The Dermal Advanced Reach Tool (dART): a Bayesian model for dermal exposure assessment

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TNO innovation for life

What is the dART?

- A tier 2 exposure model for the assessment of dermal (hands) exposure.
- Allows an estimate of exposure to be made based upon contextual information about a task (i.e. in the absence of measurements).
- Allows (higher) percentiles of the exposure distribution to be estimated.
- Quantifies uncertainty in estimates.
- Updates estimates using any available measurements on the task.

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Exposure model

- The underpinning exposure model is a log-normal mixed-effects model

$$\ln(Y_{ij}) = \mu + w_i + \varepsilon_{ij}$$

$$w_i \sim N(0, \sigma_{bw}^2)$$

$$\varepsilon_{ij} \sim N(0, \sigma_{ww}^2)$$

Exposures log-normally distributed

Task specific mean

Task specific between-worker variability

Task specific within-worker variability

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Exposure model

- Baseline estimates result from informative prior distributions

$$\mu \sim N(\log(\text{CDARTscore}), \sigma_s^2)$$

Task specific prior for the mean based upon user input.

$$\sigma_{total} \sim LN(-0.12, 0.64)$$

$$\sigma_{bw}^2 / \sigma_{ww}^2 \sim LN(-0.92, 1.44)$$

Joint prior for variance components is common to all scenarios.
- Based on the literature.

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Calibration of mechanistic model

- Dermal (hand) exposure results from three routes: deposition (D_{hands}), direct emission and direct contact (E_{hands}) and transfer (T_{hands}).
- Application of the dART mechanistic model (based upon user input) results in a score for each route.
- Scores are dimensionless with different length scales.
- Calibration is the process of converting these three scores into an estimate of exposure (mg min^{-1}).

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Calibration – data requirements

- Task-based measurement datasets
  - Mass of analyte, sampling time and analyte concentration-in-product required
- High quality contextual information accompanying each dataset, sufficient to confidently code the determinants of the dART mechanistic model.
  - Conservative judgements inappropriate for calibration: systematic bias
- A calibration model linking determinants to measurements.

Calibration – scoring

- Scenarios chosen from BEAT and BROWSE databases.
- Determinants scored by one team member based upon textual descriptions and pictures. Independently checked by a second team member.
  - Iterative process
- Final calibration dataset of 40 exposure scenarios covering five of the six activity classes.

Calibration – the model

$$\text{Exposure} = \alpha \times \text{DARTscore}$$

A re-scaling of the dART score results in an estimate of exposure (mg min^{-1})

$$\text{DARTScore} = D_{hands} + \beta_1 T_{hands} + \beta_2 E_{hands}$$

A weighting of scores required to account for relative importance of the different routes and different length scales.

Calibration – the model

Calibration model is a log-normal non-linear mixed-effect model

$$\log(Y_{ij}) = \log(\alpha) + \log(D_{hands} + \beta_1 T_{hands} + \beta_2 E_{hands}) + I_G \times Glove + s_i + \varepsilon_{ij}$$

$$s_i \sim N(0, \sigma_s)$$

$$\varepsilon_{ij} \sim N(0, \sigma_r)$$

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Particular challenges

- Measurements above and beneath PPE.
- Saturation of hands/sampling device in some scenarios.
- Measurements beneath LOD/LOQ in some scenarios.
- Complex form of calibration model – parameters within the log term.
- Relatively flat likelihood.

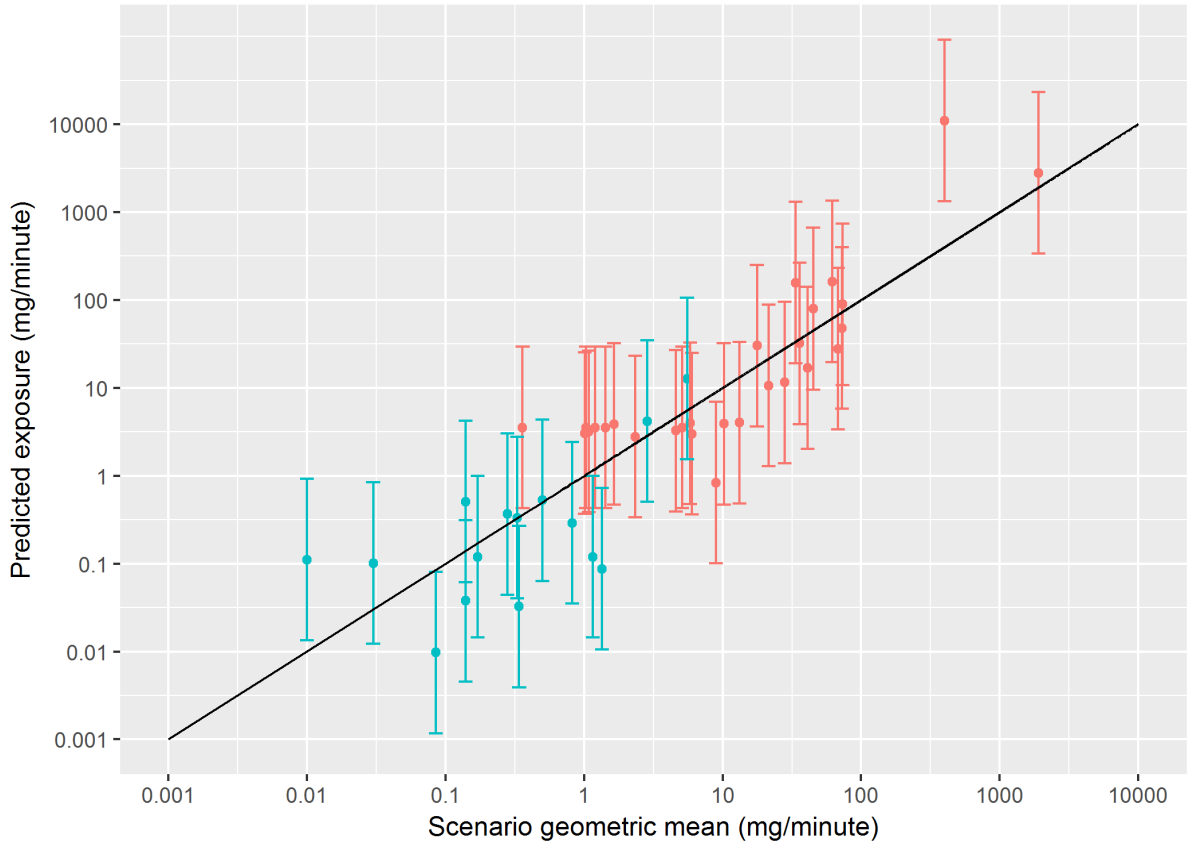
Calibrated model

- Exposure to product (mg min^{-1}).
- Central estimate of 1.14*(D_{hands}+ 87.4*T_{hands} + $5.02 * E_{hands}$).
- Between scenario standard deviation of $\sigma_s = 1.08$.
- 95% multiplicative interval of approx. 1/8 to 8 the central estimate.
- Multiply by the weight fraction for exposure to the analyte-in-product.

Post fitting checks

Satisfactory overall fit

Unbiased predictions for the five activity classes in the calibration data



Example calculation

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Potential Dermal Exposure during the Painting Process in Car Body Repair Shops

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Example calculation

$D_{hands} = 0.05, T_{hands}$= 0.00075, E_{hands} = 0.225 (from Goede et al. (2018))

CDARTSCORE = 1.14*(D_{hands}+ 87.4*T_{hands} + 5.02 $*$ E_{hands}) = 2.04 mg min^{-1}

Direct emission (63%) and Transfer (36%) are the important routes.

Approx. 95% interval of (0.3, 16.3) mg min^{-1}

Exposure to Aluminum (at weight fraction of 2%) of 0.04 (0.005, 0.34) mg min^{-1}

Summary

- Exposure model underpinning the dART has been presented.
  - Central estimate of exposure (GM) based upon a calibrated mechanistic model.
  - Priors for variance components based upon the literature.
- Methodology for calibration explained.
- Demonstration through example calculation

Next steps

- Publish!
- Retention not yet accounted for – likely to be much lower on skin/PPE than cotton sampling gloves
- Further testing and validation required
- Workflow required to integrate in the ART software platform
- Extend to other substance classes.