PBPK model outputs Readme

The following is a listing of model scripts (.m files) and corresponding output files which create results in Tables 2 and 3 of the manuscript, "Issues in Assessing the Health Risks of n-Butanol", authors: D. Segal, A. S. Bale, L. J. Phillips, A. Sasso, P. M. Schlosser, C. Starkey, S. L. Makris.

The output files have the extension ".csv", should open directly in Excel, or can be opened using any text editor.

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* "CALC\_STUDY\_DMS\_INH.m" produces RAT\_DMs\_inh.out.csv: outputs of rat inhalation simulations in Table 2.
  + Columns are:
    - nbutylacet ppm: inhaled ppm of n butyl acetate (if applicable)
    - nbut ppm, inhaled ppm of n butanol (if applicable)
    - peak nbut, peak n butanol blood concentration (this is not presented in Table 2)
    - auc nbut, AUC24 for n butanol (internal dose)

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* "CALC\_STUDY\_DMS\_ORAL.m" produces RAT\_DMs\_oral.out.csv: outputs of rat oral simulations in Table 3.
  + Columns are:
    - bolus nbut,bolus n butanol dose (not applicable)
    - dw nbut, drinking water n butanol dose
    - auc nbut, AUC24 for n butanol (internal dose)
    - "HECnDcalc\_inhstudies.m" produces HUM\_HECs\_inhstudies.out.csv and HUM\_HEDs\_inhstudies.out.csv; i.e., sets of HECs and HEDs where the internal doses are estimated for rat inhalation studies.

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* HUM\_HECs\_inhstudies.out.csv: HEC results in Table 2.
  + columns are:
    - targDM,target internal dose metric value
    - calc AUC, value of AUC24 internal dose metric
    - calc peak, value of peak n butanol internal dose metric (not applicable)
    - ppm nbut, human equivalent concentration of n-butanol (ppm inhaled)
* HUM\_HEDs\_inhstudies.out.csv: HED results in Table 2.
  + columns are:
    - targDM,target internal dose metric value
    - calc AUC, value of AUC24 internal dose metric
    - calc peak, value of peak n butanol internal dose metric (not applicable)
    - nbut dose , human equivalent dose of n-butanol (mg/kg-d ingested)

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* "HECnDcalc\_oralstudies.m" produces HUM\_HECs\_oralstudies.out.csv and HUM\_HEDs\_oralstudies.out.csv; i.e., sets of HECs and HEDs where the internal doses are estimated for rat oral studies.

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* HUM\_HEDs\_oralstudies.out.csv: HEC results in Table 3.
  + columns are:
    - targDM,target internal dose metric value
    - calc AUC, value of AUC24 internal dose metric
    - calc peak, value of peak n butanol internal dose metric (not applicable)
    - nbut dose, human equivalent dose of n-butanol (mg/kg-d ingested)

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* HUM\_HECs\_oralstudies: HED results in Table 3.
  + columns are:
    - targDM,target internal dose metric value
    - calc AUC, value of AUC24 internal dose metric
    - calc peak, value of peak n butanol internal dose metric (not applicable)
    - ppm nbut, human equivalent concentration of n-butanol (ppm inhaled)