



Modelling pollutants transport scenarios based on the X-Press Pearl disaster

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ABSTRACT

The MV X-Press Pearl accident near Sri Lanka in May 2021 released several pollutants into the ocean, including 1843.3 t of urea, raising concerns about the impact on the region. This study uses a coupled ocean (NEMO)–biogeochemistry (ERSEM) model to simulate urea dispersion under various scenarios. While it doesn't directly reflect the real accident, it provides insights into the potential impact of similar chemical spills. By adjusting tracer release rates and timing, we assessed their impact on the distribution of the chemical plume. Findings show slower release rates prolong higher urea concentrations, potentially causing phytoplankton blooms, while monsoon conditions significantly affect dispersal patterns. Due to a lack of publicly available urea observations, we used particle tracking experiments validated with data on plastic nurdle beaching. This research shows how a simpler, affordable scenario approach could inform the management of chemical spills without a fully developed operational oceanographic system.

1. Introduction

Shipping accidents and wreckage are unpredictable and can lead to great environmental disasters if polluting cargo or fuel is released into the sea. These accidents need fast responses to limit the damages. Direct intervention is usually carried by governmental bodies (e.g. armed forces) or third parties with operative capacity (e.g. specialised salvage companies or experienced voluntary groups) once an accident has occurred. To maximise the benefits of these interventions, it is important to be able to understand and predict where pollutants are likely to spread in case of an accident and what the potential impact of a shipwreck may be. Here we use a real shipping accident (Fig. 1) as case study to demonstrate methods that can be used to simulate pollutants transport in coastal regions for hypothetical scenarios of passive tracer release. In particular, we will look at the role that the timing of the events can have in determining the footprint of such a disaster. In May 2021, the MV X-Press Pearl cargo ship caught fire and sank near the coast of Colombo, the capital of Sri Lanka. It is reported that the first fumes were noted on the ship on the 20th of May, and then developed in

an intense fire which led to a major explosion on board on the 25th of May (Partow et al., 2021).

The vessel was at the time located about 17 km from Colombo's port, though there has been an attempt to move the ship further offshore in the week following the accident (Partow et al., 2021). The ship was transporting 1486 containers, 81 of which were loaded with 15 types of dangerous substances (Partow et al., 2021; Vithanage et al., 2023a), some of which were released into the water from the shipwreck location. These included 25 t of nitric acid (Partow et al., 2021), which is believed to be the most likely cause of the fire in the first place after leaking from a faulty container (Vithanage et al., 2023a), and around 1680 t of microplastics in the form of nurdles or pellets and several chemicals many of which are considered hazardous or noxious (Partow et al., 2021). Previous studies have mostly focused their attention on the dispersion and impact of the microplastics pollution (Karthik et al., 2022). In this work we will primarily focus on the dispersion of chemicals and in particular of urea, an organic nitrogen compound increasingly used as agricultural fertiliser (Glibert et al., 2006). We focus on urea because this was the most abundant chemical in the ship (1843.3 t

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Fig. 1. MV X-Press Pearl ship approaching Colombo, with visible emanating smoke/vapour (Vithanage et al., 2023a). Image credit to: Ajith Priyal de Alwis.

(Partow et al., 2021)). Nitrogen is a key element in the ocean to sustain marine life. While dissolved inorganic nitrogen is the main source of nitrogen for phytoplankton growth, urea can be used as nutrition by bacteria as well as many phytoplankton species, including some that are noxious to the other marine species and human health (Glibert et al., 2006; Glibert et al., 2005). A release of urea from the containers could therefore trigger a bloom of planktonic species that could have cascading effects on other species (Maitra and Nath, 2014; Ofojekwu et al., 2008; Ranasinghe and Sugandhika, 2016; MFARD, 2023). Furthermore, urea can also have a direct toxic effect on marine life with lethal effects being observed when concentration exceeds a few g l^{-1} (Maitra and Nath, 2014; Ofojekwu et al., 2008; Gupta and Kumari, 2021). Studies following the MV X-Press Pearl accident observed that the most abundant species of phytoplankton present in proximity of the wreck were harmful diatoms and dinoflagellates (Pathmalal et al., 2023). For these reasons it is important to study how the urea on board of the ship might have dispersed in the environment, how big the area affected could be, and how quickly the concentration could have been reduced to background values. The event coincided with the beginning of the southwest monsoon, which developed over the Andaman Sea on 21st May 2021 and set in over the accident site on 25–26 May 2021 (IMDC-SR/11) as well as with the time of tropical cyclone Yaas (Sil et al., 2021; Mohanty et al., 2022), which formed in the Bay of Bengal around the 22nd May 2021 and had landfall on 26th May 2021. The onset of First Inter Monsoon is a transition period for the northerly current to reverse southerly at around the accident site. The pre-monsoon transition and the very severe cyclonic storm might have impacted on the transport of the released cargo, which raises the question of the importance of the accident timing for the magnitude of the impact. In this study we set-up a high-resolution coastal ocean numerical model by coupling a physical ocean model with a biogeochemistry model, to simulate the release of urea from the location of the shipwreck near the Sri Lanka coast. The work aims to assess the potential dispersion of urea from an accident of the same magnitude of the MV X-Press Pearl. It addresses the following questions: (1) How is the footprint, concentration, and exceedance duration of chemical (urea) pollution affected by different rates of tracer release? (2) How important is the role of the accident's timing in driving the pollutant's dispersal (chemical and particles)? It is important to note that there are no data available in the public domain on the chemical composition of the water following the accident. For this reason, we were only able to do an indirect validation of the footprint of the pollution (Section 3.4) and therefore this work does not aim to provide a comprehensible impact assessment of the real accident.

2. Method

2.1. Model set-up

To answer those questions, we used a coupled model system based on the NEMO ocean model (Gurvan et al., 2019) with the biogeochemical model ERSEM (P. M. L., 2022; Butenschon et al., 2016), coupled through the Framework for Aquatic Biogeochemical Models (FABM) (Bruggeman and Bolding, 2023). The system set up over the Sri Lanka region (Fig. 2) is referred to as SRIL34 model. It was built following the relocatable NEMO framework (Polton et al., 2022) and all essential files used to build this system (on the Archer2 HPC), and instructions to reproduce the set-up are publicly available via the zenodo repository (Rulent, 2022), or the corresponding github repository. The model is built at $1/60^\circ$ (approximately 1–2 km) horizontal resolution grid and uses terrain following hybrid vertical coordinates with 31 vertical levels. The model uses ERA5 data (Hersbach et al., 2024) as atmospheric forcing, and FES tides (FES2014, 2024) at the boundaries, while boundary conditions of temperature, salinity and currents are built from a CMS Global reanalysis product (CMS, n.d.). Initial conditions come from an uncoupled physics simulation (NEMO only), starting in January 2019 which gives more than one year spin-up time for the physics (Rulent et al., 2024a). All coupled simulations were conducted with a one-minute time step and lasted up to 90 days.

To simulate urea in ERSEM we used the simple approach of considering urea as a passive tracer (using only the module pelagic base, (P. M. L., 2022)). While we acknowledge that urea is chemically and biologically reactive, the passive tracer assumption allowed us to use a minimal implementation of ERSEM and therefore reduce our dependency on external datasets to adequately initialise the concentration of urea. Furthermore, rates of consumption of urea vary significantly with environmental condition (e.g. temperature and abundance and type of planktonic organisms, (Solomon, 2019)), and in the absence of these data is difficult to provide a best estimate for this important parameter. In order to assess the impact of such assumption we have performed a sensitivity test, removing the assumption of passive tracer. Finally, the passive tracer assumption allow for a conservative estimate of the footprint and it allows to extend the results on urea dispersion from this study to many other contaminants that can be considered at first instance as passive. In the simulations used for this study, the release of urea has been simulated by adding a constant flux of urea in the deepest

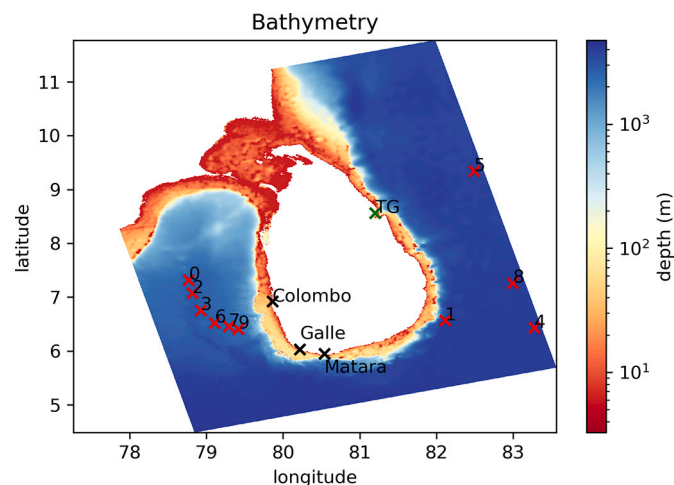


Fig. 2. Domain's bathymetry. Note the logarithmic colourbar, which allows to see in details both shallow and deep regions of this shelf. The Location of the EN4 data sampling points are indicated with a red cross, the Trincomalee TG is marked with a green cross. The cities named in the discussion are also marked on the map. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

water cell at the accident's location (approx. coordinates 7.0546°N 79.7589°E).

2.2. Experiment set-up

2.2.1. chemical tracers experiments

Different types of experiments are conducted with the coupled model with the tracer release set-up at different rates, or at different dates. In the immediate aftermath of the event, little information about the accident's circumstances was made publicly available and it was not possible to establish the exact amounts of chemical transported, or how fast they were being released into the environment. The initial information referred to 1100 t transported from the ship, which was used in our simulations. Once the official data on the cargo were released (Partow et al., 2021), we scaled all simulations by a factor of 1.68 to account for the higher amount. The assumption of linearity was successfully tested repeating one simulation with the correct release rate. Furthermore, no information about the speed of the release of contaminant was available and therefore we opted to define a set of five different hypothetical scenarios (Table 1), where different urea release rates and duration are assumed so that the 1843.3 t of urea are released over 1 h, 6 h, 1 day, 7 days, and 15 days. For the two fastest release experiments, outputs are stored hourly to conduct a more detailed analysis of these specific cases as they may exhibit noticeable changes on an hourly time scale (Rulent et al., 2024b). The values are then averaged daily to consistently compare these two runs to the 1 day, 7 days and 15 days release scenario for which outputs are saved as daily mean (Rulent et al., 2024c).

The five simulations are compared, and the concentration of urea is analysed as a function of distance from the ship. The analysis also encompasses the footprint covered by tracers in all scenarios. For this analysis, we define the footprint as the area where the model has computed a non-zero tracer value. In the absence of in-situ information about urea concentration in Sri Lankan coastal waters, we have used a value of 0.12 µM as a threshold representative of the background concentration. This value comes from the previous study of (Sipler and Bronk, 2015), which summarises the outcomes from a range of studies on dissolved organic nitrogen concentration, including urea, in the

Table 1
Summary the SRIL34 simulation and experiments of 1843.3 t tracers released at different rates/dates.

Summary of simulations			
Run date	Release rate	Output frequency	Notes
May–Jul 2021	1 h	Hourly	Post processed as daily mean before comparing with other outputs
May–Jul 2021	6 h	Hourly	Post processed as daily mean before comparing with other outputs
May–Jul 2021	1 day	Daily mean	Can be compared to run with Jan/Sep/Oct start dates
May–Jul 2021	7 days	Daily mean	
May–Jul 2021	15 days	Daily mean	
Jan–Mar 2021	1 day	Daily mean	
Sep–Nov 2021	1 day	Daily mean	
Oct–Dec 2021	1 day	Daily mean	
May–Jul 2021	1 day	Daily mean	Active tracer test $k = 0.01 \text{ d}^{-1}$
May–Jul 2021	1 day	Daily mean	Active tracer test $k = 0.1 \text{ d}^{-1}$
May–Jul 2021	1 day	Daily mean	Active tracer test $k = 0.5 \text{ d}^{-1}$
May–Jul 2021	1 day	Daily mean	Active tracer test $k = 0.9 \text{ d}^{-1}$

ocean and coastal areas. Their average value is of $1.24 \pm 1.12 \mu\text{M}$ (Sipler and Bronk, 2015). We use the lowest value of the range (0.12 µM) as a threshold to estimate the exceedance duration of tracers above plausible conditions, by estimating the number of days in which the tracer concentration remains higher than 0.12 µM. Because of the lack of site-specific information about the background concentration of urea, we are not able to properly assess the potential cascading of impacts on the ecosystem and therefore we focus on understanding how the urea added to the system can alter local chemical condition, and how spread in space and time such perturbation could be. We estimated the extent of the coastal strip reached by urea by extracting all the ocean cells bordering the land regions of the domain and estimating the number of cells above the 0.12 µM threshold. Given the horizontal resolution is between 1 and 2 km, we estimated the length of coast impacted by the polluting event by multiplying the number of cells by 1.5 km.

To assess the influence of the phase of the monsoon regime on the dispersion of urea, we defined further scenarios. The release rate is kept constant at 1843.3 t of urea over one day. However, we vary the day of the release from the 25th of May 2021, which aligns with the onset of Yala, the southwest monsoon phase (Geetha et al., 2021), to the 25th of January, representing the weakest northeast monsoon phase (Maha). Additionally, we consider release dates on the 25th September 2021, marking the transition phase between Yala and Maha, and 25th October 2021 during the most intense phase of Maha (Table 3).

All simulations begin on the first of the month of the release and are run for three months. This means that in the simulation starting in September the tracers will disperse throughout the end of September/start of October, during the transition phase between the northeast and southwest monsoon while the simulation starting in October will simulate the impact of an accident during the northeast monsoon. Finally, the end of January will cover a quiet period. We then repeat the analysis on tracer concentration, footprint, and exceedance duration of tracers.

2.2.2. Sensitivity analysis

In order to test the impact of the passive tracer assumption on the shape and persistence of the footprint, we have implemented a sensitivity test where we simulate the dispersion of urea as an active tracer being consumed following a first order kinetic with a constant specific rate (k) varying between 0.01 d^{-1} , 0.1 d^{-1} , 0.5 d^{-1} and 0.9 d^{-1} (Table 1). These values were selected to encompass the range of uptake rates reported in (Mulholland and Lomas, 2008; Solomon et al., 2010; Painter et al., 2008). The sensitivity test has been implemented only for the 1-day leak scenario on the date of the accident. Similarly to the passive assumption run, the tracers are release from the bottom cell closest to the accident's location on the 25th May 2021 and we estimate the maximum concentration, length of coast reached by tracers (above 0.12 µM), as well as the mean and maximum residence time of tracers above 0.12 µM (Table 2). We also compare the results from these simulations to that of the 1-day run by showing the difference between the 1-day release passive tracer outputs and the active tracer tests, estimating the mean difference between the runs for all value above $0.001 \mu\text{M}$. Note that this limit is chosen to avoid accounting for the widespread areas where all runs are estimating similar values very close to zero, which skews the results. We also estimate the differences between the overall maximum values found.

2.3. Validation of physical model

The model sea surface height (SSH) was validated against the tide gauges (TG) of Trincomalee and Colombo during the months of May and June using the physics outputs from a run with hourly output. The Trincomalee TG data are publicly available through EMODnet (E. M. Viewer, 2024) from the National Aquatic Resources Research and Development Agency (NARA) providers. The Colombo TG belongs to IOC sea level monitoring (maintained by NARA), and can be accessed via

Table 2
rmse of EN4 data to model for temperature (Temp.) and salinity (Sal.) at each station.

Station	0	1	2	3	4	5	6	7	8	9
Temp. (°C)	0.94	0.95	0.87	0.85	0.75	1.18	0.64	0.8	0.76	0.81
Sal. (PSU)	0.2	0.17	0.14	0.16	0.12	0.18	0.18	0.21	0.27	0.17

(VLIZ, Flanders Marine Institute. Intergovernmental Oceanographic Commission (IOC), 2024). Upon visual inspection of the TGs data, all values above 3 m and below 1.5 m were removed as evident outliers in the observations. The mean sea level was then estimated from the remaining TG values and removed from the time series. This was compared to the model's SSH at the closest point to the TG. For consistency, the mean sea level estimated from the model data was also removed from the model time series. A set of EN4 (Good et al., 2013) temperature and salinity profiles was also used for validation; this is publicly available from the Met Office Hadley Centre. The dataset was processed through the COAST analysis toolbox (Polton et al., 2022) for the analysis to be tractable and reproducible (Polton et al., 2023). Ten data points were available within the model domain to compare to the simulated temperature and salinity (Fig. 2). The model data values were interpolated at the observation depths before being compared to estimate the mean bias, and root means square error (rmse).

2.4. Particle tracking set-up

Since the only publicly available information on the spread of the impact of the MV X-Press Pearl disaster is the beaching of plastic nurdles (Jayathilaka et al., 2022), in order to provide a further validation of the ability of the model to assess the potential footprint of the accident, we have implemented some particle tracking experiments using the physical condition predicted by the model described in the previous section.

Particle tracking using a Lagrangian approach is often preferred over a Eulerian approach for predicting plastic dispersal due to its ability to track individual particles, providing a more detailed representation of their movement. Where the Eulerian method regards the particle phase as a continuous medium and formulates its conservation equations based on control volumes, resembling those for the fluid phase, in contrast, the Lagrangian method treats particles as discrete entities, following the trajectory of each individual particle (Zhang and Chen, 2007). Moreover, the Lagrangian approach allows for the incorporation of additional factors such as buoyancy (e.g. (Kaandorp et al., 2023)), enabling a comprehensive modelling of plastic behavior under hydrodynamic conditions. Lagrangian approaches are better equipped to handle transport barriers like eddies and currents (Davis, 1994), which significantly influence dispersal patterns (Chang et al., 2018; Ward et al., 2023). Additionally, they yield more accurate results in scenarios involving turbulent flow fields or complex geometries (Nordam et al., 2023), as they directly simulate particle movement through these environments. Overall, the Lagrangian approach offers a detailed and flexible framework for capturing the diverse movements of individual plastic particles, such as nurdles, in dynamic environmental conditions.

Here we used the physical conditions described by the NEMO model to drive a 3D Lagrangian model, OceanPARCELS (v2.0: (Delandmeter and van Sebille, 2019)), exploring the potential trajectories of particles released from the X-Press Pearl in the days following the disaster. Particles were constrained to the surface waters to reflect the buoyant nature of the nurdles, and advected using a 4th order Runge-Kutta advection scheme. Stochastic horizontal diffusivity was implemented using a Milstein scheme of order 1. Multiple particles ($n = 1000$) were released hourly from the disaster site starting at midnight on May 25th 2021 until 23:00 on 31st May 2021 and tracked until the 30th June 2021.

To determine the location and timing of beaching particles, a land

mask was created from the NEMO model outputs and a custom function was built within OceanPARCELS to include a binary identifier of whether a particle was on land at each timestep. The time and location of hitting land for each beached particle was then recorded and the haversine formula was used to calculate the Eulerian distance travelled by each particle from release site to land. Finally, a kernel density estimation (KDE) was calculated on the beached particles to provide insight into the spatial intensity of pollution.

To test the validity of the model, survey data from Jayathilaka et al. (2022) reporting the plastic pollution index (PPI) calculated from the number of plastic pellets found on beaches after the disaster was overlaid on the KDE.

3. Results

3.1. Validation of physical model simulations

Here we validate the robustness of the prediction of the physical dynamics in the period close to the date of the accident. Comparison of the SSH to the Trincolmalee TG (Fig. 3) shows an absolute mean difference of -0.017 m between model and observation during May. The rmse in the May–June 2021 period is 0.16 m; this drops to 0.07 m when correcting for a two hour phase offset that can be noted between model and observations. This offset can be attributed partly to the hourly temporal resolution of the model and to output data being hourly averages, in contrast with the instantaneous observation. Moreover, the TG is located within a harbour, which is not resolved by the model, and this will necessarily induce some bias. Similarly, the Colombo TG (Fig. 4) shows a rmse of 0.12 m during the May–June 2021 period, which drops to 0.06 m when corrected for 1 h phase. We therefore consider the model to be adequately resolving the sea level for the purpose of this research.

Comparison to EN4 data shows that the bias in temperature between model and observation is greater near the surface (Fig. 5). Within the first 10 m depth, the mean temperature difference across all stations is -1.55 °C, while the bias across all depths is -0.15 °C. The rmse across all sites varies between 0.64 °C and 1.18 °C (Table 2). On the contrary, salinity bias (Fig. 6) near the surface (0.02 PSU) is lower than the average bias across the water column (0.09 PSU). The rmse across the ten sites varies between 0.12 PSU and 0.27 PSU (2).

3.2. Assessment of the footprint of the MV X-Press Pearl disaster

Here we analyse the potential footprint of the accident by looking at the surface concentration of the pollutant in the first set of scenarios, where the date of the accident is kept at the 25th of May 2021, but the period over which urea is released varies. The fastest leak simulated is that of all tracers being released in a one hour leak (Fig. 7). In this case the maximum hourly averaged surface concentration of tracer found is of 52.97 μM , which occurs 23 h after the release in the location of the shipwreck. This is because the tracer is released at the bottom of the ocean (about 20 m depth), which means it takes some time to reach the surface (about 1 h in this simulation) and start accumulating. After 48 h from the release (27th of May at 00,00), the maximum concentration found at surface has already reduced by more than 50 %, dropping to 22.18 μM still in proximity of the release location. After 72 h (28th May at 00,00), the concentration is below 7.77 μM , and after five days it is below 2.63 μM . By the end of May, a week after the release, the tracer

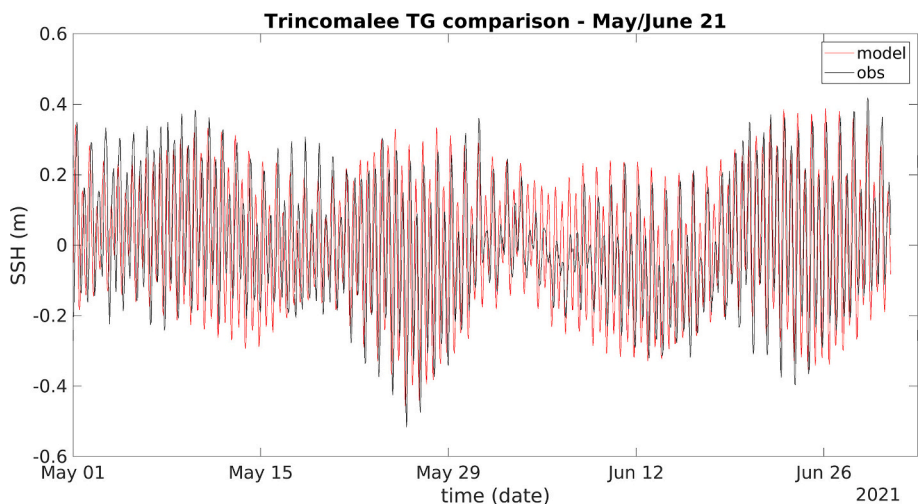


Fig. 3. Model vs TG validation at Trincomalee station.

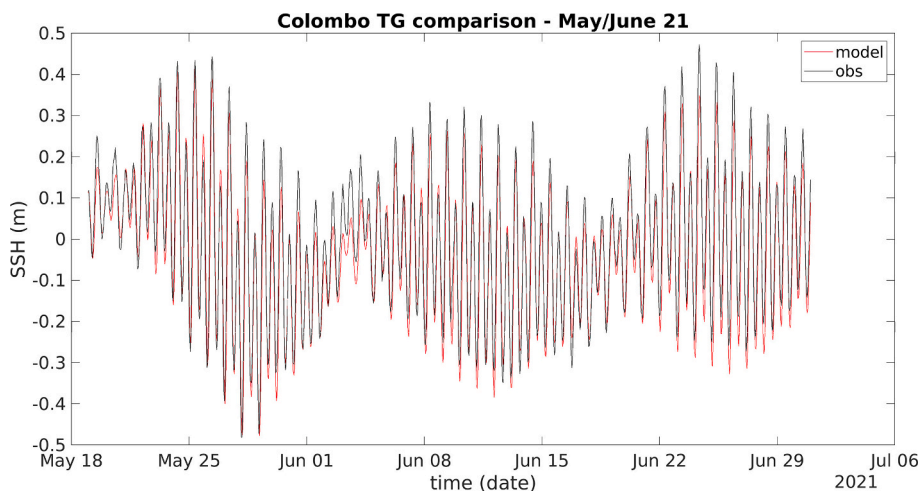


Fig. 4. Model vs TG validation at Colombo station.

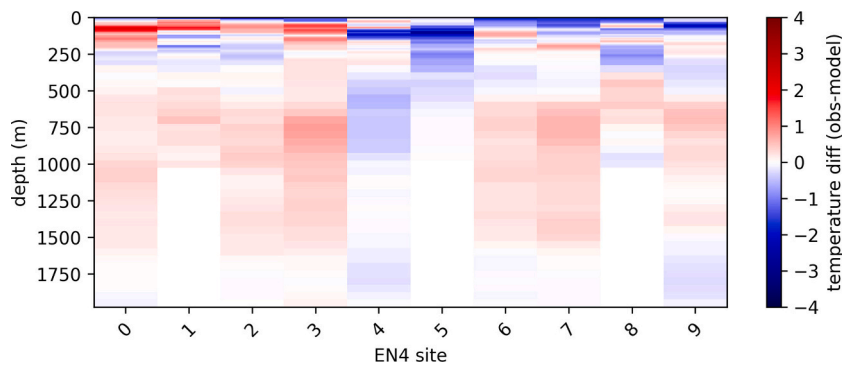


Fig. 5. Model comparison to EN4 temperature data.

concentration has dropped below $0.9 \mu\text{M}$. The tracer is directed south-east from the release location, reaching the southwestern coast of Sri Lanka. To compare the worst case scenario with the other simulations we look at the daily mean concentration rather than the hourly mean, as this is a more appropriate timescale to assess the longer duration scenarios. The worst case scenario has a peak daily mean concentration of urea in surface waters of $17 \mu\text{M}$. This concentration is higher than the peak concentration observed in the other scenarios, but the tracers

disperse faster. The slower the release rate, the lower the peak concentration is (Fig. 8). Slowing the release from 1 h to a day is enough to halve the maximum concentration in the surface domain, while slowing it down to two weeks reduces the maximum concentration by an order of magnitude. The impact is particularly evident in the area around the tracer release point; in the first 50 km from the shipwreck, the difference in maximum concentration between the different scenarios is up to an order of magnitude (Fig. 8). Conversely, the duration of the exceedance

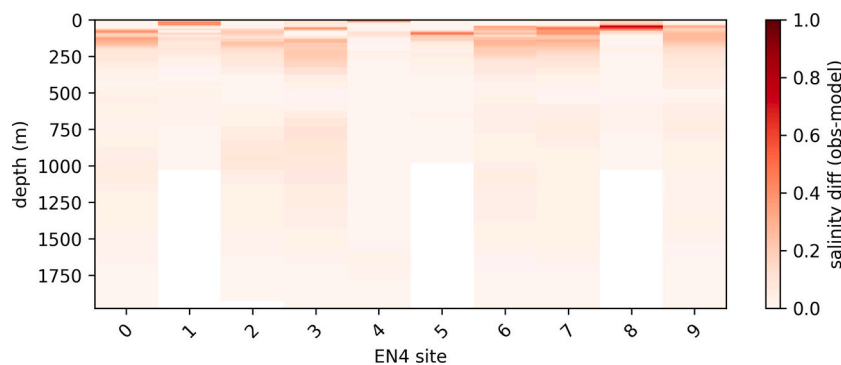


Fig. 6. Model comparison to EN4 salinity data.

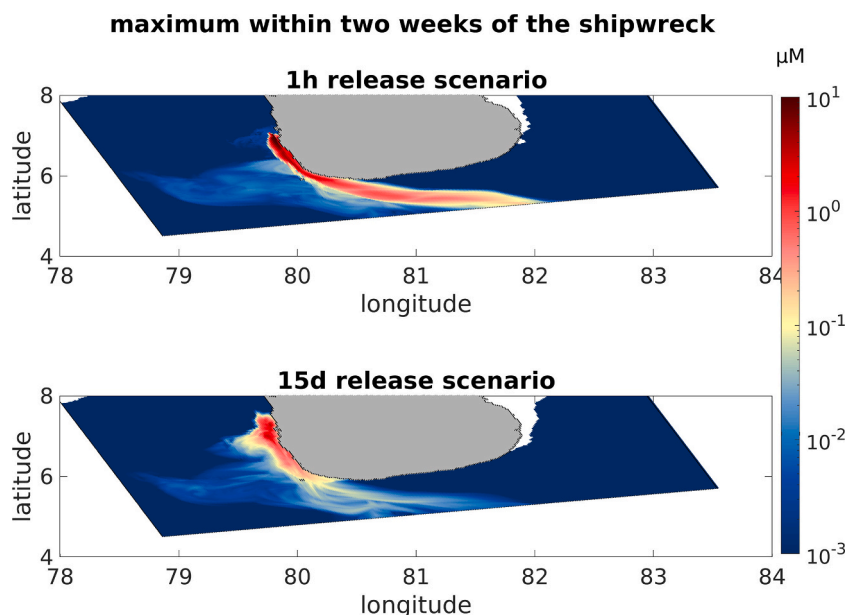


Fig. 7. Maximum surface concentration of the tracer in the domain, at any time within the first two weeks from the release in the 1 h release (top) and the 15 days release (bottom) case scenarios. These are the fastest and slowest release scenario that were simulated. Note that the blue regions are areas where the model calculates low values of tracers, while the white regions are where no tracer is simulated by the model. Land regions are shaded in grey. The abrupt end of the blue region at the northern boundary is due to the cropping of the data to zoom into the image. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of the threshold concentration is longest in the slower release scenarios (7d and 15d), where the concentration remains above the reference value of $0.12 \mu\text{M}$ for more than a month (Fig. 9). This means that even though the overall maximum concentration is lower, the tracers remain in the coastal waters for a longer time period when they are released gradually. It is interesting to note that the 7d release case (not 15d) has the overall greater exceedance duration of tracer. Results also show that reducing the release rate of the tracers only mildly affects the shape of the footprint covered by the pollutants. In all scenarios, regardless of the release rate, the area reached by the pollutants is similar with little difference in the tracer's footprint. After a week from the release, the length of coastal strip reached by the tracers (above the $0.12 \mu\text{M}$ threshold concentration) varies between 175.5 km in the 1 h release case and 219 km in the 7d release case. However, it is clear that in the longer release scenarios (7 days and 15 days) the footprint extends more northwards than in the shortest release scenarios.

Sensitivity tests of the model performance when using active tracer (Table 2, and Fig. 10) show that where k is lower than 0.1d^{-1} the maximum difference against the passive tracer scenario is below $1.33 \mu\text{M}$, while on average the difference is of $1.8 \times 10^{-3} \mu\text{M}$ (Fig. 12). The tracer's footprint is nearly identical (Fig. 11), and similar length of

coastline reached by the tracers (up to 10.5 km difference). The mean residence time is similar (2.1 days for $k = 0.1 \text{d}^{-1}$ as opposed to 2.2 days for the passive tracer scenario) though the maximum residence time is lower (decreasing to 9 days for $k = 0.1 \text{d}^{-1}$ as opposed to 21 days). For uptake rates higher than 0.5d^{-1} , the maximum difference against the passive tracer run is higher, up to $6 \mu\text{M}$ for maximum values. The coastal region reached by pollutant is more than half for $k = 0.5 \text{d}^{-1}$ and down to 45 km for $k = 0.9 \text{d}^{-1}$ as opposed to the 163.5 km resulting from the passive tracer assumption (Table 2). The residence time of tracers in the water is also reduced up from 21 days to as little as 3 days for maximum values, and from 2.2 days to 1.5 days for average values. Overall these sensitivity tests show little difference from passive tracers when considering a urea uptake rate below 0.1d^{-1} , while concentration, exceedance duration and footprint of pollutants can be significantly lower for uptake rates greater than 0.5d^{-1} .

3.3. Role of monsoon phase

The X-Press Pearl shipwreck occurred on the 25th May 2021, coinciding with the onset of Yala, the Southwest monsoon phase (Geetha et al., 2021). To understand how the footprint and concentration of

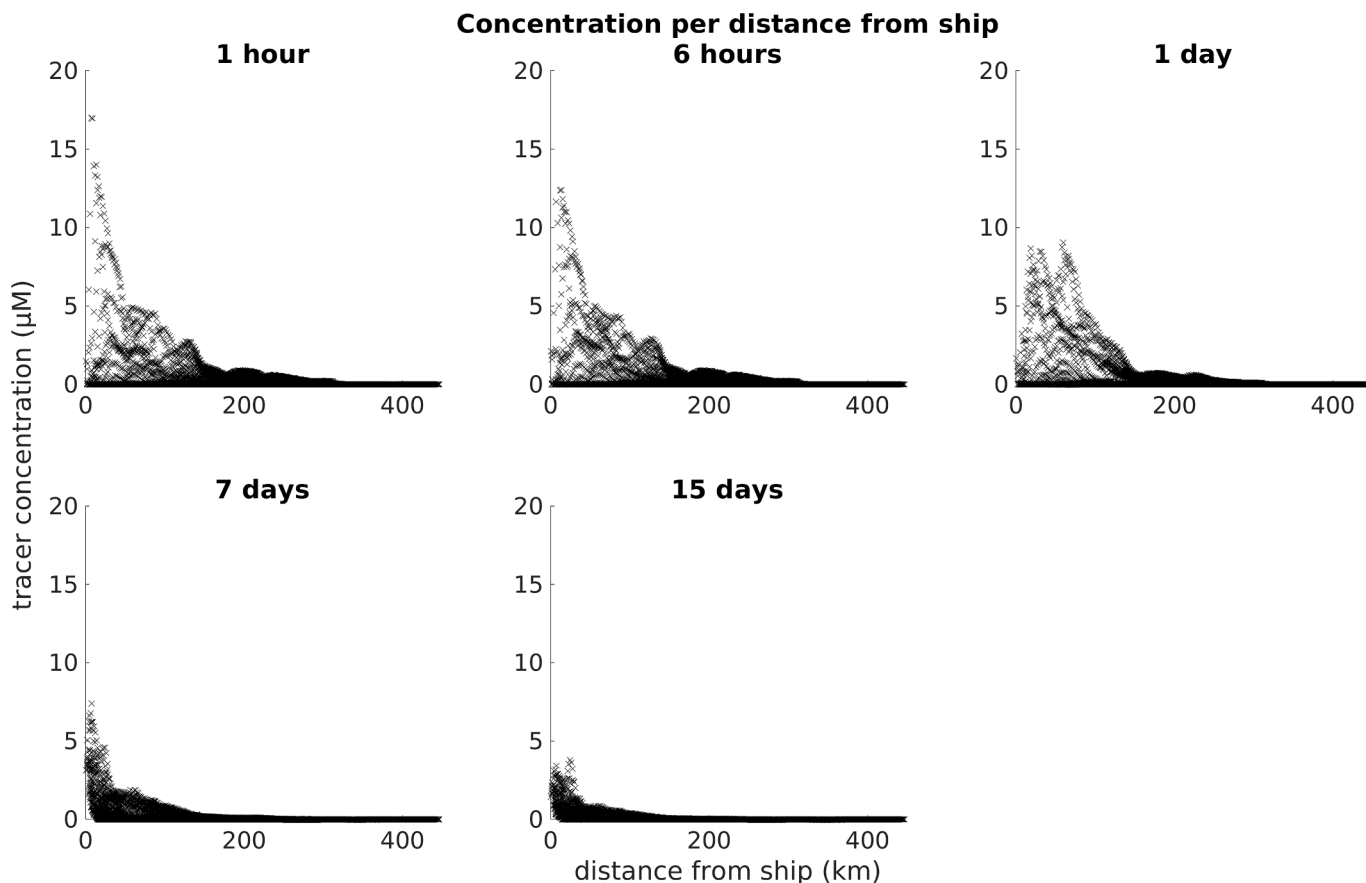


Fig. 8. Maximum tracers concentration at each domain grid point, each day, for two weeks from the tracers release. Results over the different rates of release scenarios as a function of distance from the shipwreck location.

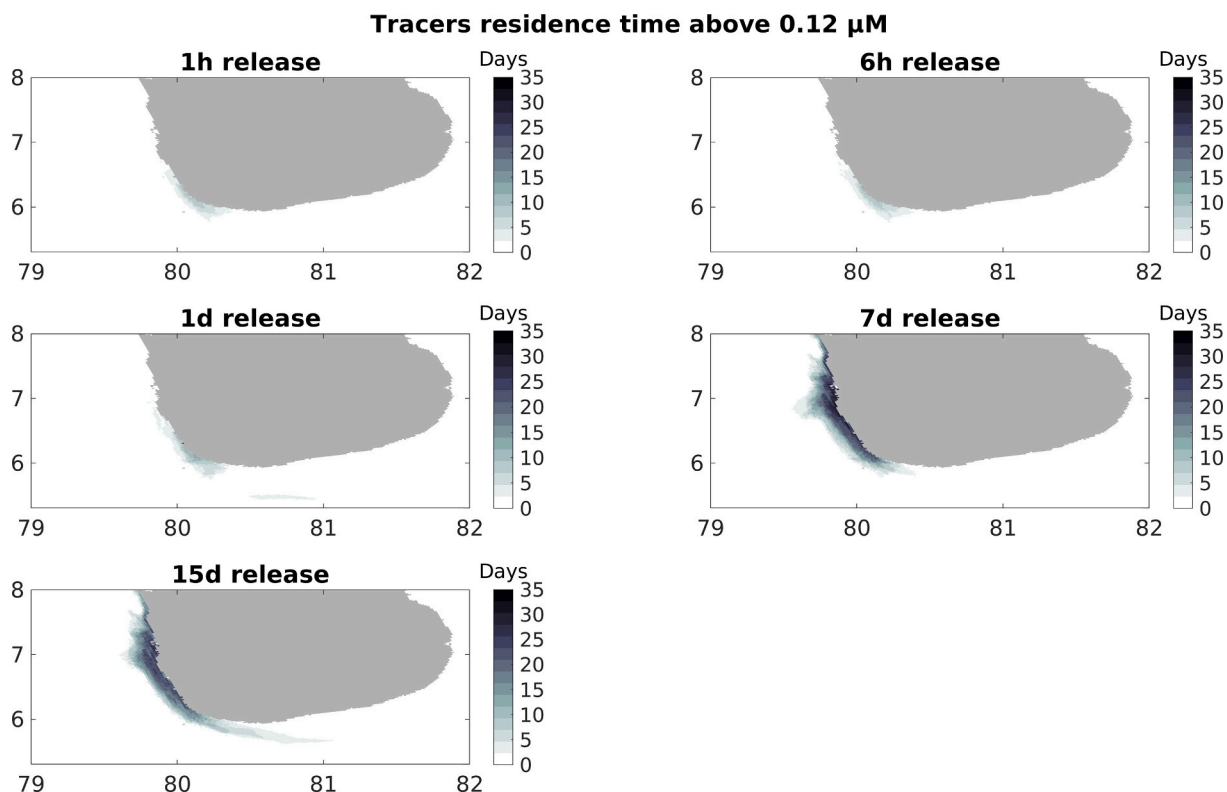


Fig. 9. Exceedance duration of tracers above 0.12 µM for all in different rate of release scenarios.

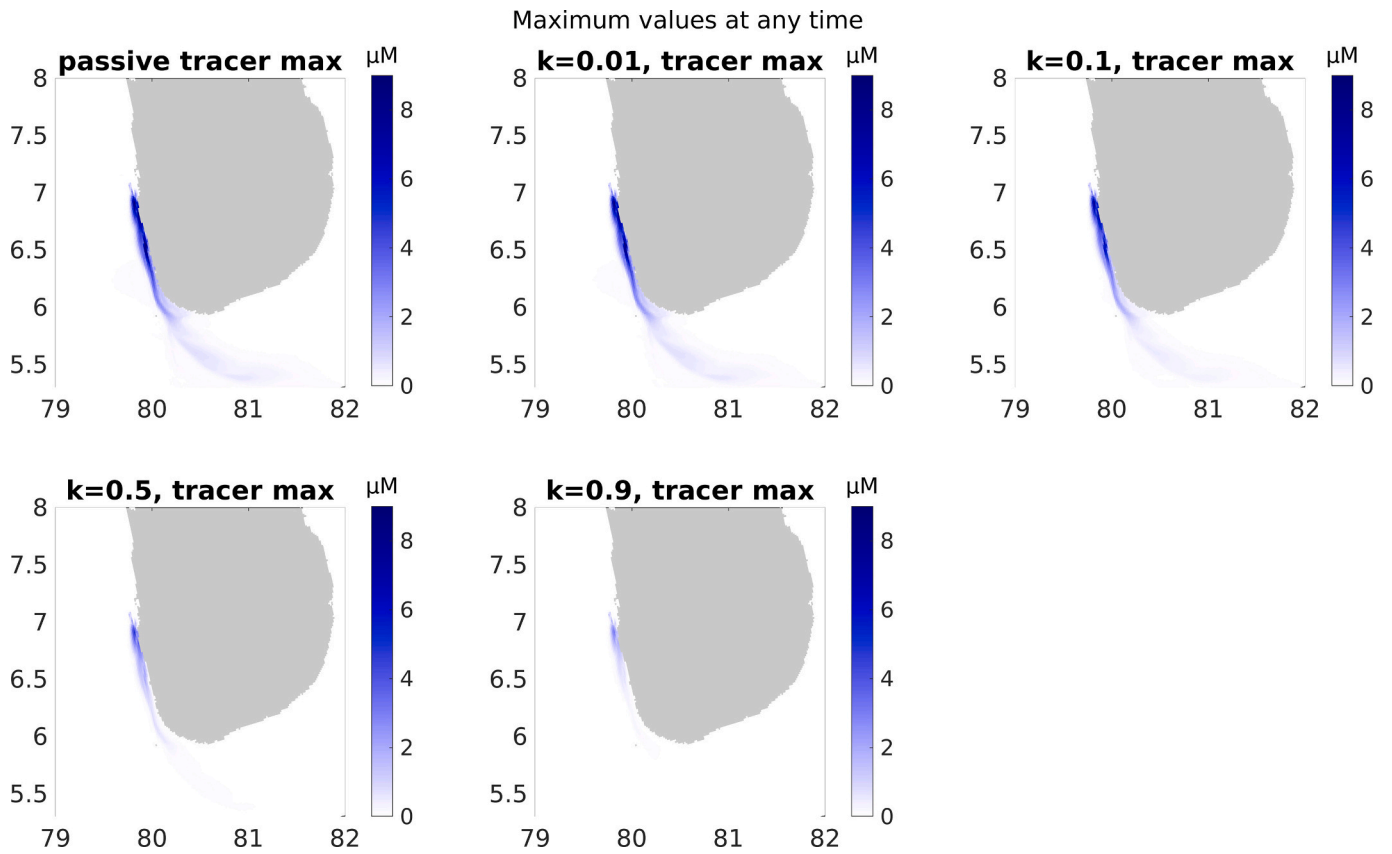


Fig. 10. Maximum values from passive tracer (1 day release) scenario and the active tracer sensitivity tests (for $k = 0.01 \text{ d}^{-1}$, 0.1 d^{-1} , 0.5 d^{-1} and 0.9 d^{-1}).

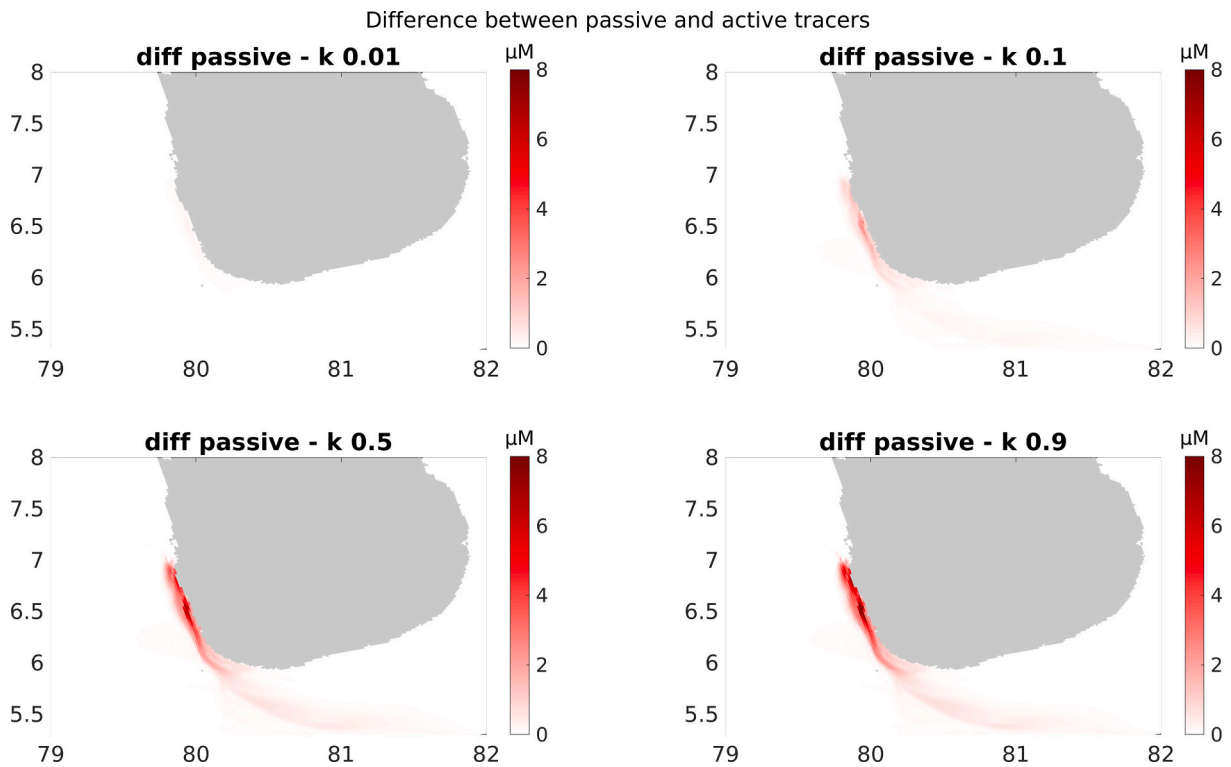


Fig. 11. Differences in maximum values between passive tracer (1 day release) scenario and the active tracer sensitivity tests (for $k = 0.01 \text{ d}^{-1}$, 0.1 d^{-1} , 0.5 d^{-1} and 0.9 d^{-1}).

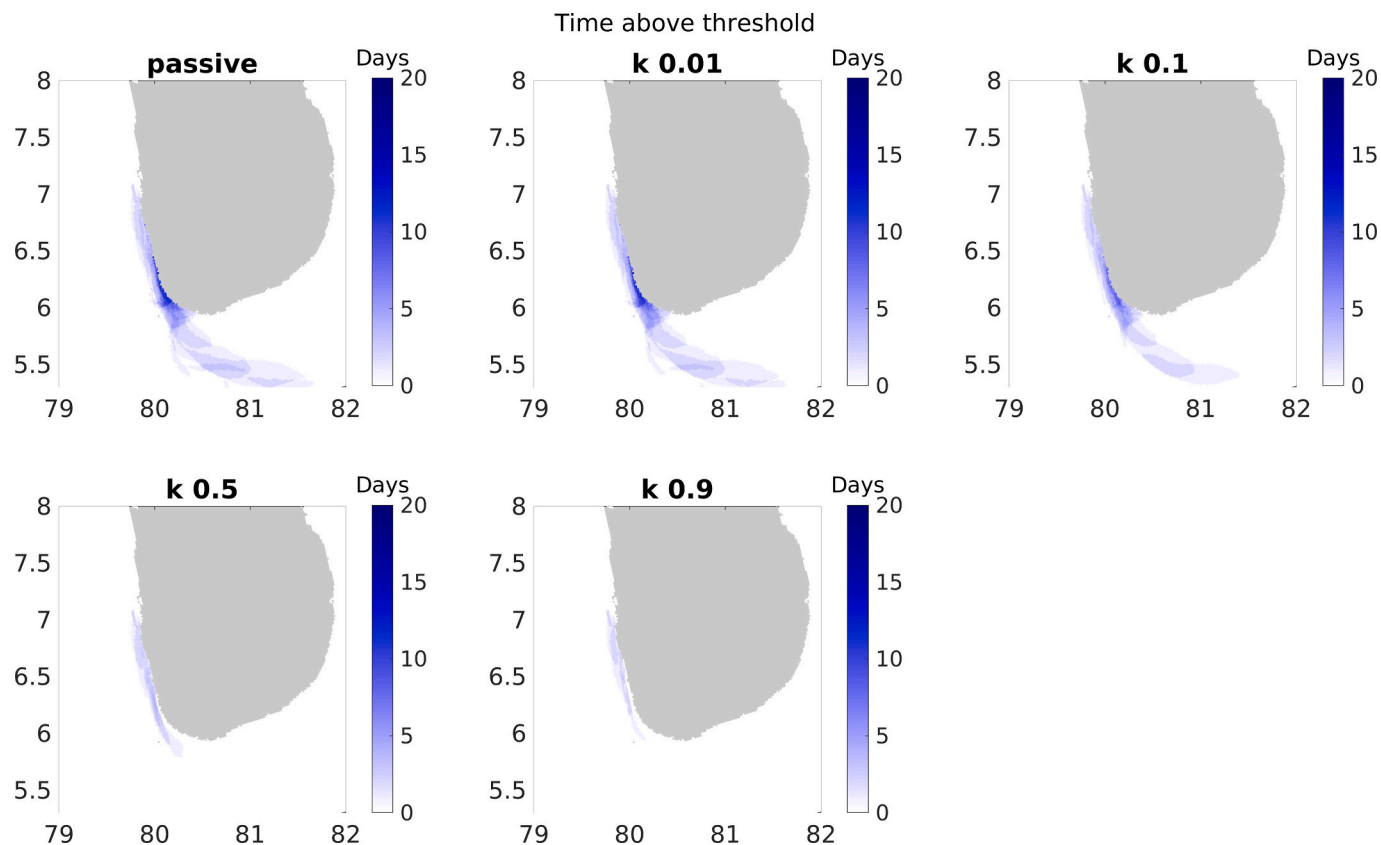


Fig. 12. Residence time of tracers in the passive tracer (1 day release) scenario and the active tracer sensitivity tests (for $k = 0.01 \text{ d}^{-1}$, 0.1 d^{-1} , 0.5 d^{-1} and 0.9 d^{-1}).

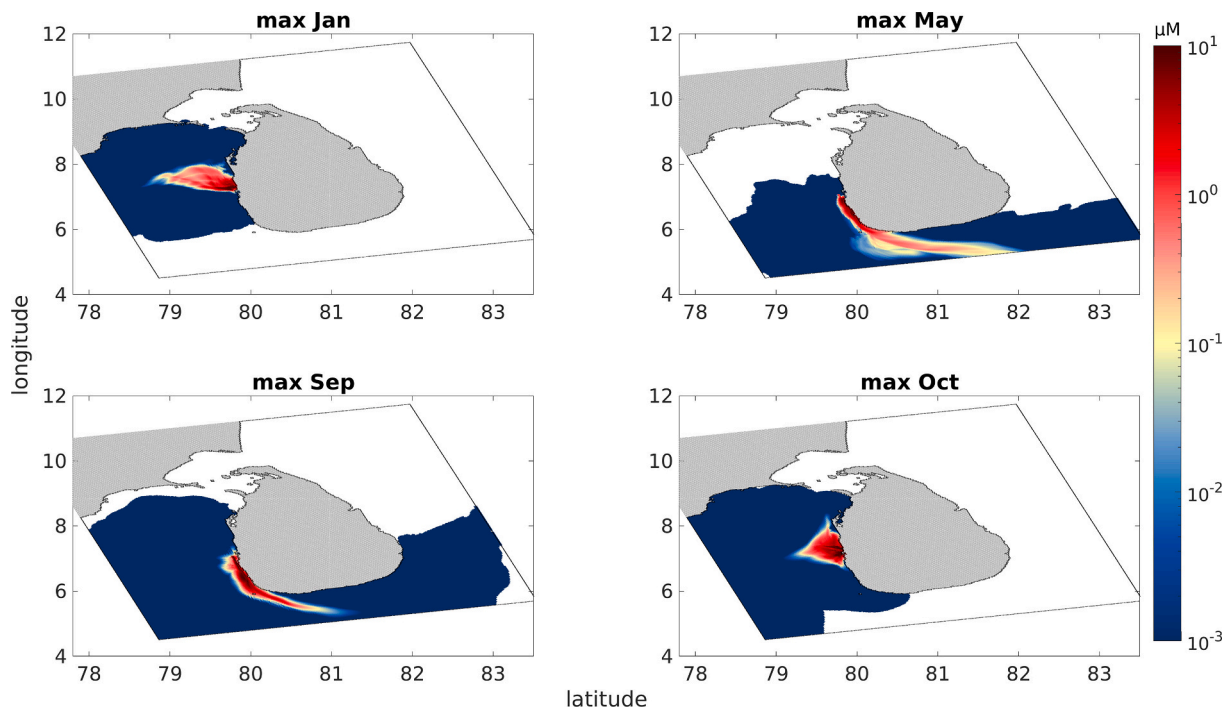


Fig. 13. Maximum daily concentration within a week for different dates of release scenarios. Note that the overall maximum was recorded on the 28th January, 28th May, 27th September, and 29th October.

pollutants could have changed if the accident happened in a different season, hypothetical scenarios were simulated by changing the date of the tracer release. Results show that the footprint of tracers is

significantly affected by changing the release date of the simulation, while the average concentration of the tracer does not vary much (Figs. 13 and 14). After only one week, the tracers in simulations

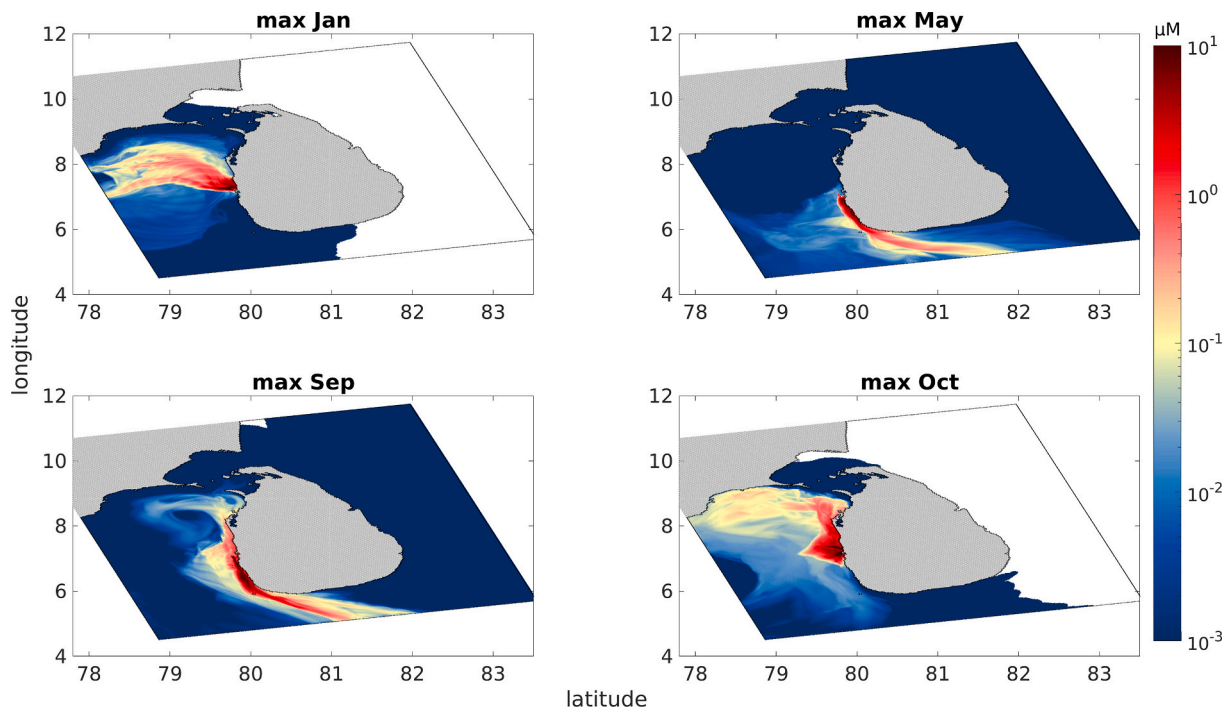


Fig. 14. Maximum concentration within a month for different dates of release scenarios.

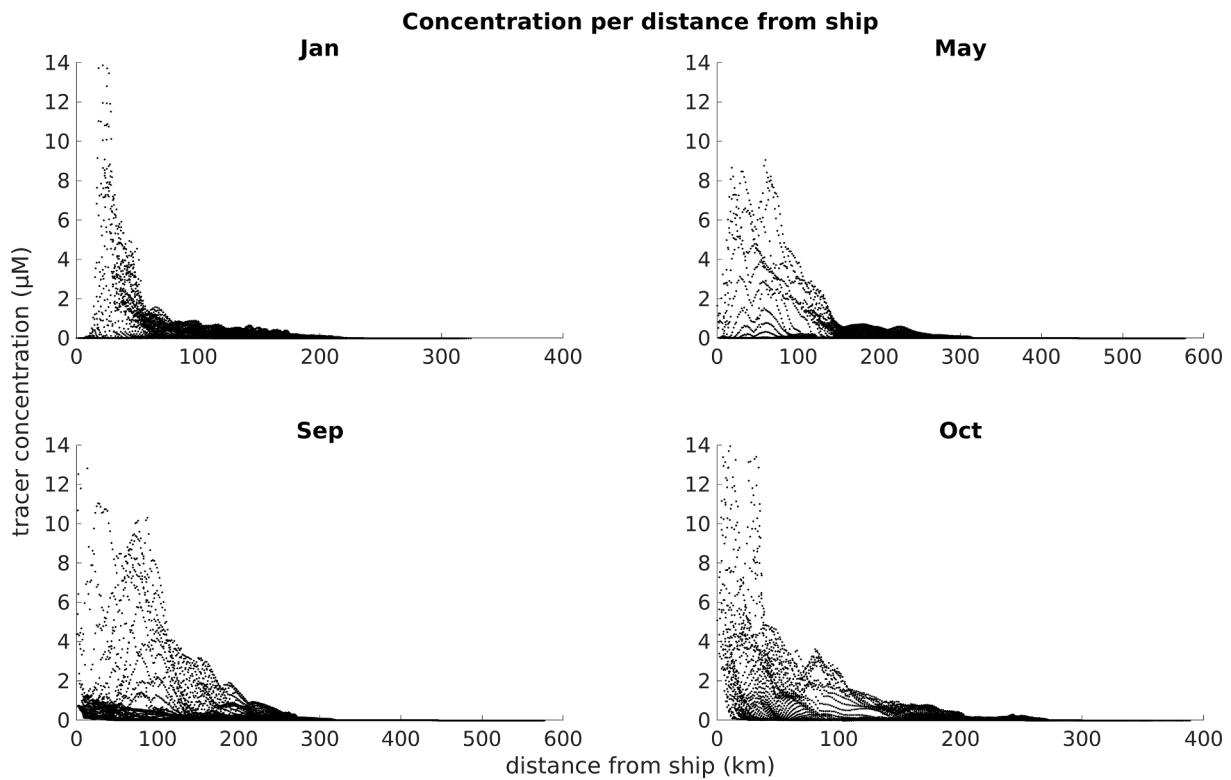


Fig. 15. Maximum tracer concentration at each domain grid point, each day, for two weeks from the tracers release. Results for different dates of release scenarios are displayed as a function of distance from the shipwreck location.

occurring near the Yala monsoon (release in May and September) reach the southwest coast of Sri Lanka, while during the Maha monsoon (release in January and October), tracers are transported northward towards the Palk strait and Gulf of Mannar (Fig. 13). On a longer time horizon (Fig. 14), in the original scenario (May 2021) the Yala monsoon phase drives the tracer southeastwards from the area near Colombo,

along the coast up to the region between Galle and Matara. When the tracer is released in October, during the opposite phase of the monsoon, it is transported by the currents in the opposite direction: the pollutants move northward along the coast, then deviate westwards reaching the coast of southern India. Similarly, during the quietest period of the Maha monsoon (release in January) the tracers also move from the release

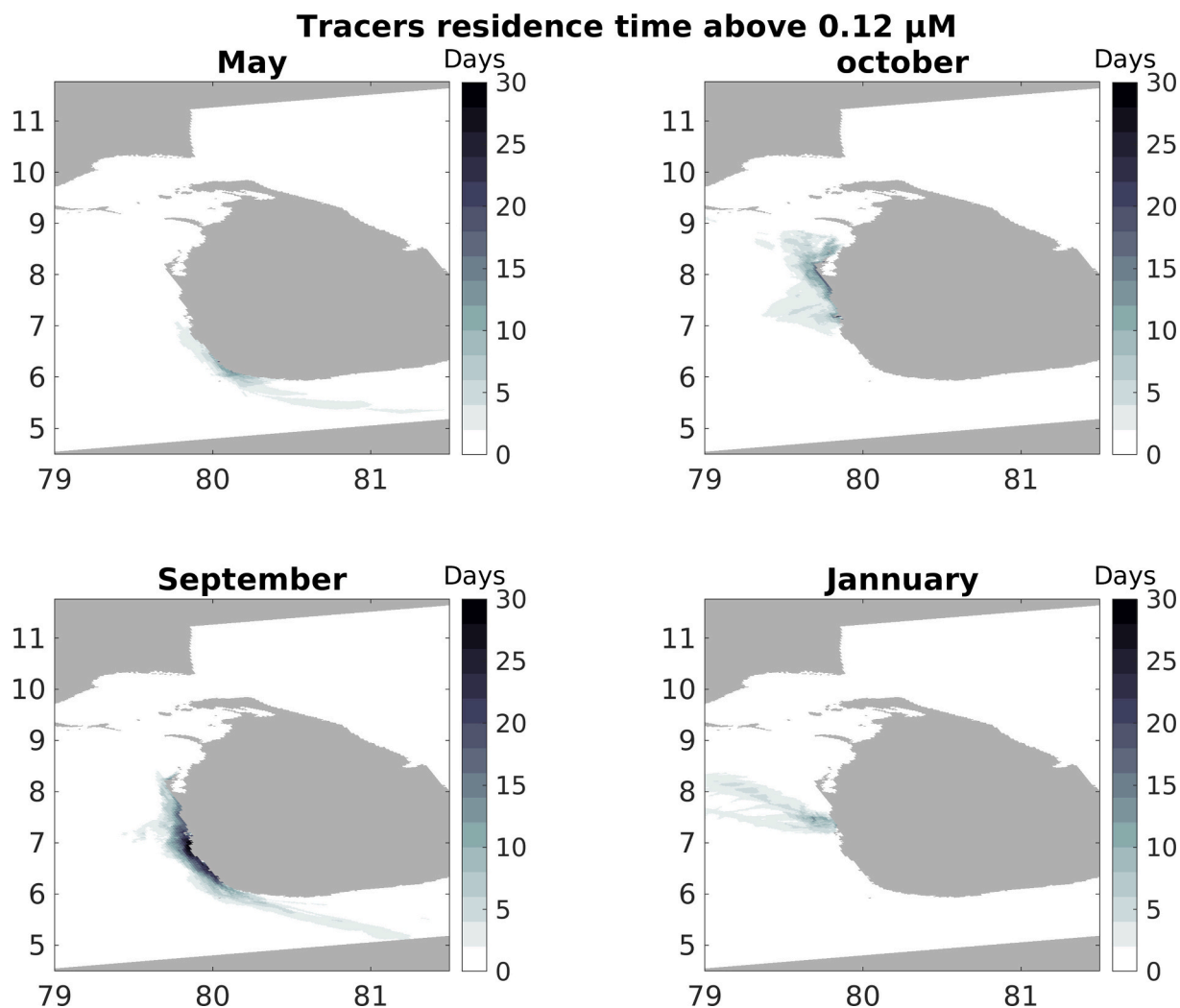


Fig. 16. Exceedance duration of tracers above 0.12 μM for all in different dates of release scenarios.

region into the Gulf of Mannar, however in this case they do not reach the Indian coast. Finally, during the transition phase between Maha and Yala, the impact of both monsoons phases is visible at once, with the tracer diffusing along the coast both north and south: after one month from the release, more than 325 km of coast have been reached by the tracers. In all cases the highest concentration of tracers is within the first 50–100 km from the release location (Fig. 15). The highest concentration peak is reached in the October release case (20.38 μM), while May shows the lowest surface concentration extremes. This could in part be due to the impact of cyclone Yaas that intensified the currents during the end of May. The duration of the period of exceedance is longer in the September-release scenario, when the concentration near the coast remains above 0.12 μM for up to a month after the release (Fig. 16). In all other instances the daily mean concentration stays above this threshold for less than two weeks.

3.4. Particle tracking experiments

To assess that the model captures correctly the dispersion patterns, we simulated the trajectory of 168,000 particles released from the MV X-press Pearl disaster site between May 25th 2021 and May 31st 2021. In these simulations, 71,154 particles were 'lost' to the outer boundaries of the model domain (42.4 % of total particles) by the end of the simulations (June 30th 2021). Only 4163 particles (2.5 % of total particles) remained 'waterborne' by the end of the simulations, leaving 92,683

particles (55.1 % of the total particles) reaching land within the simulation window. Beached particles were first identified in the simulations on the 26th May and continued to beach up until the end of the simulation, suggesting extended periods in the water prior to beaching events, with the maximum recorded Eulerian distance travelled for a beached particle being 306.6 km.

Date of particle release had a pronounced impact on the distribution of beached particles (Fig. 17). Particles released within the first 3 days of the disaster travelled south of the release site (Fig. 17a–c), with particles released on May 27th reaching the southern parts of the Sri Lanka (Fig. 17c). From May 28th onwards, however, we see a split in the distribution of particles along the coast from the release site (Fig. 17d–g), with some particles following the same trajectories as in the earlier releases, and some travelling up the coast, resulting in beaching northwards of the release site.

Fig. 18 shows the comparison between the Kernel Density Estimation of the beached particles broadly and the PPI from Jayathilaka et al. (2022). The model predicted the greatest intensity of pollution to occur along the coast between 6.6–7.2 N and 79.9–80 W, in good agreement with the area of highest PPI. The model is also able to reproduce the latitudinal spread of the observations, with the exception of the higher PPI value near the Southernmost tip of Sri Lanka.

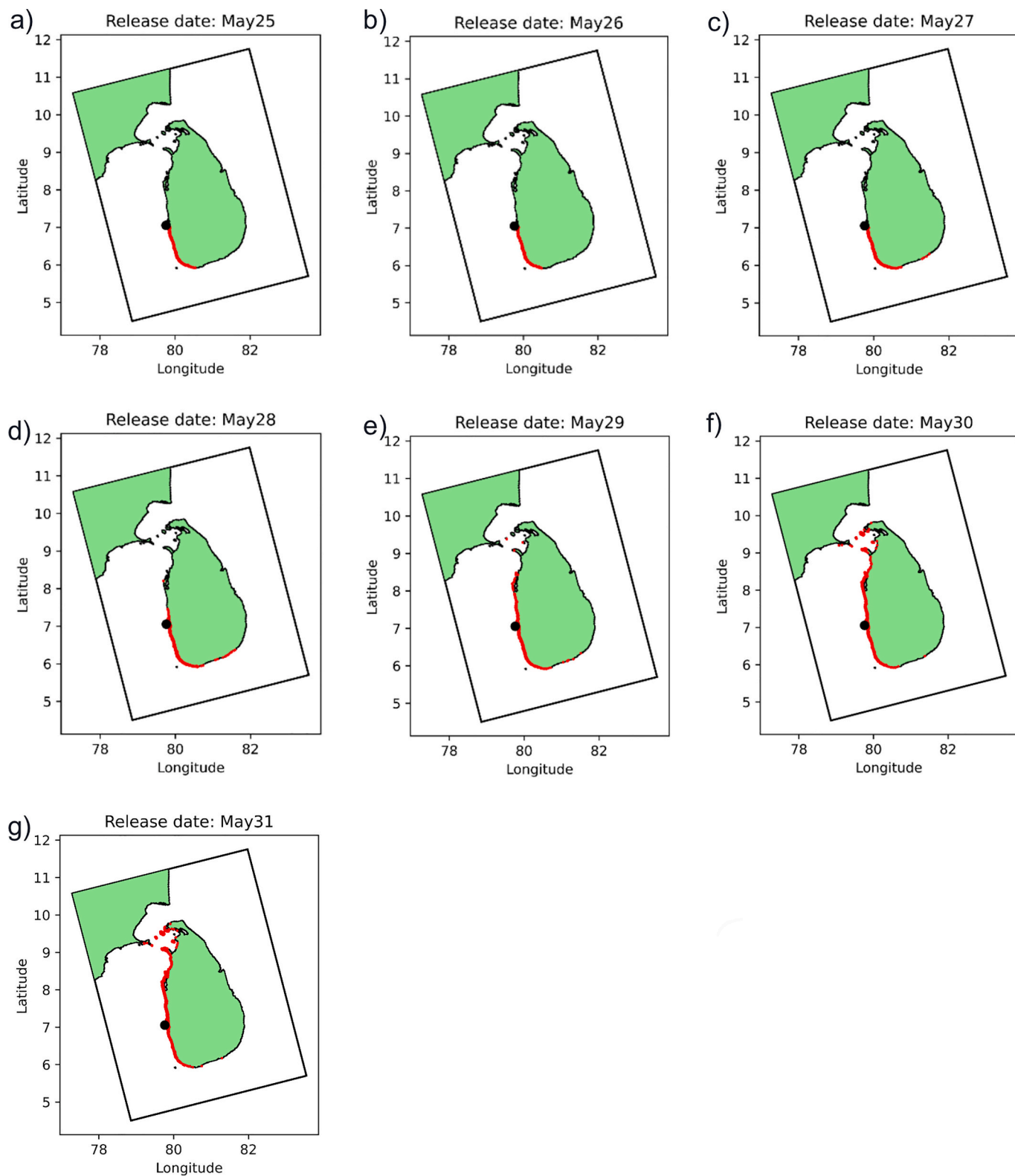


Fig. 17. Beaching locations of particles for each release date (25th–31st May). Particles could beach at any point between their release date and the end of the simulation (30th June). Large black dot denotes the location of the release site (i.e. the location of the X-Press Pearl).

4. Discussion

Some of the possible impacts on marine life and human activities following the disaster are discussed in [Vithanage et al. \(2023b\)](#). In order to use our modelling framework to support the quantification of those

impacts, a more detailed model able to represent the dispersion of the complex mixture of compounds present on board of the ship at the moment of the accident and especially of their chemical reactions in seawater would be needed. Furthermore, information on the rate of release of those compounds from the containers would be required,

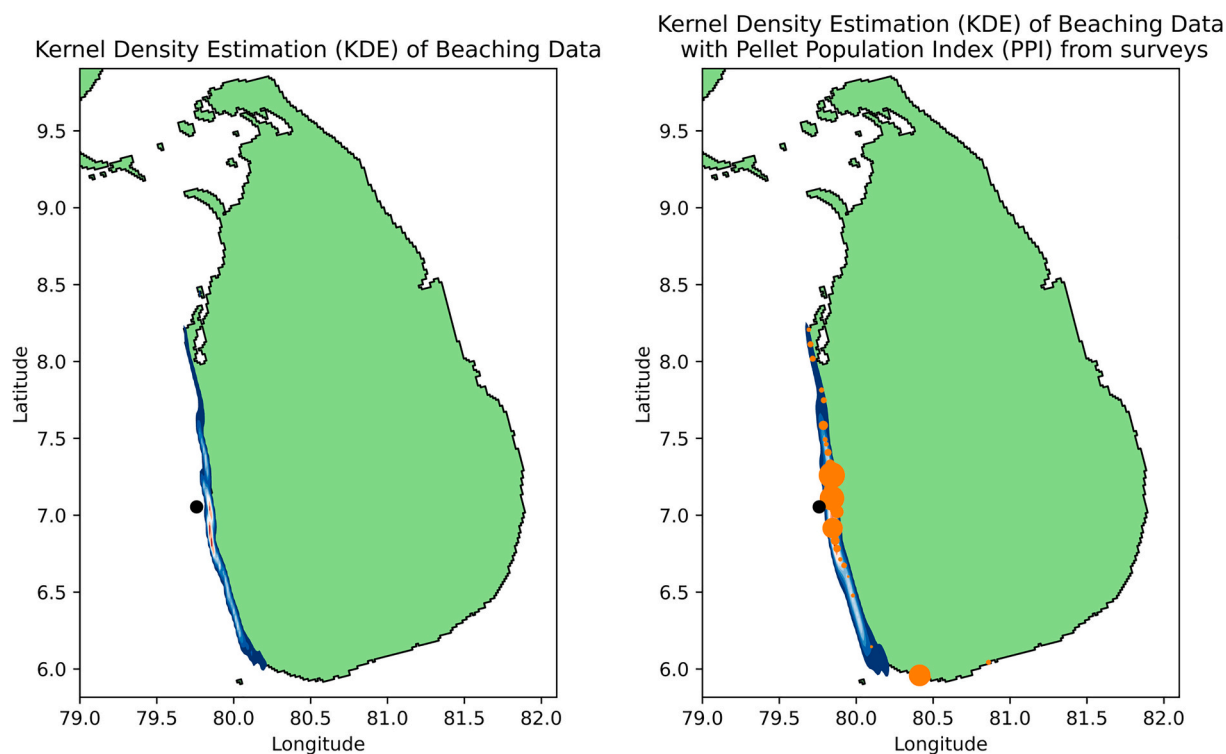


Fig. 18. Kernel Density Estimation (KDE) of the beached particles (left): red thicker band highlights the area where the model predicts a higher concentration of particles, compared to the blue thinner band. On the right, the Pellet Pollution Index (orange dots, with larger dots corresponding to higher values of PPI) is overlaid to the KDE. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

information that was not available in this case, and might also be difficult to obtain in other cases due to the difficulty in monitoring the location of the disaster.

For this reason, in this study we build a series of hypothetical tracer release scenarios based on the X-Press Pearl accident (Tables 1 and 3). The aim is to understand the potential impact over the coastal region of the accident as well as those of future similar accidents by understanding how the footprint and the concentration of the pollutant is affected by the release rate and how sensitive the dispersal is to environmental condition. This research focuses on the release of 1843.3 t of passive tracer amounting to the estimated value of urea transported by the MV X-Press Pearl.

It is important to note that few observations can be found on the concentration of the chemical components in Sri Lankan waters, especially following the accident and for urea. This lack of information makes it impossible to fully validate whether the distribution of urea simulated in our scenarios is representative of the real accident and to make any quantification of the impact. An alternative approach to increase the confidence in the model ability to reproduce pattern of dispersion has been implemented, using a particle tracking model driven by the same physical model and comparing the density of particle beached along the coasts with observations of plastic nurdles beached (Jayathilaka et al., 2022). While this approach cannot fully substitute the traditional validation against in-water observations of pollutants, it can be a good alternative when data are not available either for lacking of marine sampling (e.g. due to financial or weather constraints) or for administrative hurdles (e.g. court cases). Observations of beaching of pollutants like plastics are indeed undoubtedly easier and cheaper to collect and could be more easily available in the public domain.

Results show that the footprint of the accident (occurred on the 25th May) is not significantly affected by the rate of release: the urea (and all other dissolved chemical pollutants with similar properties) are transported south eastwards along the coast of Sri Lanka. The pattern followed by pollutants is representative of the seasonal patterns related to

the monsoon phase that characterise this region (Rath et al., 2019) and it aligns with some of the areas, specifically the southwest region, reached by plastic nurdles lost at sea from the ship's cargo (Karthik et al., 2022; Vos et al., 2022) and by the micro-plastics resulting from the pellets degradation (Karthik et al., 2022). Plastic nurdles, however, also spread further north along the west coast in both observations (Karthik et al., 2022; Vos et al., 2022) as well as our particle release experiment, in particular for particles released on or after the 29th of May (Fig. 17e, f, g). In the simulations with NEMO-ERSEM, such northward transport of late released urea is only marginally visible. Figs. 7 and 9 show indeed that when the release extends until the 29th of May and beyond (in the 7-days and 15-days release scenario) both the footprint of the maximum concentration and the duration of the exceedance of the threshold extend from the location of the accident, although it does not extend as far as the particles, that reach the Gulf of Mannar and the northernmost part of Sri Lanka. This is mostly due to the different approaches used for simulating the transport of the urea versus the buoyant particles. The Lagrangian approach focuses on the fate of every single particle, and therefore the coastline impacted by beaching appears more extended towards the Northern region than the tracer simulation when the release has been assumed to last more than the initial few days (Fig. 7, bottom). However, when the data from the Lagrangian experiment are analysed in term of density (hence more similar to the Eulerian approach of concentration), both approaches agree in highlighting a similar area of impact (south of 8°N), giving confidence in the model runs. Further less important differences can also be ascribed to the different treatment of the dissolved chemical and the buoyant particles.

Most of the tracer is transported along the southwestern coast of Sri Lanka, one of the most densely populated area of the island (DCS, 2023). Fishery and tourism are important components of the Sri Lankan economy (Ranasinghe and Sugandhika, 2016; MFARD, 2023), and urea is known to be a factor in promoting harmful algal blooms (Glibert et al., 2006; Glibert et al., 2005) that can affect both sectors. Such blooms have been observed in southwestern regions of Sri Lanka after the MV X-Press

Table 3

Summary information on all runs. The table shows the maximum concentration at any point in time (Overall max concentration), the length of the coastal stripe reached by tracers in concentration above 0.12 μM (Coast reached), the maximum exceedance duration of tracers at any point in time (max res.) and the average exceedance duration of tracers in concentration above 0.12 μM (mean res.). Note that results presented for the 1 h and 6 h case are daily average values, consistent with the rest of the simulations. Moreover note, that the table also shows statistics for the active tracer tests where the value of k is indicated in the 'Run' column.

Summary statistics				
Run	Overall max concentration (μM)	Coast reached (km)	Max res. (d)	Mean res. (d)
May-Jul 2021 1 h release	17	175.5	10	1.83
May-Jul 2021 6 h release	12.39	180	12	1.89
May-Jul 2021 1d release	9.023	163.5	21	2.2
May-Jul 2021 7d release	7.39	219	34	9.49
May-Jul 2021 15d release	3.79	166.5	32	7.90
Jan-Mar 2021 1d release	18.30	51	14	2.10
Sep-Nov 2021 1d release	10.65	363	30	4.92
Oct-Dec 2021 1d release	20.38	238.5	25	2.75
May-Jul 2021 1d release $k = 0.01 \text{ d}^{-1}$	8.76	163.5	19	2.2
May-Jul 2021 1d release $k = 0.1 \text{ d}^{-1}$	7.69	153	9	2.1
May-Jul 2021 1d release $k = 0.5 \text{ d}^{-1}$	4.80	78	4	1.8
May-Jul 2021 1d release $k = 0.9 \text{ d}^{-1}$	3.02	45	3	1.5

Pearl's spill (Pathmalal et al., 2023). The eastern and northeastern coasts however are not reached by the tracers during the first week and, within a month from the release, the tracer's concentration in these regions is extremely low (below $10^{-2} \mu\text{M}$). Although, it should be noted that the domain used is not wide enough to capture the full impact of the Sri Lanka Dome, an upwelling re-circulation feature which leads to currents being redirected northwest (Cullen and Shroyer, 2019). In these simulations, the tracer exits the domain in the southern boundary, but it is possible that part of it would be recirculated towards the east coast of Sri Lanka in a larger model domain. However, the tracer disperses fast in all release rate scenarios hence the urea concentration in the plume recirculated by the Sri Lanka Dome might be quite low; the fact that field-based studies on plastic transport found little traces of the MV X-Press Pearl's nurdles cargo over the east coast supports this assumption. It should also be noted that at the end of May 2021 Sri Lanka was struck by cyclone Yaas (Sil et al., 2021; Mohanty et al., 2022), which impacted on the tracer's dispersion. This means these results are not representative of 'typical' May conditions, however shifts in cyclones seasonality primarily driven by climate change suggest these events could become more common in pre-monsoon periods (Sil et al., 2021).

While the tracer's footprint is similar when changing the rate of release, the concentration varies by up to an order of magnitude. The greatest difference is in the area around the tracer release location and reduces away from the ship. The highest concentration of urea is of 52.97 μM , in the hourly release scenarios (this occurs 23 h after the start of the run). The highest daily mean concentration is also found in the 1 h release scenario (17 μM). These urea concentration values are

uncommon of coastal waters, where previous studies find values between 0.10 μM to 2.06 μM (Sipler and Bronk, 2015; Seeyave et al., 2013; Bradley et al., 2010), and similar values can be found in eutrophic estuaries (Glibert et al., 2006). In estuarine and coastal environments, urea can be a significant nutrient for phytoplankton (Glibert et al., 2006; McCarthy, 1972; Furnas, 1983; Glibert et al., 1991); in particular some studies show an increase in harmful phytoplankton bloom over regions where there has been an increase in the agricultural applications of nitrogen and urea (Glibert et al., 2006; Anderson et al., 2002; Glibert, 2017; Kudela et al., 2008; Olesen et al., 2020). In the fastest (1 h) release scenario however, the tracer disperses quite rapidly, and remains above the average reference level of 0.12 μM for up to a week. While this potentially limits the period of impacts, it is still enough for a significant increase in phytoplankton biomass: data from the Eastern Indian Ocean showed a phytoplankton growth rate ranging between 0.1 d^{-1} and 1.14 d^{-1} under natural environmental condition and between 0.92 d^{-1} and 1.94 d^{-1} under nutrient enrichment (Jiang et al., 2022), corresponding to a doubling time shorter than a day. Conversely, slower release scenarios lead to longer tracer exceedance duration in the water (Fig. 8), which could lead to a more significant impact over the local growth of biomass than a short burst of highly concentrated nutrients. This highlights a potential trade-off between two alternative typologies of pollution: the first type is an acute but short lived event following a sudden outburst of the pollutants from the containers after the disaster, while the second is weaker but long lasting event as a consequence of a slower release of pollutants. Both can have a significant consequences on organisms and ecosystem, with the first more likely to lead to immediate critical impacts, while the second causing prolonged cumulative effect. Our sensitivity test shows how the concentration simulated by the model under the passive tracer assumption are not too dissimilar when specific uptake rate of urea are lower than 0.1 d^{-1} and that concentration and areas of exceedance could be significantly lower for uptake rate higher than 0.5 d^{-1} . Specific uptake rates of urea in coastal area can vary in a range of several order of magnitude depending on various environmental factor like the abundance and composition of the planktonic community and temperature. The estimates we used to drive our sensitivity test are all from the Atlantic. Observations of uptake rate of urea in the Indian Ocean are available (Prakash et al., 2015; Singh and Ramesh, 2015; Kumar et al., 2004) but unfortunately no concurrent observation of urea concentration were reported and therefore it was impossible to estimate the specific uptake rate. Comparing the absolute uptake rate from the Indian ocean with those from the Atlantic, they tend to be on the lower end of the range, suggesting that the passive tracer assumption might not be too simplistic in this case. It is important to note that a faster uptake means that urea is quickly assimilated fostering plankton growth and therefore the resulting smaller chemical footprint would come at the expenses of a potentially bigger biological impact.

Our model suggests that the impact of the accident remained confined to the Sri Lankan coastal region because it happened to occur in May, which led to the seasonal monsoon coastal currents to direct the tracers southward along the coast, and then towards the open ocean. Had the accident occurred in a different period, it could have potentially impacted a larger area including the surrounding regions of the Gulf of Mannar, and in some cases could reach the Indian coast (Fig. 14). Being able to predict the potential evolution of the plume of pollutants can indeed allow to better plan an effective response to disaster, especially when it risks to extend beyond national jurisdiction. Operational models based on a similar modelling framework are usually developed and routinely run to provide this type of predictions in near real time to support environmental monitoring and management of pollution events (Karapanagioti and Takada, 2023; Cucco et al., 2024). However, the computational and financial requirements to set-up and maintain such operational framework prevents their massive expansion, especially in mid- and low income countries. For this reason, this type of scenarios-based information could be useful to a useful first base of information

to develop any risk analysis linked to maritime transport or mitigation and adaptation plans to prevent or limit the damage of similar accidents in future. While this approach still requires a relevant amount of computational power and investment, these are significantly lower and does not require a continuous investment. To facilitate further the uptake of such approach, the set-up of the Sri Lankan domain used in this study is publicly available online, along with guidelines on how to compile the modelling framework on different computing platform and initiate the simulation. The method used in this study to develop the model, set-up the domain and simulate the scenarios are in principle re-applicable to any area of the world, provided access to HPC facilities. Facilitating the work required to compile and run coupled systems of this kind means they will develop faster, leaving space for more effort to be focused on improving configurations and post-processing methods (Polton et al., 2023).

5. Limitations and future work

This work focuses on simulating the release of 1843.3 t of urea in different case scenarios, with a simple passive tracer approach. While this approach means that the direction and shape of the footprint shown here are largely valid for any of the chemical components released by the ship, on the other hand any chemical reactions between urea and the environment are not taken into account, and therefore no direct assessment of the impact can be inferred. Moreover, limited information is available about the region studied to validate the model outputs. Due to the constraints on the public availability of data, we were unable to access observations on pollutants or biochemistry data in the area, making it impossible to validate the urea tracer experiments at the moment. Comparison to a tide gauge in Trincomalee and EN4 data gives confidence in the model's ability to reproduce the physical parameters. A model-to-model comparison between our data and the CMS reanalysis also show consistent features (not shown), but more model validation is required, both in the physical parameters as well as the contaminants. However, the positive validation of the particle tracking experiments with the observation of the beached plastic nurdles from Jayathilaka et al. (2022) supports the finding of this work. The threshold value of 0.12 μM used in the study as indication of potential relevant impact comes from a publication averaging coastal values of urea found globally in previous literature (Sipler and Bronk, 2015). While this is a reasonable value, it is not specific to Sri Lanka and it does not consider the difference in background values between the near shore and the more open water areas. Results shown in this paper focus on the surface layer of the water column, because of the relative shallow water column where the accident occurred. Further work could be done by implementing the full ERSEM configuration to assess the potential implication of the urea release on the phytoplankton growth and to compare any emerging impact with ocean colour data from satellite. So far, Earth Observations have been used to detect and map oil spills from the accident (Welikanna, 2024) but they could be used to detect impacts on the phytoplankton biomass.

This accident, that followed the one occurring on the MT New Diamond in September 2020, has highlighted the high risk that the Sri Lanka is exposed to from the intense shipping activity happening near its coast (Vithanage et al., 2023a). Several proposals have been made to strengthen the national policy on maritime safety (e.g. (Ratnayake and Perera, 2022)) and to streamline the environmental impact assessment of complex mixture of contaminants like the one released by the MV X-Press Pearl (Zhang et al., 2023) and an ocean forecasts system is being established at the National Aquatic Resources Research and Development Agency (NARA) with the technical assistance of the University of Western Australia and funding from the Australian government (<http://www.nara.ac.lk/?pageid=17573>, last access 8/4). In addition to the short term forecast that such a system will provide, extending the scenario approach used in this paper to a long-term period or a climatological year would allow to identify regions at major risk from

accidents occurring near major ports or shipping routes, or 'hot spots' during specific seasons. This could be developed into a first order look-up reference as a preventive and/or impact mitigation measure in the areas that are likely to require support in case of accident during specific periods.

6. Conclusions

After the X-Press Pearl accident occurred on the 25th May 2021, approximately 1843.3 t of urea and other pollutants were released near the coast of Sri Lanka. This is a densely populated area where fishery and tourism represent a major source of income, therefore pollution affecting the local ecosystem could have important consequences. Not enough information and observation on the MV X-Press Pearl shipwreck were available to us to quantify the direct impact of the accident in this study, however this event highlighted how important it is to be prepared in a similar situation. Being able to prevent and react to events like the MV X-Press Pearl shipwreck relies partly on a good understanding of what the risks involved are and what could happen in extreme cases. In this study, we analyse what the potential impact of the MV X-Press Pearl accident could be under hypothetical scenarios. Using a coupled ocean (NEMO) - biogeochemistry (ERSEM) numerical model configuration, we simulate the release of 1843.3 t of passive tracers representing the urea transported on the ship. The tracers are released at the shipwreck location on the date of the accident at different rates (1 h, 6 h 1d, 7d and 15d), or at a constant rate during different periods of the years (January, February, May, July, October, September). We show that:

- (1) Regions affected by pollutants are independent from the release rate. The areas reached by tracers are similar whether 1843.3 t are inputted in the ocean in just 1 h, or gradually released over a period of up to two weeks. Conversely, pollutant pathways are significantly influenced by the timing of the release, and in some cases, they may reach neighboring countries, such as the Indian coast during the northeast monsoon. We show that, in principle, the affected regions - assuming specific release locations/dates (e.g. major harbour in a peak traffic period) - could be predicted in advance, regardless of the intensity of pollutants release in a hypothetical accident. This implies that some of the impacted regions could be targeted before pollutants reach the coast. In the absence of a fully implemented operational oceanographic framework, a scenario approach like the one presented here could provide critical information to improve the planning of the response and monitoring of future disasters.
- (2) Under the simplifying assumption of passive tracer, when 1843.3 t of urea is released within 1 h, the concentration peaks at 52.97 μM after 23 h, a level that could influence phytoplankton blooms, including potentially harmful species. Such concentrations are uncommon in coastal regions and are more characteristic of eutrophic estuaries. On the other hand, slower release scenarios result in prolonged exceedance of threshold concentrations, whereas rapid releases lead to faster dispersion. In the case of urea, slower releases might have a more extended impact on phytoplankton blooms, as the nitrogen remains in the water longer, allowing for greater uptake. This behavior may differ with other chemicals, particularly those that could be more dangerous in short-term high concentration bursts.
- (3) Our sensitivity test shows that the simplifying assumption is reasonable for a range of urea uptake rate lower than 0.1 d^{-1} , a value that is within the observed range.
- (4) We could assess the confidence in the simulated footprint of pollution even in absence of in situ observations on the dispersion of dissolved pollutants in the water column, by mixing the traditional Eulerian approach used for dissolved substances with a Lagrangian approach used to simulate the dispersion of

particles that can be more easily validated with land based observations of beached particle.

- (5) This research is not intended to give a quantitative assessment of the MV X-Press Pearl accident; rather, it aims to demonstrate the potential impact of various plausible scenarios. Incorporating similar information in policies development could be useful to setup preventive measure limiting the impact of accidents like the MV X-Press Pearl. Working towards facilitating the set-up of similar models, making them faster and more versatile to set-up and run could also allow to use scenarios run for quick first order analysis of conditions after an accident. This could help identifying regions to where to target actions.

CRedit authorship contribution statement

Julia Rulent: Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Molly K. James:** Writing – original draft, Visualization, Validation, Methodology, Formal analysis. **Ponnambalam Rameshwaran:** Writing – review & editing, Writing – original draft, Validation, Supervision, Methodology, Conceptualization. **Jennifer E. Jardine:** Writing – review & editing, Software, Methodology. **Anna Katavouta:** Writing – review & editing, Software, Methodology. **Sarah Wakelin:** Writing – review & editing, Validation, Supervision, Methodology. **Ruchira Jayathilaka:** Writing – review & editing, Validation. **Kanapathipillai Arulananthan:** Writing – review & editing. **Jason Holt:** Writing – review & editing, Project administration, Funding acquisition. **Mark A. Sutton:** Writing – review & editing, Project administration, Funding acquisition, Conceptualization. **Yuri Artioli:** Writing – review & editing, Writing – original draft, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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During the preparation of this work the author(s) used ChatGPT in order to improve the English. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Data availability

Numerical modeling data are publicly available and published, with links provided within the paper.

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