of the developed formulations reveals that the uncertainty in estimating Zn and Cd is the minimum (1.04%) and the maximum (5.05%), respectively. Hence, the remote sensing based approach developed herein can effectively be used in many world rivers for real-time monitoring of heavy metal pollution.

Keywords: Heavy metal; Landsat; MODIS; Pollution; STARFM; Turbidity

1. Introduction

For environmental water pollution assessment in the river system and its source management, measurement of water quality parameters at fine spatio-temporal scales is of utmost importance now-a-days. However, the conventional methods of laboratory testing and digital in-situ sensing methods are costly, time consuming and tiresome procedures; especially at fine spatio-temporal scale (Schoellhamer, 1996). Conversely, several researchers have tested the capability of remote sensing methods as an alternative to estimate the water quality parameters (Dewidar and Khedr, 2005).

Unlike total suspended solids (TSS) and turbidity (T_u), most heavy metal pollutants do not have direct impact on the optical properties of water; however, their distributions influence the surrogate properties of water, viz., chlorophyll, pH, temperature, TSS and T_u (Ritchie et al., 2003; Ritchie and Cooper, 2001). Generally, the transportation and distribution of heavy metals occur along with the suspended particles, especially, the fine particles, due to their binding capacity (Yuan et al., 2001), surface area and high cation exchange capacity (Liebens, 2001; Ujevic et al., 2000). Therefore, the concentration of TSS can be used to indirectly assess the heavy metal (HV) concentrations in the water body (e.g., Herngren et al., 2005; Hallberg et al., 2007). Similarly, turbidity is the most efficient measurement of TSS in natural rivers (Christensen et al., 2001; Schwarz et al., 2011; Stubblefield et al., 2007; Ginting and Mamo, 2006; Loperfido et al., 2010; Navratil et al., 2011; Rügner et al., 2013, 2014). Hence, the heavy metal concentrations can be indirectly estimated using the HV-TSS and TSS- T_u relationships (Nasrabadi et al., 2016).

Dispersal of turbidity due to erosion and human activities in the vicinity of water body makes it impractical for its measurement at finer spatio-temporal resolutions (Heyes et al., 2004). The presence of suspended solids, phytoplankton and benthic algae increase the cloudiness of water or turbidity; and hence, it affects the optical properties of water (Nechad

et. al., 2009). The optical properties of turbidity are related to the back scattering coefficient of light and reflectance (Dogliotti et al., 2015) and side scattering of light at wavelengths of 860 nm to Formazin (International Standards Organization, 1999). Hence, many studies estimated the turbidity using the remote sensing approach of Landsat TM-bands (Chebud et al., 2012; Song et al., 2011; Zhao et al., 2011), AVHRR (Woodruff et al., 1999; Aguirre-Gomez, 2000), and MODIS bands (Chen et al., 2007). The Red (wavelength=631-692 nm) and NIR (wavelength=772-898 nm) bands of Landsat (Bustamante et al., 2009; Brezonik, 2005), red band of LISS-I (wavelength=620–680 nm) (Choubey, 1992), and MODIS band of wavelength 645 nm (Chen et al., 2007) are found to be strongly correlated with the turbidity concentration.

The application of 30 m resolution Landsat images is limited due to its 16-days revisit period (Gao et. al., 2006; Roy et al., 2008). While the 1-day resolution MODIS image could have been an alternative to Landsat images, its application is also limited due to its low spatial resolution of 250 m to 1 km. Hence, for monitoring turbidity of water at finer spatiotemporal scales, it is required to fuse both the Landsat and MODIS satellite imageries. To blend the multi-sensor satellites, a variety of spatiotemporal data fusion methods have been advocated for forest mapping (Arai et al., 2011; Hilker et al., 2009; Xin et al., 2013), phenological studies (Senf et al., 2015; Feng et al., 2013; Walker et al., 2012; Hwang, 2011) and biophysical assessment studies (Anderson et al., 2011; Gao et al., 2006, 2012; Singh, 2011). However, there is no such study existing in the literature for river water quality assessment. Furthermore, there is no study carried out to monitor the heavy metals using the remote sensing images at daily temporal and finer spatial scales.

Hence, this study is conducted with the objectives: (i) To develop relationships between each heavy metal (Fe, Zn, Cu, Cr, Pb, Cd) and TSS; between TSS and turbidity; and between turbidity and Landsat spectral bands (red, NIR); (ii) To develop a spatiotemporal adaptive

reflectance fusion model (STARFM)-based algorithm by blending the MODIS bands of 250 m resolutions with the spectrally similar bands of Landsat images of 30 m resolutions; (iii) To map the real-time water quality parameters at 30m×1-day spatiotemporal resolutions using the heavy metal pollution index (HPI) values; and (iv) To analyze the model sensitivity and uncertainty associated with all the developed formulations.

The whole study is framed as follows: Methodology of the study is described in Section 2; the study area and the performance evaluation measures are explained in Section 3 and 4, respectively; the results and discussion of the study are illustrated in Section 5; and the conclusions of the study are mentioned in Section 6.

2. Methodology

2.1 Development of HV-TSS and TSS- T_u relationship models

A total of six heavy metals, viz., Fe, Zn, Cu, Cr, Pb and Cd are chosen for developing relationships of their concentrations with the TSS concentration. To develop non-linear relationship between HV-TSS and TSS- T_u , the Genetic algorithm (GA) evolutionally optimization approach, as illustrated in **Fig. 1**, is used herein. The assumed form of the non-linear relationships of the HV-TSS and TSS- T_u formulations can be generalized, respectively, as

$$HV_i = \alpha_{1,i}(TSS)^{\beta_{1,i}} + c_{1,i} \quad (1)$$

$$TSS = \alpha_2(T_u)^{\beta_2} + c_2 \quad (2)$$

where α and β are the multiplication and power coefficients, respectively; HV_i is the i^{th} heavy metal concentration; T_u =turbidity concentration; and c = constant.

The model parameters α , β and c are evaluated using the GA non-linear optimization model (e.g., Swain and Sahoo, 2015). In simulating the GA model, the mutation and crossover rates of 0.01 and 0.9 are considered, respectively. The objective and stop criteria of the GA model is given by

$$\text{Minimize } E = \sum_{i=1}^n (OC_i^j - SC_i^j)^2 \quad (3)$$

where OC_i^j and SC_i^j are the observed and simulated concentrations of the i^{th} datasets in each j^{th} evolution of the GA; and n = number of data sets. The evolutions are continued till the E value remains unchanged for 5000 evolutions.

2.2 Development of regression models between turbidity concentration and Landsat surface reflectance (T_u - L_s)

As discussed in section 1, it is presumed that surface reflectance of the red (L_3) (0.631-0.692 μm) and NIR (L_4) (0.772-0.898 μm) Landsat bands are mostly influenced by the change in turbidity concentration. Along with these two individual bands, the band ratio is also considered as the input parameter in developing the formulation between the turbidity concentration (T_u) and Landsat surface reflectance (L_s). Note that the band-ratio technique is a popular correction method for the topographic complications of slope, aspect, altitude and illumination differences on the surface reflectances (Metternicht et al., 2005; Cheng et al., 2004). Therefore, the relationship is set up for each water quality parameter by relating the log-transformed turbidity concentrations with a total of seven possible combinations of the two Landsat bands (L_3 , L_4) and band ratio (L_3/L_4). A total of 250 observed coincident data sets of turbidity concentration and Landsat surface reflectance are collected to set up the formulation. First, to develop the relationships between T_u - L_s , the multivariate linear regression models are analyzed by applying the Statistical Package for the Social Sciences (SPSS) software (version-17.0). Corresponding to the maximum value of correlation coefficient, and post analysis of the analysis of variance (ANOVA) table, including student t-distribution, F-distribution and failure (p) significance tests, the best model relating the turbidity concentrations and Landsat surface reflectances are selected. The significance of

these models is tested with the popular two-tailed t-test with the maximum 5% failure probability ($p < 0.05$). The relationships are considered significant only if the t-value of each variable of the model lies in the outside range of $\pm$ critical t-value ($\pm t_{\text{critical}}$), when $p < 0.05$ and $F\text{-value} > F_{\text{critical}}$. The best formulations between T_u - L_s , derived using the SPSS regression model, are further simulated using the Genetic algorithm (GA) evolutionally optimization approach to obtain the higher non-linear relationship model. The framework of the methodology is illustrated in **Fig. 1**. The form of the multivariate and non-linear relationships of the T_u - L_s formulations can be generalized as

$$\text{Log}(T_u) = \sum_{i=1}^n \alpha_i L_i^{\beta_i} + c \quad (4)$$

where T_u = Turbidity concentration; L_i = Surface reflectance of the i^{th} Landsat band or combination bands; α_i and β_i = multiplication and power coefficients of each input variable, respectively; and c = model intercept.

2.3 Spatio-temporal data fusion of Landsat and MODIS satellite bands

To blend the similar spectral bands of MODIS and LANDSAT satellite imagery, the STARFM spatio-temporal fusion algorithm is used herein. STARFM algorithm is based on the assumption that the difference in the surface reflectance values between each pure pixels of coarse (MODIS) and fine (Landsat) imagery of the same land cover type remains constant (Emelyanova et al., 2013; Zhu et al., 2010; Hilker et al., 2009; Roy et al., 2008; Gao et al., 2006). This difference in the surface reflectances, derived from a base pair of concurrent Landsat–MODIS images, can be added directly to a MODIS imagery surface reflectance data to estimate the Landsat-like synthetic surface reflectance on a prediction date (Zhu et al., 2016; Gevaert and García-Haro, 2015; Gao et al., 2006). However, for the mixed pixels and if land cover changes between the date of base image pair and date of prediction, a weightage function is applied. The weightage function depends on the differences of surface reflectances between the base Landsat-MODIS imagery pair on the base date (t_1), between

the MODIS images on the base (t_1) and prediction (t_2) dates, and the spatial Euclidian distance between the central and neighbor pixels. Herein, the in-situ locations of turbidity concentration are measured at the center of the river water pixel, for which the corresponding MODIS and Landsat surface reflectances are derived. The land cover at the central pixel does not change with respect to time along the river reach; hence, the pixels considered are pure and the ideal situation is satisfied. Therefore, the surface reflectance of the synthetic Landsat-like imagery with spatial coordinates of x and y is estimated at any time t_2 as (Gao et al., 2006; Zhu et al., 2016)

$$L_i(x, y, t_2) = M_i(x, y, t_2) + L_i(x, y, t_1) - M_i(x, y, t_1) \quad (5)$$

where (x, y) is the location of pixels; t_1 and t_2 are the date of base image pair and date of prediction, respectively; $M(x, y, t_1)$ and $M(x, y, t_2)$ are the MODIS surface reflectances at time t_1 and t_2 , respectively; and $L(x, y, t_1)$ and $L(x, y, t_2)$ are the Landsat surface reflectances at t_1 and t_2 , respectively.

The MODIS-aqua product of surface reflectance bands 1 and 2, namely, MYD09GQ with 250m×1-day resolution, and Landsat (ETM+ and OLI) images for the period 2007-2015 are used herein. The wavelengths of the MODIS band-1 (M_1) and band-2 (M_2) lie in the range of 620-670 nm and 841-876 nm, respectively. Similarly, the wavelengths of red (L_3) and NIR (L_4) bands of Landsat lie in the range of 0.631-0.692 μ m and 0.772-0.898 μ m, respectively. Since, the spatiotemporal fusion can be possible only for spectrally similar bands of MODIS-Landsat imagery, the fusion is carried between M_1 - L_3 and M_2 - L_4 bands by using the basic procedures as advocated by Gao et al. (2006). Before applying the STARFM model for estimating the Landsat-like surface reflectance and, then estimating the real-time turbidity concentration, the model is validated by applying to the three pairs of MODIS-Landsat satellite imagery data. The Landsat surface reflectance is predicted from the MODIS surface reflectances for the typical dates of 29th December, 2013, 15th February, 2014 and 4th April,

2014 using the base Landsat-MODIS pair data of 13th December, 2013, 30th January, 2014 and 19th March, 2014, respectively. The procedure to apply the STARFM algorithm for water quality estimation at daily scale is shown in **Fig. 1**.

2.4. Estimation of HPI values

The HPI (Balakrishnan and Ramu, 2016; Giri and Singh, 2014; Sirajudeen et al., 2014; Yankey et al., 2013) is generally used to assess the collective impact of heavy metals on the river water quality accounting for the standard and ideal threshold limits of these heavy metal concentrations for drinking water use. The HPI (Balakrishnan and Ramu, 2016) is expressed as

$$HPI = \frac{\sum_{i=1}^n w_i q_i}{\sum_{i=1}^n w_i} \quad (6)$$

where q_i and w_i are the sub-index and unit weightage of the i^{th} water quality parameter, respectively, and n is the number of heavy metal parameters considered. The q_i of the parameter is estimated as

$$q_i = \begin{cases} \sum_{i=1}^n \frac{|x_{mi} - x_{ii}|}{(x_{si} - x_{ii})} \times 100, & x_{si} \neq x_{ii} \\ \sum_{i=1}^n \frac{x_{mi}}{x_{si}} \times 100, & x_{si} = x_{ii} \end{cases} \quad (7)$$

where x_{mi} , x_{ii} , and x_{si} are the actual, highest desirable, and standard permissible values of the i^{th} heavy metal parameter, respectively. Depending upon the importance of each heavy metal, the value of w_i is estimated by considering w_i to be inversely proportional to its recommended standard value (Prasad and Bose, 2001). The Indian standard of permissible and highest desirable (IS 10500: 2012) threshold concentration values of the heavy metals are shown in **Table 1**. The classification of the HPI values by Edet and Offiong (2002) as low, medium and high when HPI values are <15, 15–30 and >30, respectively, is followed here. The critical value of HPI for drinking water is 100.

Table 1

2.5. Uncertainty and sensitivity analysis

There is always uncertainty involved in the spatial distribution of water quality parameters in any natural river channel in addition to errors in the sampling and laboratory measurements. There could be some uncertainty in the Landsat surface reflectance due to the effect of atmosphere and biased optical properties of different suspended matters in the river. Therefore, it is important to study the uncertainties of both the input and output variables of the developed models. The popular Monte-Carlo method of uncertainty calculation (Verbeeck et al., 2006), as illustrated in **Fig. 2**, is used herein. The independency of the input variables is verified using the correlation analysis. Note that, in the Monte-Carlo uncertainty (MCU) estimation, if the input variables are independent with each other, the input variable combinations are not required to be considered because of zero-impact on the output variable distribution (Burmaster and Anderson, 1994). In the MCU framework, the best-fit probability distribution functions (pdfs) of input variables are evaluated by testing 56 different types of pdfs with the Chi-squared rank test. The descriptive statistics of mean, standard error, 95% confidence interval, and uncertainty percentage of both the input variables L_3 and L_4 are estimated. Extensive random data are generated for L_3 and L_4 using the best-fit pdfs and their shape, scale, and location parameters. According to the ‘Guide to the Expression of Uncertainty in Measurement’ (GUM-JCGM 100:2008) of ISO standard Uncertainty of measurement: Part 3, the minimum number of random simulations (k) is given by (BIPM et al., 2010)

$$k = \frac{10^4}{1-p} \quad (8)$$

where p =selected probability (here, $p=0.95$; $k=200,000$)

The Turbidity concentration is estimated using the generated random values of L_3 and L_4 using Eq. (4). The best-fit pdf, the descriptive statistics and the 95% confidence intervals of the estimated turbidity concentrations are evaluated using the Chi-squared rank test of the 56 types of pdfs. Similarly, the TSS and heavy metal (viz., Fe, Zn, Cu, Cr, Pb, Cd) concentrations are estimated using the developed Landsat-turbidity, TSS- T_u and HV-TSS algorithms.

To determine the most influencing input variable (out of L_3 and L_4) in the T_u - L_s model that estimate the turbidity concentration and, subsequently, TSS and heavy metal concentrations, the One-parameter-at-a-time method of sensitivity analysis is performed. The absolute sensitivity coefficient (S_a) and relative sensitivity coefficient (S_r) of each input variable is calculated as (Sattar and Gharabaghi, 2015)

$$S_a = \frac{\partial V_0}{\partial V_i} ; \quad S_r = \frac{V_i}{V_0} \frac{\partial V_0}{\partial V_i} \quad (9)$$

where V_i and V_0 are the input and out variables, respectively.

It is to be noted that the variable having the highest unsigned S_r value is the most sensible variable.

3. Study Area and Data Processing

The Brahmani River (39,033 km²) in Odisha state of the eastern India is chosen for the study because of its heavy point and non-point pollution from more than 37 industries, mining, urbanization and agricultural activities in the catchment (**Fig. 3**). The State Pollution Control Board (SPCB), Bhubaneswar, Odisha is the authorized government organization to measure the concentrations of different water quality parameters. During the year 2007-2009, the SPCB was measuring the physical and biological water quality parameters of pH, biological oxygen demand (BOD), chemical oxygen demand (COD), dissolve oxygen (DO),

NH₄, Nitrate, and total coliform at monthly-scale; whereas the parameters of TSS, turbidity, total dissolved solids (TDS), sulphate, sodium, and heavy metals of Fe, Zn, Cu, Cr, Pb, and Cd were measured at 3-monthly scale. From the year 2010 onwards, the SPCB is measuring all these parameters at monthly-scale at 27 number of water quality gauging stations in the 480km main stretch of the Brahmani River (**Fig. 3**). This water quality measurement at such coarser spatio-temporal resolutions makes it nearly impossible to regulate the pollution sources in such a highly dense industrial catchment. Hence, there is a need to monitor the water qualities including the heavy metals at very fine spatio-temporal scales which can help to study the environmental impact assessment and its management.

The data collected from the SPCB for the period of 2007-2015 contains a total of 1300 number of concurrent datasets of Fe, Cr, TSS, and T_u; and 670 number of concurrent datasets of Zn, Cu, Pb, Cd and TSS. Since the revisit period of Landsat satellite is 16-days, a total of 250 coincident datasets of T_u-L_s within the study period are identified. The SPCB carries out water sampling at 30 cm depth below the water surface (e.g., ‘Guidelines for Water Quality Management’, Central Pollution Control Board, 2008) at well-mixed central locations of the river. From the year 2007 to 2015, all the cloud-free images of Landsat (L7 ETM+ and L8 OLI/TIRS) surface reflectances are downloaded from the USGS website <<http://earthexplorer.usgs.gov/>>. The surface reflectance data are extracted from the Landsat images using the ArcGIS 9.3 and ENVI 5.0 software packages.

4. Performance Evaluation Measures

The accuracy of the developed TSS-T_u, HV-TSS, Landsat surface reflectance-turbidity concentration models, and STARFM fusion algorithm are assessed by the performance

evaluation measures of Nash–Sutcliffe criterion of model efficiency, *NSE* (Nash and Sutcliffe, 1970), Coefficient of determination (r^2), Root mean square error (*RMSE*) and Index of agreement *IOA* (Willmott, 1982).

5. Results and Discussion

5.1 Evaluating the HV-TSS and TSS- T_u relationship models

As discussed in section 2.1, the 60% of the 1300 number of observed concurrent datasets of Fe-TSS and Cr-TSS; and 660 datasets of Zn-TSS, Cu-TSS, Pb-TSS, and Cd-TSS are used in calibrating the linear and non-linear regression models using the SPSS and GA optimization models, respectively. The remaining 40% of the datasets are used for validating the developed HV-TSS models. The developed formulations between each heavy metal and TSS concentration are given in **Eqs. [8(a-f)]**. The performance evaluation measures during the calibration and validation of the relationship models are shown in **Fig. 4**. **Figure 4** illustrates the *NSE*, r^2 , *IOA*, and *RMSE* values in calibrating the HV-TSS formulation that vary from 73.29-92.45%, 0.76-0.93, 92.48-98.15%, and 4.13-33.77 μ g/l, respectively. Similarly, during the validation, the values of *NSE*, r^2 , *IOA*, and *RMSE* vary from 73.92-90.78%, 0.76-0.91, 92.69-97.50%, and 3.76-38.72 μ g/l, respectively. **Figure 4** also shows that during calibration phase, Cd concentration is very well estimated with the maximum *NSE* and r^2 values of 92.45% and 0.93, respectively; whereas Cr concentration is reasonably well-estimated with the minimum *NSE* and r^2 values of 73.29% and 0.76, respectively. Similarly, during the validation phase, Cd is estimated with the maximum *NSE* and r^2 values of 90.78% and 0.91, respectively; whereas Cr is estimated with the minimum *NSE* value of 73.92%, and Fe is estimated with the minimum r^2 value of 0.76, respectively. The performances evaluation measures can be visualized in the scatter plots between the estimated and observed values shown in **Fig. 5**.

$$Fe = 20.27(TSS)^{1.008} \quad (10a)$$

$$Zn = 3.98(TSS)^{0.43} + 0.16 \quad (10b)$$

$$Cu = 1.084e^{0.013(TSS)} \quad (10c)$$

$$Cr = 0.0005(TSS)^{2.20} + 3.69 \quad (10d)$$

$$Pb = 2.87e^{0.01(TSS)} \quad (10e)$$

$$Cd = 0.306e^{0.017(TSS)} \quad (10f)$$

where TSS concentrations is expressed in mg/l; and the concentration of Fe, Zn, Cu, Cr, Pb, and Cd are in $\mu\text{g/l}$.

A similar procedure is also followed to develop the in-situ TSS- T_u relationship models using the SPSS regression and GA optimization technique with the 1300 number of datasets. This formulation reveal that TSS is the best correlated with the three separated ranges of turbidity concentrations of 0-50 NTU, 50-200 NTU and >200 NTU by different regression models. The formulations developed in the three ranges of turbidity values using the combined SPSS and GA optimization method are given by

$$TSS = \begin{cases} 2.73(T_u)^{0.98} + 4.63, & T_u \leq 50 \\ 4.37(T_u)^{0.83}, & 50 < T_u < 200 \\ 0.22(T_u)^{1.12} + 135.84, & T_u \geq 200 \end{cases} \quad (11)$$

where T_u is the turbidity expressed in Nephelometric Turbidity Unit (NTU); and TSS is expressed in mg/l.

The performance evaluation measures in estimating TSS during the calibration and validation phases are also shown in **Fig. 4**. The NSE , r^2 , IOA , and $RMSE$ error measures in calibrating the TSS- T_u relationship models are found to be 89.71%, 0.90, 97.38%, and 19.27 mg/l, respectively; whereas during the validation phase, the estimated values of NSE , r^2 , IOA , and $RMSE$ are 85.44%, 0.86, 95.86%, and 28.27 mg/l, respectively. The scatter plots between the estimated and observed TSS concentrations during the calibration and validation are shown in **Fig. 5**.

5.2. Evaluation of T_u - L_s relationship

As discussed in sections 1 and 2.2, only the red (L_3) and NIR (L_4) spectral bands of Landsat satellite imagery are selected for developing the relationship with turbidity concentration. Out of the total of 250 number of coincident Landsat-turbidity datasets collected, 150 numbers of datasets are used for calibrating the model and the remaining 100 number of data sets are used for validation. The multivariate linear and non-linear regression analyses are carried out between the turbidity concentration with each of the seven combinations of two Landsat bands and their ratios (L_3 , L_4 , L_3/L_4). The procedure followed in developing the HV-TSS and TSS- T_u relationships (section 2.1 and 2.2) is also followed herein to formulate the T_u - L_s relationship. The developed coupled SPSS regression-GA optimization technique-based T_u - L_s relationship model is expressed as

$$\text{Log}(T_u) = -30L_3^{1.02} + 29.99L_4^{0.62} - 4.67(L_3/L_4)^{-0.72} + 2.24 \quad (12)$$

where Turbidity (T_u) is in NTU.

Figure 4 illustrates the performance evaluation measures in estimating turbidity from Landsat imagery by using Eq. (12) during both the calibration and validation. It can be noted from **Fig. 4** that the T_u concentrations are well estimated by Eq. (12) with the NSE , r^2 , IOA and $RMSE$ estimates of 88.66%, 0.89, 96.07% and 27.75 NTU during the calibration phase, respectively. Similarly, during validation, the values of NSE , r^2 , IOA and $RMSE$ are 89.74%, 0.90, 97.34% and 27.28 NTU, respectively. The scatter plots between the estimated and the observed turbidity concentrations are shown in **Fig. 5**. These results reveal that T_u is very well estimated from the Landsat reflectance values.

Figs. 4 & 5

5.3. Spatio-temporal data fusion between Landsat and MODIS imagery

As discussed in Section 3, a total of six pair of typical coincident MODIS-Landsat imagery available on the dates of 13th December, 29th December, 2013, 30th January, 2014, 15th February, 2014, 19th March, 2014 and 4th April, 2014 are used for testing the STARFM spatio-temporal fusion algorithm. During calibration, the synthetic Landsat-like surface reflectance values at 400 locations along the center axis of the Brahmani River are estimated on the dates of 29th December, 2013, 15th February, 2014 and 4th April, 2014 using the base coincident Landsat-MODIS image pair of closely antecedent available dates of 13th December, 30th January, 2014, and 19th March, 2014 respectively. During validation, the performance evaluation measures estimated between these synthetic Landsat-like surface reflectances and the observed Landsat surface reflectances of the spectral bands L_3 and L_4 on the three dates 29th Dec, 2013, 15th Feb, 2014 and 4th Apr, 2014 are shown in **Fig. 6**. **Figure 6** illustrates that, in estimating the synthetic Landsat-surface reflectance of band L_3 for the image dated 29th Dec, 2013, the values of NSE , r^2 , IOA and $RMSE$ are found to be 80.31%, 0.85, 95.53% and 0.02, respectively; which are 72.72%, 0.77, 93.13%, and 0.03 for the image dated 15th Feb, 2014, respectively; and 75.41%, 0.77, 93.43% and 0.03 for the image dated 4th Apr, 2014, respectively. Similarly, in estimating the synthetic Landsat-like surface reflectance of spectral band L_4 for the image dated 29th Dec, 2013, the values of NSE , r^2 , IOA and $RMSE$ are 85.57%, 0.89, 96.70%, and 0.03, respectively; 74.68%, 0.80, 93.12% and 0.05 for the image dated 15th Feb, 2014, respectively; and 83.46%, 0.84, 95.37 5, and 0.04 for the image dated 4th Apr, 2014, respectively. The average values of NSE , r^2 , IOA and $RMSE$ in estimating L_3 of the three dated images are 76.15% 0.80, 94.03% and 0.02, respectively; which are 81.24%, 0.84, 95.06% and 0.04 in estimating L_4 of these images, respectively. The scatter plots between the observed and estimated Landsat-like surface reflectances of both the L_3 and L_4 spectral bands for these three images at different locations are shown in **Fig. 7**,

which reveal that the MODIS images of 250m resolution are effectively downscaled to the synthetic Landsat-like images of 30m resolution by the STARFM algorithm.

Figs. 6 & 7

5.4. Real-time estimation of daily-scale heavy metal pollutant concentrations for river water quality mapping

The models developed between the HV-TSS [Eqs. (10a)-(10f)], TSS- T_u [Eq. (11)], T_u-L_s [Eq. (12)] and the STARFM spatiotemporal fusion algorithm [Eq. (5)] are applied at the Talcher gauging station of the Brahmani River. For estimating Turbidity, and hence, TSS and heavy metals at daily-scale, the 250m×1-day resolution MODIS images (MYD09GQ) from Jan 01-Jun 15, 2015 are downloaded from the USGS website <<http://glovis.usgs.gov/>>. The close antecedent Landsat images of these MODIS imageries between Jan 01-Feb 28, 2015 are also downloaded from the USGS website <<http://earthexplorer.usgs.gov/>>. The synthetic Landsat-like surface reflectance values and, subsequently, the model simulated turbidity, TSS and heavy metal concentrations are shown in **Fig. 8**. **Figure 8** reveals that for the time period Jan 01-Jun 15, 2015, the values of turbidity, TSS, Fe, Zn, Cu, Cr, Pb and Cd concentrations vary from 0.24 to 473.19 NTU, 5.30 to 353.84 mg/l, 108.80 to 7517.20 $\mu\text{g/l}$, 8.31 to 49.80 $\mu\text{g/l}$, 1.16 to 107.84 $\mu\text{g/l}$, 3.71 to 206.16 $\mu\text{g/l}$, 3.03 to 98.77 $\mu\text{g/l}$, and 0.33 to 125.36 $\mu\text{g/l}$, respectively.

Similarly, the water quality mapping at daily-scale is carried out by estimating the turbidity, TSS and heavy metals at 1 km spatial interval along the 320 km long Brhamani River reach between the confluence section of the Sankh-Koel Rivers and Jenapur for the typical month of January, 2015. **Figure 9** describes the average concentration values for the month of January, 2015 at 1-km spatial interval. The average values of turbidity, TSS, Fe, Zn, Cu, Cr, Pb, and Cd concentrations during January, 2015 from the confluence section of the

Sankh-Koel Rivers to Jenapur reach is varying from 19.46-112.49 NTU, 52.84-153.84 mg/l, 1108.01-3253.90 $\mu\text{g/l}$, 20.42-31.83 $\mu\text{g/l}$, 2.471-21.13 $\mu\text{g/l}$, 9.02-55.70 $\mu\text{g/l}$, 5.27-23.91 $\mu\text{g/l}$, and 0.95-20.12 $\mu\text{g/l}$, respectively. Using the estimated average concentrations, the water quality mapping is carried out for each water quality parameter. **Figure 10** shows the water quality mapping of a typical 110 km long Talcher-Jenapur sub-reach of the Brahmani River. **Figure 10** also reveals that the concentrations of turbidity, TSS and heavy metals are high near the Talcher station and Sankh-Koel confluence section due to the presence of a large number of heavy industries (**Fig. 3**).

Figs. 8, 9, 10

5.5. *Spatio-temporal mapping of HPI*

As described in Section 2.4, the HPI values are estimated using the 1-day $\times$ 1-km scale heavy metal concentrations calculated in Section 5.4. **Figure 11** demonstrates the variation of HPI values at the Talcher gauging station from Jan 01-Jun 15, 2015 at daily-temporal scale. **Figure 11** illustrates that the HPI at the selected gauging station varies from 9.26 to 246.88 (low to critical HPI) with an average value of 77.99 (high HPI). These ranges of HPI values in the river are obvious as there are a number of industries and mines situated at the peri-urban areas of Talcher, releasing industrial and solid wastes to the river.

Fig. 11

The spatial variation of HPI values in the reach between the Sankh-Koel confluence section to Jenapur gauging station is illustrated in **Figure 12**. These HPI values are estimated using the real-time average heavy metal concentrations calculated for the month of January, 2015 along this reach as given in Section 5.4. **Figure 12** reveals that the values of HPI for this selected reach varies from 6.61 to 193.07 which is recommended as 'low to critical' with

an average value of 71.87, recommended as high HPI value. The HPI mapping is carried out along the selected Brahmani River reach and, for better visualization, the mapping of the typical Talcher-Jenapur sub-reach is shown in **Fig. 13**. **Figure 13** classifies the HPI values as low, medium, high and critical as described in Section 2.4. Hence, **Figs. 12-13** confirm that a major part of the river reach is under high to critical HPI values which means that the Brahmani River is highly polluted with heavy metal. Hence, there is an urgent need of implementing pollution control measures in this river.

5.6 Uncertainty analysis

The correlation coefficient of 0.0031 between the input parameters of spectral reflectances of L_3 and L_4 for the T_u-L_s model reveals that these parameters are independent from each other. As described in Section 2.4, after testing the 56 types of pdfs, the best-fit pdfs identified for L_3 and L_4 are found to be Pearson 6 (4-parameter) and Beta distributions, respectively. The estimated mean, standard error, 95% confidence interval, and uncertainty percentage for the spectral bands of L_3 and L_4 are obtained as 0.132, 0.001, 0.002%, and 1.852%; and 0.148, 0.002, 0.005%, and 3.073, respectively.

Similarly, a total of 200,000 numbers of simulations are carried out to estimate the turbidity concentration using the T_u-L_s relationship [Eq. (12)] and the random spectral reflectances of L_3 and L_4 . Subsequently, the concentrations of TSS and heavy metals are estimated using Eq. (11) and Eqs. (10a)-(10f), respectively. The descriptive statistics, viz., mean, standard error, median, range, 95% confidence interval and uncertainty (%) of all the water quality parameters given in **Table 2** reveal that all these water quality parameters are well-estimated with <4% uncertainty, except Cd (5.05%). The corresponding histograms and the best-fit pdfs are shown in **Fig. 14**.

Table 2 **Fig. 14**

5.7 Sensitivity analysis

Sensitivity analysis of the developed T_u - L_s model [Eq. (12)] in estimating the turbidity concentration using the observed mean reflectances of L_3 and L_4 Landsat bands is carried out using the procedure as described in Section 2.4. The results reveal that the absolute sensitivity coefficient (S_a) and relative sensitivity coefficient (S_r) estimates of L_3 and L_4 are -626.93 and -0.24, and 4749.19 and 2.04, respectively. It shows that the L_4 spectral band of Landsat is highly sensitive as compared to the L_3 spectral band in estimating the turbidity, and hence, in estimating the TSS and the selected heavy metal concentrations.

6. Conclusions

In this study, the SPSS and GA based linear and non-linear spectral relationships between the T_u - L_s , TSS- T_u and HV-TSS are developed to estimate the concentrations of turbidity, TSS and heavy metals (viz., Fe, Zn, Cu, Cr, Pb, Cd) using the Landsat surface reflectance of 30 m spatial and 16-days temporal resolution. The STARFM fusion algorithm is used to blend the spectrally similar bands of MODIS and Landsat satellite imageries, so that the aforementioned water quality concentrations could be estimated at 30m×1-day spatiotemporal resolutions. The scatter plots and the values of performance evaluation measures of the developed water quality models show that the TSS transportation occurs with the heavy metals, and the turbidity is affected by the TSS concentration; and hence, TSS transportation occurs by the heavy metal concentrations indirectly. Further, the T_u - L_s model shows that the optical properties of water are highly influenced by its physical-cum-surface

properties, i.e., turbidity. The validation of the STARFM model confirms that the MODIS surface reflectance values of 250 m resolution can effectively be downscaled to synthetic Landsat-like surface reflectance values of 30 m resolution. These daily-scale water quality mapping can be helpful in water management decision making and pollution impact assessment studies, such as, selection of water treatment locations, scale of water purification systems, regulation of industrial water pollution control and water supply for irrigation. According to the WHO international standards, the values of the concentrations of Fe, Zn, Cu, Cr, Pb and Cd should be below 3 mg/l, 2 mg/l, 50 µg/l, 10 µg/l, and 3 µg/l, respectively for drinking water supply. The high to critical values of HPI at the majority length of the Brahmani River reach concludes that there is an urgent need to advocate river basin and contaminated site management plans to mitigate these pollution hazards for sustainable riverine ecosystem.

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FIGURE CAPTIONS

Fig. 1. Framework of daily water quality monitoring at finer spatiotemporal scales by fusing the MODIS and Landsat satellite imageries.

Fig. 2. The Monte-Carlo of uncertainty analysis framework.

Fig. 3. Index map of the Brahmani River Basin showing in-situ water quality monitoring stations and location of major industries and mines.

Fig. 4. Performance evaluation measures of the eight water quality parameters during calibration and validation. The RMSE of T_u , TSS, Fe, Zn, Cu, Cr, Pb, and Cd are in NTU, mg/l, $\mu\text{g/l}$, $\mu\text{g/l}$, $\mu\text{g/l}$, $\mu\text{g/l}$, $\mu\text{g/l}$, and $\mu\text{g/l}$, respectively.

Fig. 5. Scatter plots between the observed and estimated water quality parameters.

Fig. 6. Performance evaluation measures of L_3 and L_4 Landsat bands for surface reflectances.

Fig. 7. Scatter plots between the observed Landsat and estimated synthetic Landsat-like surface reflectances of L_3 and L_4 spectral bands of three different satellite images.

Fig. 8. Daily-scale temporal distribution of the estimated water quality parameters at Talcher gauging station.

Fig. 9. Spatial distribution of averaged daily-scale water quality parameters along the Brahmani River reach (from Sankh-Koel river confluence to Jenapur) for the typical month of January, 2015.

Fig. 10. Water quality mapping of Talcher-Jenapur reach of the Brahmani River based on IS 10500: 2012 for a typical month of Jan., 2015.

Fig. 11. Temporal distribution of the estimated HPI values at Talcher gauging station.

Fig. 12. Spatial distribution of estimated HPI values of averaged daily-scale heavy metals along the Brahmani River reach (from Sankh-Koel confluence to Jenapur) for a typical month of Jan., 2015.

Fig. 13. Heavy metal pollution index (HPI) mapping of Talcher-Jenapur reach of the Brahmani River.

Fig. 14. Histograms and the best-fit pdfs of selected water quality parameters used in Monte-Carlo analysis.

Figure 1

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Table 1. The Indian Standard of permissible and desirable heavy metal concentrations for drinking water use (IS 10500: 2012)

Heavy metals	Standard permissible value (x_{si}) in $\mu\text{g/l}$	Highest desirable value (x_{ii}) in $\mu\text{g/l}$	Unit weightage ($w_i=1/x_{si}$)
Fe	300 (No relaxation)	300	0.0033
Zn	15,000	5,000	0.000067
Cu	1,500	50	0.00067
Cr	50 (No relaxation)	50	0.02
Pb	10 (No relaxation)	10	0.1
Cd	3 (No relaxation)	3	0.33

Table 2. Uncertainty estimation of water quality parameters using Monte-Carlo simulations

	Turbidity (NTU)	TSS (mg/l)	Fe ($\mu\text{g/l}$)	Zn ($\mu\text{g/l}$)	Cu ($\mu\text{g/l}$)	Cr ($\mu\text{g/l}$)	Pb ($\mu\text{g/l}$)	Cd ($\mu\text{g/l}$)
Mean	44.01	81.31	1714.53	22.65	7.58	24.67	10.77	5.60
Median	14.76	42.81	894.14	20.18	1.89	5.63	4.40	0.63
Minimum	0.00	4.63	95.01	7.85	1.15	3.70	3.01	0.33
Maximum	369.99	354.82	7538.03	49.86	109.21	207.38	99.73	127.45
Standard Error	0.68	0.88	18.67	0.12	0.14	0.39	0.15	0.14
95% Confidence Level	1.32	1.73	36.60	0.24	0.28	0.76	0.29	0.28
Uncertainty (%)	3.01	2.12	2.13	1.04	3.72	3.08	2.69	5.05