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Huntsman Polyurethanes outfall discharge assessment

Dispersion modelling for IC17

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Executive summary

Huntsman Polyurethanes (UK) Ltd (Huntsman) manufactures aniline at its site in Wilton, Teesside. Huntsman is pursuing a derogation and draft permit review for the site, and required hydrodynamic/dispersion modelling to assess the mixing and dilution of its effluent streams.

Effluent is discharged into Dabholm Gut, a tidal channel 1.4 km long that leads to the River Tees. There are two discharges to Dabholm Gut – one from Northumbrian Water's Bran Sands wastewater treatment works (WwTW) and another from the Wilton site drain operated by Sembcorp.

There are two main effluent discharges from the Huntsman site itself, referred to as "S1" and "S2":

- **S1** relates to two effluent streams from the Huntsman plant that discharge to the Wilton site drain.
- **S2** relates to the effluent stream from Huntsman's plant that is sent to Bran Sands WwTW for treatment. The discharge from the WwTW is made up of treated wastewater from domestic and industrial sources including Huntsman.

Two improvement conditions in the permit variation need to be considered:

- IC17 – Derogation for chromium and nickel associated with S1.
- IC18 – Surface water pollution risk assessment associated with both S1 and S2.

This document describes the hydrodynamic and dispersion modelling of the effluent discharge for IC17 only.

Using HR Wallingford's established TELEMAC-3D model of the Tees estuary, two sets of simulations were carried out with the following inputs to Dabholm Gut:

1. Huntsman S1 discharge, plus the Wilton site drain and Bran Sands WwTP effluent (assuming zero pollutant concentrations in the site drain and Bran Sands effluent);
2. Huntsman S1 discharge only.

The aim of the second set of simulations was to determine how the S1 effluent would be dispersed without any dilution in the drain or by the Bran Sands effluent.

The substances in the Huntsman effluent were represented in the model using a conservative (non-reacting, non-decaying) pollutant or "tracer". The concentrations of each substance are then derived by appropriate scaling of the representative tracer concentration.

Dispersion was simulated for 60 days to allow for potential build-up of pollutants in the estuary, and to include the effects of a range of spring and neap tides. Three sets of river flow conditions were also examined: low flow (5th-percentile), median flow (50th-percentile) and high flow (95th-percentile).

IC17 – Derogation for chromium and nickel associated with S1

Chromium VI

For the case including potential dilution by the other effluent streams:

- The maximum chromium VI concentration contours predicted for the low and median river flows are very similar, while the high flow case shows a slightly smaller plume extent into the estuary.
- The Maximum Acceptable Concentration (MAC) Environmental Quality Standard (EQS) is not exceeded as the chromium VI in the S1 effluent is sufficiently diluted in the drain (assuming zero chromium VI concentration in the additional flows).

- The predicted mean concentration contours are largely similar for all flows, and exceed the Annual Average (AA) EQS only in the upper 1000 m of the Gut, corresponding to an area of 0.058 km^2 at the water surface.

For the case without the potential dilution by the Bran Sands and drain flows:

- The MAC for chromium VI is predicted to be exceeded in the upper 1000 m of the Gut, corresponding to an area of 0.051 km^2 at the water surface.
- The AA is predicted to be exceeded along the whole Gut, but not in the estuary itself, corresponding to an area of 0.091 km^2 at the water surface.

Nickel

For the case including potential dilution by the other effluent streams:

- The maximum nickel contours predicted for the low and median rivers flows are very similar, while the high flow case shows smaller extent into the estuary.
- Neither the MAC or AA value are predicted to be exceeded, as the S1 effluent is sufficiently diluted in the drain (assuming zero nickel concentration in the additional flows).

For the case without the potential dilution by the Bran Sands and drain flows:

- The MAC for nickel is predicted to be exceeded in upper 1300 m of the Gut, corresponding to an area of 0.093 km^2 at the water surface.
- The AA is predicted to be exceeded in upper 1000 m of the Gut.

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1 Introduction

Huntsman Polyurethanes (UK) Ltd (Huntsman) manufactures aniline at its site in Wilton, Teesside. Huntsman is pursuing a derogation and draft permit review for the site, and requires hydrodynamic/dispersion modelling to assess the mixing and dilution of its effluent streams.

Effluent is discharged into Dabholm Gut, a tidal channel 1.4 km long that leads to the River Tees. There are two discharges to Dabholm Gut – one from Northumbrian Water's Bran Sands wastewater treatment works (WwTW) and another from the Wilton site drain operated by Sembcorp. The locations of these discharges are indicated in Figure 1.1.

There are two main effluent discharges from the Huntsman site itself, referred to as "S1" and "S2":

- **S1** relates to two effluent streams from the Huntsman plant that discharge to the Wilton site drain.
- **S2** relates to the effluent stream from Huntsman's plant that is sent to Bran Sands WwTW for treatment. The discharge from the WwTW is made up of treated wastewater from domestic and industrial sources including Huntsman.

Figure 1.1: Effluent discharges to Dabholm Gut
Source: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO

Two improvement conditions in the permit variation need to be considered:

- IC17 – Derogation for chromium and nickel associated with S1.
- IC18 – Surface water pollution risk assessment associated with both S1 and S2.

This document describes the hydrodynamic and dispersion modelling of the effluent discharge for IC17 only. Modelling results for IC18 are presented in a separate report (Reference 1).

2 Hydrodynamic study input data

2.1 Site hydrodynamic characteristics

The River Tees near Dabholm Gut is a tidal estuary, with its tidal limit at the Tees Barrage. On the flood (rising) tide, seawater from the North Sea flows upstream towards the barrage. After High Water the tide then begins to ebb (fall), and the water flows downstream towards the sea, until Low Water. The time between successive High Waters is about 12.5 hours. Tidal currents are stronger on the larger (spring) tides and weaker on the smaller (neap) tides. The full spring-neap cycle lasts around 15 days.

The freshwater discharge from the River Tees enters the estuary at the barrage. The salinity difference between the river discharge and the seawater means that the water is usually stratified in the middle part of the estuary, with a layer of fresher water near the surface and saltier water near the bed. When the river is discharging, there is a net flow out of the estuary towards the North Sea.

2.2 Bathymetry

HR Wallingford holds bathymetry data based on a combination of measurements from a 2004/2005 bathymetry survey conducted by PD Teesport covering most of the estuary, and Admiralty chart data. This was supplemented by data from a 2009 bathymetry survey conducted by PD Teesport near Billingham Reach Quay.

No bathymetry data are available for Dabholm Gut, but information on bed levels above low water were taken from the Environment Agency's LiDAR data from 2020. These data do not indicate the water level within the Gut, although it is known to be shallow. At the mouth of the Gut, there is a sill which can be seen in satellite images. This effectively maintains a moderate depth around Low Water, even when the tidal level in the estuary has fallen below the bed level in the Gut. From the LiDAR data we estimate that the level of this sill must be no lower than 0.45 to 0.5 m below Ordnance Datum Newlyn (ODN).

Figure 2.1: LiDAR data in Dabholm Gut
Source: https://environment.data.gov.uk/DefraDataDownload/?Mode=survey

2.3 Tidal levels

Tidal levels for the model were synthesised from tidal harmonics for Teesport, derived from long term tide gauge measurements in HR Wallingford's tidal database. A long record (60 days) was extracted for use in the modelling described in Section 3.

Mean High and Low Water levels at Teesmouth (from Admiralty Tide Tables) are shown in Table 2.1.

Table 2.1: Mean water levels at Teesmouth

Tide state	Water elevation (m ODN)
Mean High Water Springs	2.65
Mean High Water Neaps	1.45
Mean Low Water Neaps	-0.85
Mean Low Water Springs	-1.95

Source: *UKHO*

2.4 River flows

The river discharge was modelled using data from the National Rivers Flow Archive (NRFA) for the rivers Tees and Leven (https://nrfa.ceh.ac.uk/). Appropriate flow rates for modelling were derived from almost 50 years of measured flow data. The data were combined and analysed to derive the statistical properties of the river flow and are shown in Table 2.2. As an example, the 5th-percentile is 3.4 m^3/s. This means that river flows are up to 3.4 m^3/s for about 5% of the time (or *greater than* 3.4 m^3/s for 95% of the time).

Table 2.2: River discharge data (Tees and Leven combined)

Percentile	Discharge (m^3/s)
2nd	3.0
5th	3.4
10th	4.0
50th	12.0
90th	51.1
95th	73.5
98th	112.1

Source: *NRFA, 1969-2016*

For modelling, it is assumed that these flows correspond to the flows through the barrage into the estuary. In practice, during and after periods of very low flows, the barrage gates may be operated such that not all of the river flow will pass through the barrage in order to maintain or restore the upstream water level.

2.5 River and seawater salinities

The upstream model boundary is at the barrage. It is assumed that all water passing over the barrage into the estuary is fresh, or has negligible salinity.

Salinity is also measured during routine estuary sampling by the Environment Agency. Salinities at the estuary mouth (The Gares) are typically around 34 ppt, except during periods of exceptionally high river flow when values can reduce to about 15 ppt.

Salinities further upstream can vary spatially and over the tidal cycle, particularly during periods of high river flow.

2.6 Discharges to Dabholm Gut

Two effluent discharges are included in the model. One represents the discharge from the Wilton Site Drain (operated by Sembcorp), and the other the Bran Sands WwTW. Both discharges are at the eastern end of Dabholm Gut (Figure 1.1). The Wilton Site Drain effluent includes the S1 effluent from the Huntsman site.

The effluent flows and concentrations are described in the data review report (Reference 2). The flowrates applied at the two sources are:

- Huntsman: **3,731** m^3/d (daily mean flow from the H1 assessment provided by Huntsman);
- Sembcorp drain (excluding Huntsman): **17,998** m^3/d (mean flow during 2022, minus the mean Huntsman flow);
- Bran Sands WwTW: **139,137** m^3/d (mean WwTW plant flow (2005-2022), plus the mean flow from an industrial effluent treatment plant (IETP for 2007-2011).

3 Hydrodynamic model approach

3.1 TELEMAC system

Pollutant dispersion was modelled using TELEMAC-3D, an industry-standard finite element modelling system. TELEMAC represents the areas of interest using a completely flexible ("unstructured") mesh of triangular elements. This represents complex coastlines and other important structures accurately. HR Wallingford has wide experience of simulating currents in the Tees estuary, and elsewhere around the UK and worldwide, using the TELEMAC-3D system.

The model solves the 3D equations of motion and transport, including the important effects of buoyant spreading, inhibition of vertical mixing associated with sharp density gradients, and shear of wind-driven currents. These processes are essential to obtain a good representation of plume dispersion. HR Wallingford has validated the TELEMAC-3D model using real field measurements for a range of discharge plumes.

The Tees model has been calibrated against observed data in studies previously presented to the Environment Agency.

3.2 Mesh and bathymetry

The model covers the entire tidal extent of the estuary and is approximately 20 km long and up to 10 km wide in Tees Bay. The model mesh (Figure 3.1) was enhanced in the vicinity of Dabholm Gut. Fine resolution was used in Dabholm Gut, with a minimum horizontal grid spacing of about 5 m.

Vertical variations were represented using 13 horizontal planes, each representing a fixed proportion of the water depth (known as 'sigma planes').

The model bathymetry was updated using the new data described in Section 2.2, and is shown in Figure 3.2 and Figure 3.3 (Dabholm Gut).

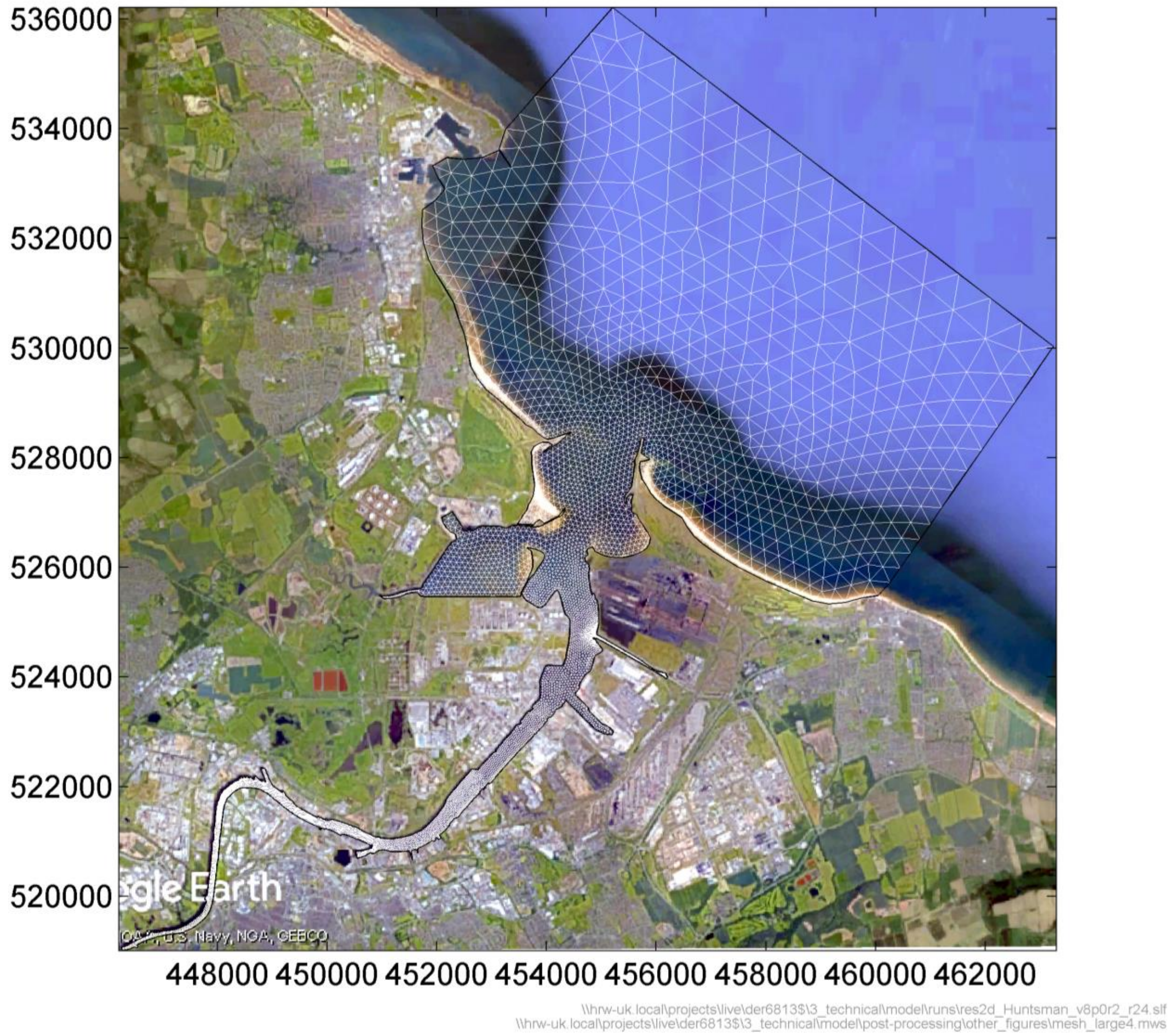

Figure 3.1: Model mesh

Source: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO

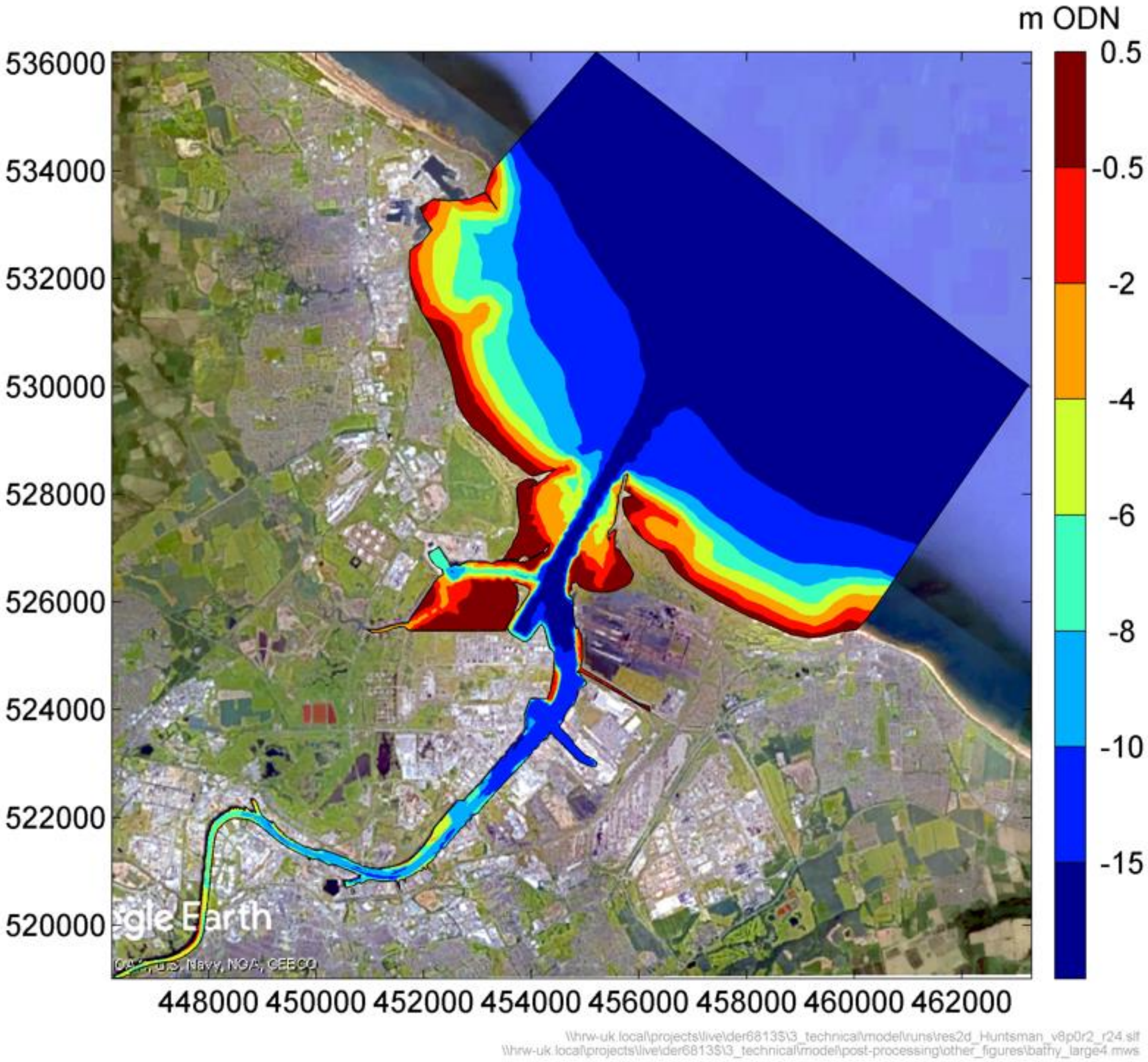

Figure 3.2: Model bathymetry

Source: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO

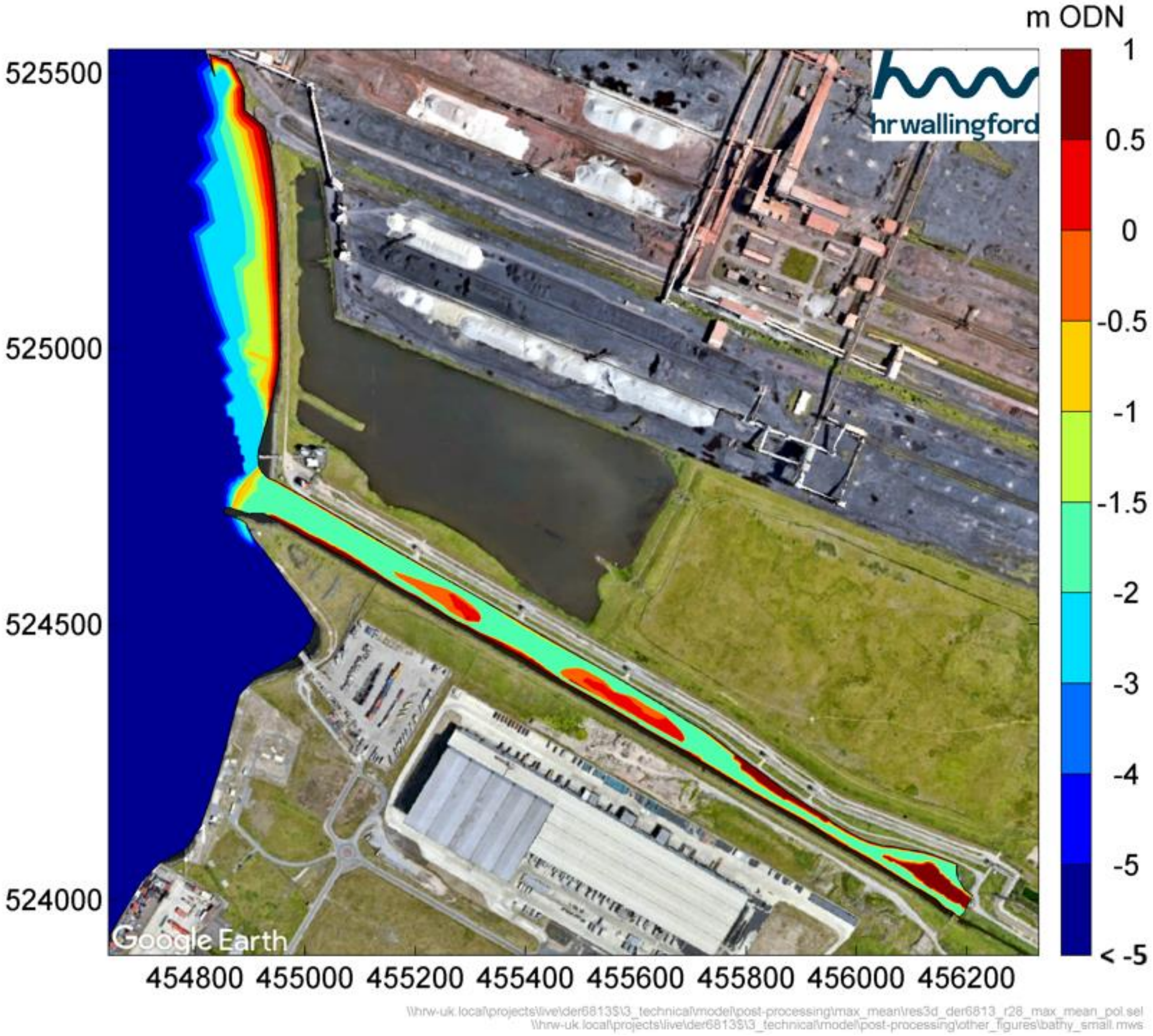

Figure 3.3: Model bathymetry in Dabholm Gut (different contour levels to Figure 3.2 to show detail)

Source: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO

3.3 Boundary conditions

Tidal levels were applied as boundary conditions at the eastern sea boundary of the model (Section 2.3). Freshwater river discharges were applied at the western river boundary at the Tees barrage, based on the data described in Section 2.4.

The salinity was set to 34 ppt at the open sea boundary, and to 0 ppt in the incoming river discharge at the barrier.

3.4 Modelled scenarios

3.4.1 Huntsman and other discharges to Dabholm Gut

Two sets of simulations were carried out with following inputs to Dabholm Gut:

1. Huntsman S1 discharge, plus the Wilton site drain and Bran Sands WwTP effluent (assuming zero pollutant concentrations in the site drain and Bran Sands effluent);
2. Huntsman S1 discharge only.

The aim of the second set of simulations was to determine how the S1 effluent would be dispersed without any dilution in the drain or by the Bran Sands effluent.

The substances in the Huntsman effluent were represented in the model using a conservative (non-reacting, non-decaying) pollutant or “tracer”. The concentrations of each substance are then derived by appropriate scaling of the representative tracer concentration.

3.4.2 River flows

The two discharge cases were applied for three river flow conditions:

- Low (5th-percentile) flow rate: 3.4 m^3/s;
- Median (50th-percentile) flow rate: 12 m^3/s;
- High (95th-percentile) flow rate: 73.5 m^3/s.

These represent the combined flows of the rivers Tees and Leven at the Tees Barrage.

3.4.3 Tidal levels

A period of 60 days was simulated using tidal data during April and May 2010. This period covers several spring-neap cycles, including tides with ranges close to the mean spring and mean neap tidal ranges.

4 Model results

Model results are shown as the maximum and mean concentrations at the water surface over the last 30 days over each 60-day simulation. The run-in period of 30 days allows for the flows and pollutant concentration fields settle down and establish a dynamic equilibrium. The final 30-day period allows for a variety of tidal ranges to be allowed for in the dispersion analysis.

It should be noted that the plots of maximum and mean concentrations show the maximum/mean predicted values at each model node over the course of the simulation. As the maxima/means do not occur at the same time at each location, these plots should be thought of as overall plume “footprints”.

The values plotted are determined by scaling modelled concentrations according to the concentration in the S1 effluent.

4.1 IC17: Derogation for chromium and nickel

The concentrations of chromium VI and nickel in the S1 effluent are shown in Table 4.1. The Environmental Quality Standards (EQS) in the estuary for the two substances are also shown. AA is the annual average, and MAC is the maximum allowable concentration.

Table 4.1: Chromium and Nickel S1 effluent concentrations, and associated marine EQS values

Substance	Effluent concentration (µg/l)		Marine EQS (µg/l)	
	Mean	Maximum	AA	MAC
Chromium VI (95th-percentile, dissolved)	52	176	0.6	32
Nickel	88	229	8.6	34

Source: ERM

The plots of the mean concentration were derived by scaling the mean tracer concentrations by the <u>mean</u> effluent concentrations. The maximum concentrations were derived by the scaling the maximum tracer concentrations by the <u>maximum</u> effluent concentrations.

Where relevant, the predicted extents of the AA or MAC mixing zone predicted for each case are highlighted on the plots using black contour lines.

4.1.1 Chromium VI

Predicted dispersion patterns for chromium VI are shown in Figure 4.1 (Huntsman discharge diluted by the other effluent streams) and Figure 4.2 (Huntsman discharge only, i.e. undiluted).

For the case including potential dilution by the other effluent streams:

- The maximum chromium VI concentration contours predicted for the low (5^{th} percentile) and median (50^{th} percentile) river flows are very similar, while the high (95^{th} percentile) flow case shows a slightly smaller plume extent into the estuary.
- The MAC value is not exceeded as the chromium VI in the S1 effluent is sufficiently diluted in the drain (assuming zero chromium VI concentration in the additional flows).
- The predicted mean concentration contours are largely similar for all flows, and exceed the AA value only in the upper 1000 m of the Gut, corresponding to an area of 0.058 km^2 at the water surface.

For the case without the potential dilution by the Bran Sands and drain flows (Figure 4.2):

- The MAC for chromium VI is predicted to be exceeded in the upper 1000 m of the Gut, corresponding to an area of 0.051 km^2 at the water surface.
- The AA is predicted to be exceeded along the whole Gut, but not in the estuary itself corresponding to an area of 0.091 km^2 at the water surface.

4.1.2 Nickel

Predicted dispersion patterns for nickel are shown in Figure 4.3 (Huntsman discharge diluted by the other effluent streams) and Figure 4.4 (Huntsman discharge only, i.e. undiluted).

For the case including potential dilution by the other effluent streams:

- The maximum nickel contours predicted for the low and median rivers flows are very similar, while the high flow case shows smaller extent into the estuary.
- Neither the MAC or AA value are predicted to be exceeded, as the S1 effluent is sufficiently diluted in the drain (assuming zero nickel concentration in the additional flows).

For the case without the potential dilution by the Bran Sands and drain flows (Figure 4.4):

- The MAC for nickel is predicted to be exceeded in upper 1300 m of the Gut, corresponding to an area of 0.055 km^2 at the water surface.
- The AA is predicted to be exceeded in the upper 1000 m of the Gut corresponding to an area of 0.039 km^2 at the water surface.

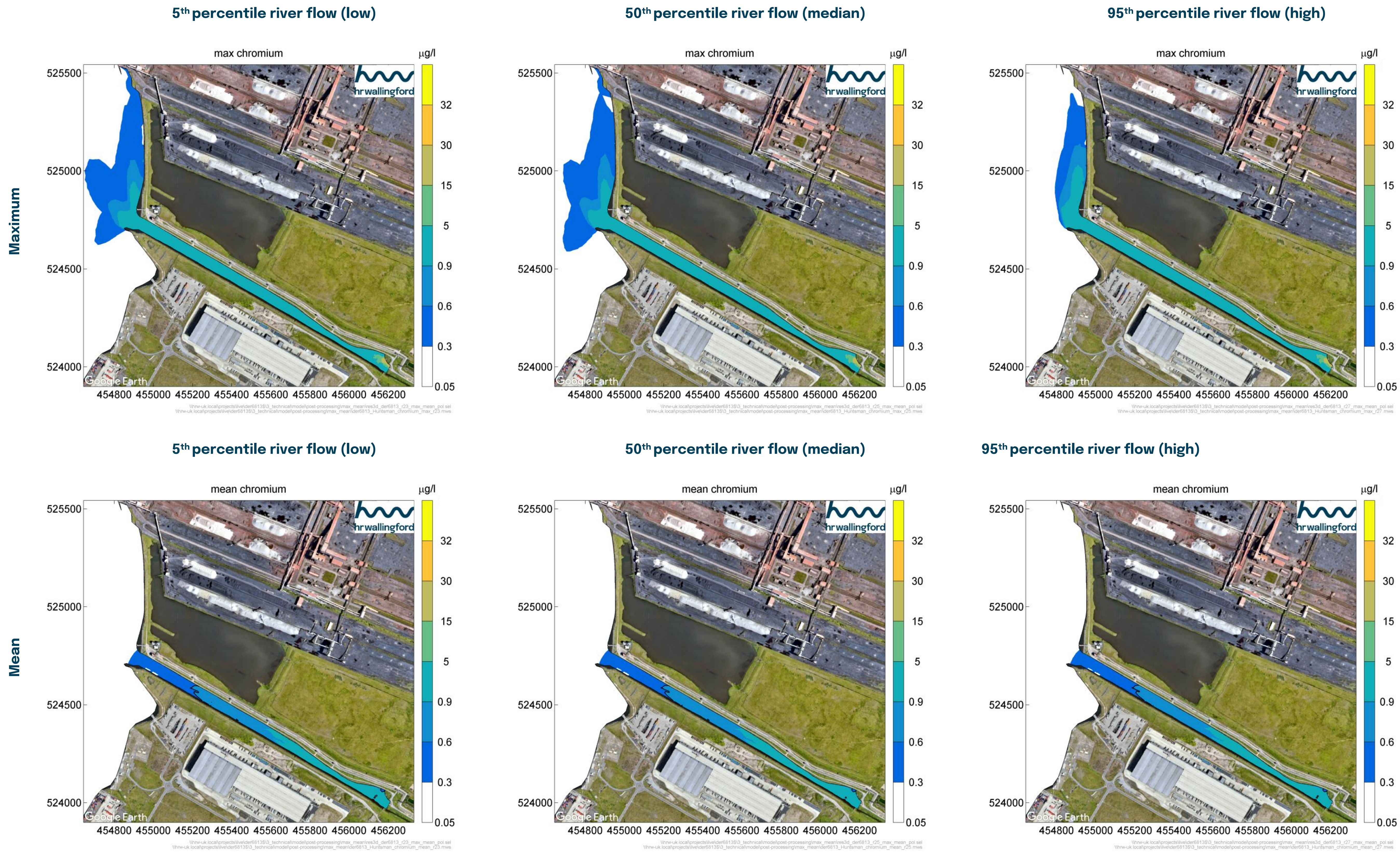

Figure 4.1: Maximum and mean surface chromium VI concentrations for three river flows (Huntsman discharge diluted by the other effluent streams)

Notes: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO
EQS values (AA = 0.6 µg/l, MAC = 32 µg/l) highlighted by black contour lines

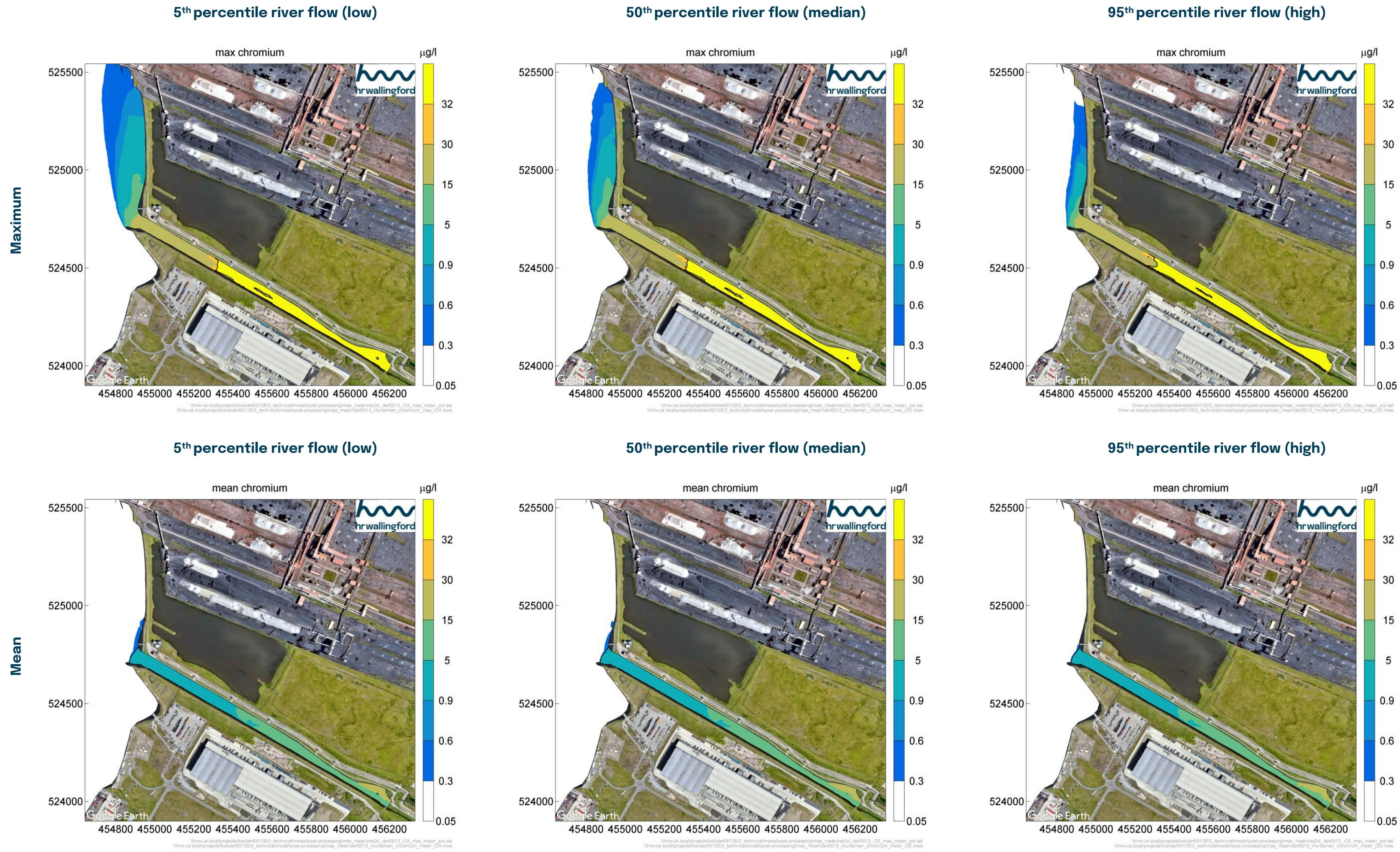

Figure 4.2: Maximum and mean surface chromium VI concentrations for three river flows (Huntsman discharge only, i.e. undiluted)

Notes: Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO
EQS values (AA = 0.6 µg/l, MAC = 32 µg/l) highlighted by black contour lines

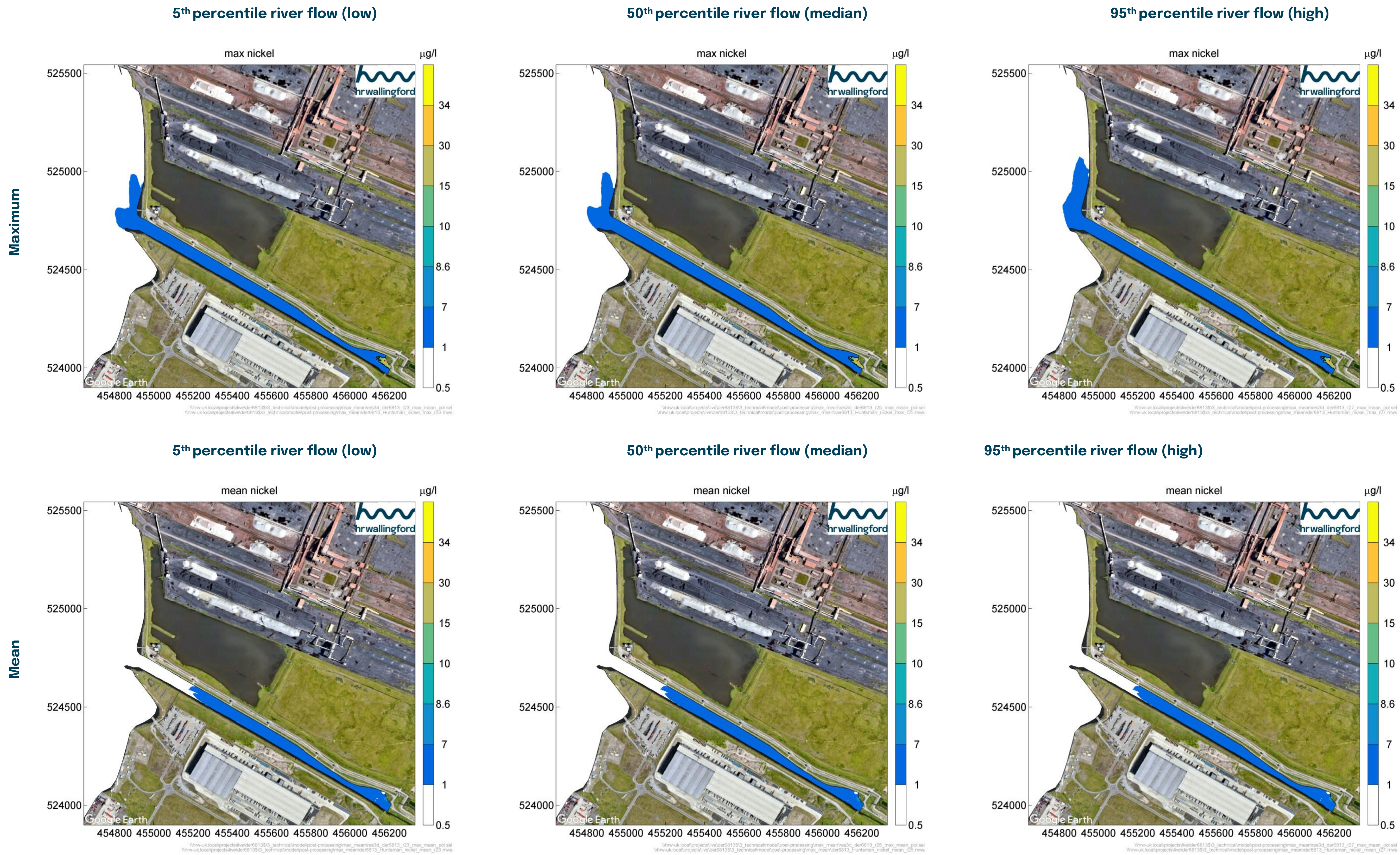

Figure 4.3: Maximum and mean surface nickel concentrations for three river flows

Notes: *Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO*
EQS values (AA = 8.6 µg/l, MAC = 34 µg/l) highlighted by black contour lines

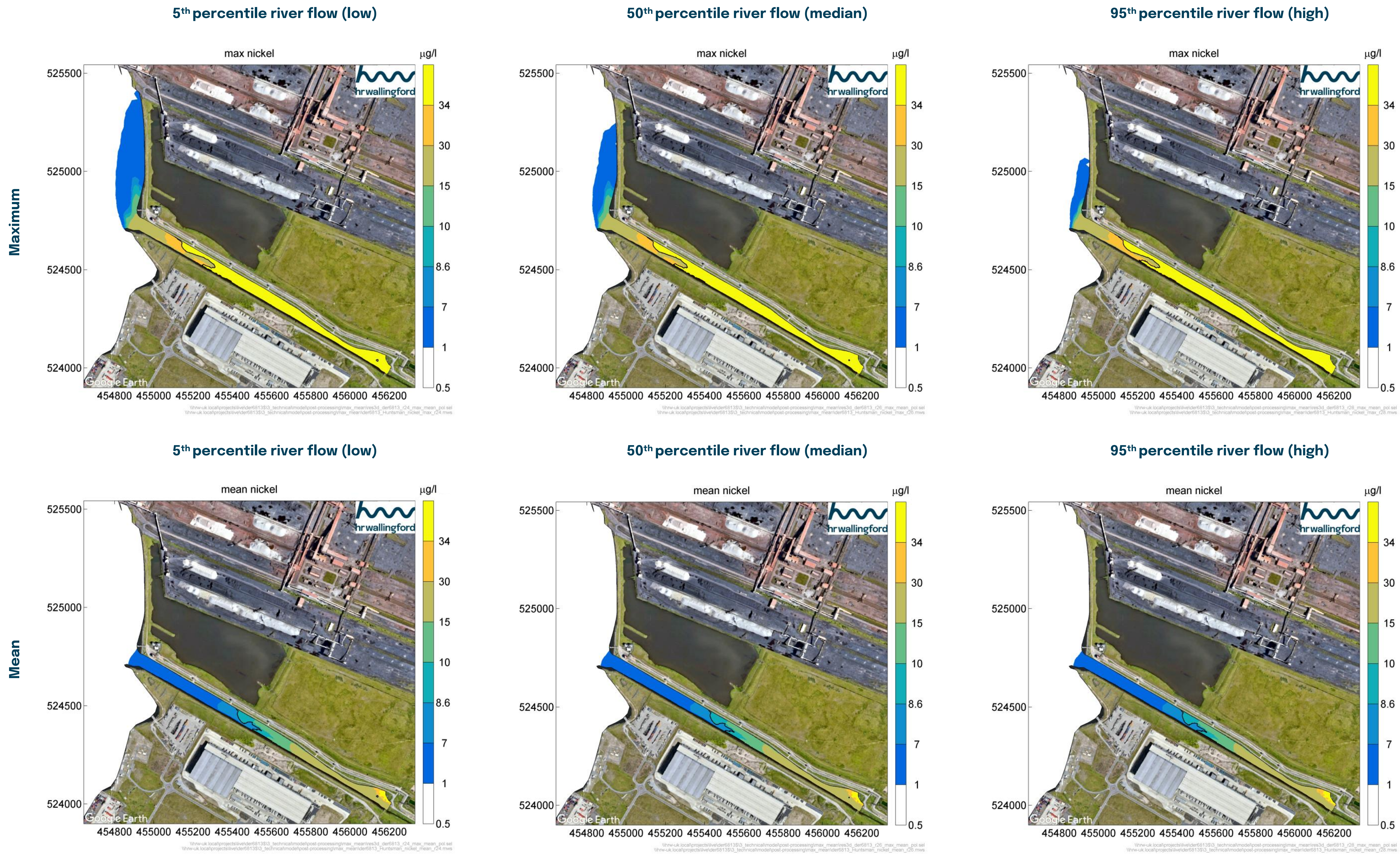

Figure 4.4: Maximum and mean surface nickel concentrations for three river flows (undiluted source)

Notes: *Background image: Google Earth with Data: SIO, NOAA, US Navy, NGA, GEBCO*

EQS values (AA = 8.6 µg/l, MAC = 34 µg/l) highlighted by black contour lines

5 References

1. Huntsman Polyurethanes outfall discharge assessment. Dispersion modelling for IC18. HR Wallingford Report DER6813-RT003-R01-00. May 2023.
2. Huntsman Polyurethanes outfall discharge assessment. Data review. HR Wallingford Report DER6813-RT001-R01-00. March 2023.

We design smarter, more resilient solutions across both the natural and built environment to help everyone live and work more sustainably with water.

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