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.

[This is a blank line]

* "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)

[This is a blank line]

* "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.

[This is a blank line]

* 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)

[This is a blank line]

* "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.

[This is a blank line]

* 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)

[This is a blank line]

* 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)