

MEMORANDUM

To: Ted Palma, U.S. Environmental Protection Agency

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Subject: Development of Penetration and Proximity Microenvironment Factor Distributions for the HAPEM5 in Support of the 1999 National-Scale Air Toxics Assessment (NATA)

Project: EPA Contract No. GS-10F-0124J

Introduction

The Hazardous Air Pollutant Exposure Model, version 5 (HAPEM5), is a screening-level human exposure model designed to estimate inhalation exposures of population subgroups to hazardous air pollutants (HAPs). HAPEM5 is being used to determine national inhalation exposure concentrations for approximately 200 HAPs as part of the 1999 National Air Toxics Assessment (NATA) national-scale assessment (Table 1; note that all tables are provided at the end of this memo). A previous version of the model (HAPEM4) was run in support of the 1996 NATA national-scale assessment for 33 HAPs.

HAPEM5 calculates microenvironmental concentrations of HAPs in 37 indoor, outdoor, and in-vehicle microenvironments (MEs) (Table 2). HAPEM5 uses HAP-specific ME factors (MEFs) to account for the contribution of indoor sources and ambient HAP concentrations to pollutant levels in the MEs. For the 1996 NATA, HAPEM4 used point estimates of MEFs for the 33 HAPs modeled. HAPEM5 is designed to incorporate distributions of MEF values to represent the variability in MEFs and improve model estimates.

This memorandum describes the development of MEF distributions for the two factors relating to ambient concentrations: the penetration factor (*PEN*) and the proximity factor (*PROX*). Below is a background section, a description of the methodology used to develop the *PEN* and *PROX* distributions, and the resulting data.

For more background on NATA and HAPEM, including more detailed definitions and history of the *PEN* and *PROX* MEFs, see the 1996 NATA documentation (USEPA, 2001 and 2002a) and the HAPEM5 User's Guide (USEPA, 2002b).

Background

MEF Definitions. HAPEM5 estimates microenvironmental pollutant concentrations using the formula:

$$C_{me} = ADD + (PEN) (PROX) (C_{amb}) \quad (1)$$

where

| | | |
|-----------|---|--|
| C_{me} | = | microenvironmental concentration |
| ADD | = | additive factor representing sources within the ME |
| PEN | = | penetration factor for the ME |
| $PROX$ | = | proximity factor for the ME |
| C_{amb} | = | ambient concentration. |

The PEN factor is obtained from the literature. It accounts for the penetration of pollutants from the exterior to the interior of indoor or in-vehicle microenvironments. PEN is defined as the ratio of indoor or in-vehicle pollutant concentration to the outdoor concentration in the immediate vicinity, absent any indoor pollutant sources. PEN is similar to the frequently reported indoor-outdoor (I/O) ratio, except that the I/O ratio often includes an indoor emission component. Thus, the I/O ratio can be greater than 1.0, but PEN must be less than or equal to 1.0. Penetration factors are not applicable to outdoor MEs, and thus all PEN factors for outdoor MEs have been set to 1.0 for HAPEM5. PEN is defined mathematically in Equation 2.

$$PEN = (\text{ME conc.}) / (\text{outdoor conc. in immediate vicinity of ME}) \quad (2)$$

The $PROX$ factor also is obtained from the literature. It is an estimate of the ratio of the outdoor concentration in the immediate vicinity of the ME to the outdoor concentration represented by the air quality data. For most situations, the $PROX$ value is 1.0, i.e., an outdoor concentration contribution in the immediate vicinity of the microenvironment is equal to the census tract average concentration contribution. However, when assessing exposure to motor vehicle emissions for MEs near roadways (e.g., in-vehicle), the pollutant concentration contribution in the immediate vicinity of the ME is expected to be higher than the average pollutant concentration contribution over the census tract, i.e., $PROX$ is expected to be greater than 1.0. $PROX$ is defined mathematically in Equation 3.

$$PROX = (\text{outdoor conc. in immediate vicinity of ME}) / (\text{air quality file conc.}) \quad (3)$$

All $PROX$ factors for MEs located away from roads have been set to 1.0 for HAPEM5.

The ADD factor represents the contribution of emission sources within the ME to the HAP concentration. The ADD factor is not addressed in this memorandum but rather is the subject of separate documentation (under development).

In HAPEM, C_{amb} has been obtained from the Assessment System for Population Exposure Nationwide (ASPEN) and represents a population-weighted average for each census tract analyzed.

Grouping of HAPs and MEs. $PROX$ and PEN distributions are needed for the approximately 7,400 possible HAP-ME combinations in HAPEM5 (i.e., 200 HAPs x 37 MEs). Because valid

data are not available for all of these combinations, a grouping approach similar to that used in HAPEM4 was needed whereby similar HAP-ME combinations are grouped together to allow assignment of the limited number of available MEFs to the groups based on the best data. Thus, each ME was assigned to one (or more) of five groups: indoors-residence; indoors–other building; outdoors–near road; outdoors–away from road; and in vehicle. These groupings were based on location for outdoor MEs and building type for indoor MEs, i.e., *PROX* factors are assumed to be influenced by ME location relative to roadway sources and *PEN* factors are assumed to be affected by the structural design and usage patterns of indoor microenvironments.

Also previously, each HAP had been assigned to one of three main atmospheric lifetime groups — short (<1 day), medium (1-5 days), and long (>5 days) — based on atmospheric lifetime and the assumption that this parameter has a major effect on infiltration of the pollutant from the outdoor to the indoor environment and removal within the indoor microenvironment, i.e., *PEN*. Under the assumption that the emission source category influences the *PROX* factor, each HAP also was assigned to one of four emission source groups — area sources (e.g., residential fireplaces), line sources (e.g., roadways), point sources-densely distributed (e.g., dry cleaning establishments), and point sources-sparsely distributed (e.g., smelters, manufacturing facilities) — based on the predominant emission source contribution for the pollutant. In HAPEM4 only the line source group was assigned a *PROX* factor different from 1.0, and this *PROX* factor was applied to the line source emissions of the pollutant.

ICF and TRJ (2000) describes these previous approaches to the grouping of MEs and HAPs in more detail.

Comments. EPA received four sets of comments on the MEF used for the previous NSA. Appendix A of the HAPEM4 User's Guide (USEPA, 2002a) discusses these comments in detail, how they were addressed in the previous NATA national-scale assessment, and plans for future related activities (including those described in this memo). These comments and the current responses are summarized below. Implementation of the responses are described in the Methodology, as appropriate.

1. *Comment:* Indoor factors should have been included, or at least their approximate relative contribution to exposure should have been indicated.

Response: EPA investigated whether there were sufficient data to characterize the distribution of ME concentration contributions from indoor sources, and determined that such data did exist for a limited number of HAPs. Thus, HAP-specific distributions for the *ADD* factor were developed based on the use frequency and duration of consumer products and indoor combustion sources, as well as the prevalence of attached garages and various types of building materials (documentation under development).

2. *Comment:* Although the ME grouping indicates that all residential MEs should have the same *PEN* factor, the MEs provided in the MEF report show a systematic difference between ME 13 (Residence - no gas stove) and other residential MEs.

Response: No data sets were identified to suggest any differences between these MEs, and thus EPA assigned identical *PEN* factors (or distributions) to ME 13 (Residence - no gas stove), ME 14 (Residence - gas stove), ME 15 (Residence - attached garage), and ME 16 (Residence - gas stove and attached garage).

3. *Comment:* The reported MEFs are inconsistent with the proposed pollutant lifetime groupings, since they show virtually no difference among the groups in range or average of *PEN* values.

Response: Insufficient data were available to reduce the uncertainty of the *PEN* factors in this regard, and thus EPA decided to dispense with the use of the pollutant lifetime groupings at this time and instead base the groupings only on physical form (gases, particles).

4. *Comment:* The *PROX* factor for mobile sources is applied only to the mobile source contribution to the ambient concentration, although because it was estimated based on the aggregate ambient concentration, it should be applied to the aggregate ambient concentration.

Response: Two options for potential improvement are: (1) apply the factors developed from aggregate concentration contributions to aggregate concentrations rather than the mobile source contribution, as suggested by one of the reviewers; and (2) estimate mobile source-specific *PROX* factors based on contributions of mobile source emissions to the near roadway concentration and "average" ambient concentration. We selected the second option because it likely provides the most accurate estimate of *PROX*, and data were identified for developing these estimates.

5. *Comment:* The *PROX* factor for mobile sources is applied only to a subset of HAPs with substantial mobile source contributions.

Response: We will apply the mobile source *PROX* factor to all HAPs for which any mobile source emissions exist.

6. *Comment:* A number of cited studies were not included in the literature review.

Response: The citations provided were added to the literature review for revising the MEFs for the 1999 NSA.

7. *Comment:* (a) Insufficient information was provided about the quality of the studies selected, (b) all studies appear to have been weighted equally, in spite of potential differences in quality, and (c) insufficient information was presented about the derivation of specific MEFs by the grouping method.

Response: Additional details are included below about the quality of the data, the selection criteria, and the procedures for extrapolating data.

Sensitivity Analysis. In response to peer review of HAPEM and the 1996 NATA national-scale assessment, ICF (2002) conducted a case study on benzene within a limited geographical area (Houston, TX) in order to meet two objectives:

1. Evaluate the sensitivity of HAPEM predictions to the uncertainty in MEFs and air quality data. For this part of the study, the range of uncertainty was specified by the range of values found in the literature review of MEFs and the range of ambient concentrations predictions within each census tract. This part of the case study provided a screening-level analysis to indicate which uncertainties for these inputs have the greatest potential to influence model predictions and, therefore, warrant more detailed study.

2. Evaluate the full range of variability of exposure concentrations within various demographic groups. This required characterizing variability among activity patterns, commuting patterns, air quality among census tracts, air quality within census tracts, and MEFs. In addition, alternative characterizations of distributional data were assessed, alternative approaches for extrapolating short-term activity data to annual sequences were compared, and "stochastic noise" was evaluated.

Several relevant conclusions and recommendations resulted from this study. These conclusions and an update on the recommendations—which have been incorporated into the Methodology, as appropriate—are provided below. **[correct? overboard?]**

1. *Conclusion:* The HAPEM4 exposure estimates are not very sensitive to changes in the treatment of the *PEN* factor.

Recommendation: We should not prioritize research on *PEN* factors for VOC pollutants. Since *PEN* factors for semi-volatile organic compounds (SVOCs) and particles may be substantially lower than VOCs, however, their uncertainty may show more effect. A separate sensitivity test for a representative pollutant of this type may be necessary.

2. *Conclusion:* The HAPEM4 exposure estimates are not very sensitive to the use of seasonal average concentrations.

Recommendation: We should not incorporate seasonal average concentrations into HAPEM at this time for application to VOC pollutants unless they are known to have a significant seasonal pattern of emissions. We will re-visit this issue if season-specific ME factors become available. Because SVOCs and particles are subject to deposition, however, their concentrations may be more influenced by seasonal factors, such as precipitation or wind speed. Therefore, a separate sensitivity test for a representative pollutant of this type, where both wet and dry deposition are considered, may be necessary.

3. *Conclusion:* The HAPEM4 mean total exposure is not very sensitive to changes in the treatment of the *PROX* factor, but the variance of the total exposure and the mean and variance of the onroad exposure is sensitive to changes in the treatment of the *PROX* factor. This is primarily due to the changes for the in-vehicle car ME.

Recommendation: We should make research on the *PROX* factor for the in-vehicle car ME a moderate priority for mobile source pollutants.

4. *Conclusion:* The HAPEM4 mean and variance of total exposure estimates are very sensitive to changes in the treatment of the *ADD* factor, primarily from changes to the residential MEs with or without an attached garage, particularly when the 95th percentile is used instead of the geometric mean (giving a 115 % increase in mean total exposure).

Recommendation: We should make research on the *ADD* factors for residential MEs a high priority.

5. *Conclusion:* Between HAPEM4 and an early version of HAPEM5 the mean exposure increased by only 17 % but the variance of the exposure increased by 116 %. About half

the increase in variance is attributable to the ME factors (which increases the variance by 72 % compared to HAPEM4).

Recommendation: To characterize the full inter-individual variance in exposure, we should incorporate ME factor variability into HAPEM.

Methodology

Based on reviewer comments, further examination of the data, the sensitivity analysis, and the need to streamline MEF development because of the decision to develop distributions rather than point estimates for MEFs, we are making the following changes to the previous approach:

1. The HAP lifetime grouping approach has been replaced by a physical form grouping (i.e., gas, particle, and mixed gas/particle).
2. *PROX* has been redefined and received greater emphasis during data development.
3. *PEN* for non-VOCs has received greater emphasis during data development.
4. The HAP source groups have been simplified to consider only onroad mobile sources and other sources.
5. The ME groups have been redefined to clarify the underlying rationale.

HAP Grouping Scheme. In place of the lifetime grouping approach, we developed a HAP grouping scheme based on physical state. This scheme has been combined with one for designating HAPs based on onroad vs. other sources. Thus, the HAP groups are now (1) gas, other; (2) mixed gas/particle, other; (3) particle, other; (4) gas, onroad; (5) mixed, onroad; and (6) particle, onroad. For some MEs, no literature data were available for the mixed HAP (gas/particle) groups. Therefore, these pollutants were reassigned to the particle groups based on the assumption that they tend to act more like particles than gases.

PROX Revision. We estimated *PROX* factors specifically for applying to the onroad mobile source fraction by modifying the more available aggregate *PROX* based on estimates of contributions of onroad mobile source emissions to the near roadway concentration ($C_{\text{onroad mobile source-near road}}$) and to the "average" ambient concentration ($C_{\text{onroad mobile source-ave. ambient}}$). Thus, to develop *PROX* for onroad mobile sources ($PROX_{\text{onroad mobile}}$) when as is usually the case we only have near-road concentrations for the aggregate ($C_{\text{agg.-near road ambient}}$) and average ambient concentrations for the aggregate ($C_{\text{agg.-ave. ambient}}$), we used the relative contribution fraction of the on-road mobile source category for the HAP in whichever study area the data collection took place ($f_{\text{onroad mobile-study area}}$), as shown in Equation 4:

$$PROX_{\text{onroad mobile}} = \frac{(C_{\text{agg.-near road ambient}} - [(1 - f_{\text{onroad mobile-study area}}) \times C_{\text{agg.-ave. ambient}}])}{(f_{\text{onroad mobile-study area}} \times C_{\text{agg.-ave. ambient}})} \quad (4)$$

ME Grouping. To obtain MEFs, we first developed a preliminary ME grouping scheme to guide the literature review (Table 2). We changed two groups in the scheme used in HAPEM4:

1. Two indoor MEs are now considered to be near roads (i.e., ME-5, public garage, indoors; and ME-9, service station, indoors); and

2. MEs designated “other location” and “not specified” (i.e., ME-34 and 35, respectively) that previously had been assigned a combination of near-road and away-from-road factors are now considered primarily near road.

After completion of the literature review, the ME (and HAP) grouping schemes were revised to eliminate groups for which insufficient concentration data were found and consolidate those MEs (and HAPs) into other groups.

Literature Review. Previous literature reviews have documented that few studies exist with data suitable for the calculation of MEFs (ICF and TRJ, 2000; EC/R and TRJ, 2002). For example, studies designed to measure I/O ratios often reveal the presence of indoor sources, preventing determination of the *PEN* factor. Data presentation methods may also constrain the use of study data for development of MEF distributions. Studies that report average indoor and average outdoor concentrations without individual paired ratios enable calculation of a point estimate for *PEN*, but not a distribution.

To address these issues and others raised by prior peer reviewers, we decided to focus on the single study judged to have the highest quality, most relevant data pertaining to a specific ME-HAP group combination. This study, termed the “representative group study” (RGS), was used to develop a single MEF distribution for all ME-HAP combinations included in the group. The principal advantage of the RGS approach is that it ensures that all members of the group have identical distributions based on the best information available. It also avoids the need to combine data from multiple studies, which can be problematic due to differences in methodology, data presentation, and relevance. As new, improved information becomes available, distributions can be easily revised to incorporate the new data without recalculation of multi-study parameters.

We did not conduct a broad literature search, but rather reviewed the information derived from the literature previously used to develop MEF point estimates to identify potential RGSs for developing distributions. We also reviewed several recent studies not considered in previous work, including those identified by peer reviewers. Several criteria were used to select potential RGSs. We looked for matched simultaneous measurements, absence of indoor sources (I/O ratio < 1.0), large sample size at multiple ME sites, quality assurance procedures for data reporting, good correlation results, and other evidence of high-quality research. All studies considered as candidate RGSs are included in the reference list for this memorandum.

RGS Selection and Analysis. For each ME-HAP group MEF, we selected a single study as the RGS from among the candidates identified during the literature review. Since studies often report results for multiple pollutants and microenvironments, we reviewed sample size, measurement methods, data capture rates, absence of indoor sources, correlation results, and other indicators to choose the best data set from the RGS. For studies with multiple pollutant data pertaining to *PEN* factors, we selected the pollutant with the minimum I/O ratio, indicating low influence of indoor sources. For the mixed gas/particulate HAP group, we chose a pollutant with physical properties representative of the group. We used the selected data set to develop a distribution for the relevant group MEF.

Calculation of ME Factor Distributions. HAPEM5 has the capability of representing the distribution of *PEN* or *PROX* values for a particular ME-HAP group as either (1) an empirical distribution (i.e., individual values) given that the number of values does not exceed 10 (due to limitations in the current model program and input file structure) or (2) one of four continuous distributions (normal, lognormal, uniform, and triangular). Thus, we generally used the empirical data “as is” for data sets that contained 10 or fewer values, and we developed continuous

distributions for data sets that contained greater than 10 values (with one exception, as described below). Two methods were used in fitting continuous distributions. In the case of percentiles (rather than individual values), we used regression techniques to fit the percentiles to a distribution. In the remaining cases, each data set contained from 17 to 54 individual values. We used the STATFIT™ software package to fit each of the candidate distributions to each data set. The Kolmogorov-Smirnov statistic and other goodness-of-fit criteria provided by the program were used to identify the best-fitting distribution.

As discussed above, *PEN* is defined as the indoor/outdoor ratio expected to occur in the absence of indoor sources. We had previously assumed that valid *PEN* data would not include values exceeding 1.0, as such values suggest that an indoor source may be present. However, many of the data sets judged to be otherwise good representations of *PEN* data included one or more values exceeding 1.0. In each of these cases, we set up alternative “censored” versions of the data set in which one or more of the values above 1.0 were omitted. Distributions were fit to each alternative data set and the results compared with the uncensored fit.

Censoring was also employed in fitting distributions to the *PROX* data sets. Although judged to be generally good representations of *PROX* data, each of the selected *PROX* data sets included one or more large “outlier” values that were systematically omitted and evaluated to determine the effect on the resulting distributional fits.

Results

Table 3 lists the candidate and selected RGSs and the resulting ME-HAP group MEF. This table also briefly describes the rationale for selecting the target data set. The HAP-ME grouping scheme resulted in seven ME-HAP groups for the *PEN* factor and four ME-HAP groups for the *PROX* factor. Table 4 presents the combined ME-HAP grouping scheme, together with the MEFs included in each group.

Because many of the data sets judged to be otherwise good representations of *PEN* data included one or more values exceeding 1.0, we created alternative “censored” versions of these data sets in which one or more of the values above 1.0 were omitted. In general, the best fits were obtained under moderate censoring conditions in which some—but not all—of the values exceeding 1.0 were omitted. We also found that omitting two values from the *PROX*-2 data set and one value from the *PROX*-4 data set significantly improved the resulting distributional fits.

We used the empirical distribution approach for *PEN*-1, *PEN*-2, and *PEN*-3 (Table 5). The remaining data sets were fit by continuous distributions (Table 6). Because the data sets selected for *PEN*-1 and *PEN*-2 each contained less than 10 values, these data sets were used “as is” to create the corresponding empirical distributions. The *PEN*-3 data set obtained from Rodes et al. (1998) contained 56 values, but only 26 equaled 1.0 or less. Because these 26 could not be well described with any of the parametric distribution forms available in HAPEM5, we interpreted them as an empirical distribution and interpolated to calculate 10 equally-spaced percentiles for input to HAPEM.

In the case of *PEN*-4, the data set to be fit contained five percentiles (10th, 25th, 50th, 75th, and 90th) rather than individual values. Using regression techniques, we found that these percentiles could be very closely fit by a lognormal distribution. In the remaining cases, each data set contained from 17 to 54 individual values and were fit as described above.

Table 6 presents the final continuous distribution fit to each data set. The results for each fit include the number of values in the fitted data set, the largest value retained in the data set, and the name and parameter values of the fitted distribution. With the exception of PEN-4, the results also include the Kolmogorov-Smirnov statistic and the associated p value.

MEFs for each combination of HAP and ME can be determined using Tables 1, 2, 4, and 5 or 6. For example, the appropriate *PEN* distribution for polycyclic organic matter (POM) in cars is lognormal with a geometric mean of 0.798 and a geometric standard deviation of 1.262, based on the following steps:

1. Table 1 lists POM as a particle;
2. Table 4 lists PEN-5, PEN-6, and PEN-7 as the appropriate *PEN* groups for particles;
3. Table 2 lists ME-1 as the designation for cars;
4. Table 4 lists PEN-7 as the ME-HAP group associated with ME-1 and particles; and
5. Table 6 provides the PEN-7 distribution characteristics.

As additional research is carried out to collect data useful for estimating *PEN* and *PROX* factors, the ME-HAP groups and RGSs defined in this project should be updated to reflect the new information. Although the present approach provides modelers with MEF estimates for all HAPs in all MEs, more data are needed to improve MEF distributions and the resulting modeled exposures.

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Table 1. Characteristics of HAPs to be Modeled in HAPEM5

| HAP | CAS No. | SAROAD No. ^a | Gas/ Particulate ^b | 1999 NATA |
|---|------------------------|-------------------------|----------------------------------|--------------|
| 7-PAH Group | -- | 80233 | G/P | Y |
| Acetaldehyde | 75070 | 43503 | G | Y |
| Acetamide | 60355 | 80101 | G | Y |
| Acetonitrile (methyl cyanide) | 75058 | 70016 | G | Y |
| Acetophenone | 98862 | 80103 | G | Y |
| Acetylaminofluorene (2) | 53963 | 53963 | G/P | |
| Acrolein | 107028 | 43505 | G | Y |
| Acrylamide | 79061 | 80105 | G | Y |
| Acrylic acid | 79107 | 43407 | G | Y |
| Acrylonitrile | 107131 | 43704 | G | Y |
| Allyl chloride (3-chloro-1-propene) | 107051 | 80108 | G | Y |
| Aminobiphenyl (4) | 92671 | 92671 | G | |
| Aniline | 62533 | 45701 | G | Y |
| Anisidine (o) (methoxyaniline) | 90040 | 80110 | G | |
| Antimony Compounds | 7440360 | 80111/80311 | P ^c | Y |
| Arsenic Compounds (inorganic; excluding arsine) | 7440382 (As only) | 70112/70312 | P ^c | Y |
| Arsine | 7784421 | 70001 | G | Y |
| Asbestos | 1332214 | 99049 | P | |
| Benzene | 71432 | 45201 | G | Y |
| Benzidine (diaminobiphenyl) | 92875 | 80115 | G/P | Y |
| Benzotrichloride | 98077 | 80116 | G | Y |
| Benzyl chloride | 100447 | 45810 | G | Y |
| Beryllium Compounds | 7440417 (Be only) | 80118/80318 | P | Y |
| Biphenyl | 192524 | 45226 | G | Y |
| Bis (2-ethylhexyl) phthalate (DEHP) | 117817 | 45470 | G/P | Y |
| Bis (chloromethyl) ether | 542881 | 80121 | G | Y |
| Bromoform | 75252 | 80122 | G | Y |
| Butadiene (1,3) | 106990 | 43218 | G | Y |
| Cadmium Compounds | 7440439 | 80124/80324 | P | Y |
| Calcium cyanamide | 156627 | 99061 | P | |
| Caprolactam | 105602 | -- | G | |
| Captan | 133062 | 80127 | G/P | Y |
| Carbaryl | 63252 | 80128 | G/P | Y |
| Carbon disulfide | 75150 | 43934 | G | Y |
| Carbon tetrachloride | 56235 | 43804 | G | Y |
| Carbonyl sulfide | 463581 | 43933 | G | |
| Catechol (1,2-benzenediol) | 120809 | 80132 | G | |
| Chloramben | 133904 | -- | G | |
| Chlordane | 57749 | 80134 | G/P | Y |
| Chlorine | 7782505 | 80135 | G | Y |
| Chloroacetic acid | 79118 | 80136 | G | Y |
| Chloroacetophenone (2) | 532274 | 99024 | G | Y |
| Chlorobenzene | 108907 | 45801 | G | Y |
| Chlorobenzilate | 510156 | 99073 | G/P | Y |
| Chloroform | 67663 | 43803 | G | Y |
| Chloromethyl methyl ether | 107302 | 80139 | G | |
| Chloroprene (2-Chloro-1,3-butadiene) | 126998 | 43862 | G | Y |
| Chromium III Compounds | 16065831 (Cr-III only) | 59992/59993 | P | Y |

| HAP | CAS No. | SAROAD No. ^a | Gas/ Particulate ^b | 1999 NATA |
|--|-----------------------|-------------------------|----------------------------------|--------------|
| Chromium VI Compounds | 15723281 (Cr-VI only) | 69992/ 69993 | P | Y |
| Chromium Compounds | 7440473 (Cr only) | -- | P | |
| Cobalt Compounds | 7440484 (Co only) | 80142/80342 | P | Y |
| Coke Oven Emissions | — | 80411 | G/P | Y |
| Cresol (m) | 108394 | 45605 | G | Y |
| Cresol (o) | 95487 | 45605 | G | Y |
| Cresol (p) | 106445 | 45605 | G | Y |
| Cresols/Cresylic acid | 1319773 | 45605 | G | Y |
| Cumene (Isopropylbenzene) | 98828 | 45210 | G | Y |
| Cyanide Compounds | -- | 80143/80144/ 80145 | G/P | Y |
| Hydrocyanic Acid (HCN) | 74908 | -- | G/P | Y |
| Sodium Cyanide (NaCN) | 143339 | -- | G/P | Y |
| Potassium Cyanide (KCN) | 151508 | -- | G/P | Y |
| D(2,4), salts and esters | 94757 | 80146 | G/P | Y |
| DDE | 3547044 | -- | G/P | |
| Diazomethane | 334883 | 99084 | G | |
| Dibenzofurans | 132649 | 80247 | G/P | Y |
| Dibromo-3-chloropropane(1,2) | 96128 | 92672 | G | Y |
| Dibutylphthalate | 84742 | 45452 | G/P | Y |
| Dichlorobenzene(1,4)(p) | 106467 | 45807 | G | Y |
| Dichlorobenzidene(3,3) | 91941 | 80150 | G/P | Y |
| Dichloroethyl ether (Bis(2-chloroethyl)ether) | 111444 | 80151 | G | Y |
| Dichloropropene(1,3) | 542756 | 80152 | G | Y |
| Dichlorvos | 62737 | 80153 | G | Y |
| Diesel PM | -- | 80400/80401 | P | Y |
| Diethanolamine | 111422 | 80154 | G | Y |
| Diethyl aniline (N,N) (Dimethylaniline (N,N)) | 121697 | 80155 | G | Y |
| Diethyl sulfate | 64675 | 80156 | G | |
| Dimethoxybenzidine(3,3) (Dianisidine) | 119904 | 80157 | G/P | Y |
| Dimethyl aminoazobenzene | 60117 | 92673 | G/P | Y |
| Dimethyl benzidine(3,3) | 119937 | 92675 | G/P | Y |
| Dimethyl carbamoyl chloride | 79447 | 92674 | G | |
| Dimethyl formamide | 68122 | 43450 | G | Y |
| Dimethyl hydrazine(1,1) | 57147 | 80159 | G | Y |
| Dimethyl phthalate | 131113 | 45451 | G | |
| Dimethyl sulfate | 77781 | 80161 | G | |
| Dinitro-o-cresol(4,6), and salts | 534521 | 80162 | G/P | Y |
| Dinitrophenol(2,4) | 51285 | 80163 | G/P | Y |
| Dinitrotoluene(2,4) | 121142 | 80164 | G | Y |
| Dioxane(1,4) (1,4-Diethyleneoxide) | 123911 | 80165 | G | Y |
| Diphenylhydrazine(1,2) | 122667 | 92676 | G | Y |
| Epichlorohydrin (Chloro-2,3-epoxy- propane(1)) | 106898 | 43863 | G | Y |
| Epoxybutane(1,2) (1,2-Butylene oxide) | 106887 | 80167 | G | Y |
| Ethyl acrylate | 140885 | 43438 | G | Y |
| Ethylbenzene | 100414 | 45203 | G | Y |
| Ethyl carbamate (Urethane) | 51796 | 80170 | G | Y |
| Ethyl chloride (Chloroethane) | 75003 | 43812 | G | Y |
| Ethylene dibromide (1,2-Dibromoethane) | 106934 | 43837 | G | Y |
| Ethylene dichloride (1,2-Dichloroethane) | 107062 | 43815 | G | Y |

| HAP | CAS No. | SAROAD No. ^a | Gas/ Particulate ^b | 1999 NATA |
|--|---------|-------------------------|----------------------------------|--------------|
| Ethylene glycol | 107211 | 43370 | G | Y |
| Ethylene imine (Aziridine) | 151564 | 80175 | G | |
| Ethylene oxide | 75218 | 43601 | G | Y |
| Ethylene thiourea | 96457 | 80177 | G | Y |
| Ethylidene dichloride (1,1-Dichloroethane) | 75343 | 43813 | G | Y |
| Formaldehyde | 50000 | 43502 | G | Y |
| Glycol ethers (Cellosolves) | — | 43367 | G | Y |
| Heptachlor | 76448 | 80182 | G/P | Y |
| Hexachlorobenzene | 118741 | 80183 | G | Y |
| Hexachlorobutadiene | 87683 | 80184 | G | Y |
| Hexachlorocyclopentadiene | 77474 | 80185 | G | Y |
| Hexachloroethane | 67721 | 80186 | G | Y |
| Hexamethylene-1,6- diisocyanate | 822060 | 99114 | G/P | Y |
| Hexamethylphosphoramide | 680319 | 99115 | G | |
| Hexane | 110543 | 43231 | G | Y |
| Hydrazine | 302012 | 80188 | G | Y |
| Hydrochloric acid | 7647010 | 80189 | G | Y |
| Hydrogen fluoride (Hydrofluoric acid) | 7664393 | 80190 | G | Y |
| Hydroquinone (1,4-benzenediol) | 123319 | 80191 | G | Y |
| Isophorone | 78591 | 80192 | G | Y |
| Lead Compounds | 7439921 | 80193/80393 | P | Y |
| Lindane (all isomers) | 58899 | 80194 | G/P | Y |
| Maleic anhydride (Furandione) | 108316 | 43603 | G | Y |
| Manganese Compounds | 7439965 | 80196/80396 | P | Y |
| Mercury Compounds | 7439976 | 80197/80405 | G/P | Y |
| Methanol | 67561 | 43301 | G | Y |
| Methoxychlor | 72435 | 80199 | G/P | Y |
| Methyl bromide (Bromomethane) | 74839 | 80200 | G | Y |
| Methyl chloride (Chloromethane) | 74873 | 43801 | G | Y |
| Methyl chloroform (1,1,1-Trichloroethane) | 71556 | 43814 | G | Y |
| Methyl ethyl ketone (2-Butanone) | 78933 | 43552 | G | Y |
| Methyl hydrazine | 60344 | 80205 | G | |
| Methyl iodide (Iodomethane) | 74884 | 80206 | G | |
| Methyl isobutyl ketone (Hexone) | 108101 | 43560 | G | Y |
| Methyl isocyanate | 624839 | 80208 | G | Y |
| Methyl methacrylate | 80626 | 43441 | G | Y |
| Methyl tert-butyl ether | 1634044 | 43376 | G | Y |
| Methylene bis (2- chloroaniline)(4,4) | 101144 | 80211 | G/P | Y |
| Methylene chloride (Dichloromethane) | 75092 | 43802 | G | Y |
| Methylene diphenyl diisocyanate (MDI) | 101688 | 45730 | G/P | Y |
| Methylenedianiline(4,4) | 101779 | 46111 | G/P | Y |
| Mineral fibers | — | 99106 | P | |
| Naphthalene | 91203 | 46701/46702 | G | Y |
| Nickel Compounds | — | 80216/80316 | P | Y |
| Nitrobenzene | 98953 | 45702 | G | Y |
| Nitrobiphenyl(4) | 92933 | 99035 | G | |
| Nitrophenol(4) | 100027 | 80218 | G | Y |
| Nitropropane(2) | 79469 | 80219 | G | Y |
| N-nitroso-N-methylurea | 684935 | 99143 | G | |
| Nitrosodimethylamine(N) | 62759 | 80221 | G | Y |
| Nitrosomorpholine(N) | 59892 | 80222 | G | Y |

| HAP | CAS No. | SAROAD No. ^a | Gas/ Particulate ^b | 1999 NATA |
|--|---------|---|----------------------------------|--------------|
| Parathion | 56382 | 80223 | G/P | Y |
| Pentachloronitrobenzene (Quintobenzene) | 82688 | 80224 | G/P | Y |
| Pentachlorophenol | 87865 | 80225 | G/P | Y |
| Phenol | 108952 | 45300 | G | Y |
| Phenylenediamine(p) | 106503 | 80227 | G | Y |
| Phosgene | 75445 | 80228 | G | Y |
| Phosphine | 7803512 | 99161 | G | Y |
| Phosphorus | 7723140 | 80229 | G/P | Y |
| Phthalic anhydride | 85449 | 45601 | G | Y |
| Polychlorinated biphenyls (PCB) | 1336363 | 80231 | G/P | Y |
| Polycyclic organic matter (POM) | — | 71002/72002/ 73002/74002/ 75002/76002/ 77002/78002 | G/P | Y |
| POM Group 1: Unspecified | -- | -- | G/P | Y |
| POM Group 2: no URE data | -- | -- | G/P | Y |
| POM Group 3: 5.0E-2<URE<=5.0E-1 | -- | -- | G/P | Y |
| POM Group 4: 5.0E-3<URE<=5.0E-2 | -- | -- | G/P | Y |
| POM Group 5: 5.0E-4<URE<=5.0E-3 | -- | -- | G/P | Y |
| POM Group 6: 5.0E-5<URE<=5.0E-4 | -- | -- | G/P | Y |
| POM Group 7: 5.0E-6<URE<=5.0E-5 | -- | -- | G/P | Y |
| POM Group 8: Unspecified 7-PAH | -- | -- | G/P | Y |
| Propane sultone(1,3) | 1120714 | 99012 | G | Y |
| Propiolactone(beta) | 57578 | 99055 | G | |
| Propionaldehyde | 123386 | 43504 | G | |
| Propoxur (Baygon) | 114261 | 80235 | G/P | Y |
| Propylene dichloride (1,2-Dichloropropane) | 78875 | 43838 | G | Y |
| Propylene oxide | 75569 | 43602 | G | Y |
| Propylenimine(1,2) (2-Methyl aziridine) | 75558 | 80238 | G | |
| Quinoline | 91225 | 80239 | G | Y |
| Quinone (1,4-Cyclohexadienedione) | 106514 | 80240 | G | |
| Radionuclides (including radon) | — | -- | G/P | |
| Selenium Compounds | 7782492 | 80242/80343 | P | Y |
| Styrene | 100425 | 45220 | G | Y |
| Styrene oxide | 96093 | 80244 | G | Y |
| Dioxins/Furan as tetrachlorodibenzo-p-dioxin(2,3,7,8) (TCDD) | 1746016 | 80245 | G/P | Y |
| Tetrachloroethane(1,1,2,2) | 79345 | 80246 | G | Y |
| Tetrachloroethylene (Perchloroethylene) | 127184 | 43817 | G | Y |
| Titanium tetrachloride | 7550450 | 80248 | P | Y |
| Toluene | 108883 | 45202 | G | Y |
| Toluene diamine(2,4) (2,4-Diaminotoluene) | 95807 | 80250 | G | Y |
| Toluene diisocyanate(2,4) | 584849 | 45731 | G | |
| Toluidine(o) | 95534 | 80252 | G | Y |
| Toxaphene (Chlorinated camphene) | 8001352 | 99180 | G/P | Y |
| Trichlorobenzene(1,2,4) | 120821 | 45830 | G | Y |
| Trichloroethane(1,1,2) | 79005 | 43820 | G | Y |
| Trichloroethylene | 79016 | 43824 | G | Y |
| Trichlorophenol(2,4,5) | 95954 | 99017 | G | Y |
| Trichlorophenol(2,4,6) | 88062 | 80256 | G | Y |
| Triethylamine | 121448 | 99182 | G | Y |

| HAP | CAS No. | SAROAD No.^a | Gas/ Particulate^b | 1999 NATA |
|--|----------------|-------------------------------|---|----------------------|
| Trifluralin | 1582098 | 80257 | G/P | Y |
| Trimethylpentane(2,2,4) | 540841 | 43250 | G | |
| Vinyl acetate | 108054 | 43453 | G | Y |
| Vinyl bromide | 593602 | 80260 | G | Y |
| Vinyl chloride | 75014 | 43860 | G | Y |
| Vinylidene chloride (1,1-Dichloroethylene) | 75354 | 80262 | G | Y |
| Xylene(m) | 108383 | 45102 | G | Y |
| Xylene(o) | 95476 | 45102 | G | Y |
| Xylene(p) | 106423 | 45102 | G | Y |
| Xylenes (mixed) | 1330207 | 45102 | G | Y |

Source: SAI, 1999.

^a Storage and Retrieval of Aerometric Data number.

^b G = gas phase; P = particulate phase; G/P = gas/particulate phase. This use of this designation is described in the Methodology section of this memo.

^c Changed from G/P in SAI, 1999.

Table 2. HAPEM5 Microenvironments

| ME No. | ME Designation | General ME Type | Location ^a | Building Type ^b |
|--------|--------------------------------|-----------------|-----------------------|----------------------------|
| 1 | Car | In vehicle | N | -- |
| 2 | Bus | In vehicle | N | -- |
| 3 | Truck | In vehicle | N | -- |
| 4 | Other | In vehicle | N | -- |
| 5 | Public garage | Indoors | N | NR |
| 6 | Parking lot/garage | Outdoors | N | -- |
| 7 | Near road | Outdoors | N | -- |
| 8 | Motorcycle | Outdoors | N | -- |
| 9 | Service station | Indoors | N | NR |
| 10 | Service station | Outdoors | N | -- |
| 11 | Residential garage | Indoors | -- | R |
| 12 | Other repair shop | Indoors | -- | NR |
| 13 | Residence - no gas stove | Indoors | -- | R |
| 14 | Residence - gas stove | Indoors | -- | R |
| 15 | Residence - attached garage | Indoors | -- | R |
| 16 | Residential - stove and garage | Indoors | -- | R |
| 17 | Office | Indoors | -- | NR |
| 18 | Store | Indoors | -- | NR |
| 19 | Restaurant | Indoors | -- | NR |
| 20 | Manufacturing facility | Indoors | -- | NR |
| 21 | School | Indoors | -- | NR |
| 22 | Church | Indoors | -- | NR |
| 23 | Shopping mall | Indoors | -- | NR |
| 24 | Auditorium | Indoors | -- | NR |
| 25 | Health care facility | Indoors | -- | NR |
| 26 | Other public building | Indoors | -- | NR |
| 27 | Other location | Indoors | -- | NR |
| 28 | Not specified | Indoors | -- | NR |
| 29 | Construction site | Outdoors | -- | -- |
| 30 | Residential grounds | Outdoors | -- | -- |
| 31 | School grounds | Outdoors | -- | -- |
| 32 | Sports arena | Outdoors | -- | -- |
| 33 | Park/golf course | Outdoors | -- | -- |
| 34 | Other location | Outdoors | N | -- |
| 35 | Not specified | Outdoors | N | -- |
| 36 | Train/subway | In vehicle | -- | -- |
| 37 | Airplane | In vehicle | -- | -- |

^a N = near road^b R = residence; NR = nonresidence

Table 3. Representative Group Study (RGS) Selection Process for ME Factors

| ME-HAP Group Number and Description | Selected RGS and Rationale | Candidate Representative Group Studies |
|--|---|--|
| PEN-1 Indoor, residence – gas | Crump et al. (1997). This study presented paired annual average measurements from newly constructed test houses. Data from the second and final year of the study were used as representing minimum indoor sources. Benzene was chosen as the target pollutant due to low indoor-outdoor (I/O) ratios, indicating a lack of indoor sources. | Clayton et al. (1999) Crump et al. (1997) Edwards et al. (2001) Hung & Liao (1991) Ilgen et al. (2001) Lee et al. (2002) Lewis and Zweidinger (1992) Peters (1997) Wallace (1987) |
| PEN-2 Indoor, non-residential – gas | Hisham & Grosjean (1991). This study had the largest number of directly measured I/O ratios < 1.0. Tetrachloroethylene was selected as the target pollutant due to evidence of the lack of indoor sources (low I/O ratios). | Baek et al. (1997) Brickus et al. (1998) Daisey et al. (1994) Hisham and Grosjean (1991) Lee et al. (accepted 2002) Schwar et al. (1997) |
| PEN-3 In vehicle – gas | Rodes et al. (1998). This study has the largest sample size (n=26) and the clearest data presentation. MTBE was selected from among several VOCs as the target pollutant since it had the smallest mean I/O ratio (indicating least indoor source) and one of the highest number of measurements above the reporting level. | Chan et al. (1991) Duffy and Nelson (1997) Kim et al. (2001) Lawryk et al. (1995) Riediker et al. (2003) Rodes et al. (1998) Solomon et al. (2001) |
| PEN-4 Indoor, residence – mixed | Sheldon et al. (1992). This study computed percentiles of I/O ratios for matched measurements. Fluoranthene was selected from several pollutants on the basis of physical properties (similar to other members of this HAP group), low I/O ratio, high Spearman rank correlation for indoor and outdoor measurements, and high percentage of quantifiable measurements. | Ando et al. (1996) Sheldon et al. (1992) Sheldon et al. (1993a) Sheldon et al. (1993b) |
| PEN-5 Indoor, residence – particle | Bell & Hipfner (1997). This study presents paired data for 28 residences with I/O < 1, more than any other study. Cr(VI) was the only pollutant monitored. Although the half-life of Cr(VI) in ambient air is likely to be less than 24 hours, atmospheric lifetime was not used as a criterion for MEF HAP grouping. | Bell & Hipfner (1997) Clayton et al. (1993) Clayton et al. (1999) Funasaka et al. (1996) Halpern (1978) LaRosa et al. (2000) Long et al. (2000) Mukerjee et al. (1997) Pellizzari et al. (1998) Suh et al. (1994) Wallace and Slonecker (1997) |

| ME-HAP Group Number and Description | Selected RGS and Rationale | Candidate Representative Group Studies |
|--|---|--|
| PEN-6 Indoor, non-residential – mixed, particle | Falerios et al. (1992). This study reports multiple indoor and outdoor chromium measurements at 17 sites. Total chromium was chosen as the target pollutant since it had a low mean I/O ratio. Means of multiple measurements at each site were used as input values for distribution development. | Al-Radady et al. (1994) Falerios et al. (1992) Halpern (1978) Jenkins et al. (1997) |
| PEN-7 In vehicle – mixed, particle | Rodes et al. (1998). This multi-pollutant study had the highest number of vehicles with paired interior and exterior measurements for which I/O < 1.0. Because fewer than 5% of the speciated metal HAP samples were above the reporting limit, we selected PM _{2.5} as the target pollutant (97% reportable). | Riediker et al. (2003) Rodes et al. (1998) Shikiya et al. (1989) |
| PROX-1 Outdoor/indoor, near road – gas – onroad | Rodes et al. (1998). This study has the higher number of sites with paired data. Toluene was used as the target pollutant since it had the most measurements above the reporting level. | Chan et al. (1991) Rodes et al. (1998) |
| PROX-2 In vehicle – gas – onroad | Rodes et al. (1998). This study has the highest number of vehicles with paired data. Toluene was used as the target pollutant since it had the most measurements above the reporting level. | Chan et al. (1991) Jo and Park (1998) Kim et al. (2001) Rodes et al. (1998) |
| PROX-3 Outdoor/indoor, near road – mixed, particle – onroad | Rodes et al. (1998). This is the only study available with paired data. Because fewer than 5% of the speciated metal HAP samples were above the reporting limit, we selected PM _{2.5} as the target pollutant (97% reportable). | Riediker et al. (2003) Rodes et al. (1998) |
| PROX-4 In vehicle – mixed, particle – onroad | Rodes et al. (1998). This is the only study available with paired data. Because fewer than 5% of the speciated metal HAP samples were above the reporting limit, we selected PM _{2.5} as the target pollutant (97% reportable). | Riediker et al. (2003) Rodes et al. (1998) |

Table 4. ME-HAP Groups Developed for HAPEM5

| MEF | ME-HAP Group No. | ME-HAP Group Description | MEs ^a |
|------------|------------------|-------------------------------|------------------|
| <i>PEN</i> | PEN-1 | Indoor, residence – gas | 11, 13-16 |
| | PEN-2 | Indoor, non-residential – gas | 5, 9, 12, 17-28 |
| | PEN-3 | In vehicle – gas | 1-4, 36, 37 |
| | PEN-4 | Indoor, residence – mixed | 11, 13-16 |

| MEF | ME-HAP Group No. | ME-HAP Group Description | MEs ^a |
|------|------------------|--|-------------------------|
| | PEN-5 | Indoor, residence – particle | 11, 13-16 |
| | PEN-6 | Indoor, non-residential – mixed, particle | 5, 9, 12, 17-28, 36, 37 |
| | PEN-7 | In vehicle – mixed, particle | 1-4 |
| PROX | PROX-1 | Outdoor/indoor, near road – gas – onroad | 5-10, 34, 35 |
| | PROX-2 | In vehicle – gas – onroad | 1-4 |
| | PROX-3 | Outdoor/indoor, near road – mixed, particle – onroad | 5-10, 34, 35 |
| | PROX-4 | In vehicle – mixed, particle -- onroad | 1-4 |

^a ME numbers as listed in Table 2.

Table 5. Values Included in the Empirical Distributions Developed for PEN-1, PEN-2, and PEN-3

| ME-HAP Group | Value (n = 3) | ME-HAP Group | Value (n = 5) | ME-HAP Group | Percentile | Value (n = 10) |
|--------------------|---------------|--------------|---------------|--------------|------------|----------------|
| PEN-1 ^a | 0.8 | PEN-2 | 0.33 | PEN-3 | 5 | 0.678 |
| | 0.8 | | 0.67 | | 15 | 0.773 |
| | 1.0 | | 0.71 | | 25 | 0.884 |
| | -- | | 1.0 | | 35 | 0.914 |
| | -- | | 1.0 | | 45 | 0.947 |
| | -- | | -- | | 55 | 0.971 |
| | -- | | -- | | 65 | 0.982 |
| | -- | | -- | | 75 | 0.984 |
| | -- | | -- | | 85 | 1.0 |
| | -- | | -- | | 95 | 1.0 |

^a One value > 1.0 was omitted (1.4).

Table 6. Continuous Distributions Fit to Selected Penetration and Proximity Data Sets

| ME-HAP Group | Number of values included in fit | Number of omitted values | Fit results | | | |
|--------------|---|--------------------------|-----------------------|--|------------------------|----------------|
| | | | Best fit ^a | Goodness-of-fit statistics | Parameter ^d | Value |
| PEN-4 | Percentiles (10 th , 25 th , 50 th , 75 th , 90 th) | None | Lognormal | R ² = 0.998 for regression of ln(PEN-4) vs. z value | GM | 0.781 |
| | | | | | GSD | 1.644 |
| PEN-5 | 31 | 2 (X > 1.08) | Lognormal | K-S ^b = 0.163 (p = 0.342) | GM | 0.330 |
| | | | | | GSD | 1.871 |
| PEN-6 | 11 | 6 (X > 1.25) | Lognormal | K-S = 0.151 (p = 0.933) | GM | 0.385 |
| | | | | | GSD | 1.687 |
| PEN-7 | 28 | 2 (X > 1.28) | Lognormal | K-S = 0.121 (p = 0.759) | GM | 0.798 |
| | | | | | GSD | 1.262 |
| PROX-1 | 36 | None (max = 6.43) | Triangular | K-S = 0.106 (p = 0.779) | Minimum | 0 ^c |
| | | | | | Mode | 1.572 |
| | | | | | Maximum | 7.072 |
| PROX-2 | 52 | 2 (X > 13.8) | Triangular | K-S = 0.117 (p = 0.444) | Minimum | 0 ^c |
| | | | | | Mode | 1.933 |
| | | | | | Maximum | 14.36 |
| PROX-3 | 20 | None (max = 14.7) | Lognormal | K-S = 0.159 (p = 0.639) | GM | 1.803 |
| | | | | | GSD | 2.970 |
| PROX-4 | 25 | 1 (X > 17.7) | Lognormal | K-S = 0.092 (p = 0.970) | GM | 2.518 |
| | | | | | GSD | 2.971 |

^a Tested distributions: exponential, lognormal, triangular. Data set distribution recommended for n < 10.

^b Kolmogorov-Smirnov statistic.

^c The minimum *PROX* value was set to 1.0 in the HAPEM5 input files.

^d Abbreviations: GM = geometric mean, GSD = geometric standard deviation.