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Investigations of the effects of different ventilation structures on physiologically based pharmacokinetic modeling (PBPK) simulations

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Abstract: Physiologically based pharmacokinetic (PBPK) models translate external concentrations into internal dose estimates using ordinary differential equations. Most PBPK models use multiple assumptions when modeling toxicant uptake through ventilation, but those assumptions can vary and different equations can be used. In the current study, existing human PBPK models of xylene and perchloroethylene are used to investigate the effect of the structure of air and blood concentration equations on compartmental predictions. Differences in ventilation equation structure do have an effect on model predictions and may affect parameter estimations, especially if the data used for optimization are blood concentrations. Specifically, inverse problems to determine metabolic parameters are used with simulated data to show how different model structures affect parameter estimation.