Supplemental Information for *Effect and Pathways Modifiers in a Bayesian Pathways Analysis of the National Human Exposure Assessment Survey for Arsenic in EPA Region 5*

Definitions of Input Variables and Fitted Bayesian Pathways Models

This document specifies the variables and results from all Bayesian Pathways Models fitted to the NHEXAS data in the paper *Effect and Pathways Modifiers in a Bayesian Pathways Analysis of the National Human Exposure Assessment Survey for Arsenic in EPA Region 5.* It also lists the full-conditional distributions of the model parameters used by our MCMC algorithm.

1 Media and Pathway Modifier Variables

See Tables 1 and 2.

2 Full Conditional Distributions of the Hierarchical Bayesian Subpopulation Model

2.1 Posterior distribution

Letting $\boldsymbol{\theta} = (\boldsymbol{\beta}, \boldsymbol{\tau}, \boldsymbol{\omega})$, the posterior distribution is

$$\begin{aligned} [\boldsymbol{\theta}, \boldsymbol{X} | \boldsymbol{Y}] &\propto [\boldsymbol{Y} | \boldsymbol{X}, \boldsymbol{\theta}]\ [\boldsymbol{X} | \boldsymbol{\theta}]\ [\boldsymbol{\theta}] \\ &= [\boldsymbol{Y} | \boldsymbol{X}, \boldsymbol{\omega}]\ [\boldsymbol{X} | \boldsymbol{\beta}, \boldsymbol{\tau}]\ [\boldsymbol{\beta}]\ [\boldsymbol{\omega}]\ [\boldsymbol{\tau}], \end{aligned}$$

assuming independence of the three components within $\boldsymbol{\theta}$. The distribution is not available in closed form and so we use a Gibbs sampler Markov chain Monte Carlo (MCMC), based on an augmented (including censored and missing data) joint distribution to sample from this posterior distribution.

Variable	**Type**	**Definition and Units**
UR	M	natural log of arsenic concentration in Urine ($\mu g/\ell$)
FD	M	natural log of arsenic intake in Food ($\mu g/day$)
BV	M	natural log of arsenic intake in Beverage ($\mu g/day$)
IA	M	natural log of arsenic concentration in Indoor Air (ng/m^3)
OA	M	natural log of arsenic concentration in Outdoor Air (ng/m^3)
PA	M	natural log of arsenic concentration in Personal Air (ng/m^3)
SL	M	natural log of arsenic concentration in Soil (ng/g)
SD	M	natural log of arsenic loading in Surface (Sill) Dust ($\mu g/cm^2$)
WF	m	natural log of arsenic concentration in Tap Water, Flushed ($\mu g/\ell$)
logcrtst	C	natural log of creatinine concentration ($\mu g/\ell$)
mlogcrtn	C	negative of the natural log of creatinine concentration ($\mu g/\ell$)
logcreatinine	C	the natural log of creatinine concentration ($\mu g/\ell$)
male	C, E	binary (0/1) variable indicating the participant is male
female	E	binary (0/1) variable indicating the participant is female
child4to11/Age1	C, E	binary (0/1) variable indicating the participant is between 4 and 11 years old
age	C, E	participant's age (years)
AgeAtoB	C, E	binary (0/1) variable indicating the participant's age is between A and B years old
Age2	C,E	binary (0/1) variable indicating the participant's age is between 12 and 19 years
hhold	E, P	household size
log hhold	E, P	natural log of household size
minushhold	E, P	negative of household size
hrs.home	E	average number of hours participant spends inside home/day
glass	E	average number of glasses of water participant drinks/day
tap.c	P	binary (0/1) variable indicating participant cooks with tapwater
fruit	P	binary (0/1) variable indicating participant eats fruit at least 3 days/three-months
tap.d/tapwater	E	binary (0/1) variable indicating participant drinks tapwater
c.air	E	binary (0/1) variable indicating participant's home has central air
no.c.air	E	binary (0/1) variable indicating participant's home does *not* have central air
gasequip	P	binary (0/1) variable indicating participant used gas equipment in the past week

Table 1: For each variable used in the Bayesian hierarchical analysis, the variable symbol, its use-depending on the fitted model (M = media, C = component of the creatinine adjustment, E = effect modifier, and P = pathway modifier), and its definition, including units.

Variable	Type	Definition and Units
tobacco/tobacco1	P	binary (0/1) variable indicating the participant is a current smoker
tobacco2	P	binary (0/1) variable indicating the participant is a former smoker
workshop	P	average number of minutes/day in an enclosed workshop
work20	P	binary (0/1) variable indicating participant works $\geq$ 20 min./day in a workshop
fish	P	binary (0/1) variable indicating participant eats fish
new.fish	P	binary (0/1) variable indicating participant eats fish more than once/month
no.fish	P	binary (0/1) variable indicating participant eats fish less than once/month
logBMI	C	Natural log of Body Mass Index (kg/m^2)
race3_2	C, E	a binary(0/1) variable indicating whether the participant is African-American
race3_3	C, E	binary(0/1) variable indicating the participant's race is *not* Caucasian/African-American
no.wellwater	P	binary(0/1) variable indicating the source of running water is well water
wellwater	P	binary(0/1) variable indicating the source of running water is *not* well water

Table 2: For each variable used in the Bayesian hierarchical analysis, the variable symbol, its use-depending on the fitted model (M = media, C = component of the creatinine adjustment, E = effect modifier, and P = pathway modifier), and its definition, including units.

2.2 Full conditional distributions

1. For each i and j we set/draw augmented data, Y_{ij}^*, as follows:

$$Y_{ij}^* \quad \begin{cases} = Y_{ij}, & Z_{ij} = 0; \\ \sim \text{Truncated } N(X_{ij}, 1/\omega_j) \text{ on } (-\infty, M_{ij}], & Z_{ij} = 1; \\ \sim N(X_{ij}, 1/\omega_j), & Z_{ij} = 2. \end{cases}$$

2. For the process variable $\boldsymbol{X}$, we sample each process variable $\boldsymbol{X}_j$, $j = 1 \ldots, J$, conditional on the other process variables $\{\boldsymbol{X}_k : k \neq j\}$ and the other parameters in the model. We have that

$$\begin{aligned} & [\boldsymbol{X}_j | \{\boldsymbol{X}_k : k \neq j\}, \boldsymbol{\beta}, \boldsymbol{\tau}, \boldsymbol{Y}^*, \boldsymbol{\omega}] \\ \propto \quad & \left[\boldsymbol{Y}_j^* | \boldsymbol{X}_j, \boldsymbol{\omega}\right] \left[\boldsymbol{X}_j | \{\boldsymbol{X}_k : k \neq j\}, \boldsymbol{\beta}_j, \tau_j\right] \prod_{l \in ch_j} \left[\boldsymbol{X}_l | \{\boldsymbol{X}_k : k \neq l\}, \boldsymbol{\beta}_l, \tau_l\right], \end{aligned}$$

where ch_j denotes the columns of the process variable $\boldsymbol{X}$ that depend on $\boldsymbol{X}_j$ in their definition of the conditional mean μ_{ij} (i.e., those l for which $s_{lk}^X = j$ for some k or $s_{lm}^{EX} = j$ for some m).

The above is expression is equal to

$$\prod_{i=1}^{I}\left(\left[Y^*_{ij}|X_{ij},\omega_j\right]\left[X_{ij}|\{X_{ik}:k\neq j\},\boldsymbol{\beta}_j,\tau_j\right]\prod_{l\in ch_j}\left[X_{il}|\{X_{ik}:k\neq l\},\boldsymbol{\beta}_l,\tau_l\right]\right),$$

from which we can see that we can sample each X_{ij}, $i=1,\dots,I$, independently. Now

$$\left[Y^*_{ij}|X_{ij},\omega_j\right] \quad\propto\quad \exp\Big(\frac{\omega_j}{2}(Y^*_{ij}-X_{ij})^2\Big),$$

$$\left[X_{ij}|\{X_{ik}:k\neq j\},\boldsymbol{\beta}_j,\tau_j\right] \quad\propto\quad \exp\Big(\frac{\tau_j}{2}(X_{ij}-\mu_{ij})^2\Big),$$

and for each $l\in ch_j$

$$[X_{il}|\{X_{ik}:k\neq l\},\boldsymbol{\beta}_l]\propto\exp\Big(\frac{\tau_l}{2}(X_{il}-\delta_{il}(j)-\epsilon_{il}(j))^2\Big). \tag{1}$$

In (1) we define

$$\delta_{ij}(o) \quad=\quad \alpha_j+\sum_{\{k:s^X_{jk}\neq o\}}\beta^X_{jk}X_{is^X_{jk}}+\sum_l\beta^P_{jl}P_{is^P_{jl}}+\sum_m\beta^E_{jm}E_{is^E_{jm}}+\sum_{\{n:s^{EX}_{jn}\neq o\}}\beta^{EX}_{jn}E_{is^E_{jn}}X_{is^{EX}_{jn}}$$

to be the conditional mean of X_{ij} minus the regression terms that depend on X_{io}, and

$$\begin{aligned}\epsilon_{ij}(o) \quad&=\quad \sum_{\{k:s^X_{jk}=o\}}\beta^X_{jk}X_{is^X_{jk}}+\sum_{\{m:s^{EX}_{jm}=o\}}\beta^{EX}_{jm}E_{is^E_{jm}}X_{is^{EX}_{jm}}\\ &=\quad X_{io}\left[\sum_{\{k:s^X_{jk}=o\}}\beta^X_{jk}+\sum_{\{m:s^{EX}_{jm}=o\}}\beta^{EX}_{jm}E_{is^E_{jm}}\right],\end{aligned}$$

to be the regression terms that depend on X_{io}. Always, $\delta_{ij}(o)+\epsilon_{ij}(o)=\mu_{ij}$.

Rearranging the terms of X_{ij}, the distribution of X_{ij} conditional on all other terms is $N(q/p,1/p)$ where

$$q \quad=\quad \omega_jY^*_{ij}+\tau_j\mu_{ij}+\sum_{l\in ch_j}\tau_l\left(X_{il}-\delta_{il}(j)\right)\left(\sum_{\{k:s^X_{jk}=n\}}\beta^X_{jk}+\sum_{\{m:s^{EX}_{jm}=n\}}\beta^{EX}_{jm}E_{is^E_{jm}}\right)$$

and

$$p \quad=\quad \omega_j+\tau_j+\sum_{l\in ch_j}\tau_l\left(\sum_{\{k:s^X_{jk}=n\}}\beta^X_{jk}+\sum_{\{m:s^{EX}_{jm}=n\}}\beta^{EX}_{jm}E_{is^E_{jm}}\right)^2.$$

3. For the regression parameters $\boldsymbol{\beta}$, we sample each $\boldsymbol{\beta}_j$ conditional on the other parameters in the model. Letting

$$\boldsymbol{A}_j \quad = \quad \begin{bmatrix} 1 & \left\{X_{1s^X_{jk}}\right\} & \left\{P_{1s^P_{jk}}\right\} & \left\{E_{1s^E_{jk}}\right\} & \left\{E_{1s^E_{jk}} X_{1s^{EX}_{jk}}\right\} \\ 1 & \left\{X_{2s^X_{jk}}\right\} & \left\{P_{2s^P_{jk}}\right\} & \left\{E_{2s^E_{jk}}\right\} & \left\{E_{2s^E_{jk}} X_{2s^{EX}_{jk}}\right\} \\ \vdots & \vdots & \vdots & \vdots & \\ 1 & \left\{X_{Is^X_{jk}}\right\} & \left\{P_{Is^P_{jk}}\right\} & \left\{E_{Is^E_{jk}}\right\} & \left\{E_{Is^E_{jk}} X_{Is^{EX}_{jk}}\right\} \end{bmatrix},$$

the distribution of $\boldsymbol{\beta}_j$ conditional on the other parameters is

$$\mathrm{MVN}_{r_j}\left(\boldsymbol{R}_j^{-1}\boldsymbol{q}_j, \boldsymbol{R}_j^{-1}\right),$$

where $\boldsymbol{R}_j = \tau_j \boldsymbol{A}_j^T \boldsymbol{A}_j + \boldsymbol{\Sigma}_j^{-1}$ and $\boldsymbol{q}_j = \tau_j \boldsymbol{A}_j^T \boldsymbol{X}_j + \boldsymbol{\Sigma}_j^{-1}\boldsymbol{m}_j$.

4. For each j, the conditional distribution of the process precision τ_j, given the other parameters, is

$$Ga\left(c_j + I/2,\ d_j + \sum_{i=1}^{N}(X_{ij} - \mu_{ij})^2/2\right),$$

where μ_{ij} was defined above in Equation (1) of the paper.

Models fit in "Effect and Pathways Modifiers in a Bayesian Pathways Analysis of the NHEXAS for Arsenic in EPA Region 5"

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	Clayton	Subpops	Reduced
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FD	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
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BV	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	IA	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	SD	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	WF	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	tapwater	■			■							■															■	■	■	■	■	■	■	■						■									
	tap.d																																		■	■	■	■	■		■	■	■	■	■	■		■	■
	glass	■					■					■															■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■
	tapwater*WF	■			■							■															■	■	■	■	■	■	■	■						■									
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	glass*WF	■					■					■															■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■
	glass*tapwater	■										■																																					
	glass*tapwater*WF											■																																					
IA	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	OA	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	SL	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	hhold														■	■	■	■	■	■	■	■	■	■			■		■		■	■	■	■	■	■	■	■	■	■	■	■		■	■	■		■	■
	minushhold																								■	■		■		■													■						
	hold***OA**														■	■	■	■	■	■	■	■	■	■			■		■		■	■		■	■	■	■	■	■	■	■	■		■	■	■		■	
	minushold***OA**																								■	■		■		■			■										■						
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	c.air***OA**															■	■	■	■	■	■						■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■			
OA	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
PA	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	OA	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	IA	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	tobacco	■	■									■		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■		■	■	■	■	■	■	■	■	■	■	■	■		■	
	gasequip																										■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■
	workshop																										■	■	■	■	■	■	■	■	■	■						■							
	work.cat																																				■												
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	hrs.home																											■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■
	hrs.home***OA**																											■	■	■				■	■	■	■	■	■	■	■	■	■	■	■	■		■	
	hrs.home***IA**																											■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■
	Male																																		■	■	■	■	■	■									
	tobacco1																															■		■															
	tobacco2																															■		■															

Models fit in "Effect and Pathways Modifiers in a Bayesian Pathways Analysis of the NHEXAS for Arsenic in EPA Region 5"

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	Clayton	Subpops	Reduced
SL	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
SD	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
	IA	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
WF	**Intercept**	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
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	Age2	▨	▨	▨	▨	▨	▨	▨																																									
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	age	▨	▨	▨	▨	▨	▨	▨																																									
	race3_2	▨	▨	▨	▨	▨	▨	▨																																									
	race3_3	▨	▨	▨	▨	▨	▨	▨																																									
	Female	▨	▨	▨	▨	▨	▨	▨																																									
	race3_2*Age1	▨	▨	▨	▨	▨	▨	▨																																									
	race3_3*Age1	▨	▨	▨	▨	▨	▨	▨																																									
	race3_2*Age2	▨	▨	▨	▨	▨	▨	▨																																									
	race3_3*Age2	▨	▨	▨	▨	▨	▨	▨																																									
	race3_2*Age20to50	▨	▨	▨	▨	▨	▨	▨																																									
	race3_3*Age20to50	▨	▨	▨	▨	▨	▨	▨																																									