Geospatial Visualisation of Food Contaminant Distribution: Polychlorinated Naphthalenes (PCNs) Polybrominated Diphenylethers (PBDEs) and Aflatoxins

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Introduction

The visualisation of the spatial distribution of contaminants in foods sampled across large areas allows the rapid and efficient communication of information for regulators, risk assessors and managers. This geospatial intelligence is especially relevant when multidimensional data is involved, where the sheer volume of generated data makes interpretation time-consuming and difficult. Visualisation can be applied to geo-spatial analysis outputs e.g. contaminant distribution in different regions, to provide a powerful tool for risk identification and establishment. This can promote the development of mitigation activities and identify other potential risk areas where data collection resources can be directed. Visualisation can be complemented with hierarchical cluster analyses to allow prediction of dataset correlations

Some web-based mapping resources such as Google Maps (Google Maps 2016) provide a powerful platform for the visualisation of spatial data. These platforms can be developed to efficiently represent and explore the complex inter-relationships between food contaminant occurrences, e.g. in different fish species or crop producing regions, as demonstrated in this paper. Using an interactive webpage, data points derived from occurrence data can be presented by different coloured circles or radiation patterns corresponding to their GPS position to represent different entities. This can then be superimposed with the magnitude of contaminant occurrence e.g. by varying the radii of circles,

Polychlorinated naphthalenes (PCNs) were industrial chemicals widely used, mainly as dielectrics in the 20th century and are now recognised as persistent organic pollutants (POPs), as evidenced by their listing in Annex A of the Stockholm Convention. PCNs also demonstrate properties of persistence and high bioaccumulation potential, coupled with a similarity in structural configuration to dioxins. Many congeners have been reported to contribute to dioxin-like toxicity^{1,2} eliciting a range of toxic responses such as mortality, embryotoxicity, hepatotoxicity, carcinogenicity etc. Earlier reports and a recent review of human tissue and food occurrence² show relatively higher concentrations in fish.

Once mass produced, polybrominated diphenylethers (PBDEs) are a widely studied class of brominated flame retardant. They are also recognised as POPs and listed by the Stockholm convention. Manufacturing is restricted, but they can still occur in many products either as a result of imports or recycling of older materials. PBDEs are reported to cause liver and neurodevelopmental toxicity, affect thyroid hormone levels and may be particularly harmful during a critical window of brain development during pregnancy and early childhood³. A number of studies^{4,5,6} have established their widespread occurrence in food, and particularly, fish. It is possible that PBDEs may be regulated in food within the EU.

Aflatoxins are contaminants that are produced by the moulds, *Aspergillus flavus* and *Aspergillus parasiticus*. Aflatoxin B1 is recognised as a genotoxic carcinogen and is the most potent of the 14 aflatoxins that are natural products of these fungi. Within crops such as maize and groundnuts, the growth of these moulds is promoted by poor storage conditions combined with ambient humidity and temperature. Although hepatocellular carcinogenesis is generally recognised as the most lethal biological effect, the stunting of growth in childhood

(affecting 165 m. children world-wide) that occurs in some countries in the African continent, may show an association with dietary aflatoxin occurrence^{7,8}. High levels of childhood aflatoxin exposure were observed during a study on three regions of Tanzania in $2010^{9.10}$

This paper focusses on the geospatial mapping of these contaminants to provide effective visualisation of their distribution within geographical regions. For PCNs and PBDEs, occurrence is mapped for different edible marine fish species from locations in the North Atlantic Ocean. For Aflatoxin B1, visualisation is demonstrated by human exposure as measured in blood AF-alb biomarkers (or occurrence in stored maize and food commodities) in 3 rural locations in Tanzania. Visualisation can be enhanced by superimposition with related variable data e.g. socio-economic status.

Experimental

The generation of the occurrence data for the fish species has been described elsewhere¹¹. For PBDEs, data for 135 samples of Sea Bass, Herring, Mackerel, Mullet and Sardine was used, whereas for PCNs, 75 data points were identified. Samples were collected from waters around the UK and the European coastal North Atlantic. Samples were analysed for contaminants including PCNs and PBDEs as described earlier^{12,13}.

The following PCN congeners were included in this study - PCN-52/60, 53, 66/67, 68, 69, 71/72, 73, 74, & 75. The PBDE congeners were – BDE-17, 28, 47, 49, 66, 71, 77, 85, 99, 100, 119, 126, 138, 153, 154, 183 and 209. The analyses are fully validated, with ISO17025 accreditation for the PBDEs, and successful participation in inter-laboratory testing. The aflatoxin data is derived from a study¹⁰ that investigated 3 regions in Tanzania (Iringa, Tabora and Kilimanjaro). Validated methodology was used to measure aflatoxin–albumin adducts (AF-alb), as biomarkers in blood plasma taken from 166 children. Dietary intake data and anthropometric indicesbody weight, recumbent length, etc. were recorded.

For the geo-spatial mapping, an interactive webpage based on Google Maps was used¹⁴ to integrate sample location (GPS), with contaminant concentration data. The webpage primarily consisted of control fields such as species selection, contaminant selection, factor selection (scaling), colour legend of selected species/contaminants and a help field. Each sample was presented with a circle centred at its GPS coordinate location. The magnitude of occurrence was indicated by the radius of each circle (ng/kg for PCNs; μ g/kg for PBDEs; pg/mg for AF-alb). The design allows multiple species or congeners to be selected, differentiated by colour coding and line type (solid, dashed, dotted) as applied to relevant circle representations. The aflatoxin study used plasma AF-alb biomarker data and/or contaminant levels within maize/other foods at the designated sampling region together with hazard indicators such as child weight z-scores. Magnitude levels are indicated by the radii of scalable circular plots which can be simultaneously colour coded to variables such as socio-economic status. This approach offers efficient data exploration without full statistical analyses.

Where sufficient data exists, Hierarchical Clustering (HC) can complement the above approach, a feature which would allow the user to investigate if certain locations or species/individuals are susceptible to concentration levels of concern. HC is a typical algorithm to analyse the similarities (or dissimilarities) of objects in variable space¹⁵. In the fish study, to have a better understanding of the geographical distribution, or independence of occurrence of the congeners, HC was employed (e.g. by dividing the fish samples into 3 clusters with the PBDE congener concentration as input variables) to investigate if correlations existed between the species and spatial locations.

Results and Discussion

PBDEs occurred in all fish samples with concentrations ranging from 0.09 to 8.9 μ g/kg whole weight for the sum of all measured congeners. Congeners showing high occurrence were BDE-47, BDE-49, BDE-100, BDE-99 and BDE-154. Species occurrence in descending order of magnitude was herring, sea bass, mullet, mackerel and sardine. The patterns of occurrence showed that fish species and congener types would affect the geographical distribution, so the data was analysed by individual species in order to avoid the mixing the two variables. The resulting visualisation, e.g. BDE-47, is shown in Figure 1a. This is complemented by HC analysis, Figure 1(b), where the larger circles denote areas of greater concentration. Both analyses concur that

for sea-bass, the occurrence of BDE-47 is highest at the coasts where the English Channel meets the North Sea. Similarly for herring, both spatial analysis as well as HC showed that the occurrence of PBDE congeners was most prominent in the Irish Sea, off the western coast of England, north of Wales.

The results of the PCN analysis showed concentrations (sum of twelve measured congeners) ranging from 0.7 ng/kg ww (turbot) to 265 ng/kg ww (sprats). Highest concentrations were recorded for sprats and mackerel with mean concentrations of 67 ng/kg ww and 68 ng/kg ww respectively. Geospatial mapping of the concentrations reveal that locations across the southern/eastern UK coasts and northern France showed a majority of the higher concentrations (Figure 2), although the highest PCN concentrations were recorded for samples from the Irish Sea.



Figure 1. BDE-47 analysis for sea-bass occurrence showing (a) Spatial distribution and (b) HC analysis.



Figure 2 Spatial distribution of PCN congeners 66/67 in sprat/mackerel from southern UK coasts and N. France

These preliminary results of aflatoxin analysis demonstrate the initial exploratory potential of the application. Geospatial analysis was applied to the distribution of the aflatoxin biomarker AF-alb in children's blood from 3 locations, to individual anthropometric or socio-economic data. The examples in Figures 3A and 3B show the magnitude of AF-alb content overlaid with socio-economic status and family size respectively and shows how potential associations for indicators may be explored. The Tabora region (located centre of Figures 3A & B) shows relatively stronger associations. Similarly, correlation to child hazard data (e.g. stunting) can be performed to evaluate biomarker to hazard indicators.

Figures 1-3 demonstrate rapid and effective geo-spatial visualisation of the large amount of data associated with these studies. Areas of higher contamination that may relate to relatively higher risk are immediately apparent from the plots and enable rapid qualitative assessment of potential associations within data. If sufficient data are available, more detailed analyses, e.g. HC, can be conducted or alternatively, where data are lacking, this allows more informed planning e.g. where additional research/data acquisition is required, and enables greater transparency across stakeholders.



Figure 3 Selected spatial distribution for the aflatoxin biomarker AF-alb in Tanzania with A. associated socioeconomic status colour coding and B. family size colour-coding, respectively.

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