

INSTRUCTIONS FOR USE OF THE PME CALCULATOR

This note gives instructions for using the PME calculator version 4.0.02, which implements the new PME developed in CRC Project RW-107-3a. The new PME uses the Yield Sooting Index (YSI) to characterize the sooting potential of hydrocarbon compounds found in gasoline. Please bring to CRC's attention problems that you find in using the calculator. Comments, corrections, and suggestions for the calculator and/or these notes are also welcomed to improve the tool going forward.

The PME spreadsheet Template.v4.0.02 comes pre-loaded with the SwRI and SSI DHAs for the eight E-94-2 fuels as examples. The examples can be removed from tabs F 01 through F 16 by deleting the input data (red font) in columns A-C starting at row 5. The spreadsheet's 16 fuel slots are sufficient for an experiment in 4 variables at 2 levels each.

Each fuel is a separate tab into which the CAS number (when available), compound name, and wt% from a DHA are placed. Both ASTM and SSI¹ DHAs are supported. At the front is the PME calculation tab (set to print a PME report and chart on 2 pages) followed by two reference datasets: ASTM D6730-21 Table X1.2 and the CRC Master compound list (excerpted as Appendix B of the RW107-2-3a report).

All tabs are protected to guard against inadvertent changes, but no password is used. Unprotected areas are setup for the places where the user will input data. These have a gray background and use red font. Any sheet can be unlocked by clicking on "Unprotect Sheet" under the Excel Review menu option. To minimize the chance of corrupting formulas or formats, we strongly suggest that the ONLY way new data are put into the spreadsheet is by typing them in or using a "copy/paste/VALUES" operation.

A first step in learning to use the calculator would be to work through the tabs for one of the example fuels to understand how DHA data are input and handled to compute the PMI_y term (cells T4 and U4) and how that information is carried forward to the PME calculation page.

To load the spreadsheet for a new set of fuels, save it under a new filename and follow this approach:

- Go through the fuel-specific tabs and erase the DHA data already present (in red font) in columns A-C starting at row 5. Leftover data that does not belong to one of your fuels can be a source of great confusion. Leave unneeded tabs in place, but without data.
- In the PME Calculation tab, fill in the information regarding each fuel to identify it by name and its LHV and EtOH content (vol%).
- Go to the first fuel tab. Open the DHA for your first new fuel to the tab that groups the compounds. Select the columns that contain CAS number (if present), compound name, and weight percent and copy/paste/VALUES the data into cell A5. Exclude ALL unidentified compounds from this².

¹ SSI DHAs are those determined using the method developed in CRC AVFL-29 and reported in the ASTM D6730-21 standard for DHA. The term ASTM DHA refers to any DHA done according to earlier versions of the D6730 standard.

² You may also want to exclude DHA entries that are never found in your fuels. As an example, the ASTM E-94 DHAs used in RW-107-2 contained "C9-NaphthenoOlefin-6" but always with zero wt%. Such entries may or may

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The spreadsheet will update columns D-W by cross-referencing the compounds to the CRC Master tab. The CAS number is tried first. If there is no match, then the compound name is tried. If all compounds are successfully matched, the spreadsheet will complete the PME calculation and show the result in the PME calculation tab. If no match is found for a compound, the VP Source cell (column J) will display "ERROR" and turn to a red highlight. Such rows are the ones the user must manually resolve.

There are a number of reasons why an entry in a DHA cannot be matched against the CRC Master or SSI Master List tab, all of which revolve around: (a) the DHA entry does not exist in the CRC Master tab; or (b) the compound is identified differently in the DHA than in the CRC Master tab:

- If the compound has a CAS number, make sure it is correct. Search CRC Master for the compound name to find a corresponding entry. If the CRC Master entry's CAS number is different than the one used in the DHA, the problem can be fixed by changing the CAS number in the DHA to match. If the CRC Master entry does not have a CAS number (so is matched by compound name), the problem can be fixed by deleting the CAS number from the DHA.
- Some compounds are matched only by their compound name. Sometimes a compound name is truncated in the DHA (or in CRC Master) so that a match cannot be made although a corresponding entry is present. This can be fixed by editing the DHA compound name to correspond to that used in CRC Master.

There may truly be no match in the CRC Master. It contains entries for all compounds found in ASTM D6730-21 Table X1.2 and for compounds that were previously found with non-zero wt% in the DHAs used in RW-107-2 (plus additions made during development and testing).

When you have a truly non-matching compound, you will want to enter it into CRC Master. Unlock the CRC Master tab and find the first empty line at the bottom of the list. Enter the relevant data into the area highlighted in light gray and displaying in red font. Then relock the tab. The match is done using Excel's "MATCH" function which is not affected by the sort order in CRC Master; there is no need to re-sort the data. The data values needed to compute PME are VP_{443K} and YSI value. The former can be obtained from any source that provides it, while the later can be retrieved from the NREL online YSI calculator at <https://ysi.ml.nrel.gov/> using the compound's canonical SMILES.

As will become apparent in using the PME calculator, there is real potential for corrupting the spreadsheet unintentionally when resolving a non-matched compound. Information can be copied using copy/paste/**VALUES** within a tab and from an external source into a tab. Do not attempt to copy formulas within a single tab except when going down the column. In general, you have no guarantee that formulas will copy correctly from one tab to another because some cells contain sheet references that must be manually adjusted.

Please markup any errors in the CRC Master tab and bring them to CRC's attention along with any calculational errors you may find.

not appear in the CRC Master tab. If not, an "ERROR" will be reported in their line item and the contributions to PMI and PME will be forced to zero. This is an acceptable outcome once verified by the user to be appropriate.