



National Institute for Public Health  
and the Environment  
*Ministry of Health, Welfare and Sport*

# Evaluation of the ConsExpo Exposure to vapour – Evaporation model

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in collaboration with  
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# Goals

- > Evaluate correctness and usability of ConsExpo model for evaporation of liquids
- > Covers all aspects: availability of parameters and their uncertainty, validity of model assumptions, veracity of implementation
- > Next step: assess whether ConsExpo needs improvement



# Methods

- > Literature search for air concentration measurements for substances emitted by paint/lacquer and household cleaning products
- > Determination of physicochemical properties: vapour pressure or Henry's law constant, molecular weight of matrix
- > Reproduction of experiments in ConsExpo including propagation of uncertainties in vapour pressure or Henry's law constant
- > Comparison of ConsExpo model predictions against measurement data



## Details reproduction in ConsExpo

- > ConsExpo uses Raoult's law (limit of high concentrations)

$$P_{\text{eq}} = VP \times x$$

equilibrium pressure = vapour pressure  $\times$  molar fraction

- > Henry's law (limit of low conc.) is often more suitable, but value depends also on solvent

- > Henry's law constant  $H_{\text{v}}^{px}$  is drop-in replacement for VP

$$P_{\text{eq}} = H_{\text{v}}^{px} \times x$$

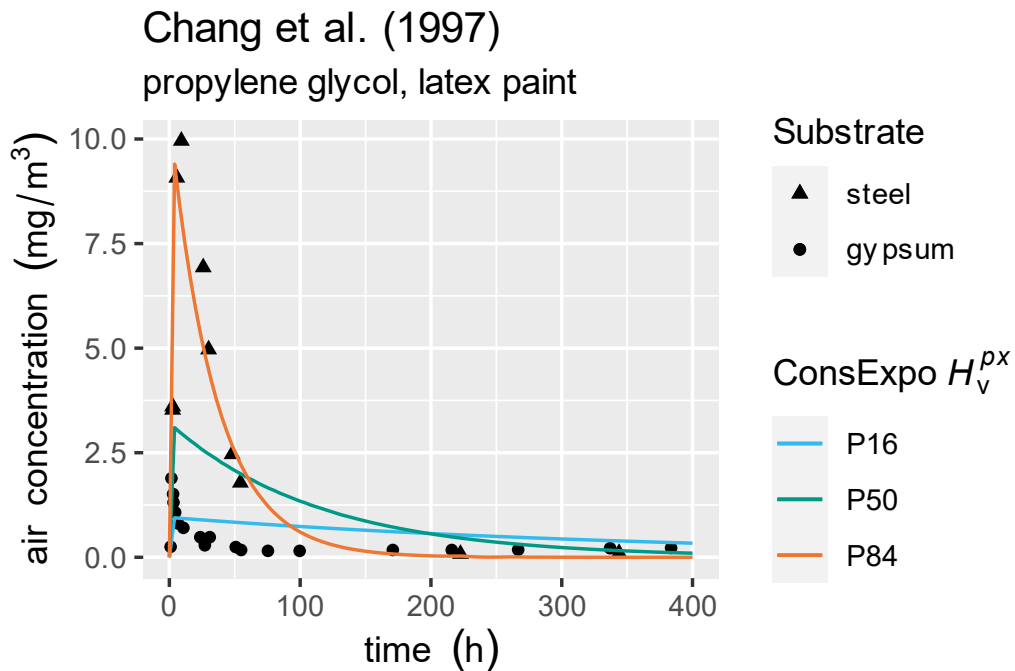
- > For water as solvent (a.o. latex paint, diluted household cleaning products) many  $H_{\text{v}}^{px}$ s can be found at [henrys-law.org](http://henrys-law.org)
- > Preference for values from measurements and literature reviews, otherwise QSPRs and VP/AS estimates
- > For oily solvents, no  $H_{\text{v}}^{px}$ s available; use VPs for lack of something better



# Several examples of model vs. data



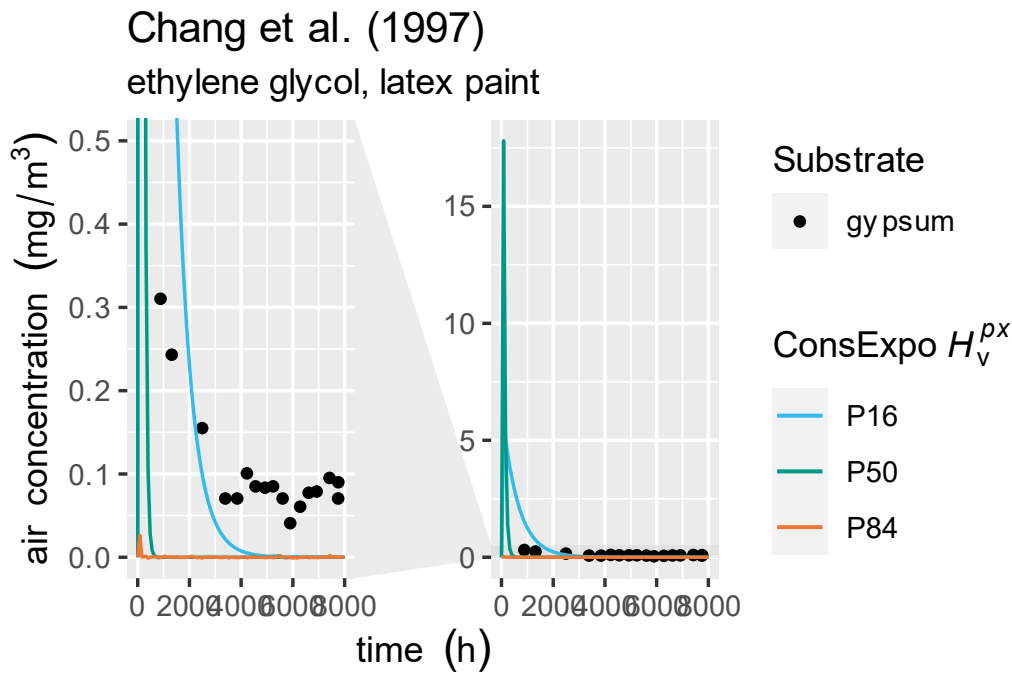
# Paint, with and without substrate effects



- > Paint on steel and other non-porous substrates: mostly consistent with data within/around 68% credible interval
- > Paint on gypsum board and other porous substrates: acute emission significantly overestimated



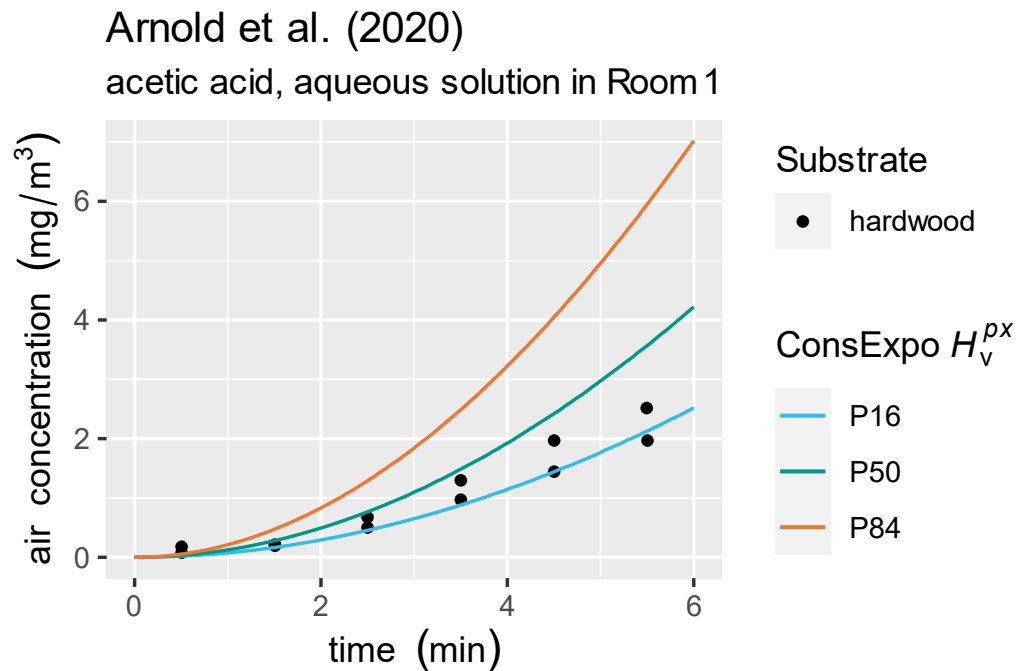
# Paint, long-term substrate effects



- > Long-term low-level emissions from paint on gypsum board or other porous substrates are not reproduced by ConsExpo
- > ConsExpo assumes 100% of substance is eventually emitted, integrated emission cannot be underestimated



# Aqueous cleaning product

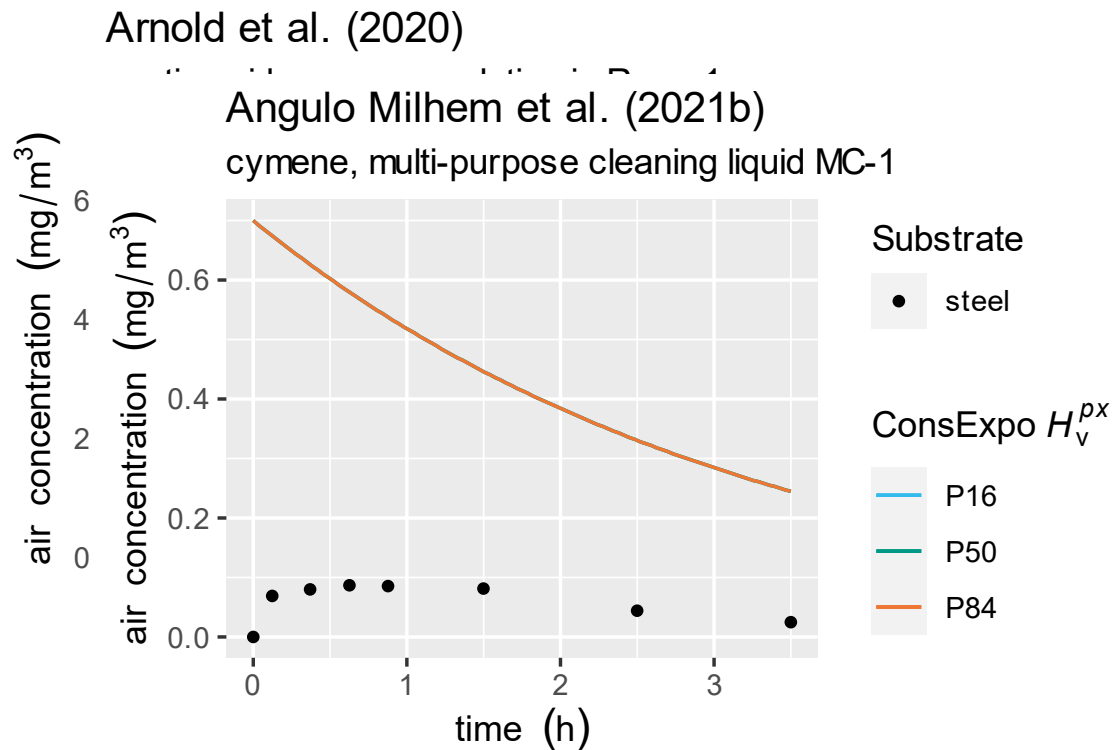


- > This category shows excellent reproduction if the matrix is indeed nearly pure water
- > For aqueous matrices with a significant fraction of other solvents, the model can be significantly off if a  $H_v^{px}$  for (pure) water is used





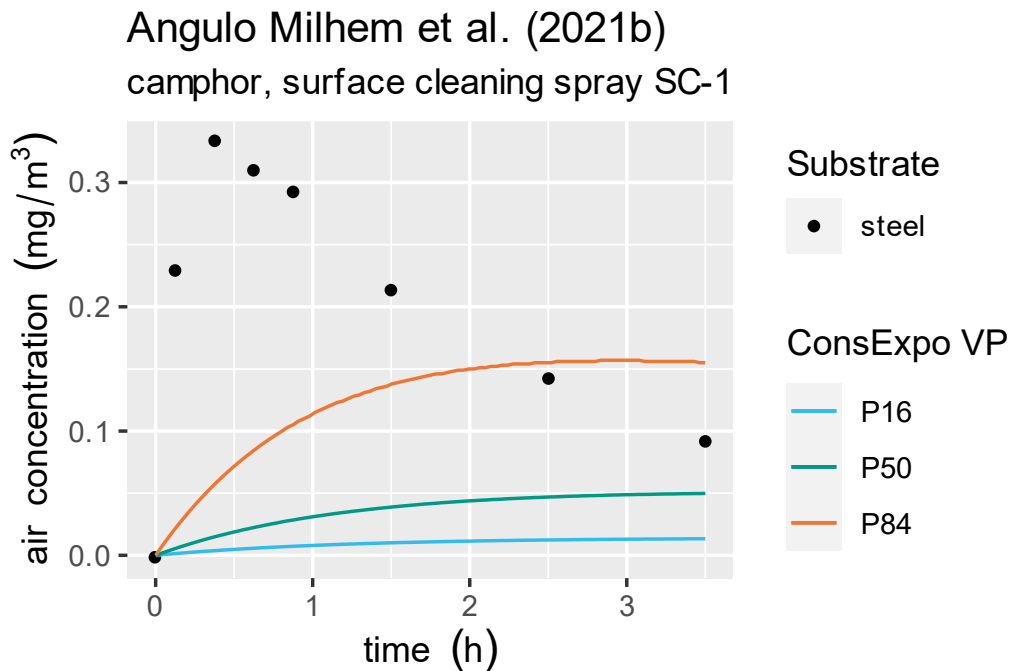
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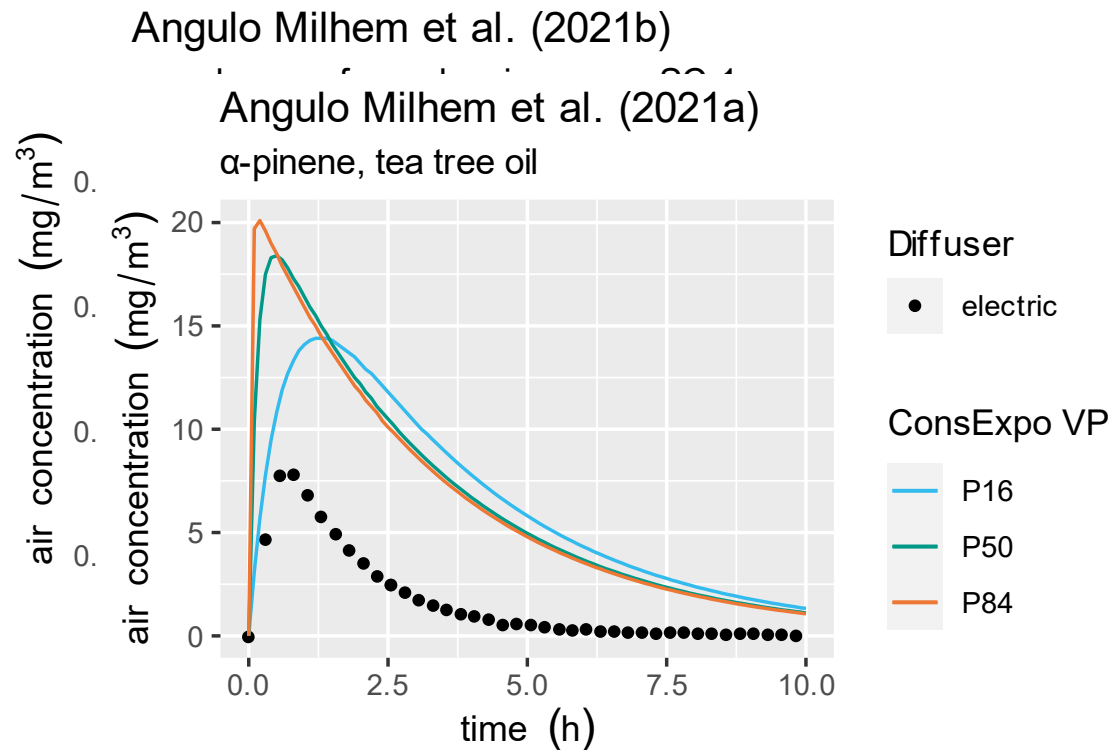
# Oily cleaning product



- > This category is very difficult
- > Poor availability of  $H_V^{px}$  for solvents other than water
- > Forced to improvise using VP
- > Diverse emission behaviour: under- or overestimation, different time scale



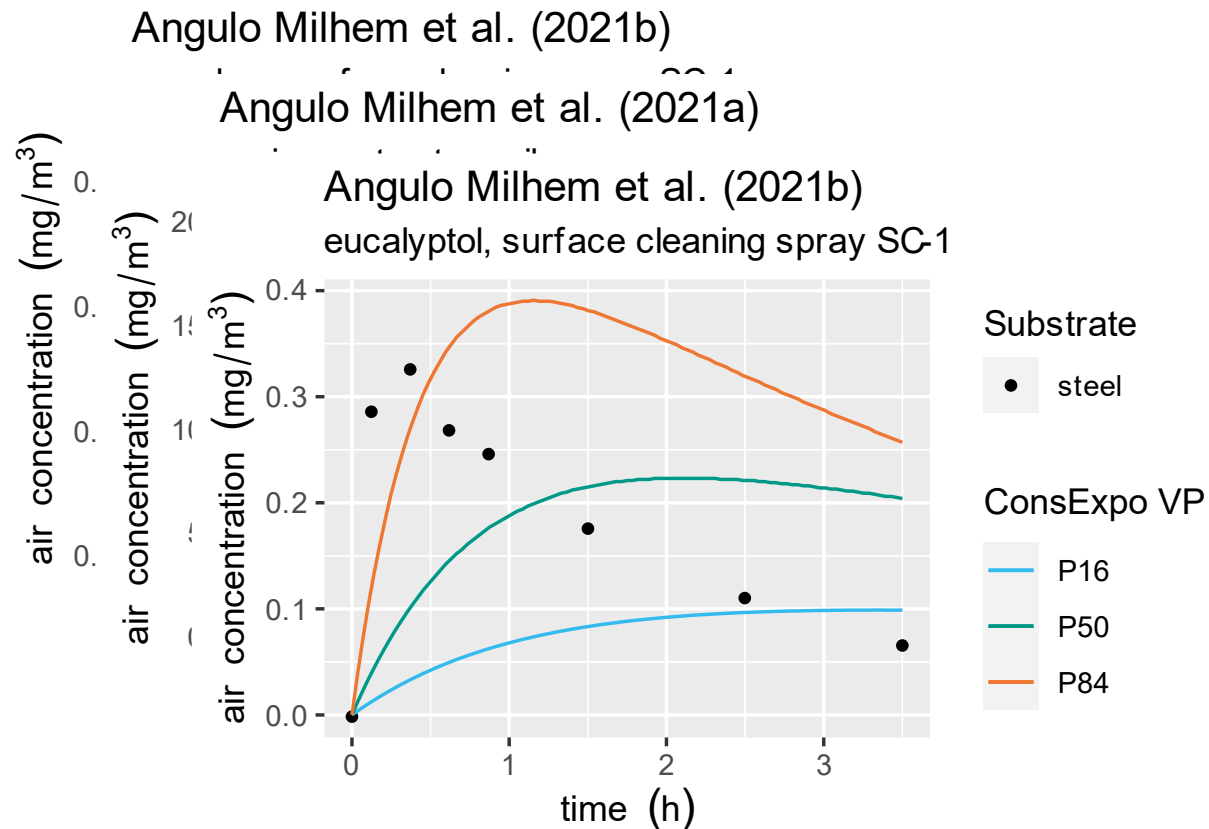
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# Conclusions

- > Good reproduction for aqueous solutions on impermeable substrates
- > When substrate is porous:
  - Overestimation of short-term emissions
  - Underestimation of long-term emissions
  - Total emissions never underestimated
- > Reproduction for matrices other than mostly water hampered by lack of (accurate) Henry's law constants



# Thank you!

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