

Linear Relationships Between Total Hydrocarbons and Benzene, Toluene, Ethylbenzene, Xylene, and *n*-Hexane during the *Deepwater Horizon* Response and Clean-up

Caroline P. Groth^{1,*}, Tran B. Huynh², Sudipto Banerjee³, Gurumurthy Ramachandran⁴, Patricia A. Stewart⁵, Harrison Quick⁶, Dale P. Sandler⁷, Aaron Blair⁸, Lawrence S. Engel^{7,9}, Richard K. Kwok^{7,10} and Mark R. Stenzel¹¹

¹Department of Epidemiology and Biostatistics, WVU School of Public Health, West Virginia University, One Medical Center Drive, Morgantown, WV 26506, USA; ²Department of Environmental and Occupational Health, Dornsife School of Public Health, Drexel University, 3215 Market St, Philadelphia, PA 19104, USA;

³Department of Biostatistics, UCLA Fielding School of Public Health, University of California –Los Angeles, 650 Charles E. Young Drive, Los Angeles, CA 90095, USA; ⁴Department of Environmental Health and Engineering, Bloomberg School of Public Health, Johns Hopkins University, 615 N Wolfe St, Baltimore, MD 21205, USA; ⁵Stewart Exposure Assessments, LLC, 6045 N. 27th. St., Arlington, VA 22207, USA; ⁶Department of Epidemiology and Biostatistics, Dornsife School of Public Health, Drexel University, 3215 Market St, Philadelphia, PA 19104, USA; ⁷Epidemiology Branch, National Institute of Environmental Health Sciences, 111 T.W. Alexander Drive MD A3-05, P.O. Box 12233, Research Triangle Park, NC 27709, USA; ⁸National Cancer Institute, 9609 Medical Center Drive, Building 9609 MSC 9760, Bethesda, MD 20892-9760, USA;

⁹Department of Epidemiology, University of North Carolina at Chapel Hill, 35 Dauer Drive, Chapel Hill, NC 27599, USA; ¹⁰Office of the Director, National Institute of Environmental Health Sciences, 9000 Rockville Pike, Bethesda, MD 20892, USA; ¹¹Exposure Assessment Applications, LLC, 6045 N. 27th. St., Arlington, VA 22207, USA

*Author to whom correspondence should be addressed. Tel: (304) 581 - 1835; e-mail: caroline.groth@hsc.wvu.edu

Submitted 13 October 2020; revised 20 June 2021; editorial decision 25 July 2021; revised version accepted 29 July 2021.

Abstract

Objectives: Our objectives were to (i) determine correlations between measurements of THC and of BTEX-H, (ii) apply these linear relationships to predict BTEX-H from measured THC, (iii) use these correlations as informative priors in Bayesian analyses to estimate exposures.

Methods: We used a Bayesian left-censored bivariate framework for all 3 objectives. First, we modeled the relationships (i.e. correlations) between THC and each BTEX-H chemical for various overarching groups of measurements using linear regression to determine if correlations derived from linear relationships differed by various exposure determinants. We then used the same linear regression relationships to predict (or impute) BTEX-H measurements from THC when only THC measurements were available. Finally, we used the same linear relationships as priors for the final exposure models that used real and predicted data to develop exposure estimate statistics for each individual exposure group.

Results: Correlations between measurements of THC and each of the BTEX-H chemicals ($n = 120$ for each of BTEX, 36 for *n*-hexane) differed substantially by area of the Gulf of Mexico and by time period that reflected different oil-spill related exposure opportunities. The correlations generally exceeded 0.5. Use of regression relationships to impute missing data resulted in the addition of >23 000 *n*-hexane and 541 observations for each of BTEX. The relationships were then used as priors for the calculation of exposure statistics while accounting for censored measurement data.

Conclusions: Taking advantage of observed relationships between THC and BTEX-H allowed us to develop robust exposure estimates where a large amount of data were missing, strengthening our exposure estimation process for the epidemiologic study.

Keywords: BTEX; correlations; *Deepwater Horizon*; determinants of exposure; *n*-hexane

Introduction

The National Institute for Environmental Health Science (NIEHS) is conducting the Gulf Long-term Follow-up STUDY (GuLF STUDY) to investigate possible adverse health effects among workers involved in the response and clean-up efforts of the *Deepwater Horizon (DWH)* oil spill in 2010. We needed to quantify airborne exposures to a variety of chemicals to evaluate possible exposure-response relationships among workers in the study.

A total of 26 161 air samples that met study inclusion criteria were taken on oil spill response and clean-up (OSRC) workers during the performance of various OSRC activities. The goal of the exposure assessment was to use these measurements, along with other information available on the OSRC activities, to develop exposure statistics that could be linked through job-exposure matrices (JEM) to the study participants through their work activities reported in the study interviews. Although measurements were available for total hydrocarbons (THC), benzene, toluene, ethylbenzene, xylene, and *n*-hexane (BTEX-H), they were sometimes insufficient to adequately characterize exposures in certain jobs/activities/tasks, locations, time periods, and vessel/vessel type. First, *n*-hexane was not measured during the initial period of the response and clean-up when exposures generally were higher, or on land, where thousands of participants worked. Second, we had previously developed THC personal estimates from VOC area direct-reading measurements on several vessels

where there were gaps (coverage of days worked) in the sampling strategy and wanted to incorporate the corresponding BTEX-H values into the estimation process (Groth *et al.*, 2021; Ramachandran, 2021). Third, many of the exposure statistics associated with exposure groups were based on a small number of measurements and/or a large number of censored measurements [below the limit of detection (LOD) of the analytical method] that needed to be incorporated in the calculation of the statistics.

Using the methods in Groth *et al.* (2017, 2018), our objectives were to apply a Bayesian linear regression model that accounted for measurements below the LOD while: (i) developing and describing the linear relationships (correlations) between measurements of THC and each of the BTEX-H chemicals (the basis of these relationships is provided in the [Supplementary Material](#), available at *Annals of Occupational Hygiene* online) for various overarching groups of measurements defined by a high level set of exposure determinants, (ii) predict BTEX-H levels when THC measurements were available but BTEX-H measurements were not (we call this imputation) using regression parameters, and (iii) incorporate these same regression coefficients as informative priors (i.e. additional information used in the analysis) to calculate parameter estimates [e.g. arithmetic means (AMs)] for our exposure groups.

Here, after describing the oil spill, we briefly describe the underlying basis for a Bayesian approach and the need for priors identified as overarching groups. Next, we

discuss the statistical background and the regression analyses performed to develop linear relationships that were used in achieving our three objectives. Finally, we present the different relationships and the impact of imputing missing measurements on the GuLF STUDY data.

Inhalation exposure estimates developed for THC and BTEX-H using these relationships for the GuLF STUDY are described in [Stewart, Groth *et al.* \(2021\)](#); [Stenzel, Groth, Huynh *et al.* \(2021\)](#); [Stenzel, Groth, Banerjee *et al.* \(2021\)](#); [Huynh *et al.* \(2021a,b,c\)](#); [Ramachandran *et al.* \(2021\)](#); [Groth *et al.* \(2021\)](#). Estimation of exposures to other airborne substances are described elsewhere: dispersants ([Arnold *et al.*, 2021](#); [Stenzel, Arnold *et al.*, 2021](#)), PM_{2.5} ([Pratt *et al.*, 2021](#)), oil mist ([Stewart, Groth *et al.*, 2021](#)); dermal exposures to THC, BTEX-H and dispersants are also discussed ([Gorman Ng *et al.*, 2021](#); [Stewart, Gorman Ng *et al.*, 2021](#)).

Background

Oil began leaking on 22 April 2010, as soon as the *DWH* sank, severing the riser pipe that connected it to the well's damaged blowout preventer (BOP) near the floor of the Gulf of Mexico. Response vessels arrived within hours to rescue survivors, search for missing personnel, and extinguish the fire. Rig vessels began arriving in the area within two weeks of the oil release. A large number of marine vessels supported the rig vessels, including marine vessels piloting remotely operated vehicles (ROV vessels). The well was mechanically capped on 15 July 2010 with the installation of a functioning BOP. In addition to the capping operation, thousands of other large and small vessels were deployed to perform other support operations and clean-up of the released oil. On 15 September 2010, the first relief well intersected the original well, and the well was sealed on September 19, 2010. Vessels started being decontaminated of oil and released from service. Land operations over this entire period included cleaning beaches and marshes, deploying boom, and, at ports and docks, decontaminating vessels and other equipment, and supporting of all the operations.

THC, measured as total petroleum hydrocarbons, is a composite measure of the volatile chemicals in the crude oil, including the BTEX-H chemicals. The proportion of these chemicals in THC at any given time or location was a function of oil weathering, that is, the chemical and physical change in the oil when exposed to the Gulf water, the elements, or dispersants ([NOAA Office of Response and Restoration, 2020](#)).

It was known that weathering affected the composition of the leaking oil from the *DWH* wellhead

differentially when the fresh oil contacted the subsea Gulf water due to the oil chemicals' differing solubilities in water and when it reached the water surface by evaporation due to the chemicals' different vapor pressures and other natural processes. The weathering process is very complicated, and factors such as time since the crude oil surfaced or the presence of dispersants can affect which of the many weathering processes are important under various conditions, and can, therefore, affect the relationships between THC and BTEX-H ([Liu *et al.*, 2012](#)). A detailed discussion of the effect of weathering and how it impacted our identification of exposure determinants is provided elsewhere ([Supplementary Material of Stenzel, Groth, Huynh *et al.*, 2021](#)).

Bayesian methods and overarching groups

The unit of estimation for the GuLF STUDY was the exposure group (EG), with each EG comprising a set of measurements on workers who were expected to have had comparable distributions of exposure based on their having the same exposure determinant characteristics ([Stenzel, Groth, Huynh *et al.*, 2021](#)). The specific exposure determinants considered in this paper are displayed in [Table 1](#) and described in detail in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online). The EGs were then normalized through a JEM to make them compatible with the work history questionnaires. We identified 3420 EGs that needed consideration for linkage to our study participants through their work histories. For 24% of the EGs actually estimated (2786), we had ≥ 100 measurements for each chemical of interest, but for 44% we had $n = 5-20$. Model-based estimates developed for many of the EGs, therefore, could have been unstable. In addition, our measurement data were characterized by high censoring (i.e. below the LOD; 11-83%, depending on the substance). Inclusion of censored data is important because if we omit these left-censored data, we introduce bias into our exposure estimates (as the estimates would be biased high). Furthermore, there may be additive or synergistic effects between these substances even at these low levels. If these measurements are not accounted for, we are not able to study these effects in the epidemiologic study.

We had previously reviewed various estimation methods that accounted for censoring and found that most estimation methods resulted in higher bias and imprecision than we desired ([Huynh *et al.*, 2014, 2016](#)). Given the characteristics of our measurement data, we found that Bayesian methods resulted in a low amount of bias and imprecision while providing credible intervals (CI, similar to confidence intervals).

Table 1. Determinants used to Develop Overarching Groups used as Bayesian Priors.

Determinant	Determinant value	Definition and description
Time period	TP1a	22 April–14 May 2010. Fresh oil leaking; first relief well started being drilled.
	TP1b	15 May–15 July 2010. Fresh oil leaking, dispersant being applied, 2 relief wells were being drilled. The well was successfully capped on 15 July 2010. Beach cleanup work started.
	TP2	16 July–10 August 2010. Relief well work continued. Beach cleanup work continued.
	TP3	11 August–30 September 2010. The relief well was successfully sealed. Decontamination of vessels started. Beach cleanup work continued.
	TP4	1 October–31 December 2010. Water operations essentially ended. Beach cleanup work continued.
	TP5	1 January–31 March 2011. Beach work continued, although with decreasing numbers of personnel.
	TP6	1 April–30 June 2011. Daily temperatures started rising; beach work being done with fewer people.
Area ^a	Hot zone	Within 1 nmi (1.8 km) radius of the wellhead.
	Source	Within 5 nmi (9 km) radius of the wellhead excluding the hot zone.
	Offshore	>5 nmi of the wellhead and >3 nmi (5.6 km) from land.
	Near shore	<3 nmi of the shoreline.
	Beaches and marshes	Shoreline where cleanup of oil and tar balls occurred.
	Ports and docks	Manmade structures for incoming and outgoing vessels. Site of vessel and boom decontamination; administration support.
	Other	Miscellaneous.
Vessel type	Rigs	4 large rig ships located in the hot zone charged with stopping the oil leak and drilling relief wells.
	ROV vessels	14 vessels piloting remotely operated vehicles (ROVs) that supported the rig vessels.
	MVs	Unknown number of marine vessels supporting the rig vessels.
	Other vessels	Thousands of smaller vessels performing cleanup: skimming, burning, boom work, etc.
Location on rig	Inside	Inside the rig vessel: living and office quarters.
	Outside	Outside the rig vessel: deck and other indoor areas, such as engine rooms.

ROV Vessels: Vessels operating remotely operated vehicles; MVs: Marine Vessels; Other Vessels: A group comprised of research vessels, and vessels other than marine vessels, rig vessels, and ROV vessels.

^aDistances are approximate.

Further research by [Groth et al. \(2017\)](#) identified that it is possible to gain additional information about each of the BTEX-H exposures by using $\ln(\text{THC})$ as a predictor in a linear regression setting (with the natural log of the BTEX-H chemical as the response). [Groth et al. \(2017, 2018\)](#) developed a Bayesian linear regression-based framework that accounts for censoring in both the predictor and response chemical and allows the estimation of exposures to BTEX-H in the same model framework. We chose THC as the predictor in our regression, as it had the lowest amount of censoring and could therefore provide the most information to inform the exposure estimates of each of the BTEX-H chemicals.

Posterior inference is the output of the model. To develop estimates of uncertainty around each estimated regression parameter (which includes regression coefficients and variance terms), we generated numerous plausible values using Markov Chain Monte Carlo

(MCMC) methods. This process provides a distribution for a large number of values (all observations are retained after a period of burn-in to ensure convergence. Burn-in is the period the model uses to discard the first set of samples that may be biased. Convergence means that the model agrees on a solution with an appropriate uncertainty level) for each parameter of interest that can be used to develop estimates of the AM, geometric mean (GM), geometric standard deviation (GSD), etc. (see, e.g. [Gilks et al., 1996](#); [Marin and Robert, 2007](#); [Carlin and Louis, 2008](#); [Gelman et al., 2013](#); [Brooks et al., 2011](#) for more information on Bayesian statistical methods).

Bayesian methods require the use of priors, that is, expected statistical characteristics of the parameters being estimated, for example, means, variances, regression coefficients, etc., to inform the analysis. Bayesian methods incorporate this information along with (in

our case) measurement data to develop the output, called posterior inference. Here, to use the methods of [Groth et al. \(2017\)](#), priors were needed on the regression parameters (including the regression coefficients and variance terms) that relate $\ln(\text{THC})$ to $\ln(\text{BTEX-H})$.

Ideally, the measurements of each EG would provide information to the model to predict or impute the missing data (while we use the word imputation/impute, this approach was a Bayesian model-based prediction method and should not be confused with multiple imputation). Using a large number of very specific priors would have resulted in many priors having small measurement numbers, which would have provided little information to the model, such that a Bayesian regression analysis would have provided results, for example, means, that were little different than simply calculating means. As almost half our EGs were associated with limited numbers of measurements, little information would be provided to the Bayesian model, resulting in wide credible intervals. Alternatively, because our data appeared to contain multiple exposure distributions, using a single broad prior for the regression parameters to represent all 3420 EGs could have resulted in severe misclassification. The misclassification, in particular, would occur among the EGs that lay outside the central part of the distribution, as it would move the EGs on the extreme ends of the distribution closer to the overall mean, reducing exposure contrast among the EGs and making it more difficult to find an association, should one exist. Thus, a balance was needed between the large heterogeneity that would have been associated with a single prior and use of too many priors, that would lead to limited additional information being provided and greater modeling complexity overall. In addition, many of our EGs had a large number of censored observations, and priors based on a limited number of larger groups of measurements that would aid in the estimation of these measurements below the LOD so that reasonable exposure estimates of each EG could be developed accounting for censored observations.

We, therefore, applied a Bayesian linear regression analysis (described in [Groth et al., 2017](#)) with informative priors to increase the stability of the regression parameters by using the linear relationships present in overarching groups. Overarching groups refer to large sets of measurements that meet particular characteristics that were deemed to be important for differentiating the many EGs', exposure levels, as defined by sets of high-level determinants. The assumption for using overarching groups is that, among the measurements assigned to an overarching group, the major source of the exposure (i.e. the oil) was roughly similar in composition

for all EGs within the group, and therefore, the relationship of THC to each of the BTEX-H chemicals was similar. [A second source of THC and BTEX-H that affected a small number of EGs was gasoline or diesel fuel, which was used to fuel vessels and land equipment. This source was considered separately from oil-based groups because the THC: BTEX-H relationships were expected to differ from those of the oil (see [Supplementary Material](#), available at *Annals of Occupational Hygiene* online)].

Because our EGs were based on unique combinations of exposure determinants ([Stenzel, Groth, Huynh et al., 2021](#)), we considered the same exposure determinants in determining our overarching groups. We selected combinations of time period ($N = 7$ values), distance from the wellhead ($N = 7$), vessel type ($N = 4$), and inside/outside of the rig vessels ($N = 2$) as likely to provide the balance between homogeneity and sufficient measurements within each group to inform the Bayesian regression ([Table 1](#)). The exposure determinants associated with the overarching groups related to the composition of the oil and its corresponding vapor concentrations; we did not consider differences in exposure determinants that were related to jobs/activities/tasks. For example, there is likely an exposure distribution associated with the activity skimming oil, but the actual exposure levels will be different if the oil skimmed was fresh crude versus somewhat weathered crude oil. In addition, use of job/activity/task also would have resulted in some groups having small numbers of measurements, which would provide little information to the model. More detail on these groups can be found in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online).

Therefore, to quantify the relationships between THC and each BTEX-H chemical by the determinants, we used the Bayesian linear regression method, as described in [Groth et al. \(2017, 2018\)](#) with overarching groups of measurements defined by combinations of exposure determinants in three situations here: first to develop correlations/linear relationships between THC and each of the BTEX-H chemicals, second to impute missing data, and finally to calculate our exposure statistics (using overarching priors) while accounting for censored data. See the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online) for the statistical background on the method.

Methods

Development of correlations

To evaluate our selection of determinants for the overarching groups, we extended a simple linear

regression model for censored data (Groth *et al.*, 2017) to a multiple linear regression for censored data (analyses not shown) that allowed us to determine if linear relationships differed from one determinant value to another within the context of all the determinants. If differences were identified, this suggested that different regression analyses should be performed to characterize the EGs. Modeling the determinants of multiple EGs together, however, requires the assumption of similar variability within each group, which our preliminary data suggested was not true. The importance of the various determinants (as reflected in the beta regression coefficients) was found to be similar (if not identical) for both the multiple and simple linear regressions. We therefore used simple linear regression to estimate the final relationships of each overarching group to allow us to develop separate variability estimates and avoid incorporating multiple intercepts and slopes from the multiple linear regressions into the priors, which is more complicated computationally with little gain.

Therefore, for each overarching group (comprising all measurement data meeting the determinants defining the group), let Y_i be the natural log of the BTEX-H chemical of interest for observation i and X_i be the natural log of THC for observation i . Let β_0 represent the intercept, β_1 represent the slope, ε_i represent the error for observation i , and $\sigma_{Y|X}^2$ be the conditional variance of $Y|X$. Then, we can write the following linear regression equation representing the relationship between X and Y :

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i \text{ where } \varepsilon_i \overset{iid}{\sim} N(0, \sigma_{Y|X}^2) \quad (1)$$

This regression provided us with posterior inferences of each of the regression parameters. To this basic framework, we accounted for censored data in both the response and predictor. To estimate the correlation (ρ) between THC and BTEX-H, we sampled from the posterior distributions of the regression parameters 25 000 times using MCMC methods described in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online) and calculated the Pearson correlation coefficient using the relation:

$$\rho = \beta_1 \times \frac{\sigma_X}{\sigma_Y} \quad (2)$$

Thus, we sampled $\{\beta_1, \sigma_X, \sigma_Y\}$ from their posterior distributions, where σ_X and σ_Y , are the marginal standard deviations of Y and X (i.e. the variance of only X or only Y), respectively, and entered these estimates into equation 2 for ρ to obtain the posterior estimates of ρ . We note that the model in Groth *et al.* (2017) uses terms of the conditional variance of $Y|X$ (Conditional variance means that our model provides the variance of Y given we know the value

of X and the regression parameters), but in computing ρ , we calculate the marginal variance of Y from this conditional variance and the other parameters (using conditional variance formulas of bivariate normal distributions).

We identified credible differences in the overarching groups by observing non-overlapping CIs of the slopes and intercepts for independent groups (e.g. groups that do not contain the same measurements). It should be noted that if the slope is credibly different, the correlation will usually be credibly different as well since the correlation equation includes the slope (equation 2).

We performed a linear regression and estimated the Pearson correlation (using 25 000 iterations after 5000 iterations of burn-in) for each of our overarching groups. We report the median, the 2.5th quantile, and the 97.5th quantile of the posterior samples for the intercept, slope, correlation coefficient (ρ), and the median posterior estimate of the coefficient of determination (R-squared). All regression results can be found in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online) excel file ([Supplementary Tables S1–S5](#)).

Model-based imputation of missing BTEX-H measurements

BTEX-H measurements were not available for two scenarios. First, laboratory analyses of n -hexane primarily had been conducted on air samples collected on the water for time periods 1b, 2, and 3. Thus, n -hexane measurement results corresponding to those of THC and BTEX on land and in time periods 1a, 4, 5, and 6 were not available. Second, we previously had predicted THC (personal) exposures from VOC area measurements (Groth *et al.* 2021; Ramachandran *et al.* 2021), but corresponding BTEX-H measurements were not available.

We applied the same bivariate left-censored Bayesian model described in Groth *et al.* (2017), using equation 1 (using 25 000 iterations after 5000 iterations of burn-in) with: (i) the THC personal measurement corresponding to the missing value as the predictor (X_i) (if the THC value was censored, the THC value was imputed from the model using a normal distribution below the LOD with an estimated mean and variance; see Groth *et al.*, 2017, 2018), and (ii) each missing measurement's corresponding overarching group's linear regression (THC:BTEX-H) equation. That is, for every missing value, we obtained 25 000 posterior estimates of a GM-like statistic and 25 000 posterior estimates of the GSD. Since these relationships are on the natural log scale, we used the posterior distributions of these statistics to calculate AM estimates. Specifically, using the posterior distribution of the GM-like statistic and the GSD for each missing measurement and

$$AM = GM \times e^{\left(\frac{1}{2} (\ln(GSD))^2\right)} \quad (3)$$

We calculated a corresponding posterior distribution of the 25 000 AMs of each imputed value. The median of each set of the 25 000 imputed AM values (posterior samples) was considered the imputed BTEX-H value for each missing measurement.

Use of informative priors in the estimation of exposure levels

Once all missing BTEX-H measurements had been estimated, we again applied the method in Groth *et al.*, (2017) using the linear relationship of equation (1) to develop an exposure estimate for BTEX-H for each EG.

With the completed dataset for each EG of interest (i.e. the real and imputed measurements totally 26 702 across all EGs for each BTEX-H chemical; 26161 measured THC and 541 imputed THC), the model estimated the linear relationship between the natural log of THC and the natural log of the chemical of interest (one of the BTEX-H chemicals) for that EG (all EGs were modeled separately) accounting for censored information (for formal details of this, see the Supplementary Materials in Stewart, Groth *et al.* 2021). Since some EGs had limited sample sizes or many censored measurements, it was harder, however, for the model to agree on an appropriate linear relationship. Therefore, we provided additional information about the linear relationship, that is the regression parameters of the slope, intercept, and conditional variance of the overarching relationship as prior information (priors). This allowed us to develop BTEX-H exposure statistics for all of our EGs regardless of the number of measurements. The model then generated coefficient estimates of the linear relationship for the specific EG, which were used to generate estimates of the AM, GM, GSD, and 95th percentile of the chemical of interest using equations (1) and (3). For further details on the development of these priors from the correlations and the exposure statistics derived from these predictions, see Huynh *et al.* (2021a,b,c); Ramachandran *et al.* (2021); and the Supplementary Materials in Stewart, Groth *et al.* (2021).

Credible differences or statistically notable differences in correlations were identified using non-overlapping 95% CIs of the correlations. All analyses were conducted in the R statistical programming environment using the RJAGS software package (Plummer, 2003, 2016; R Core Team, 2017).

Results

The regression relationships can be found in the Supplementary Material (available at *Annals of*

Occupational Hygiene online) (Supplementary Tables S1–S5). We provide the median, 2.5th quantile, and 97.5th quantile for the intercept, slope, and correlation for each relationship along with the median posterior sample of the R-squared.

Correlations

Briefly, although the range of the Pearson correlations (ρ) was substantial among the five BTEX-H chemicals ($\rho < 0.1$ to > 0.75), the median ρ values were similar for the five chemicals (0.52–0.66; median of posterior estimate taken to be the estimate of the correlation). For benzene, the primary groups with higher ρ values (> 0.70) comprised other vessels that were primarily near shore. No time period, vessel type, or area was dominant for the toluene values. Higher correlations for ethylbenzene were primarily seen with the other vessels group and the ROV vessels group. For xylene, the other vessels group across all areas (except offshore) and the hot zone for all three vessel types were associated with many ρ values > 0.60 . For *n*-hexane, the rigs and ROV vessels in the hot zone had the highest correlations.

Time period

Figs. 1 and 2 display the BTEX-H Pearson correlations (ρ) by time period for each overarching grouping. The error bars show the 95% CI of the correlation coefficient, and the points represent the median posterior estimates. The rig and ROV vessel groups had data in only TP1a-b, 2, and 3, while the other vessels group had data in TP1a-b, 2, 3, and 4, after which most of the water operations had ended. In TP5-6, only land measurements were available. *n*-Hexane measurements were missing in TP1a and TP4-6, having measurements only in TP1b, 2, and 3. There were few land measurements for *n*-hexane, so we report an ‘all land’ category in TP1b and TP3, but not in TP2 because there were too few measurements in TP2 ($N = 5$) to conduct a stable regression analysis.

Overall, correlations were around 0.5 across all overarching groups and all chemicals and generally notably different from 0 (i.e. 0 lies outside of the 95% Bayesian credible interval). The correlations tended to decrease from TP1a-b to TP2 on the (outside) rig vessels and on the ROV vessels. Credible differences in correlations were found for rig vessels for toluene (TP1a-1b, correlation $\rho = 0.66$, 95%CI:0.62, 0.70; TP2: $\rho = 0.45$, 95%CI:0.30, 0.57), ethylbenzene (TP1a-b, $\rho = 0.78$, 95%CI:0.75, 0.81; TP2: $\rho = 0.52$, 95%CI:0.35, 0.65), xylene (TP1a-1b: $\rho = 0.85$, 95%CI:0.82, 0.87; TP2: $\rho = 0.73$, 95%CI:0.64, 0.81) and *n*-hexane (TP1b: $\rho = 0.86$, 95%CI:0.83, 0.88; TP2: $\rho = 0.52$, 95%CI:0.35, 0.65). Similarly, on the ROV vessels, credible differences in correlations existed between TP1a-b and TP2 for

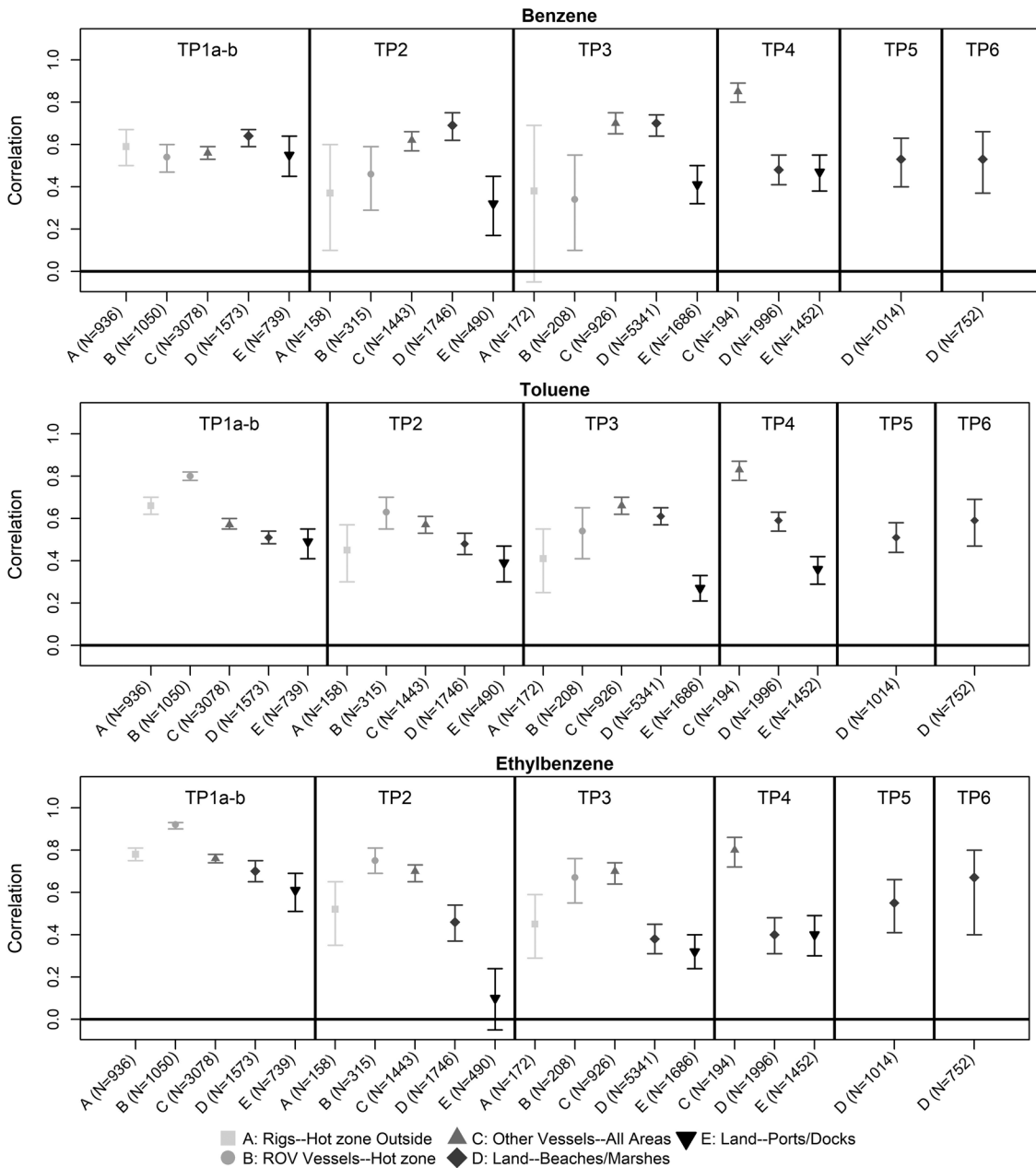


Figure 1. Benzene, toluene, ethylbenzene correlations with total hydrocarbons (THC) by time period. Correlations reflect all outside areas within a particular group. The error bars represent the 95% credible interval and the points represent the median posterior estimate.

toluene (TP1a-1b: $\rho = 0.80$, 95%CI:0.78, 0.82; TP2: $\rho = 0.63$, 95%CI:0.55, 0.70), ethylbenzene (TP1a-1b: $\rho = 0.92$, 95%CI:0.90, 0.93; TP2: $\rho = 0.75$, 95%CI:0.69, 0.81), xylene (TP1a-1b: $\rho = 0.88$, 95%CI:0.87, 0.90; TP2: $\rho = 0.74$, 95%CI:0.67,0.79), and *n*-hexane (TP1b: $\rho = 0.90$, 95%CI:0.88, 0.91; TP2: $\rho = 0.52$, 95%CI:0.42,

0.60). Differences between TP2 and TP3 for both the rig and the ROV vessels were generally small for the 5 BTEX-H chemicals.

A notable difference in the correlation for the other vessels group was the increase in correlations over TP1a-1b to TP4 for benzene (TP1a-1b: $\rho = 0.56$,

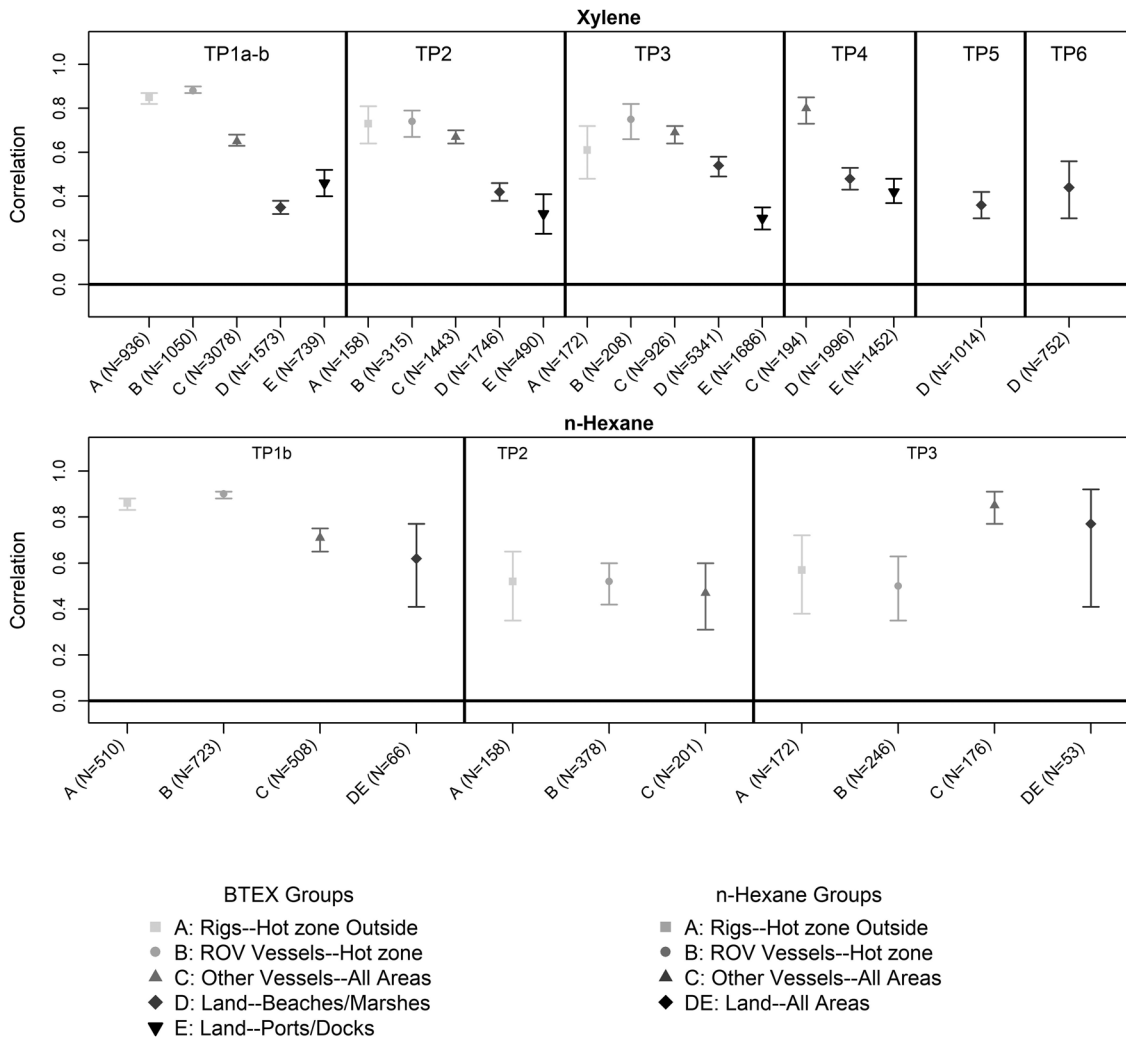


Figure 2. Xylene and *n*-hexane correlations with total hydrocarbons (THC) by time period. Correlations reflect all outside areas within a particular group. The error bars represent the 95% credible interval and the points represent the median posterior estimate. *n*-Hexane was not observed in all time periods (leading to missing measurements that we later imputed) and is therefore only shown for TP1b-3. Within land, *n*-hexane had too few measurements in TP2 to develop a relationship ($N = 5$) and had too few measurements to develop separate relationships for Beaches/Marshes and Ports/Docks. These *n*-hexane land correlations include near shore measurements due to the lack of observed *n*-hexane measurements on land. The correlations for Ports/Docks in TP5 are not shown due to limited measurements ($N = 11$).

95%CI:0.53, 0.59; TP2: $\rho = 0.62$, 95%CI:0.57, 0.66; TP3: $\rho = 0.70$, 95%CI:0.65, 0.75; TP4: $\rho = 0.85$, 95%CI:0.80, 0.89), toluene (TP1a-1b: $\rho = 0.57$, 95%CI: 0.55, 0.60; TP2: $\rho = 0.57$, 95%CI:0.53, 0.61; TP3: $\rho = 0.66$, 95%CI:0.62, 0.70; TP4: $\rho = 0.83$, 95%CI:0.78, 0.87), ethylbenzene (TP1a-1b: $\rho = 0.76$, 95%CI:0.74, 0.78; TP2: $\rho = 0.70$, 95%CI:0.65, 0.73; TP3: $\rho = 0.70$, 95%CI:0.64, 0.74; TP4: $\rho = 0.80$, 95%CI:0.72, 0.86), and xylene (TP1a-1b: $\rho = 0.65$, 95%CI:0.63, 0.68; TP2: $\rho = 0.67$, 95%CI:0.64, 0.70; TP3: $\rho = 0.69$,

95%CI:0.64, 0.72; TP4: $\rho = 0.80$, 95%CI:0.73, 0.85). The same pattern was seen for *n*-hexane, except no measurements were available in TP4 (TP1b: $\rho = 0.71$, 95%CI:0.65, 0.75; TP2: $\rho = 0.47$, 95%CI:0.31, 0.60; TP3: $\rho = 0.85$, 95%CI:0.77, 0.91). While the correlations in the other vessel group in TP1a-1b, TP2, and TP3 were derived from measurements across all water areas (i.e. near shore, offshore, source and hot zone), in TP4 the measurements were derived from only near shore observations.

In the land areas, most adjacent time periods did not have notably different correlations. However, the correlations were different from zero [other than TP5 in ports and docks, which is not shown due to limited sample size ($N = 11$)]. In the cases where we found statistically credible differences in adjacent time periods, there was no consistent trend over time across the multiple chemicals.

Area: distance from wellhead

Correlations by general area are reported in [Figs. 3 and 4](#) for BTEX. Data for *n*-hexane are not presented due to small sample sizes. Rig vessels and ROV vessels were primarily located in the hot zone, so these vessel groups do not contribute to any other area.

No pattern was seen for correlations (across all time periods) for other vessels by area for benzene. For toluene the correlation coefficient for the hot zone was notably higher than that for the source (hot zone: $\rho = 0.69$, 95%CI:0.64, 0.75; source: $\rho = 0.51$, 95%CI:0.40, 0.61) and for offshore ($\rho = 0.36$, 95%CI: 0.25, 0.47), but not for near shore ($\rho = 0.65$, 95%CI: 0.63, 0.67). For ethylbenzene, the pattern was somewhat different: the correlation coefficients for the hot zone, source and near shore areas were similar (hot zone: $\rho = 0.75$, 95%CI:0.70, 0.80; source: $\rho = 0.74$, 95%CI:0.65, 0.80; near shore: $\rho = 0.74$, 95%CI:0.71, 0.75), while that for offshore was notably lower ($\rho = 0.47$, 95%CI:0.35, 0.58). For xylene the correlation patterns were similar to ethylbenzene, that is, similar for the hot zone, source and near shore and different for offshore (hot zone: $\rho = 0.73$, 95%CI:0.68, 0.78; source: $\rho = 0.68$, 95%CI: 0.59, 0.75; near shore: $\rho = 0.68$, 95%CI:0.66, 0.69 vs offshore: $\rho = 0.45$, 95%CI:0.34, 0.54). Within land areas (over all time periods), statistically credible differences in correlations were identified for the beaches/marshes area compared to the ports/docks area for benzene (beaches/marshes: $\rho = 0.63$, 95%CI:0.61, 0.66; ports/docks: $\rho = 0.39$, 95%CI:0.34, 0.43), toluene (beaches/marshes: $\rho = 0.51$, 95%CI:0.48, 0.53; ports/docks: $\rho = 0.30$, 95%CI:0.26, 0.33), and ethylbenzene (beaches/marshes: $\rho = 0.50$, 95%CI:0.46, 0.53; ports/docks: $\rho = 0.33$, 95%CI:0.27, 0.37). The correlations of the two areas were not different for xylene.

Type of vessel

[Figs. 3 and 4](#) also allows us to compare vessel types within the hot zone (across all time periods). Credible differences in correlations existed between the rig vessels and the ROV vessels, with the latter having a higher correlation for toluene (rigs: $\rho = 0.60$, 95% CI:0.56, 0.64; ROV vessels: $\rho = 0.76$, 95% CI:0.74, 0.79) and for ethylbenzene (rigs: $\rho = 0.72$, 95% CI:0.69, 0.75; ROV vessels: $\rho = 0.86$, 95% CI:0.84, 0.87). This difference was not seen for benzene, xylene, or *n*-hexane. Correlations among rig vessels

and other vessels in the hot zone were similar across chemicals except for xylene where rigs had a notably higher correlation than other vessels (rigs: $\rho = 0.82$, 95% CI:0.79, 0.84; other vessels: $\rho = 0.73$, 95% CI:0.68, 0.78).

Inside/outside

The correlations between inside and outside measurements on the rig vessels are provided in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online), [Supplementary Tables S1–S5](#). For the combined measurements from all time periods, the inside measurement correlations were lower than the outside correlations for benzene (inside: $\rho = 0.19$, 95%CI:-0.24, 0.58; outside: $\rho = 0.55$, 95%CI:0.48, 0.62), toluene (inside: $\rho = 0.31$, 95%CI:0.05, 0.53; outside: $\rho = 0.60$, 95%CI:0.56, 0.64), ethylbenzene (inside: $\rho = 0.23$, 95%CI:-0.03, 0.46; outside: $\rho = 0.72$, 95%CI:0.69, 0.75), and xylene (inside: $\rho = 0.66$, 95%CI:0.48, 0.79; outside: $\rho = 0.82$, 95%CI:0.79, 0.84). *n*-Hexane had a similar correlation for both inside and outside (inside: $\rho = 0.85$, 95%CI:0.69, 0.93; outside: $\rho = 0.83$, 95%CI:0.81, 0.86).

Imputation of missing data

Over 23 000 measurements for *n*-hexane were imputed, primarily on land ($N = 16\,481$). [Table 2](#) describes the data used to impute *n*-hexane and the number of imputed measurements, both for the situations where the laboratory did not analyze for *n*-hexane on the air samples and where the THC estimates had been derived from the VOC area measurements. In this table, we report for each group the number of measurements originally available the determinant characteristics of the measurements (i.e. the overarching group) used to generate the linear relationship, the observed Pearson correlation coefficient calculated from the relationship, the number of imputed measurement values and the total number of measurement values after imputation and the number of the observations the linear relationship used to impute. Generally, 300–700 measurements were imputed for the groups of rig vessels, ROV vessels, and marine vessels. In contrast, the other vessels and land groups had >5000 and >16,400 imputed values respectively.

Methods: Model-based imputation of missing BTEX-H measurements above, we also imputed BTEX-H where we had predicted THC (personal) observations from VOC area measurements. This led to an additional 272 measurements for each BTEX-H chemical for the ROV vessels and 269 measurements for each BTEX-H chemical for the marine vessels ([Table 2](#); note some additional imputed measurements are included above that were not used in the 223 reported in [Ramachandran et al., 2021](#)).

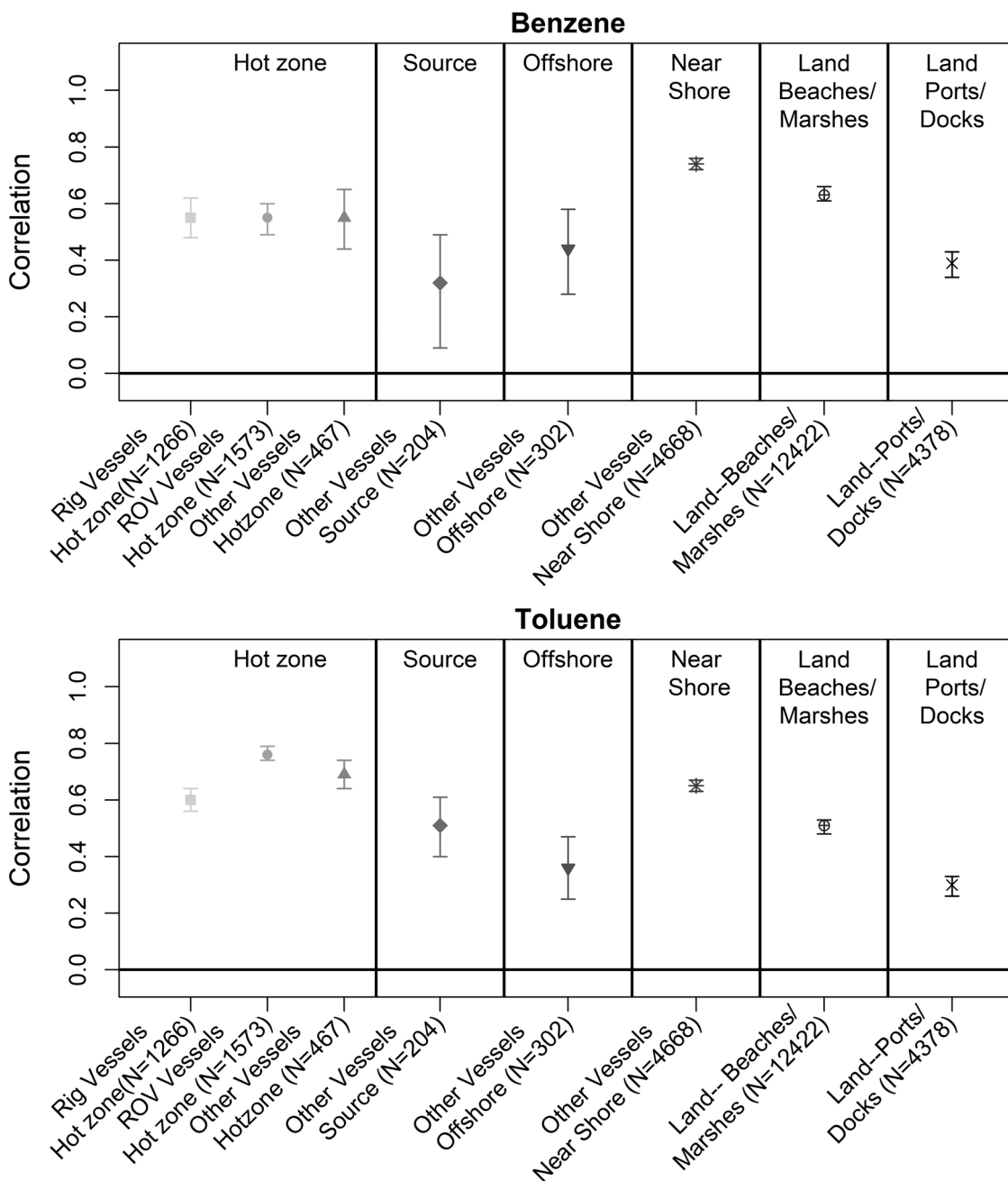


Figure 3. Benzene and toluene correlations with total hydrocarbons (THC) by area. Correlations reflect all time periods and outside measurements. The error bars represent the 95% credible interval and the points represent the median posterior estimate.

Informative priors and exposure estimates

The overarching groups, that were used as priors in the Bayesian analyses for developing BTEX-H exposure statistics are presented with their number of measurements (N), intercept, slope (and their 95% CI of the slope and intercept), correlation, and R-squared in [Tables S1–S5](#) in the [Supplementary Material](#) (available at *Annals of*

Occupational Hygiene online). For each of the BTEX chemicals, 120 overarching groups were formed (36 for *n*-hexane, due to the small number of measurements available). Some of these correlations were described above.

Exposure estimates generated using these priors ranged from <0.01 ppb to 137.02 ppb for ethylbenzene; 0.02 ppb to 187.98 ppb for toluene; 0.37 ppb to 445.35

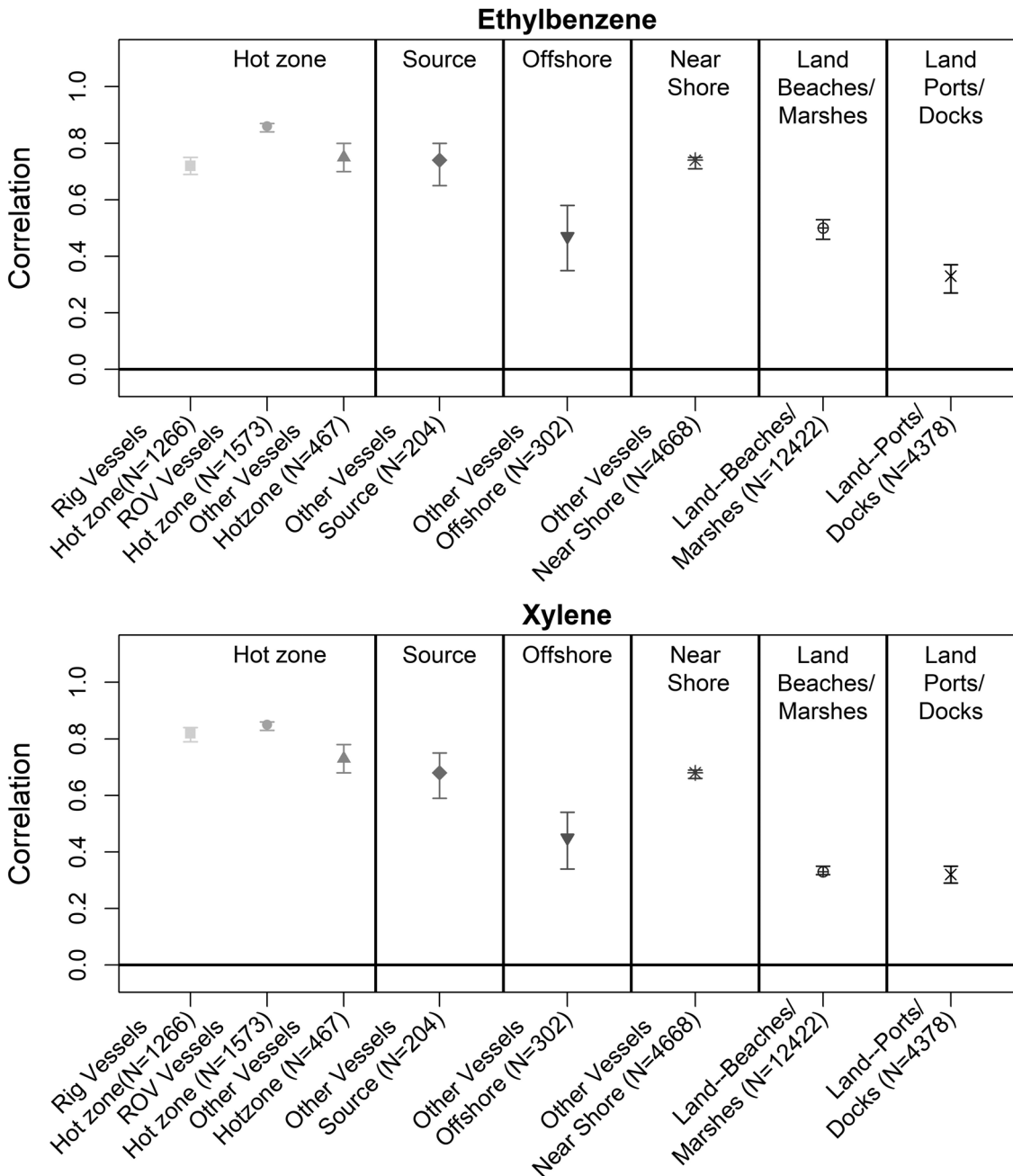


Figure 4. Ethylbenzene and xylene correlations with total hydrocarbons (THC) by area. Correlations reflect all time periods and outside measurements. The error bars represent the 95% credible interval and the points represent the median posterior estimate. *n*-Hexane is not shown since priors were not developed by area within other vessels or land categories.

ppb for xylene; and 0.02 ppb to 2441.0 ppb for *n*-hexane (Benzene was commonly highly censored for many EGs and is therefore not included in this summary). See [Huynh et al. \(2021a,b,c\)](#); [Ramachandran et al. \(2021\)](#) for more information on the exposure estimates generated for BTEX-H.

Discussion

In this study, we used Bayesian linear regression analyses with overarching groups to estimate correlations/linear relationships between THC and each of the BTEX-H chemicals and used the regression coefficients of each

Table 2. *n*-Hexane measurements available and imputation strategies. We provide the number of samples originally available in each group (Number of original measurements), the imputation regression relationship, the number of imputed values (Number of imputed values), and the total *N* for the group after imputation (Total *N* after imputation). Relationships used for imputation are described based on the time period and area used. We also provide the correlation of the regression.

Determinant characteristics			Number of original measurements	Linear regression used for imputation			Number of imputed values	Total <i>N</i> after imputation	
Group	Time period	Area		Time period	Area/group	Correlation median			
Rigs	Outside	TP1a-b	521	TP1b	Rigs	0.86	435	956	
	Inside	All	48	All	Rigs-inside	0.85	29	77	
	All ^a	All	904				464	1368	
ROV vessels	Original	TP1a-b	723	TP1b	ROVs	0.90	385	1108	
	VOC Derived	TP1a-b		TP1b	ROVs	0.90	192	192	
		TP2		TP2	ROVs	0.52	65	65	
		TP3		TP3	ROVs	0.50	15	15	
	All ^a	All	1347				657	2004	
MVs ^b	Original	TP1b	273	TP1b	Other vessels	0.71	35	308	
		TP3	152	TP3	Other vessels	0.85	3 ^c	155	
	VOC derived	TP1a-b		TP1b	Other vessels	0.71	184	184	
		TP2		TP2	Other vessels	0.47	85	85	
	All ^a	All	594				307	901	
Other vessels	TP1b	Hot zone	51	TP1b	Other vessels	0.71	52	103	
		Source	48	TP1b	Other vessels	0.71	20	68	
		Offshore	92	TP1b	Other vessels	0.71	51	143	
		Near shore	59	TP1b	Other vessels	0.71	2268	2327	
		All land areas	1	TP1b	Near shore/land	0.62	41	42	
	TP2	Offshore	36	TP2	Other vessels	0.47	31	67	
		Near shore	2	TP2	Other vessels	0.47	1152	1154	
		All land areas ^d	0	TP2-3	Near shore/land	0.66	22	22	
		TP3	Near shore	32	TP3	Other vessels	0.85	706	738
			All land areas ^d	4	TP3	Near shore/land	0.77	201	205
	TP4	Near shore	0	TP3	Other vessels	0.85	189	189	
		Ports/docks ^d	0	TP3	Near shore/land	0.77	292	292	
	Land	All ^a	All	408				5025	5433
		TP1a	Near shore	0	TP1b	Other vessels	0.71	2	2
			All land areas ^d	0	TP1b	Near shore/land	0.62	64	64
TP1b		Near shore	0	TP1b	Other vessels	0.71	77	77	
		All land areas ^d	6	TP1b	Near shore/land	0.62	5964	5970	
TP2		Near shore	0	TP2	Other vessels	0.47	69	69	
		All land areas ^d	0	TP2-3	Near shore/land	0.66	2465	2465	
TP3		Near shore	0	TP3	Other vessels	0.85	41	41	
		All land areas ^d	0	TP3	Near shore/land	0.77	3130	3130	

Table 2. Continued

Determinant characteristics			Number of original measurements	Linear regression used for imputation			Number of imputed values	Total N after imputation
Group	Time period	Area		Time period	Area/group	Correlation median		
	TP4	Near shore	0	TP3	Other vessels	0.85	5	5
		All land areas ^d	0	TP3	Near shore/land	0.77	2920	2920
	TP5	All land areas ^d	0	TP3	Near shore/land	0.77	1016	1016
	TP6	All land areas ^d	0	TP3	Near shore/land	0.77	728	728
	All ^a	All	6				16 481	16 487
Fueling ^e	All ^a						133	133
Total							23 067	26 326^f

^aThese total rows identify the number of measurements from time periods or areas where no imputation was done in the number of original measurements and Total N After Imputation columns.

^bThe IOS Pipeliner and the West Sirius did not have any valid total hydrocarbon (THC) measurements and thus counts were omitted from Ramachandran *et al.* (2021), but the counts are included here.

^cSamples analyzed by Laboratory 2 (Stenzel, Groth, Banerjee *et al.*, 2021).

^dAll Land Areas refer to Beaches/Marshes, Ports/Docks, and Other land areas.

^eFueling samples were imputed using a multiplier instead of a linear regression.

^fThe total number of measurements used in the study was 26 161 (excluding those on the ROV vessels (Ramachandran *et al.*, 2021)). The additional 165 measurements presented were not used due to their not meeting our inclusion criteria (Stenzel, Groth, Banerjee *et al.*, 2021).

N: Number of measurements; TP: Time period; VOC: Volatile Organic Compounds; VOC Derived: Measurements originally derived using the VOC database; Original: Measurements not considering VOC derived samples; ROV Vessels: Vessels operating remotely operated vehicles; MVs: Marine Vessels; Other Vessels: A group comprised of research vessels, and vessels other than marine vessels, rig vessels, and ROV vessels; Total: Reflects the totals of all measurements including fueling.

overarching group to impute values for missing BTEX-H measurements. Then, we used these overarching group relationships as priors to model exposure statistics, incorporating the recently imputed observations into each EG and accounting for censored data.

Correlations

The linear relationships (described here as correlations but modeled using linear regressions) between THC and the BTEX-H chemicals were based on the assumption that the significant source of these chemicals in the air was the evaporated oil. The oil weathered differentially for the BTEX-H chemicals over time and space, so we considered the effect of weathering on the air concentrations to decrease uncertainty in our estimates. Because we had no measurements of weathering, we identified proxies for weathering that were documented with the measurements, that is, time period (from date sampled) and area of the Gulf. In addition, two other determinants, type of vessel, and on the rig vessels, indoors/out of doors, were evaluated. As demonstrated in Figs. 1–4, many of these relationships differed notably by these determinants, as hypothesized. Correlations differed by

time period, distance from the wellhead (i.e. area of the Gulf), and vessel type, although the latter was largely confounded by distance from the wellhead. In addition, the correlations were different and were generally lower inside the rig vessels than outside.

In TP1a-1b, crude oil was continuously being released into the GuLF, leading to a pseudo-equilibrium between the fresh and weathered oil. This equilibrium was likely the cause of the higher correlations for the vessels at the wellhead at this time. After the well was mechanically capped (at the end of TP1b), the correlations differentially fell for the rig vessels and ROV vessels in TP2 and sometimes further in TP3. This differential decrease may have occurred due to the continued differential weathering and the possible presence of other sources of these substances (such as cleaning chemicals and engine exhaust) that could have contributed relatively more to the vapors' concentrations than in earlier time periods.

The other vessels group showed a different pattern, with correlations generally increasing over time. It is unclear why this occurred; it may be because the measurements in TP1a-3 were located throughout the larger area of the Gulf (hot zone, source, offshore, and near shore), whereas in TP4 the measurements primarily were collected near shore.

No patterns were seen for land measurements possibly because of the limited range of the measurements. Our ability to fully interpret these results is limited due to the extremely complex exposure situation and weathering conditions.

Correlations across areas of the Gulf varied by chemical. Analyses of toluene, ethylbenzene, and xylene found similar (ethylbenzene, xylene) or slight differences (toluene) between the hot zone, source, and near shore areas, but notable differences in the offshore area possibly due to the larger area, resulting in more variable concentrations than in the smaller areas of the hot zone, source and near shore. The consistently higher correlations at beaches and marshes compared to ports and docks may be due to 'purer' conditions (i.e. no other major sources than the weathered oil) compared to the ports and docks, which was characterized by having fueling and decontaminating operations, both of which could have contributed to the (differential) air concentrations.

We found that the type of vessel provided little additional information than area because of the high correspondence between vessel type and area. We presented correlations by type of vessel, however, because the correlations were more interpretable with that information. We also analyzed the data by the U.S. Gulf coast state in which the measurement was taken as another proxy for weathering. We did not observe statistically credible differences between most states' correlations (analysis not shown). Furthermore, analyses by state greatly diminished the sample size of these overarching relationships, particularly for *n*-hexane. Thus, we did not consider state-specific relationships/correlations.

On the rig vessels, correlations inside were lower than the correlations outside for most BTEX chemicals (although less so for benzene and xylene), suggesting that the ventilation system's particulate and charcoal filters removed differentially the chemicals or that additional sources of chemicals (e.g. cleaning chemicals or exhaust from a cooking grill) may have been present during some measurements. *n*-Hexane had a similar correlation between inside and outside measurements, which may be related to the limited sample size for measurements inside ($N = 43$ compared to $N = 75$ for BTEX) or because it is not typically present in cleaning chemicals or cooking exhaust.

While a single overarching regression or correlation could have been used across all measurements, such an approach would have not accommodated the variability seen among the various overarching EGs, and thus would have increased the uncertainty in our estimates. Nonetheless, grouping of determinants was done for the BTEX chemicals when only a small number of measurements were available. For example, we combined TP1a

with TP1b for particular areas and vessel types, due to small numbers in TP1a. We did this based on the assumption that the relationship for the overarching group would produce reasonable estimates of exposure for the smaller group, although with increased uncertainty. In addition, using a larger group (i.e. at least two time periods or multiple areas) for predicting measurements of the various members of the larger group, although less than ideal, was expected to be a valid assumption for various reasons. First, we assumed that our determinants allowed us to identify overarching groups with exposure to roughly similar degrees of weathered oil. From our findings it is clear that determinants led to different linear relationships between THC and each BTEX-H chemical (both on the log scale) as evidenced by the number of non-overlapping CIs for the slopes in [Tables S1–S5](#) in the [Supplementary Materials](#) (available at *Annals of Occupational Hygiene* online) and [Figs. 1–4](#). Second, we scientifically and statistically evaluated when new relationships were needed (using multiple linear regression); that is, we identified scientifically based determinants that were expected to influence correlations and combined them into overarching groups. We also found that relationships differed significantly [in [Tables S1–S5](#) in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online)].

These correlations should be useful in future oil spills to help guide the sampling strategy and institute measures protective of workers.

Missing data imputation

The imputation of *n*-hexane provided us with substantially greater coverage of time periods (primarily TP1a, TP1b, TP4-6) and for land. The priors for the *n*-hexane land estimation were based primarily on near shore measurements because of the few ($N \leq 30$) land measurements that were available. Using near shore measurements brought the sample sizes to $N > 50$ in all time periods except in TP2, for which we used the TP2-3 relationship [reflected in relationships shown in [Table S5](#) in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online)]. The use of near shore measurements to predict land measurements was not ideal, because it is likely that land measurements were affected to a greater degree of weathering than near shore measurements. *n*-Hexane is much more volatile than the BTEX chemicals and therefore is much more affected by the degree of weathering. However, near shore is the group most similar to the land measurements as the former measurements were collected <3 nmi (5.56 km) from land. Using these surrogate measurements for land in later time periods could have resulted in

overestimation of *n*-hexane in TP4-6. Before conducting the *n*-hexane imputation, we had 3259 measurements for *n*-hexane; after the imputation, we had 26 326 *n*-hexane measurements. Although this imputation substantially aided our estimation process, such extensive imputation means that any *n*-hexane results should be interpreted with caution.

Informative priors

The priors we used to develop exposure statistics for our EGs are the intercepts and slopes from [Tables S1–S5](#) in the [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online) along with the conditional variance (conditional variance not shown in [Tables S1–S5](#)). We used the most similar overarching group as the prior for the EG except when there were too few measurements for stable estimates. For example, for workers who worked outside on the rig vessels in TP1a, we used the TP1a-1b outside rig vessels as the prior relationship to inform the regression. Although the vessel type was highly correlated with area, we included vessel type in the characterization of the priors for clarity. Using the overarching groups allowed us to develop more stable exposure estimates for EGs with smaller numbers of measurements and/or with higher percentages of censored measurements by borrowing information from the regression analysis and from THC. These priors were used in the development of the exposure estimates (AMs, GMs, GSDs, and 95th percentiles) discussed in [Huynh et al. \(2021a,b,c\)](#); [Ramachandran et al. \(2021\)](#); [Stewart, Groth et al. \(2021\)](#).

Statistical assumptions and limitations

We assumed that all the relationships presented here were linear in nature and that the assumptions of linear regression were met [equal variances, linearity, normality of residuals (and lognormality of each chemical), and independence of observations]. These assumptions appear to be reasonable based on chemical laws [see [Supplementary Material](#) (available at *Annals of Occupational Hygiene* online) and [Stenzel, Groth, Huynh et al., 2021](#)]. In addition, while it is possible that some study participants contributed multiple measurements within any particular regression/correlation, within-participant level variability was not assessed due to insufficient information in the measurement database on which samples represented the same participant ([Stewart, Groth et al., 2021](#)). Also, other relationships or distributional assumptions were not explored. Furthermore, we also assumed that a single value of the AM, that is, the median posterior estimate derived from a Bayesian fully model-based imputation was representative of each imputed exposure measurement. Other statistics were not considered. Future work could consider

using the full posterior distributions of each missing measurement in the final exposure estimation process.

We also assumed that all linear relationships identified were representative of the particular groups studied and could be used as informative prior relationships. If a particular set of observations substantially deviated from this assumption, the exposure estimates may be more biased or imprecise than estimates that did not deviate from the assumption. However, exposure estimates were unlikely to have been influenced dramatically by the use of informative priors due to the use of a downweighting procedure to allow the real data to drive the inference when enough data were present ([Quick et al., 2017](#)). In addition, since these correlations were identified directly from the data used in the assessment of the EGs, although based on larger datasets, the overarching groups should be representative of the true exposures in the larger groups, thus providing reasonable informative prior relationships to the best degree possible, albeit possibly with broader credible intervals than preferred.

Strengths

The strengths of this analysis are several. First, this study used a Bayesian left-censored linear model that accounts for censoring in both the predictor (THC) and the response (each of the BTEX-H chemicals). For more statistical benefits of this method, see [Groth et al. \(2017 and 2018\)](#). Second, this approach used scientific principles to identify several determinants of exposure. We could have relied on a single linear relationship; however, after statistically evaluating the relationships, we found that many credibly different correlations were present, supporting the approach taken of identifying different sets of exposure determinants to represent different exposure conditions. Thus, use of the different correlations allows us to further differentiate exposures, likely narrowing our credible intervals from what they would have been had we used only a single group of all observations. Third, imputation of the missing measurements increased our overall number of observations in many EGs, particularly for *n*-hexane, although, in TP4-6 the *n*-hexane estimate may have a marginally positive bias. The newly imputed values for BTEX-H were developed after deriving the correlations because we wanted the correlations to reflect the real data. As a result, the relationships used for imputation were based only on real observed data. Finally, the use of these relationships as informative priors allowed EGs with limited information (small number of measurements and/or high censoring) to borrow strength from overarching relationships in the data. This process likely further increased the robustness of our exposure estimates and potentially made them more accurate.

Conclusion

We used physical/chemical principles to develop relationships (correlations) between our known data (THC) and each of the BTEX-H chemicals and evaluated those relationships for statistical credibility. Correlations between THC and each of the BTEX-H chemicals generally exceeded 0.50 and differed notably across various time periods, areas, vessel type, and of inside versus outside on the rig vessels. Most of these findings were likely due to the degree of weathering in oil.

These correlations were used to impute missing data, resulting in >23 000 additional *n*-hexane observations and >500 BTEX additional observations that were used in the exposure estimation process. Because of the large number of imputed *n*-hexane values, however, caution should be used when interpreting any health outcome-*n*-hexane relationship.

Finally, these correlations provided information as priors in the application of the Bayesian method to develop exposure statistics for EGs even when the number of measurements were limited or a substantial percentage of the BTEX-H measurements were censored by borrowing strength from a similar overarching relationship. This procedure likely enabled us to develop more stable estimates for the exposure statistics used in the investigation of exposure-response relationships in the epidemiologic study.

Supplementary data

Supplementary data are available at *Annals of Work Exposures and Health* online.

Acknowledgments

This study was funded by the NIH Common Fund and the Intramural Research Program of the NIH, National Institute of Environmental Health Sciences (ZO1ES102945). Dr. Sudipto Banerjee would like to acknowledge funding from the following grants: National Institutes of Health/National Institute of Environmental Health Sciences (R01ES027027-01, R01ES030210-01), National Science Foundation (DMS-1513654, IIS-1562303, and DMS-1916349). Dr Tran Huynh was also supported, in part, by Center for Disease Control/National Institute for Occupational Safety and Health K01OH011191 award.

Conflict of interest

The authors declare no conflict of interest relating to the material presented in this Article. Its contents, including any opinions and/or conclusions expressed, are solely those of the authors.

Data availability

The data underlying this article will be shared on reasonable request, consistent with protections for the privacy of study participants and existing multi-party agreements. Requests should be made following instructions on the study website <https://gulfstudy.nih.gov>.

References

- Arnold S, Stewart PA, Pratt GC *et al.* (2021) Estimation of aerosol concentrations of oil dispersants COREXIT™ EC9527A and EC9500A during the *Deepwater Horizon* oil spill response and clean-up operations. *Ann Work Expo Health*; **66**: i188–i201.
- Brooks S, Gelman A, Jones G *et al.* (2011) *Handbook of Markov chain Monte Carlo*. 1st edn. Boca Raton, FL: Chapman & Hall/CRC. ISBN 1420079417.
- Carlin BP, Louis TA. (2008) *Bayesian methods for data analysis*. 3rd edn. Boca Raton, FL: Chapman & Hall/CRC. ISBN 1584886978.
- Gelman A, Carlin B, Stern HS *et al.* (2013) *Bayesian data analysis*. 3rd edn. Boca Raton, FL: CRC Press. ISBN 1439840954.
- Gilks WR, Richardson S, Spiegelhalter D. (1996) *Markov chain Monte Carlo in practice*. Boca Raton, FL: Chapman & Hall/CRC. ISBN 0412055511.
- Gorman Ng M, Cherrie JW, Sleuwenhoek A *et al.* (2021) GuLF DREAM: a model to estimate dermal exposure among oil spill response and clean-up workers. *Ann Work Expo Health*; **66**: i218–i233.
- Groth CP, Banerjee S, Ramachandran G *et al.* (2021) Methods for the analysis of 26 million VOC area measurements during the *Deepwater Horizon* oil spill clean-up. *Ann Work Expo Health*; **66**: i140–i155.
- Groth CP, Banerjee S, Ramachandran G *et al.* (2017) Bivariate left-censored bayesian model for predicting exposure: preliminary analysis of worker exposure during the *Deepwater Horizon* oil spill. *Ann Work Expo Health*; **61**: 76–86.
- Groth CP, Banerjee S, Ramachandran G *et al.* (2018) Multivariate left-censored Bayesian modeling for predicting exposure using multiple chemical predictors. *Environmetrics*; **29**: 1–16.
- Huynh TB, Groth CP, Ramachandran G *et al.* (2021a) Estimates of occupational inhalation exposures to six oil-related compounds on the four rig ships responding to the *Deepwater Horizon* oil spill. *Ann Work Expo Health*; **66**: i89–i110.
- Huynh TB, Groth CP, Ramachandran G *et al.* (2021b) Estimates of inhalation exposures to oil-related components on the supporting vessels during the *Deepwater Horizon* oil spill. *Ann Work Expo Health*; **66**: i111–i123.
- Huynh TB, Groth CP, Ramachandran G *et al.* (2021c) Estimates of inhalation exposures among land workers during the *Deepwater Horizon* oil spill clean-up operations. *Ann Work Expo Health*; **66**: i124–i139.

- Huynh T, Quick H, Ramachandran G *et al.* (2016) A comparison of the β -substitution method and a Bayesian method for analyzing left-censored data. *Ann Occup Hyg*; 60: 56–73.
- Huynh T, Ramachandran G, Banerjee S *et al.* (2014) Comparison of methods for analyzing left-censored occupational exposure data. *Ann Occup Hyg*; 58: 1126–42.
- Kwok RK, Engel LS, Miller AK *et al.*; GuLF STUDY Research Team. (2017) The GuLF STUDY: a prospective study of persons involved in the *Deepwater Horizon* oil spill response and clean-up. *Environ Health Perspect*; 125: 570–8.
- Liu Z, Liu J, Ahu Q, Wu W. (2012) The weathering of oil after the *Deepwater Horizon* oil spill: insights from the chemical composition of the oil from the sea surface, salt marshes and sediments. *Environ Res Lett*; 7: 035302.
- Marin J, Robert C. (2007) *Bayesian core: a practical approach to computational Bayesian statistics*. 1st edn. New York, NY: Springer. ISBN 038738972.
- NOAA Office of Response and Restoration. Weathering processes affecting spills [Internet]. 2020. Available at <https://response.restoration.noaa.gov/oil-and-chemical-spills/oil-spills/weathering-processes-affecting-spills>. Accessed 18 August 2020.
- Plummer M. (2003) JAGS: a program for analysis of Bayesian graphical models using Gibbs sampling. In Proceedings of the 3rd International Workshop on Distributed Statistical Computing (DSC 2003), March 20–22, Vienna, Austria. ISSN 1609-395X.
- Plummer M. (2016) rjags: Bayesian graphical models using MCMC. R package version 4–6. Available at <https://CRAN.R-project.org/package=rjags>
- Pratt GC, Stenzel MR, Kwok RK *et al.* (2021) Modeled air pollution from *in situ* burning and flaring of oil and gas released following the *Deepwater Horizon* disaster. *Ann Work Expo Health*; 66: i172–i187.
- Quick H, Huynh T, Ramachandran G. (2017) A method for constructing informative priors for Bayesian modeling of occupational hygiene data. *Ann Work Expo Health*; 61: 67–75.
- R Core Team (2017) *R: a language and environment for statistical computing*. Vienna, Austria: R Foundation for Statistical Computing. <https://www.R-project.org/>
- Ramachandran G, Groth CP, Huynh TB *et al.* (2021) Using real-time area VOC measurements to estimate total hydrocarbons exposures to workers involved in the *Deepwater Horizon* oil spill. *Ann Work Expo Health*; 66: i156–i171.
- Stenzel MR, Groth CP, Huynh TB *et al.* (2021) Exposure Group Development in support of the NIEHS GuLF STUDY. *Ann Work Expo Health*; 66: i23–i55.
- Stenzel MR, Groth CP, Banerjee S *et al.* (2021) Exposure assessment techniques applied to the highly censored *Deepwater Horizon* Gulf oil spill personal measurements. *Ann Work Expo Health*; 66: i56–i70.
- Stenzel MR, Arnold SF, Ramachandran G *et al.* (2021) Estimation of airborne vapor concentration of oil dispersants COREXIT™ EC9527A and EC9500A, volatile components associated with the *Deepwater Horizon* oil spill response and clean-up operations. *Ann Work Expo Health*; 66: i202–i217.
- Stewart PA, Gorman Ng M, Cherrie JW *et al.* (2021) Estimation of dermal exposure to oil spill response and clean-up workers after the *Deepwater Horizon* disaster. *Ann Work Expo Health*; 66: i234–i246.
- Stewart P, Groth CP, Huynh TB *et al.* (2021) Assessing exposures from the *Deepwater Horizon* oil spill response and clean-up. *Ann Work Expo Health*; 66: i3–i22.