Characterizing Exposure to Indoor VOCs and SVOCs using Simple Mass-Transfer Models

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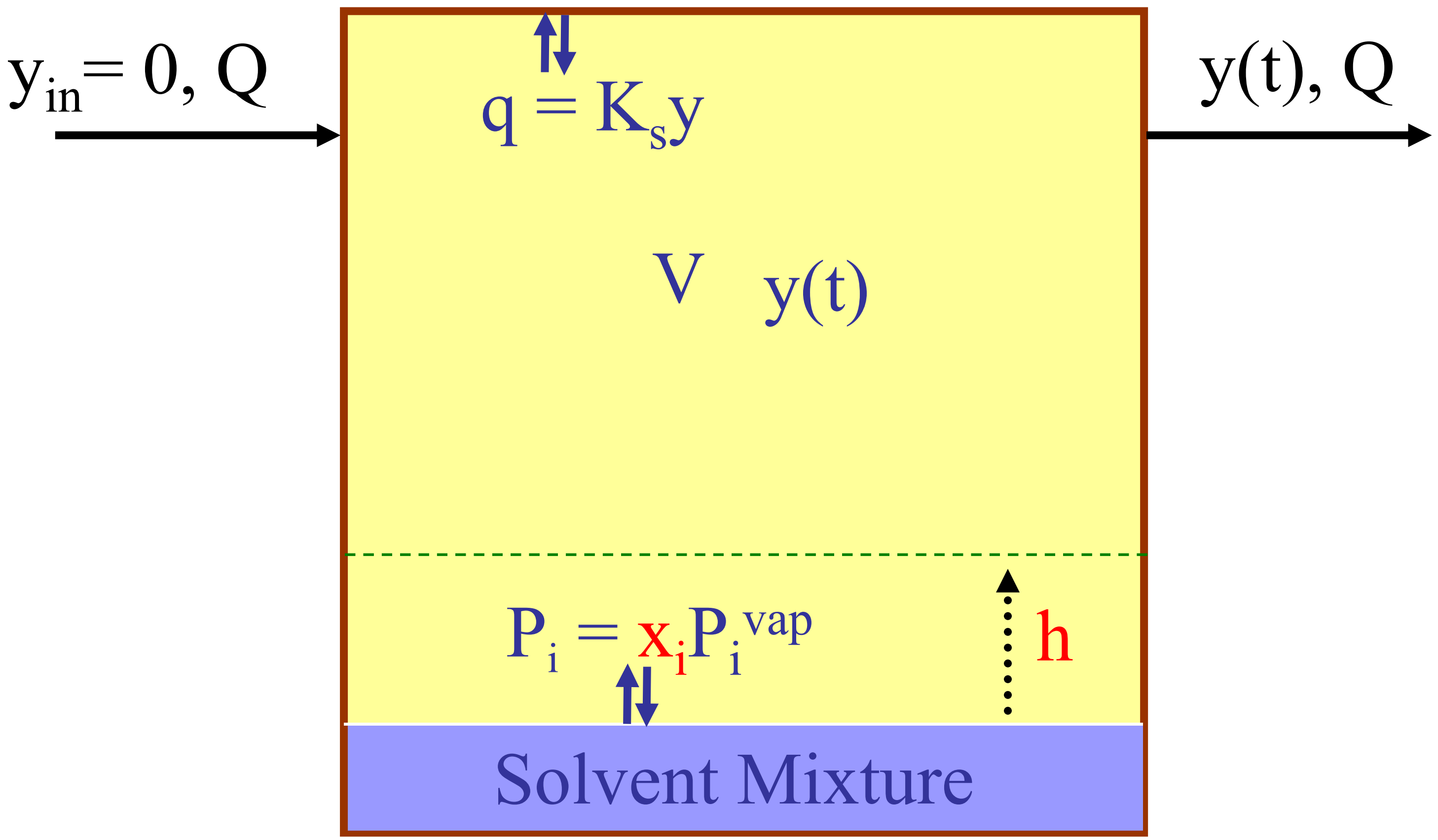
Characterizing Sources

- Too many materials and products for emissions to be individually measured
- Develop mechanistic mass-transfer models for generic source types
- Independently measure model parameters
- Collect experimental data in small chambers to validate models
- Develop correlation equations to predict model parameters based on compound properties (molecular weight and vapor pressure)
- Use models to predict exposure

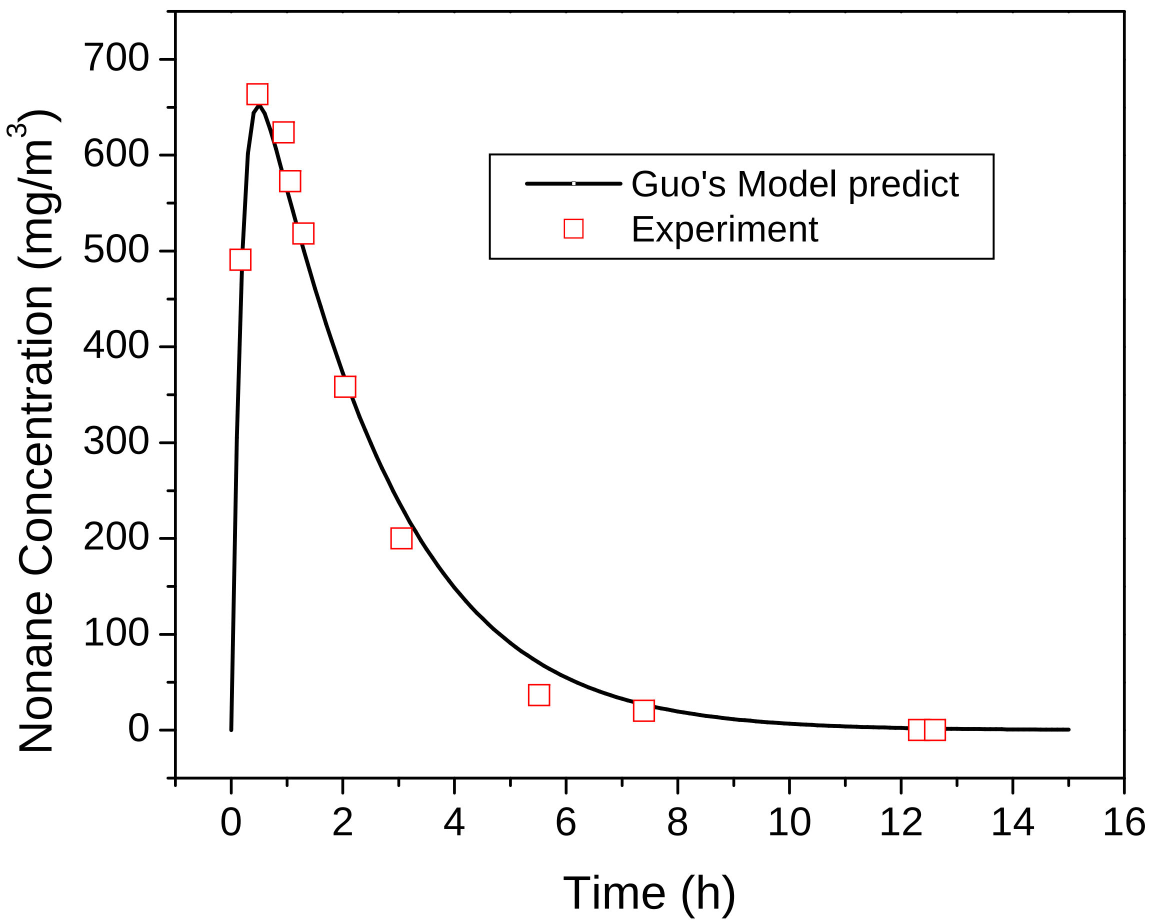
Three Generic Source Models

- **Liquid Source** → **VOC** – Nonane in Coating Materials (Guo et al., 1999)
- **Solid Source** → **VOC** – Phenol in Vinyl Flooring (Cox et al., 2002)
- **Solid Source** → **SVOC** – DEHP in Vinyl Flooring (Xu and Little, 2006)

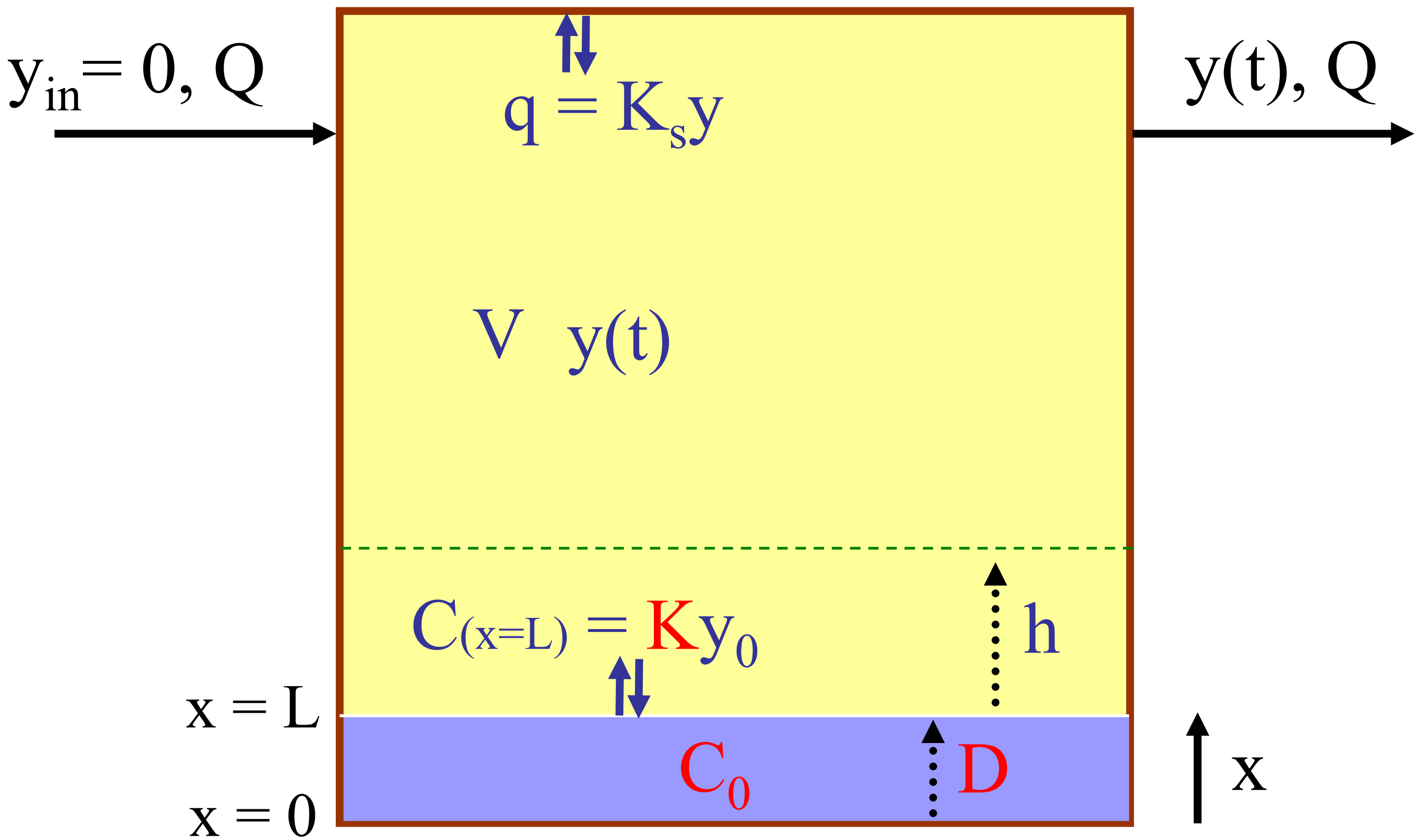
Liquid Source → VOC



Model Validation
(Nonane in Coating Material)

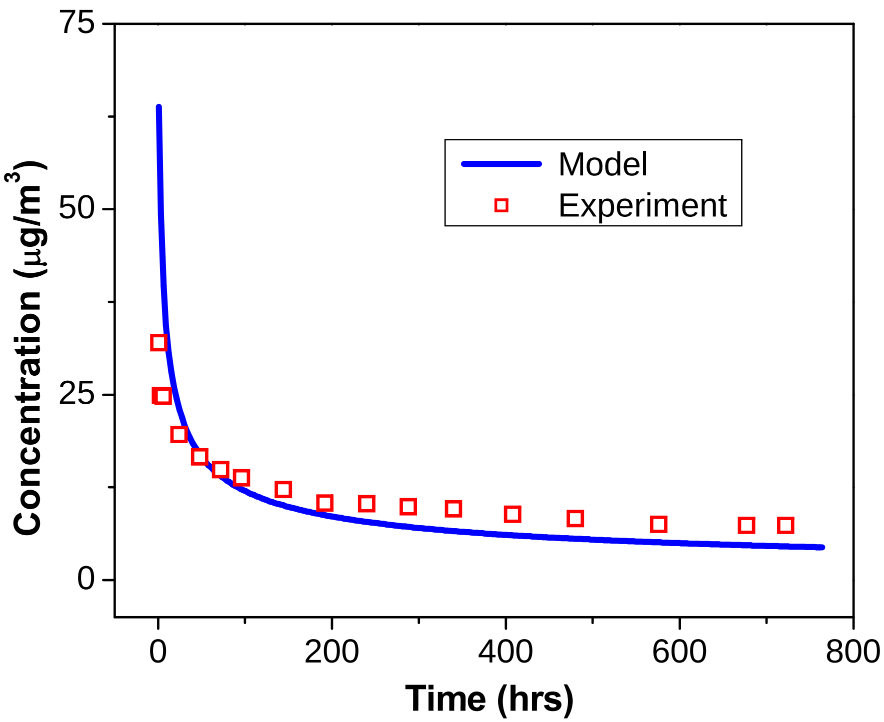


“Solid” Source → VOC

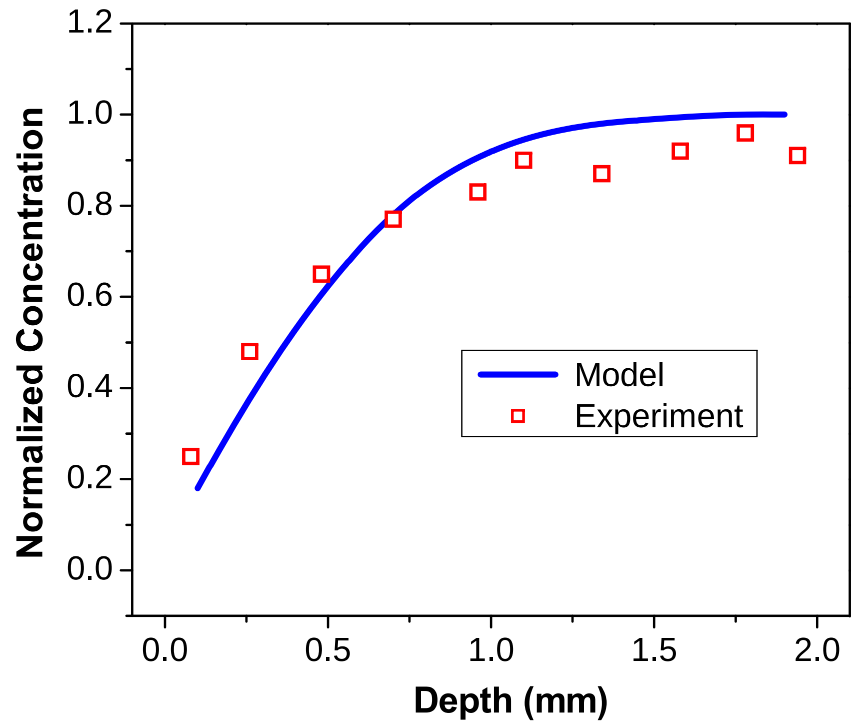


Model Validation
(Pentadecane in Vinyl Flooring)

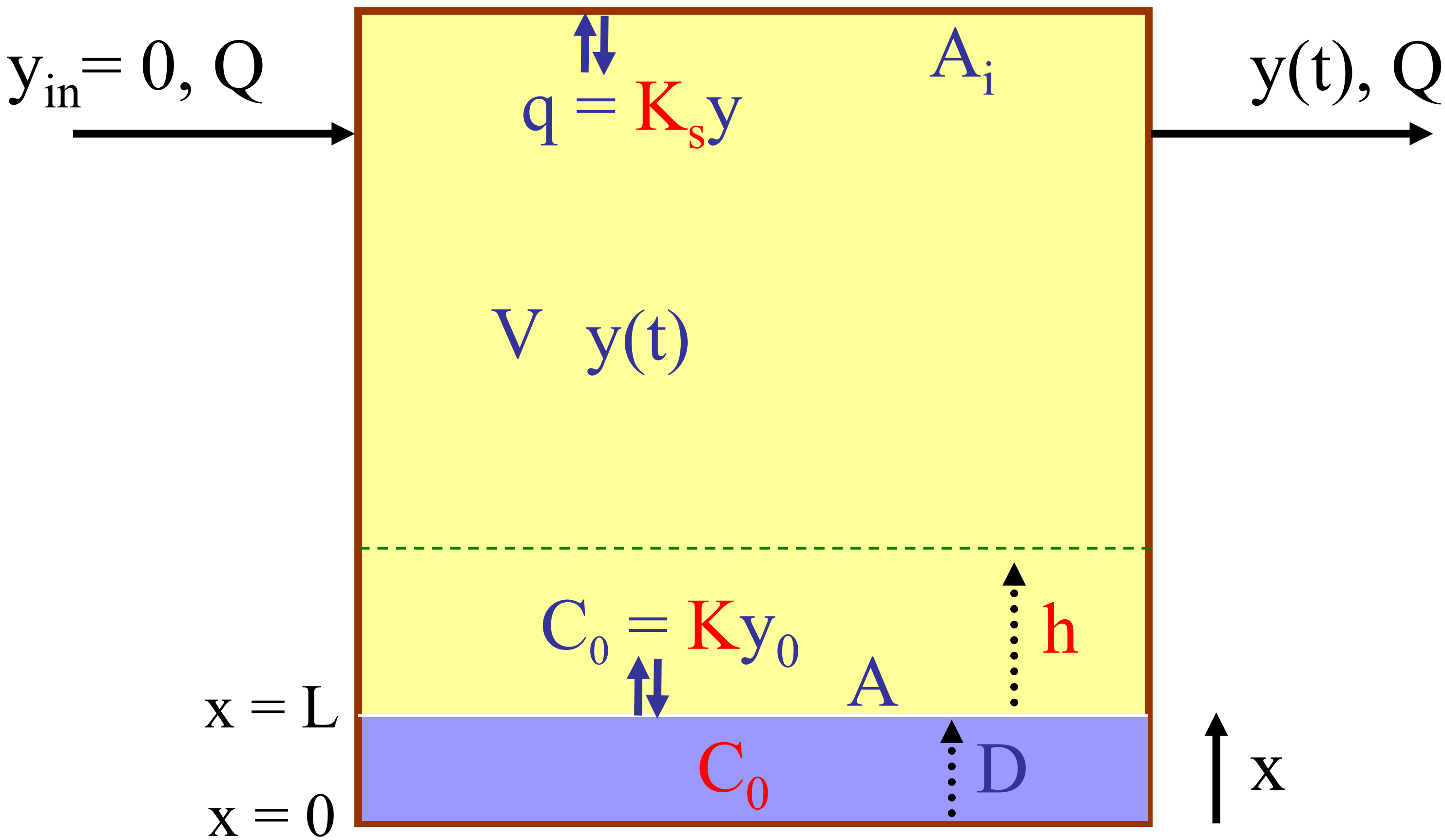
Gas-phase Concentration



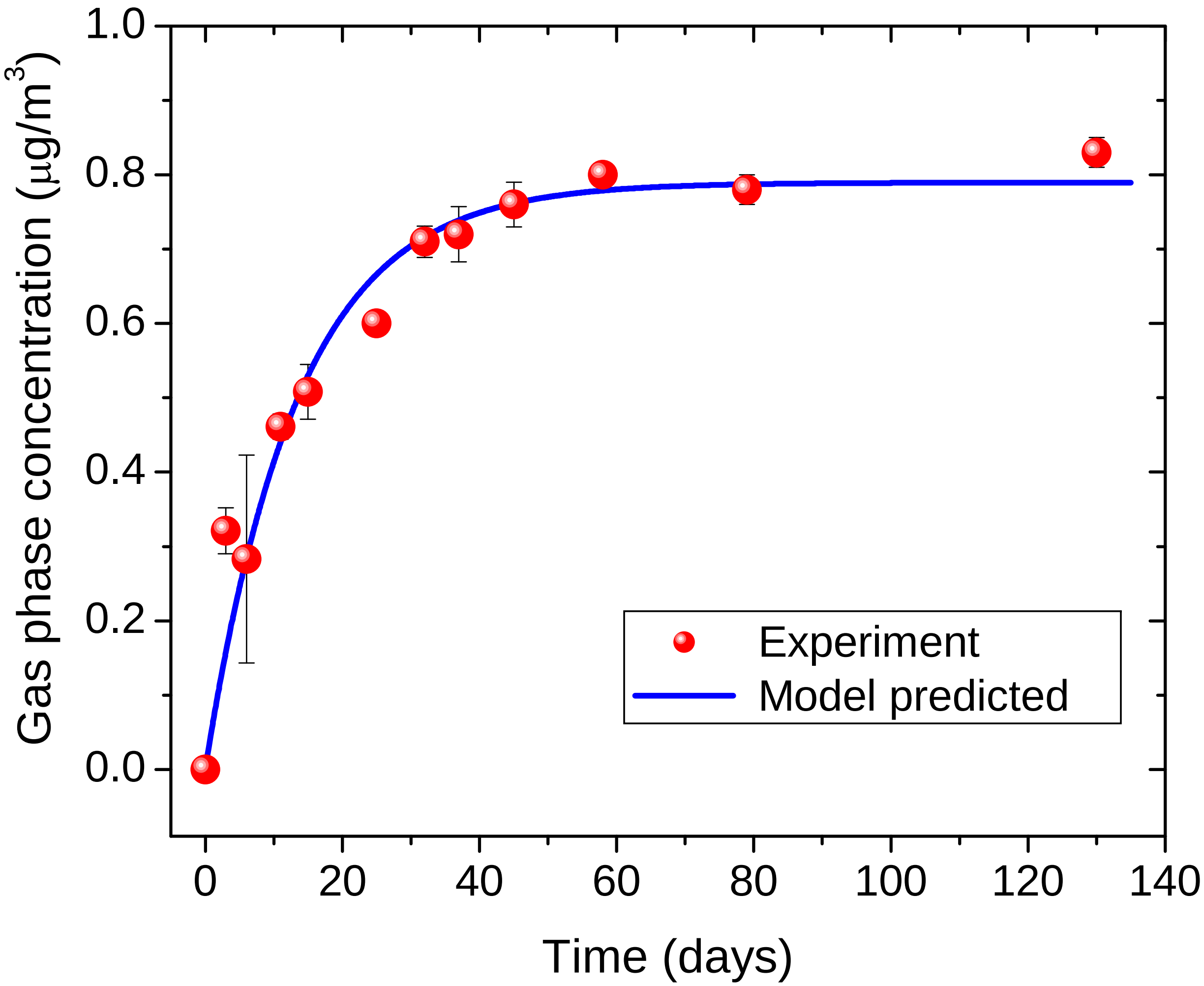
Material-phase Concentration



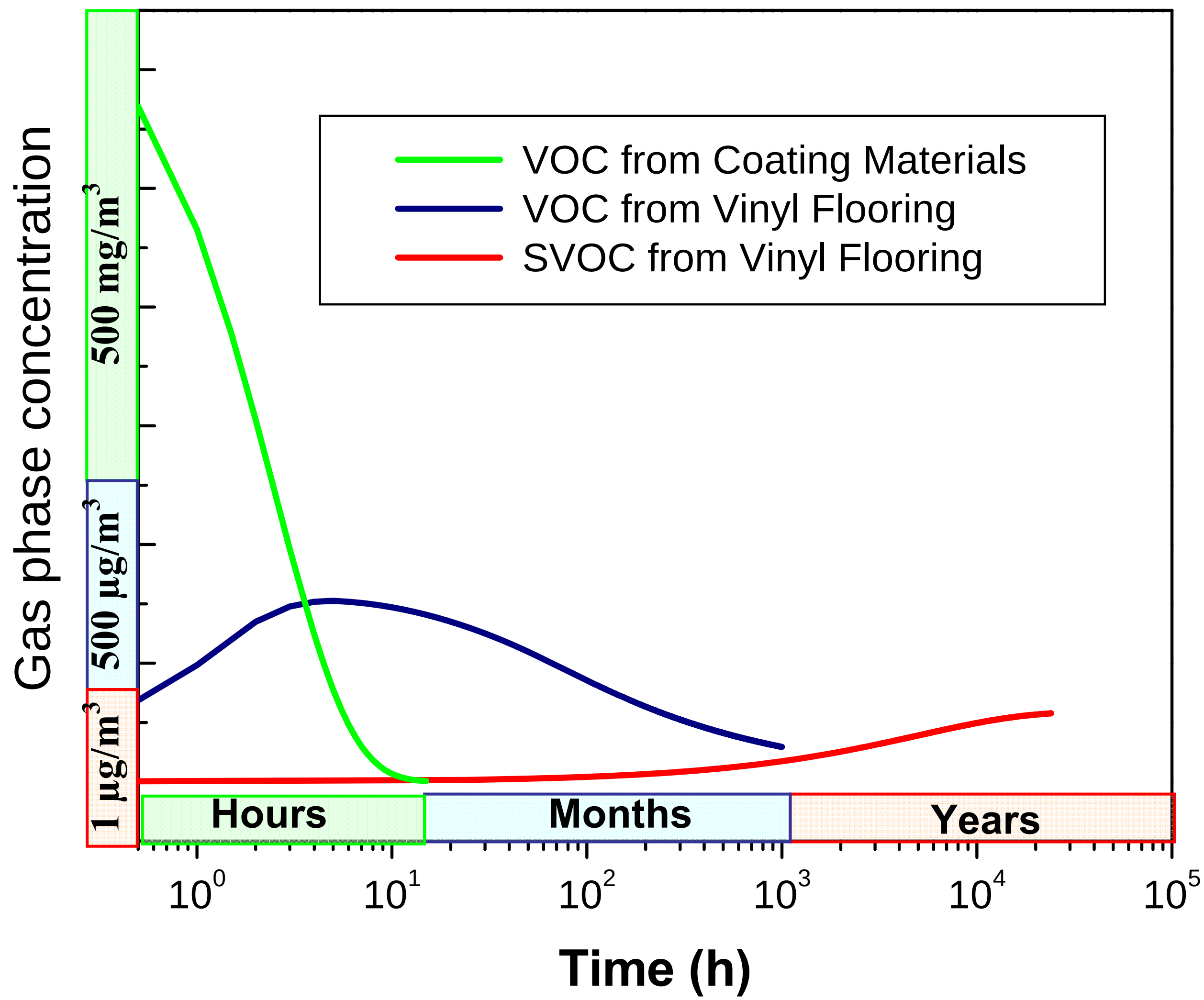
“Solid” Source → SVOC



Model Validation
(DEHP in VF)



Comparison of Three Models
(nonane, phenol, and DEHP)



Mechanistic Insights

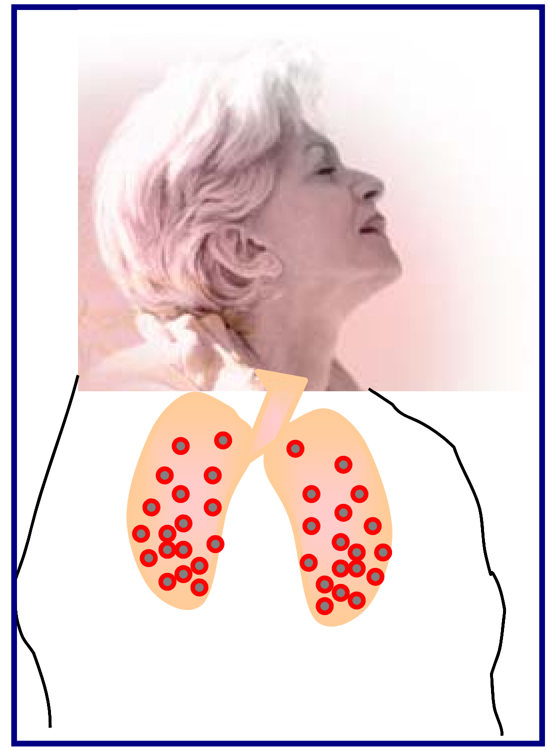
- Gas-phase concentration is proportional to material-phase concentration, so x_i and C_0 are the most important parameters.
- External mass-transfer coefficient (h) can be estimated.
- Diffusion coefficient (D) correlates with molecular weight, while partition coefficients (K and K_s) correlate with vapor pressure. Once values are known for a few compounds, can develop correlations and predict others.
- Because of strong surface sorption, emission and transport of SVOCs depend more on specific residential environment than for VOCs.

Example of SVOC Emissions

- Di-ethylhexyl phthalate (DEHP) used as plasticizer in vinyl flooring.
- Emits slowly, but over very long period.
- Toxicity of phthalates is of concern.
- Extend model validated for small chamber to predict emissions and exposure in residential environment.
- Account for sorption of DEHP by airborne particles as well as interior surfaces.

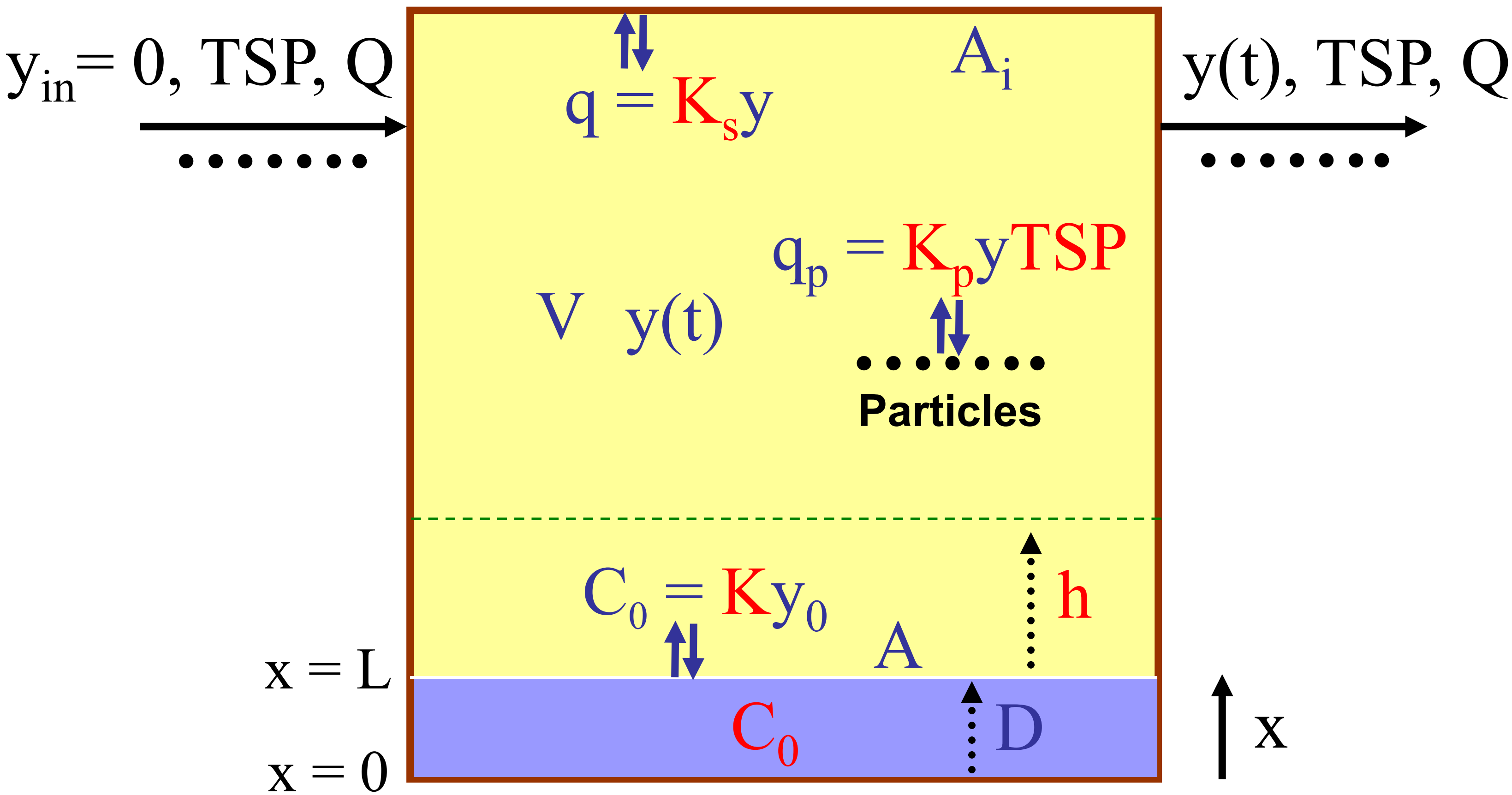
Effect of Airborne Particles

VOCs



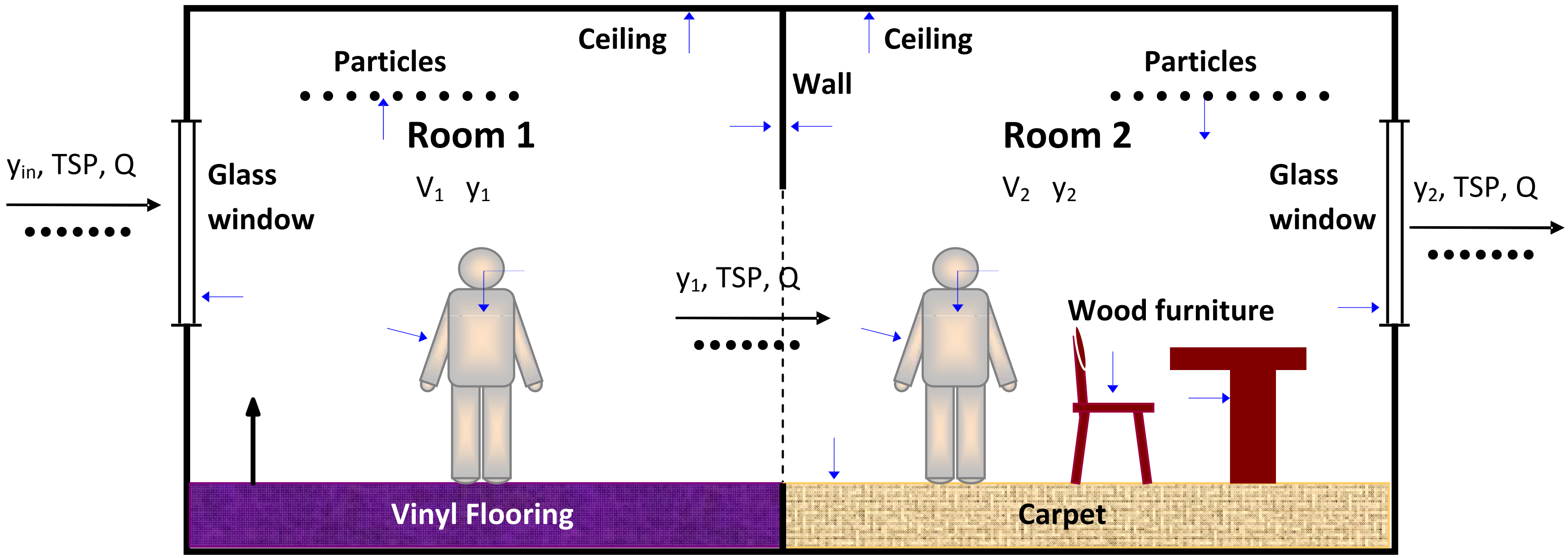
SVOCs

DEHP Emissions + Airborne Particles



Making model more representative of real indoor environment

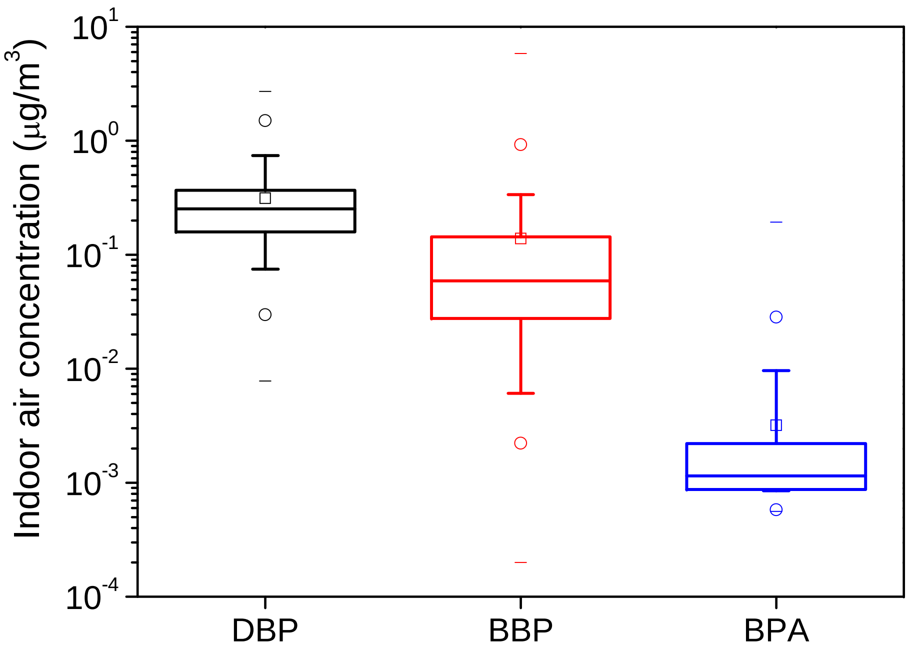
Two-Room Model

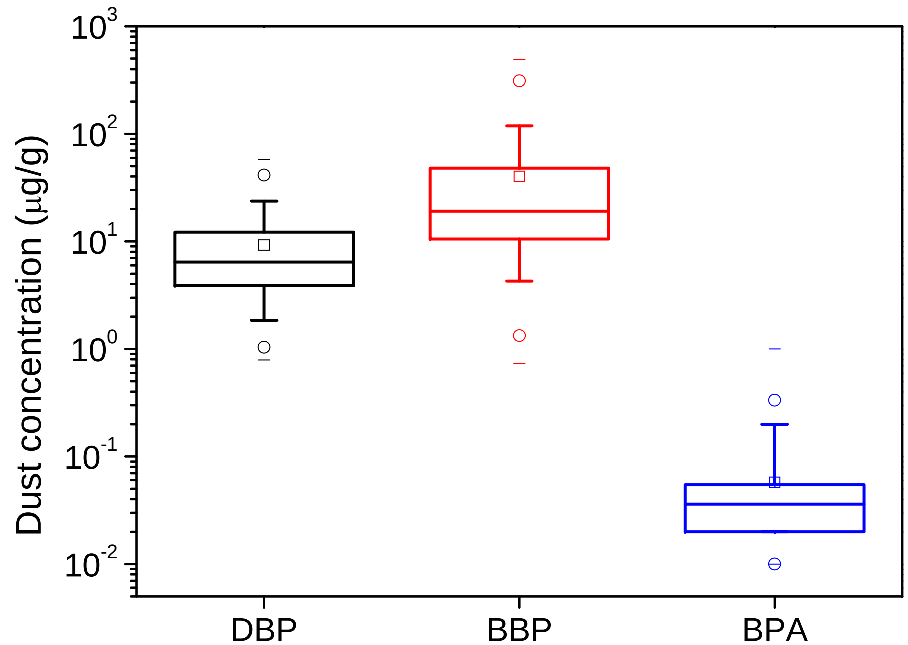


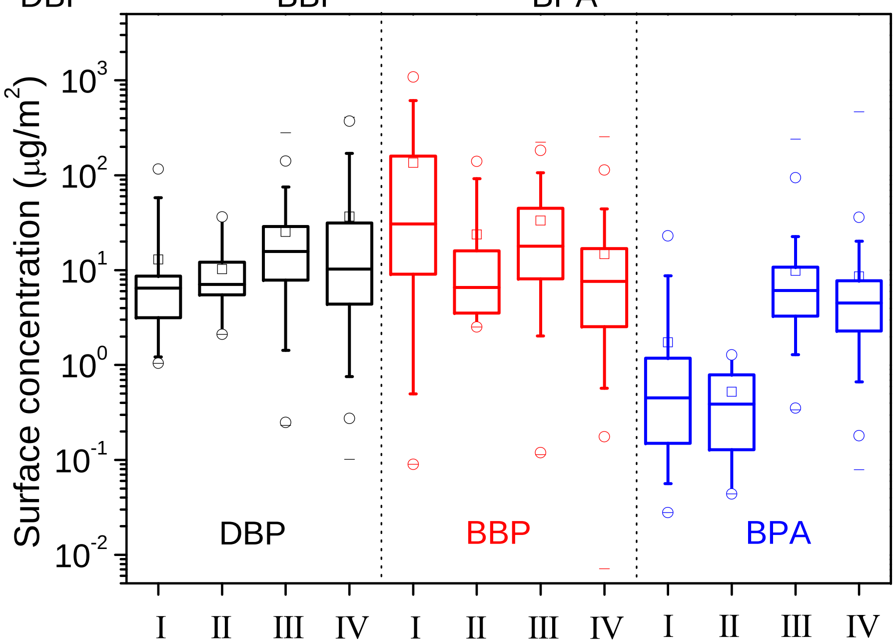
Sorption of DEHP to Interior Surfaces and Dust

- **EPA CTEPP study**
  - 300 homes and day care centers in NC and OH
  - 50 pollutants
  - air, house dust, interior surfaces, and dermal wipe samples
- **Top three high surface conc.**
  - BBP, benzyl butyl phthalate
  - DBP, dibutyl phthalate
  - BPA, bisphenol-A
  - No DEHP data

CTEPP Data







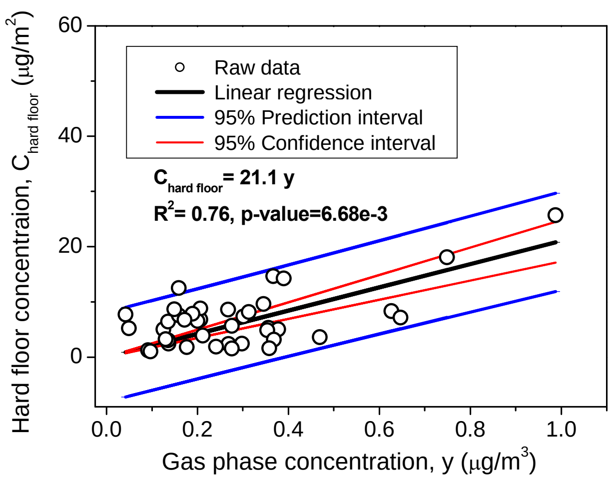
I: hardwood floor surface

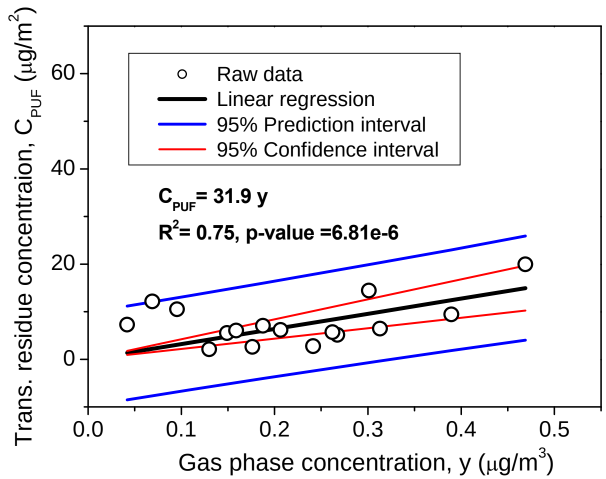
II: transferable residues from carpet

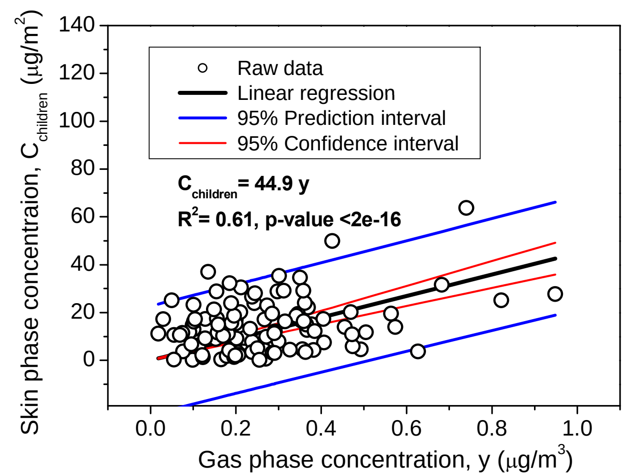
III: hand wipe of children

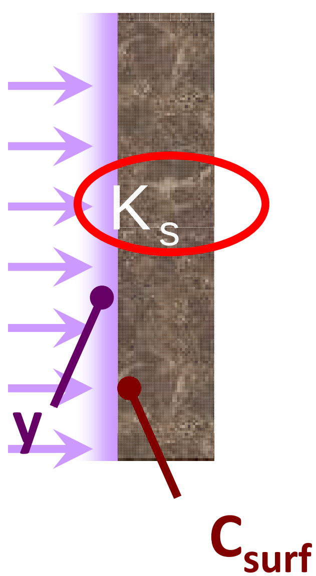
IV: hand wipe of adults

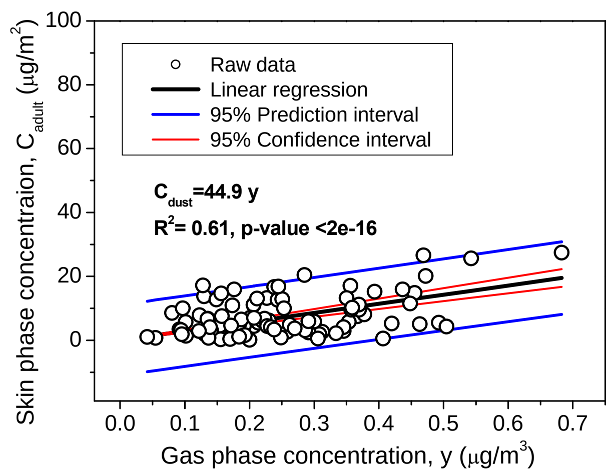
Linear regression to obtain K_s for DBP

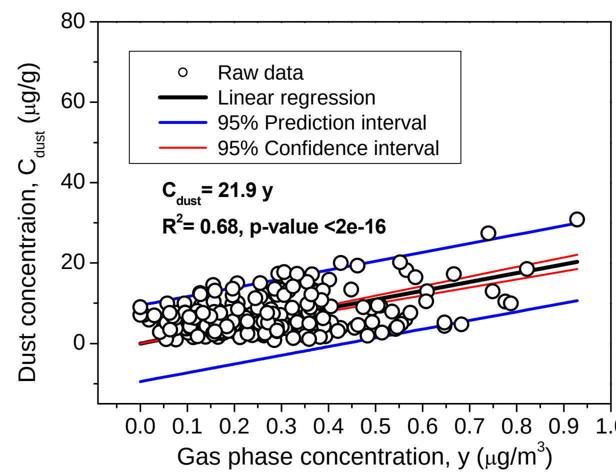




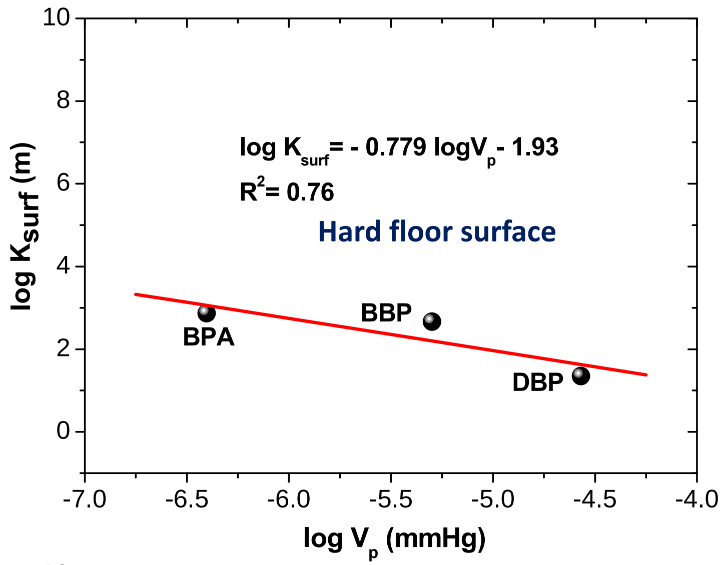


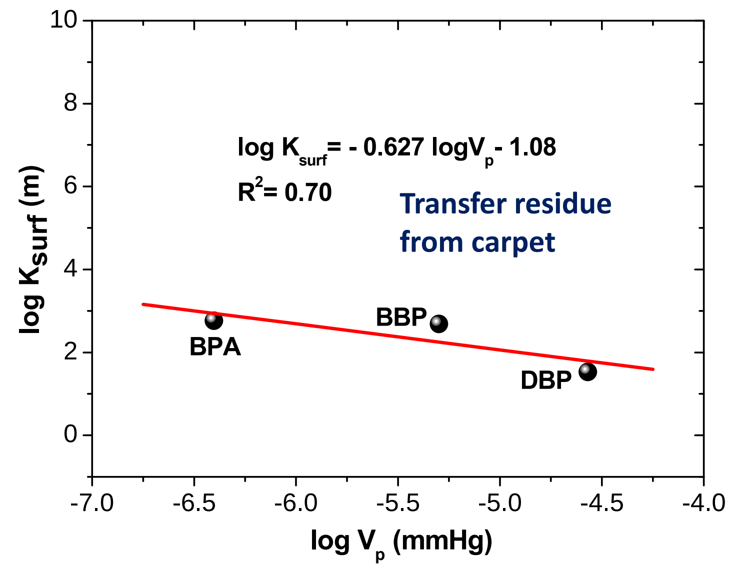


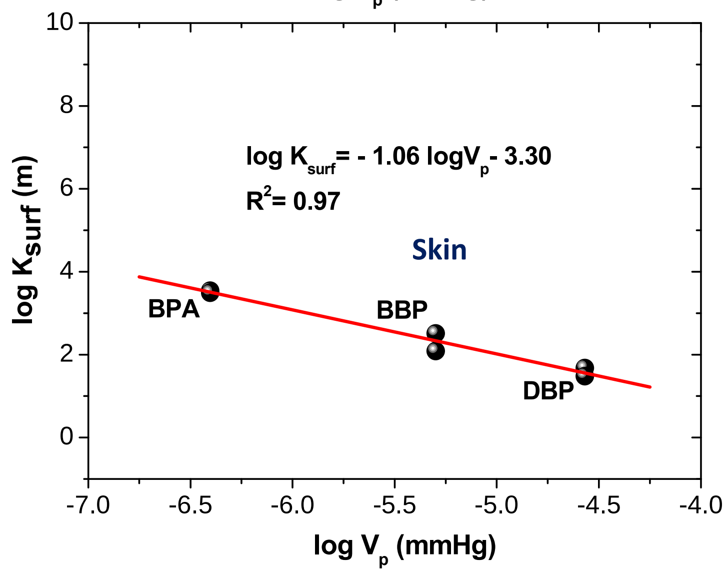


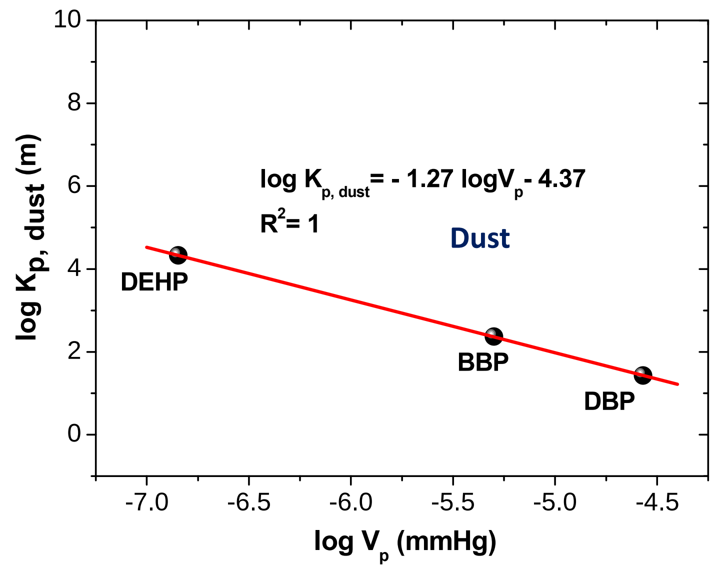


Correlation of partition coefficient with V_p

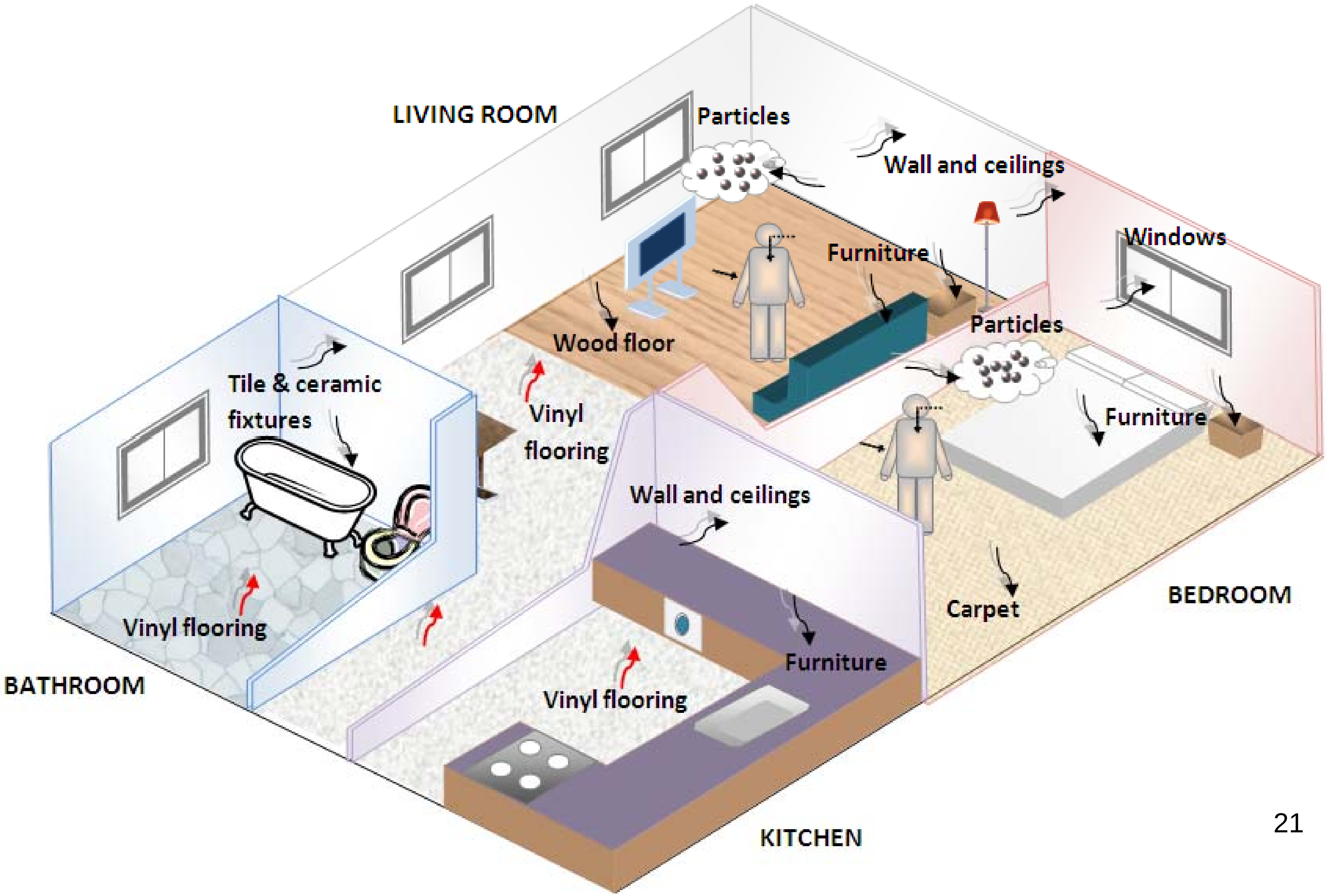




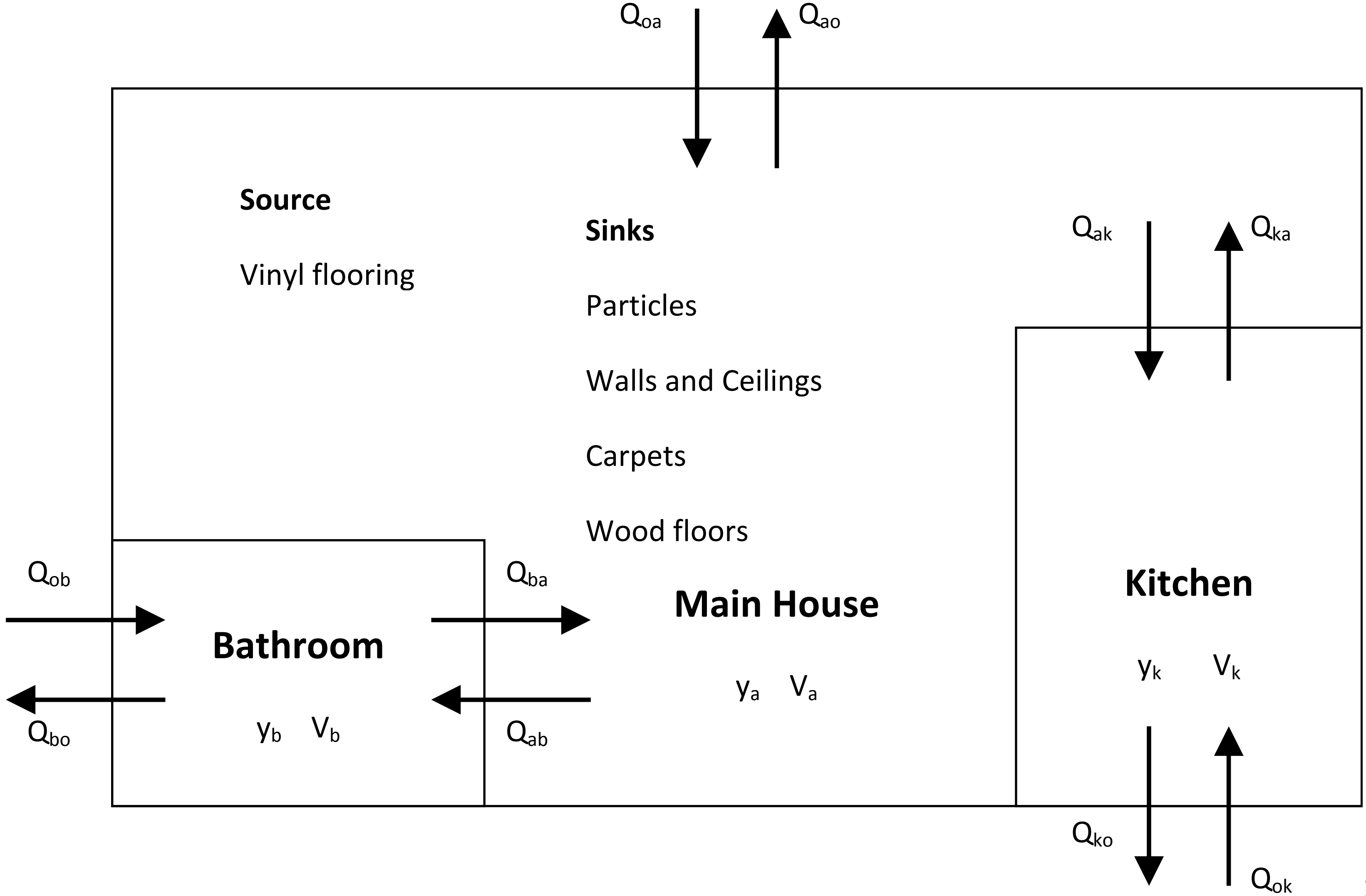




Residential Environment



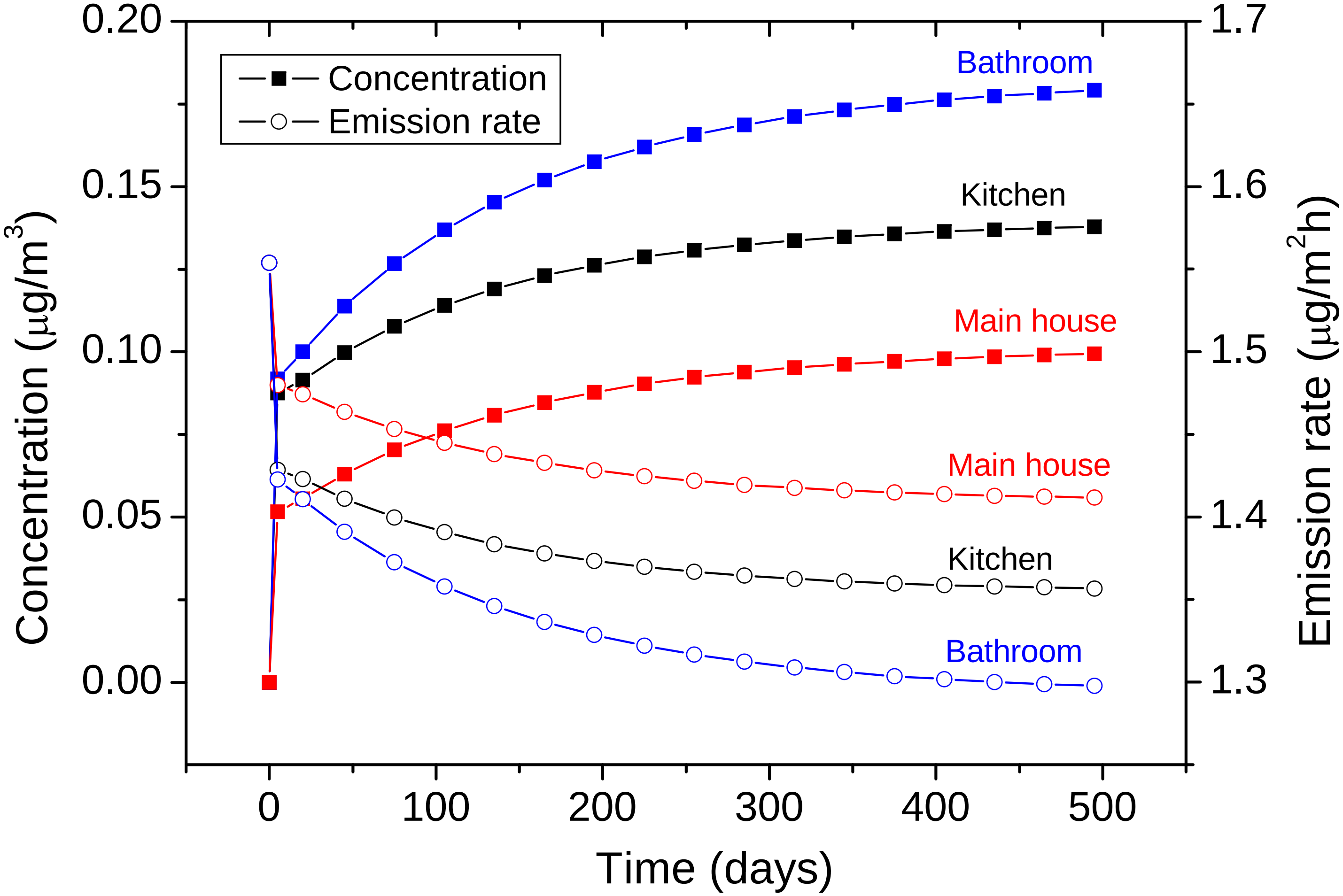
Residential Environment



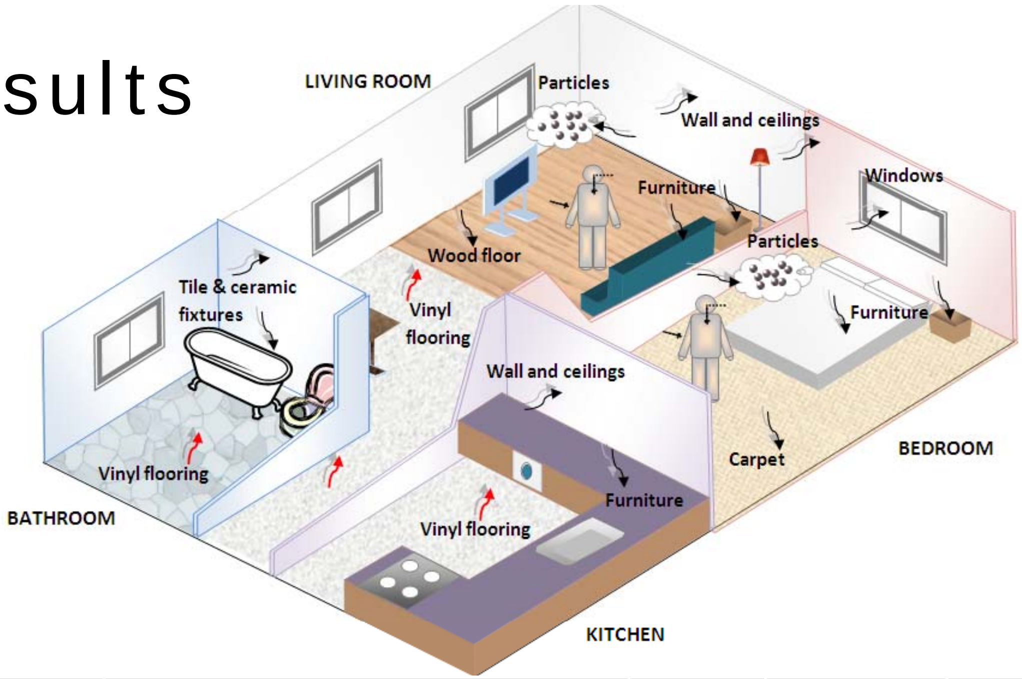
Residential Environment

Compartment	Main house		Kitchen		Bathroom	
Volume	128		35		15	
Flowrate	Q_{oa}	65	Q_{ok}	12	Q_{ob}	1.1
	Q_{ao}	44	Q_{ko}	32	Q_{bo}	2.1
			Q_{ak}	44	Q_{ab}	14
			Q_{ka}	24	Q_{ba}	13
Surface area						
Vinyl flooring	19.2		14.4		6.20	
Walls & Ceilings	124		34.0		23.3	
Carpet	35.8		--		--	
Wood floor	32.0		--		--	
Hard surface furniture	61.4		12.6		5.40	
Windows & mirrors	5.12		1.75		1.05	
Tile & ceramic fixtures	5.12		3.50		16.5	
TSP	20.0		20.0		20.0	

Model results



Model results

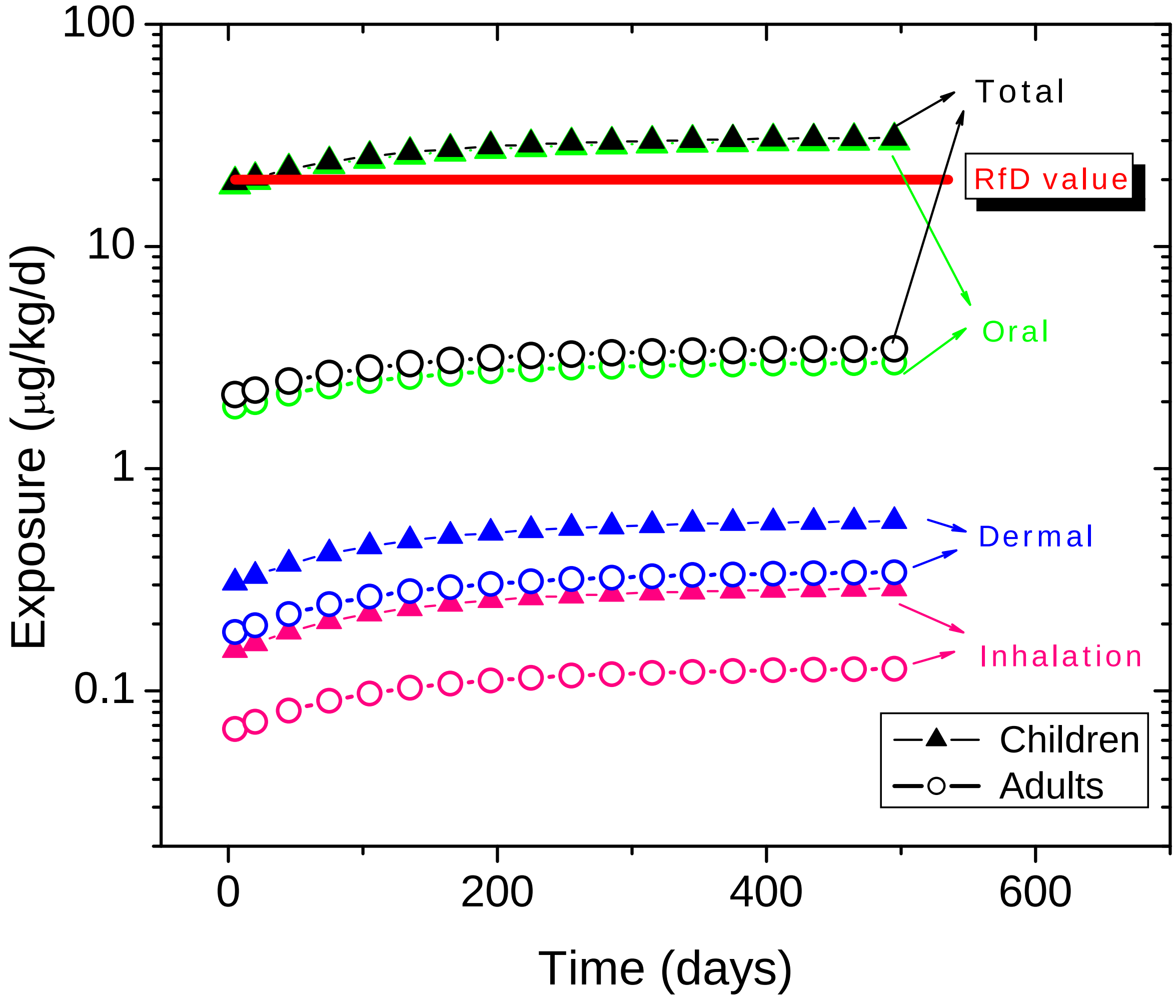


DEHP	References	n	Mean	Max	Our study
Gas phase Conc. ($\mu g/m^3$)	Bauch,1991	40	**0.4**	**1.6**	**0.1~0.18**
	Sheldon et al., 1994	125	**0.14**	**--**	
	Rudel et al., 2003	102	**0.07**	**1.0**	
	Fromme et al., 2004	59	**0.19**	**0.4**	
Dust phase Conc. ($\mu g/g$)	Bauch, 1991	12	**950**	**3100**	**2000~3500**
	Mattulat et al., 2002	600	**1200**	**3500**	
	Rudel et al., 2003	101	**340**	**7700**	
	Fromme et al., 2004	30	**780**	**1800**	

Exposure in Residential Environment

Exposure pathways:

- **Inhalation of vapor and particles**
- **Dermal absorption of DEHP from air**
- **Oral ingestion of household dust**



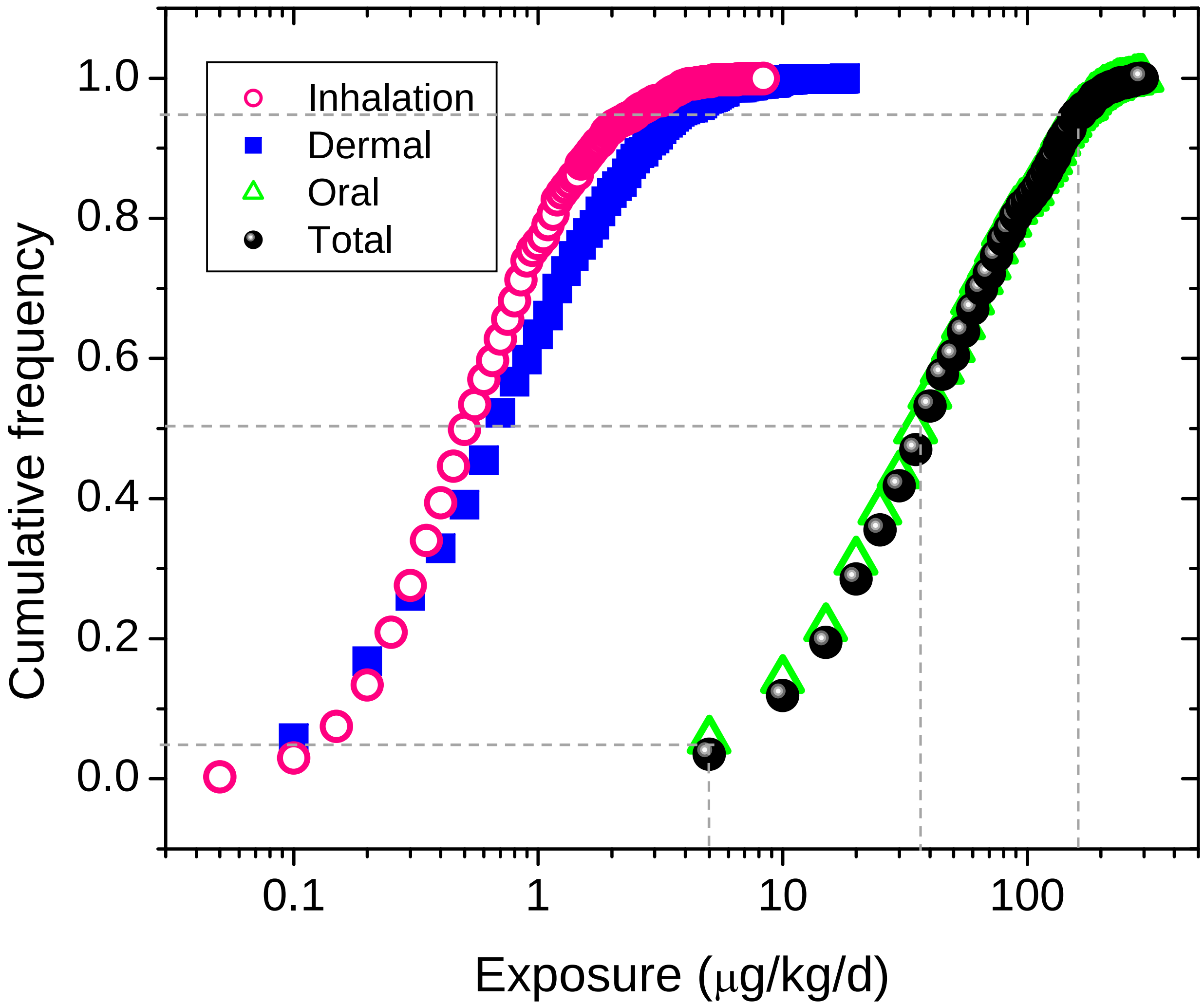
Sensitivity Analysis

Variables	Baseline Value	Exposure pathway			
		Inhalation	**Dermal**	**Oral**	**Total**
DEHP concentration in vinyl floor (C_0, μg/m^3)	2.55×10^{11}	1.00	1.00	1.00	1.00
Vinyl floor thickness (L, mm)	2	0.00	0.00	0.00	0.00
Partition coefficient ($K_{vinyl/air}$)	2.3×10^{11}	-0.50	-0.50	-0.50	-0.50
Mass transfer coefficient for flat surfaces (h, cm/s)	0.1	0.82	0.82	0.79	0.79
Total suspended particle concentration (TSP, μg/m^3)	20	0.07	-0.42	-0.41	-0.41
Partition coefficient ($K_{particle/air}$, m^3/μg)	0.25	0.07	-0.42	-0.41	-0.41
Mass transfer coefficient for particles (h_p, cm/s)	14	0.00	0.00	0.00	0.00
Partition coefficient ($K_{dust/air}$, m^3/g)	21100	0.00	0.00	1.00	0.97
Inhalation rate (IR, m^3/day)	6.8	1.00	0.00	0.00	0.01
Exposure duration in kitchen (ED_1, hr/day)	1	0.07	0.07	--	--
Exposure duration in bathroom (ED_2, hr/day)	0.5	0.05	0.05	--	--
Exposure duration in main house (ED_3, hr/day)	16.5	0.88	0.88	--	--
Skin surface area (SA, m^2)	0.59	0.00	1.00	0.00	0.02
Overall skin permeability coefficient of gases (P, cm/hr)	580	0.00	1.00	0.00	0.02
Daily intake rate of dust (DIR, mg/kg/day)	10.3	0.00	0.00	1.00	0.97
Body weight (kg)	11	-0.50	-0.50	--	--
Air exchange rate for three compartments	0.5	-0.46	-0.46	-0.46	-0.46

Uncertainty Analysis

Variables	Min	Max	References
DEHP concentration in vinyl floor (C_0, μg/m^3)	2.25×10^{11}	6.0×10^{11}	Clausen et al., 2004; Deisinger et al., 1998
Partition coefficient ($K_{vinyl/air}$)	2.05×10^{11}	5.45×10^{11}	--
Mass transfer coefficient for flat surfaces (h, cm/s)	0.03	0.29	Huang et al., 2004; Lin et al., 2004; Carmeliet et al., 2003
Total suspended particle concentration (TSP, μg/m^3)	12	66	Weschler et al. 2007
Partition coefficient ($K_{particle/air}$, m^3/μg)	0.215	0.28	Naumova et al. 2003
Partition coefficient ($K_{dust/air}$, m^3/g)	2000	4×10^4	Rudel et al. 2001; Weschler et al. 2007
Inhalation rate (IR, m^3/day)	5	14.5	Pastenbach, 2000
Exposure duration in main house (ED_3, hr/day)	12.6	18.1	Hubal et al., 2000
Skin surface area (SA, m^2)	0.59	1.7	EPA, 1997
Overall skin permeability coefficient of gases (P, cm/hr)	56	1035	De Dear et al. 1997
Daily intake rate of dust (DIR, mg/kg/day)	1.03	10.3	Wensing et al., 2005
Body weight (kg)	9.15	62.2	EPA, 1997
Air exchange rate for three compartments	0.1	1.1	Wallace et al., 2002
Vinyl flooring area in kitchen (A_{1vinyl}, m^2)	11.9	47.6	Hodgson et al., 2004
Vinyl flooring area in bathroom (A_{2vinyl}, m^2)	5.1	20.4	Hodgson et al., 2004
Vinyl flooring area in main house (A_{3vinyl}, m^2)	2.56	44.8	Hodgson et al., 2004

Uncertainty Analysis



Concluding Remarks

- Several generic models have been developed and rigorously validated
- Initial material-phase concentration is most important model parameter
- Other parameters are either not so important or could be quickly estimated once a few values are known
- Procedures to measure model parameters are available or are being developed
- With some investment, this approach could be applied to rapidly estimate screening-level exposure to wide range of compounds in many materials and products
- Couple with screening-level toxicity estimates from ToxCast to estimate risk and prioritize further action

Key References

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- Little, J. C. Mass Transfer Modeling of Volatile Organic Emissions from Building Materials, National Science Foundation – CAREER Award, 7/15/96 – 6/30/02, BES 9624488.
- Little, J. C. Designing Panelized Systems to Minimize Impact on Indoor Air Quality in Tightly-Sealed Buildings, National Science Foundation – PATH Award, 9/15/01 – 2/28/06, CMS 0122165.
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