Transport of volatile organic molecules through paper

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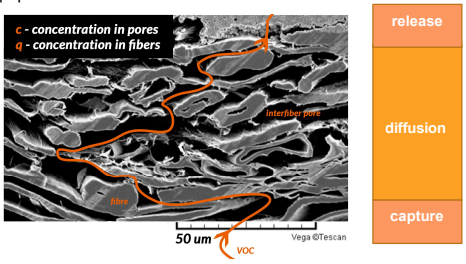
Motivation

- To the date there is lack of context-based numerical models that provide guidance to characterize and predict volatile organic compounds (VOCs) concentrations when transported through cellulose-based materials, i.e., paper
- Therefore, we put our focus on a mathematical model suitable to predict transport process of VOCs through paper
- Paper: **porous material**
- Consists of solid fibrous cellulose-lignin based matrix and interfiber space
- **Transport** of VOCs is possible **over gas** and **solid phase**.



Schematics of VOCs transport through paper, SEM [1]

Aim of the Study

- **Evaluate and understand diffusion of volatile organic compounds (VOCs) through the porous paper matrix**
- **Establish a mathematical model to simulate the VOCs transport**
- **Verify the model for test systems**
- **Understand the role of polar properties of migrants in the transport processes**

Application

- Results will allow to predict amounts of the volatiles transported through paper over a given time
- It will be possible to calculate the amounts of migrants sorbed by fibrous matrix of the paper material
- These results can be used to optimize paper structure at the production stage

Proposed Methodology

Stage I

- **Gain the knowledge about diffusion processes in porous media**
- **Collect data about existing results [2], [3], [4]**
- **Define the main bottle neck problems in application to transport of VOCs through paper**

Defining the crucial parameters influencing the transport process:

- **Diffusion coefficients** – *do we have to distinguish between gas and solid phases?*
- **Sorption constant**
- **Paper porosity**
- **Saturation concentrations** in fibers and interfibrous space
- **Partition coefficients** with environment

Proposing a mathematical description in a form of a PDE system:

$$\epsilon_p \frac{\partial c}{\partial t} = \epsilon_p D_p \frac{\partial^2 c}{\partial x^2} - (1-\epsilon_p)\frac{\partial q}{\partial t}$$ mass conservation

$$\frac{\partial q}{\partial t} = k(q_{sat} - q)$$ uptake by fiber

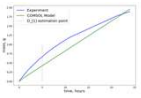
$$c_{environment} * K = c_{paper}$$

$$J_{in} = J_{out}$$ boundary conditions

$$Initial\ conditions$$

ϵ_p - porosity, D_p - diff. coeff. for pores, k – sorption rate, q_{sat} – saturation concentration in fibers, K - partition coefficient, $c_{environment}$ - concentration outside of paper

Verifying applicability of the model for a known system: **water vapor transport** through paper [5]

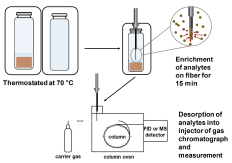


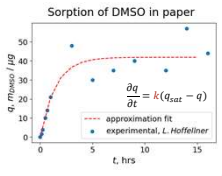
Simulations via commercially available **FEM** packages AKTS, COMSOL **and PINNs**, e.g. DeepXDE [6]

Stage II

Experimental and simulation setups to **determine sorption constants** which are unique for each pair "VOC – paper type"

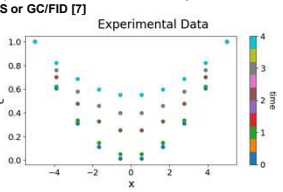
Sorption studies – Solid phase microextraction and **GC/MS or GC/FID***
*Lisa Hoffellner, ACFC TU Graz



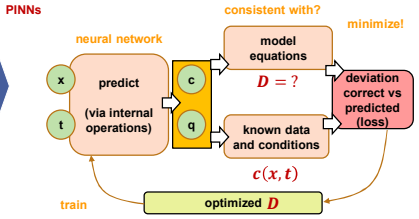


Determination of Diffusion Coefficients is challenging

Obtain **experimental data** on **concentrations** of a migrant in a paper stack **resolved in time and space** domains via **GC/MS or GC/FID [7]**

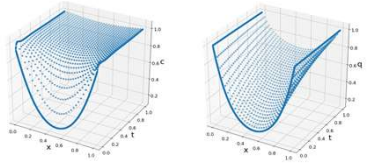


Use the experimental data to derive the Diffusion Coefficients by solving inverse problem



Stage III

Verifying obtained parameters by solving direct problem via simulations



Gas phase and solid phase dimensionless concentrations distributions in space and time

- **Optimizing simulation procedures – by better FEM routines & PINNs**
- **Long time-scale predictions via the model**
- **Testing our approach on further systems of VOCs**
- **Refining and tuning the model**

Questions:

- **How can we optimize paper microstructure to influence the diffusion of VOCs?**
- **Can we make predictions about diffusion of mixtures?**

References

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[2] V.I. Triantafyllou et al., 2005, doi: 10.1016/j.chroma.2005.04.061
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[4] E. Hellen et al., Diffusion through fibre networks, 2002
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[7] L. Hoffellner et al., 2020, doi: 10.35812/CelluloseChemTechnol.2020.54.52

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