D.5.2.1 – Simulations for the validation of the Alert Tool

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INDEX

1. INTRODUCTION

In this report, we describe the validation of a relocatable modelling system (Alert Tool) for assessing microbial pollution in coastal areas which consists of a hydrodynamic model, a transport and diffusion model and a microbial decay model. The adopted approach realises a seamless transition between different spatial scales, from the river mouth to the open sea, and adopts a high spatial and temporal resolution of the forcing and boundary conditions that drive the simulations. The hydrodynamic model, the transport and diffusion model and the microbial decay model have been applied to the five pilot sites in the Adriatic Sea for a total of 15 simulations. The model is evaluated against observations in the coastal areas, illustrating the capability of this tool in simulating the water circulation as well as the dispersion and decay of microbial pollutants. The model evaluation is limited by the availability of site-specific observations.

2. The observational datasets

The different study areas are monitored by several observational networks which differ for the observed parameters, type of monitoring instruments and frequency of acquisition. The monitored parameters used in the validation procedures are grouped into the following three categories:

- hydrodynamic: water levels;
- physicochemical: water temperature and salinity;
- microbial: faecal bacteria (E. coli and intestinal enterococci) concentration.

The main characteristics of the available dataset in the five study areas are presented in Table 1.

Table 1: Description of the available observational datasets.

Study area	***Hydrodynamic***	***Physico-chemical***	***Microbial***
Fano coast and Arzilla stream	Water levels measured in the Arzilla stream at a 15-min frequency (2021)	Mid-column water temperature and salinity from water samples collected at the river mouth and along three coastal transects with points at 50, 100, 150, 200 and 250 m from the coastline. Nine monitoring surveys were performed in the summer of 2019 and 2020.	Mid-column *E. coli* concentration from water samples collected at the river mouth and along three transects with points at 50, 100, 150, 200 and 250 m from the coastline. Nine monitoring surveys were performed in the summer of 2019 and 2020.
Pescara coast and Pescara River	Water levels measured in the Pescara harbour at a 15-min frequency (2020)	Surface water temperature values measured in the Pescara harbour at a 15-min frequency (2020)	Surface *E. coli* concentration from water samples collected in 9 points at the river mouth and along Pescara coast in the summer 2021
Raša River canal	Water discharge of river Rasa at daily frequency (2019-2020)	Surface water temperature and salinity from water samples collected at the river mouth and along three transects with points at 200, 400 and 600 m from the river mouth, and at two popular touristic sites located at 1.5 and 3.4 km from the river mouth. Four monitoring surveys were performed in October and November 2020.	Surface *E. coli* concentration from water samples collected at the river mouth and along three transects with points at 200, 400 and 600 m from the river mouth, and at two popular touristic sites located at 1.5 and 3.4 km from the river mouth. Four monitoring surveys were performed in October and November 2020.
Omiš coast	Water discharge of	Surface water temperature and	Surface *E. coli* concentration

and Cetina River	river Cetina at daily frequency (2019-2020)	salinity from water samples collected in the 6 sea points in the summer 2021	from water samples collected in 6 sea points in the summer 2021 along Omis coast
Ploče coast and Neretva Estuary	Water discharge of river Neretva at daily frequency (2019-2020)	Surface water temperature and salinity from water samples collected in the 9 sea points at Neretva River mouth in the summer 2021	Surface *E. coli* concentration from water samples collected in 9 sea points at Neretva River mouth in the summer 2021

3. Model assessment

The model performance was evaluated in terms of the difference between the average of simulated and observed values (BIAS), the root mean squared error (RMSE) and the Pearson product-moment correlation coefficient (R). For the concentration of *E. coli*, the root mean squared logarithmic (base 10) error (RMSLE) was used instead of RMSE (Locatelli et al., 2020).

The model suite has been applied to the five pilot sites in the Adriatic Sea for a total of 15 numerical simulations covering the summer period of years 2019 and 2020. The model evaluation is here presented following the subdivision proposed for the observations (hydrodynamics, physicochemical, microbial pollution) and considering the availability of site-specific forcing conditions and observational datasets.

3.1. Hydrodynamic assessment

Concerning the hydrodynamic assessment, the model results were compared with water levels recorded in Pescara, Omiš-Cetina and Ploče-Neretva study areas. The water level is here used to evaluate the hydrodynamic model performance. Observed and simulated time series were processed with a tidal harmonic analysis tool based on the least-squares fitting (Codiga, 2011) to separate the tidal and the residual contributions to the total sea level. The statistics of the simulated values (total and tidal water levels) for the three study sites are reported in Table 2.

Table 2: Statistical analysis of simulated water levels at three study areas in terms of RMSE, BIAS and R. Statistics are reported for both the total water level and tidal level.

Study area	***Station name***	***RMSE (m)***	***BIAS (m)***	***R***
Pescara	Pescara harbour	0.17 / 0.02	0.02 / 0.	0.81 / 0.99

Omiš-Cetina	Omiš	0.09 / 0.03	0.04 / 0.	0.72 / 0.96
Ploče-Neretva	Ušće	0.08 / 0.02	-0.07 / 0.	0.79 / 0.98
	Opuzen	0.09 / 0.02	-0.07 / 0.	0.77 / 0.98

The model well reproduced the water levels variability observed in Pescara (top panel in Fig. 1), even if it is not able to capture the very high-frequency fluctuations, probably generated inside the harbour by resonance phenomena. RMSE, BIAS and R for the total water level are 0.17 m, 0.02 m and 0.81, respectively. However, the model simulated the tidal fluctuation (bottom panel in Fig. 1), which is the main driver of the sea-level variability in this area, with very high accuracy (RMSE=0.02 m and R=0.99).

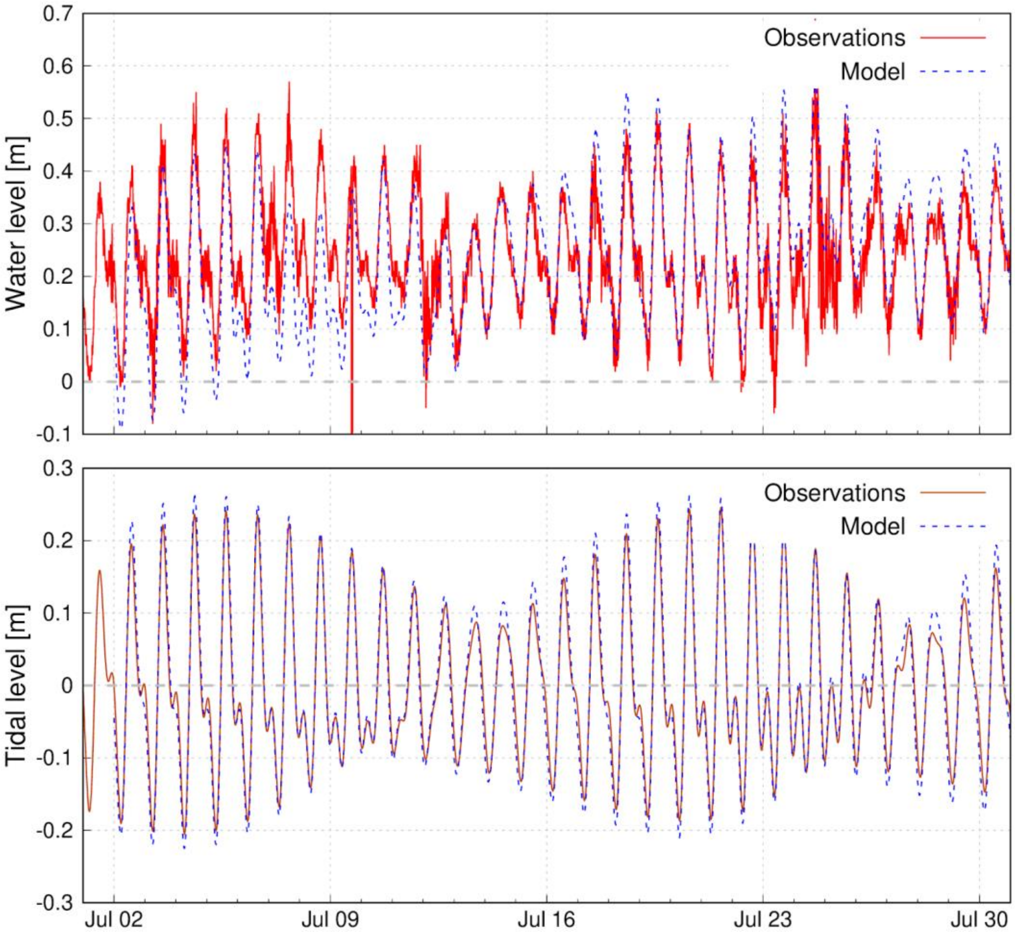

Figure 1: Measured and observed water levels in the Pescara harbour (summer 2020). The top panel presents the total water levels, while the bottom panel reports the tidal levels.

The results of the model application to the Omiš-Cetina were compared with the water level continuously measured near the city of Omiš. The statistical parameters reported in Table 2 demonstrate that the model captures the sea-level variability in the investigated area, which was mostly determined by the tidal action. RMSE and R are 0.09 and 0.72 for the total water level and 0.03 and 0.96 for the tidal level.

The numerical model well reproduced the water level also in the Ploče-Neretva study area (Table 2) with an RMSE is 0.08 and 0.02 m for the total water level and the tidal level, respectively. The results of the tidal harmonic analysis revealed that the model captures the observed tidal amplification along the river estuary, even if it is slightly overestimating the amplitude of the K1 diurnal constituent. Generally, the comparison with the tide gauge data confirmed the good performance of the SHYFEM model in simulating sea levels and tidal propagation in the Adriatic Sea (Ferrarin et al., 2017; Ferrarin et al., 2019).

3.2. Physicochemical assessment

The water temperature and salinity values observed in the Fano-Arzilla, Pescara and Raša study areas were used to assess the capacity of the modelling system in reproducing heat fluxes, transport dynamics and mixing processes. Fig. 2 shows scatter plots of simulated and observed water temperature (panel a) and salinity (panel b) for the Fano-Arzilla study area. The obtained BIAS and RMSE for salinity are 3.1 and 2.5 psu, and -0.1 °C and 1.2 °C for water temperature. The correlation coefficient resulted to be 0.95 and 0.64 for salinity and water temperature, respectively. The analysis of the results reveals that, despite the large uncertainty on the boundary conditions, the numerical model compares reasonably well with the measurements acquired in Fano coastal waters and reproduces the observed spatial and temporal variability of both water temperature and salinity. Model slightly overestimated salinity.

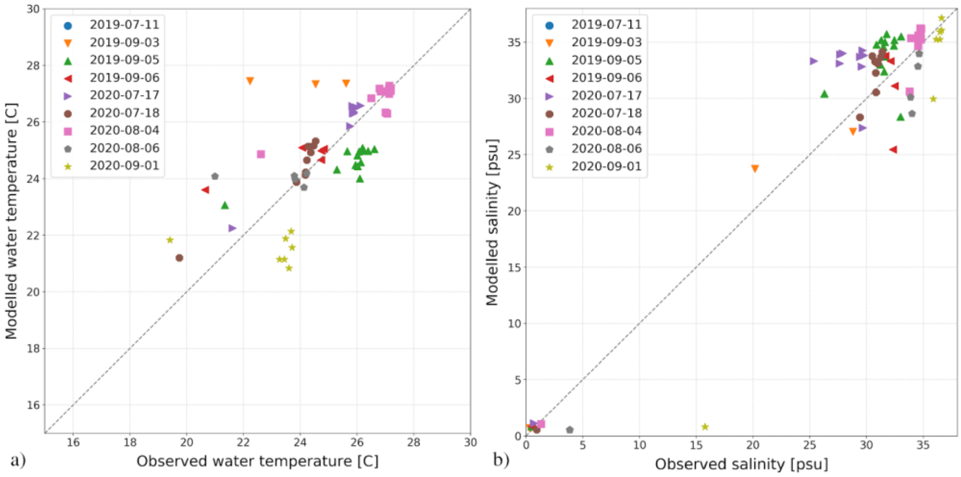

Figure 2: Scatter plot of observed and simulated water temperature (a) and salinity (b) in the Fano-Arzilla study area (2019 and 2020 samples).

As shown in Fig. 3, model results were generally in good agreement with the continuous water temperature values measured in the Pescara harbour. The model well captured the observed weekly variability of the water temperature during the summer of 2020, as well as the daily cycle. RMSE, BIAS and R between modelled and observed water temperatures in Pescara are 0.50 °C, 0.46 °C and 0.93, demonstrating the good performance of the finite element modelling suite for this study site.

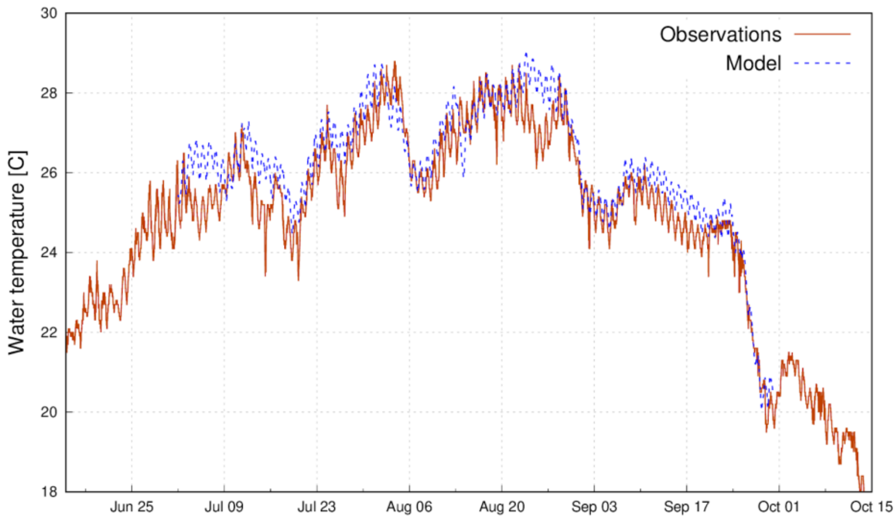

Figure 3: Measured and simulated water temperature in Pescara harbour (summer 2020).

Despite the sparse data and the complexity of the system, the model seems to be able to reproduce the observed salinity and water temperature distributions in the Raša River canal (Fig. 4). Salinity ranged from 3 to 38 psu and was generally increasingly moving from the river mouth to the sea, even if during the 18 September 2020 survey all observations have values around 37 psu. This is due to the temporal fluctuation of the Raša River discharge which in a few days passed from less than 1 m3 s-1 to 15 m3 s-1 as a consequence of an intense rainy event. The obtained BIAS, RMSE and R for the salinity are 1.3 psu, 7.1 psu and 0.71, and -0.4 °C, 1.7 °C and 0.67 for the water temperature. Generally, the model underestimated salinity near the river mouth and overestimated it at the two touristic sites located at 1.5 and 3.4 km from the river mouth. The mismatch could be due to the uncertainty on the bathymetry of the very shallow (less than 1 m) area in front of the river mouth and which was not monitored during the bathymetric survey.

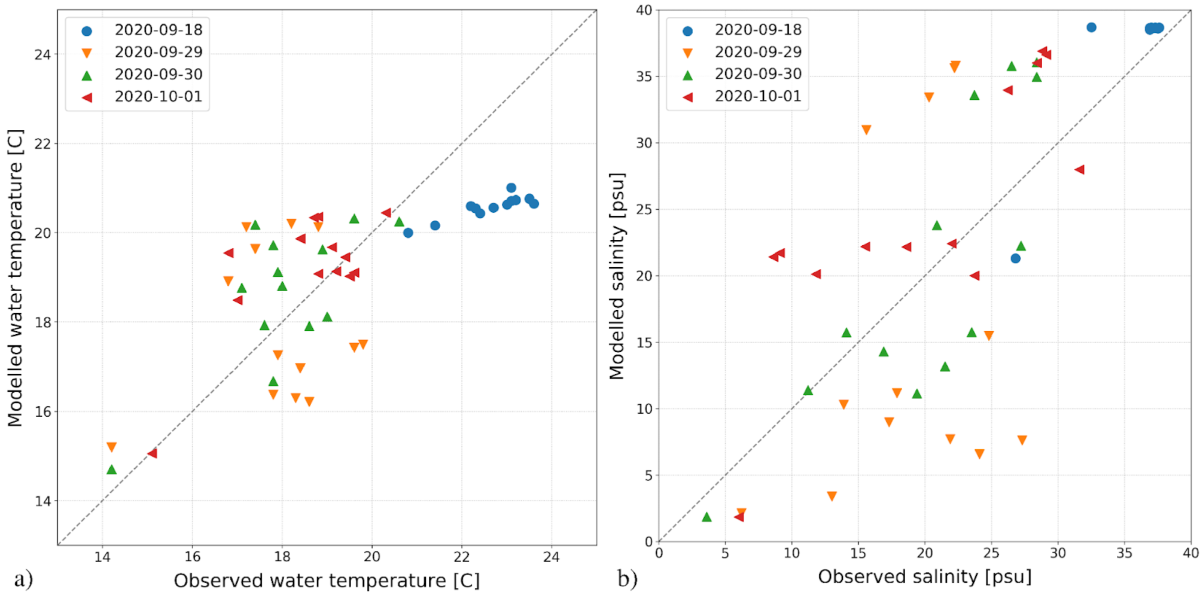

Figure 4: Scatter plot of observed and simulated water temperature (a) and salinity (b) in the Raša study area (2020 samples).

3.3. Microbial pollution assessment

Regarding microbial pollution, the numerical model results were compared with the *E. coli* concentration measured in the Fano-Arzilla and Raša study areas for assessing the capacity of the model in reproducing the dispersion and decay of faecal bacteria in nearshore waters. E. coli concentration is reported as CFU 100 ml^{-1} of water.

In the Fano-Arzilla site, the *E. coli* concentration was monitored with nine sampling surveys in the summer of 2019 and 2020. More details about the sampling strategy and the microbial analysis can be found in Penna et al., (2021).
As shown in Fig. 5a, the numerical model provides a realistic representation of the *E. coli* distribution in the nearshore waters, describing the marked decrease in the bacteria concentration observed from the river mouth towards the open sea. This is mostly due to the effect of dilution with sea waters and decay induced by solar radiation and salinity.
According to the scatter plot presented in Fig. 5b, the modelling system well described (mostly within an order of magnitude precision) the observed *E. coli* concentration measured in the two years of sampling activity. RMSLE for E. coli concentration in Fano-Arzilla is 0.18, a value below the ones reported in other studies (Thupaki et al., 2010; Liu et al., 2012; Locatelli et al., 2020; Weiskerger and Phanikumar, 2020), and the correlation coefficient is 0.93.

During some events, e.g., on 5 September 2019 and 17 July 2020, the model underestimated the bacterial concentration in coastal waters. Such discrepancy could be related to the occasional formation of ephemeral stagnant freshwater pools at the river mouth, not reproduced by the model, where bacteria proliferate before reaching the sea.

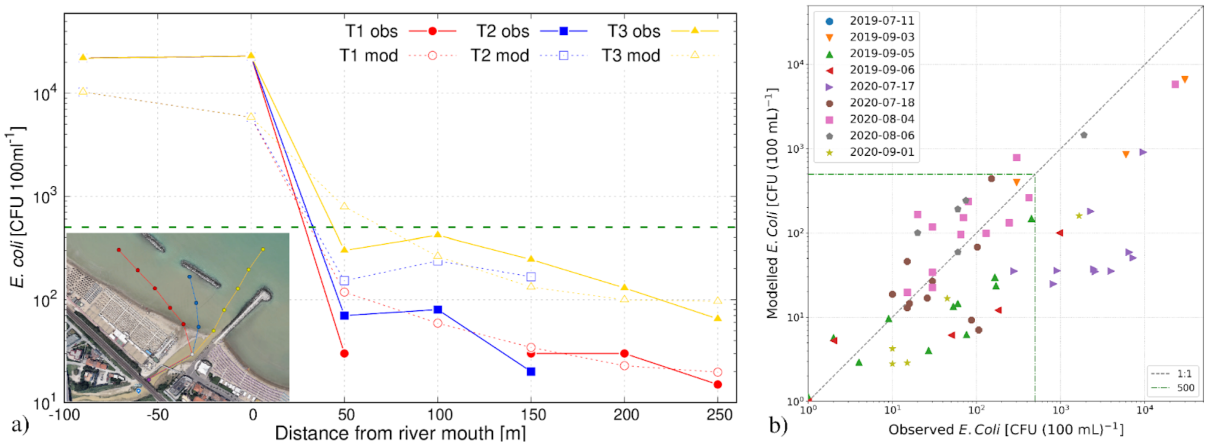

Figure 5: Observed (obs) and simulated (mod) E. coli concentration in Fano. a) Simulated (dashed lines) vs. observed (solid lines) concentration along the three river-sea transects monitored on 4 August 2020. b) Scatter plot of simulated versus observed values (2019 and 2020 samples). The green dashed line indicates the 500 CFU 100 ml^{-1} value.

In the Raša River canal, the model is reproducing the observed *E. coli* concentrations with a satisfactory agreement (Fig. 6a). RMSLE and R for *E. coli* concentration in Raša are 0.44 and 0.68, respectively. E. coli concentrations at the mouth of the Raša River and adjacent touristic locations were below 10 CFU 100 ml^{-1} on 18 September 2020 and increased up to the bathing limit of 500 CFU 100 ml-1 as a consequence of the rainfall rain event of 29 September 2020. As shown in Fig. 6b, the polluted waters coming from the Raša River tended to flow along the western coast. The model slightly underestimated the faecal bacterial concentration in Trget and Blaz.

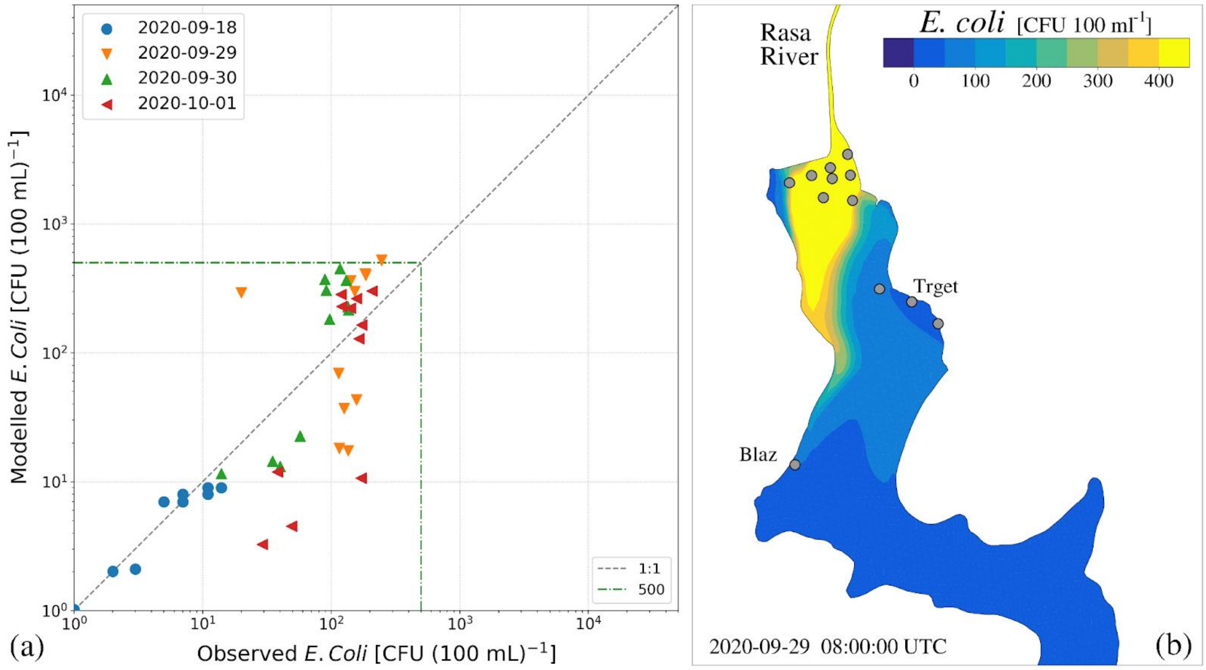

Figure 6: a) Scatter plot of simulated versus observed E. coli concentrations (2020 surveys). b) Simulated distribution of E. coli on 29 September 2020 at 08 UTC. The grey dots mark the sampling stations.

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