Design Project – SIE 2025

EPFL
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Sciences et ingénierie de l'environnement

# GENERATION AND CHARACTERIZATION OF PLASTIC ADDITIVES IN LIQUID AEROSOLS FOR HUMAN TOXICOLOGICAL RESEARCH

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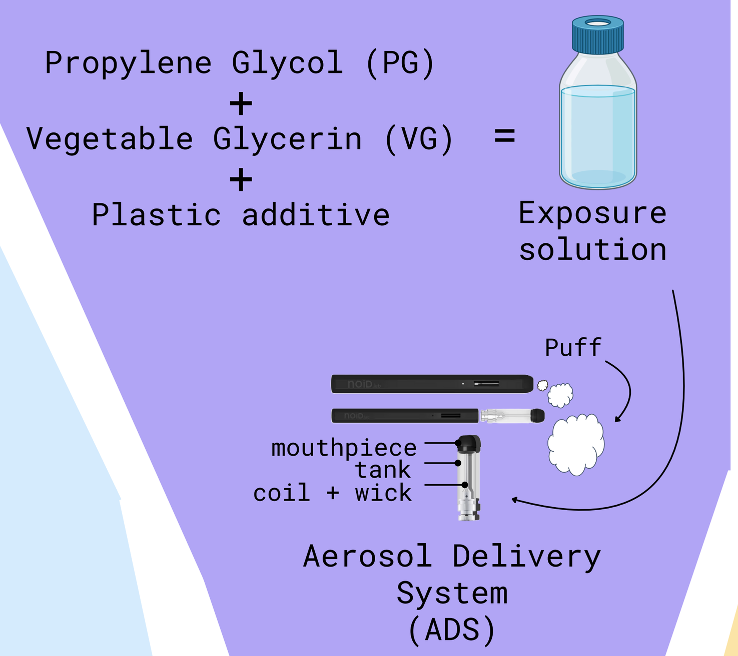
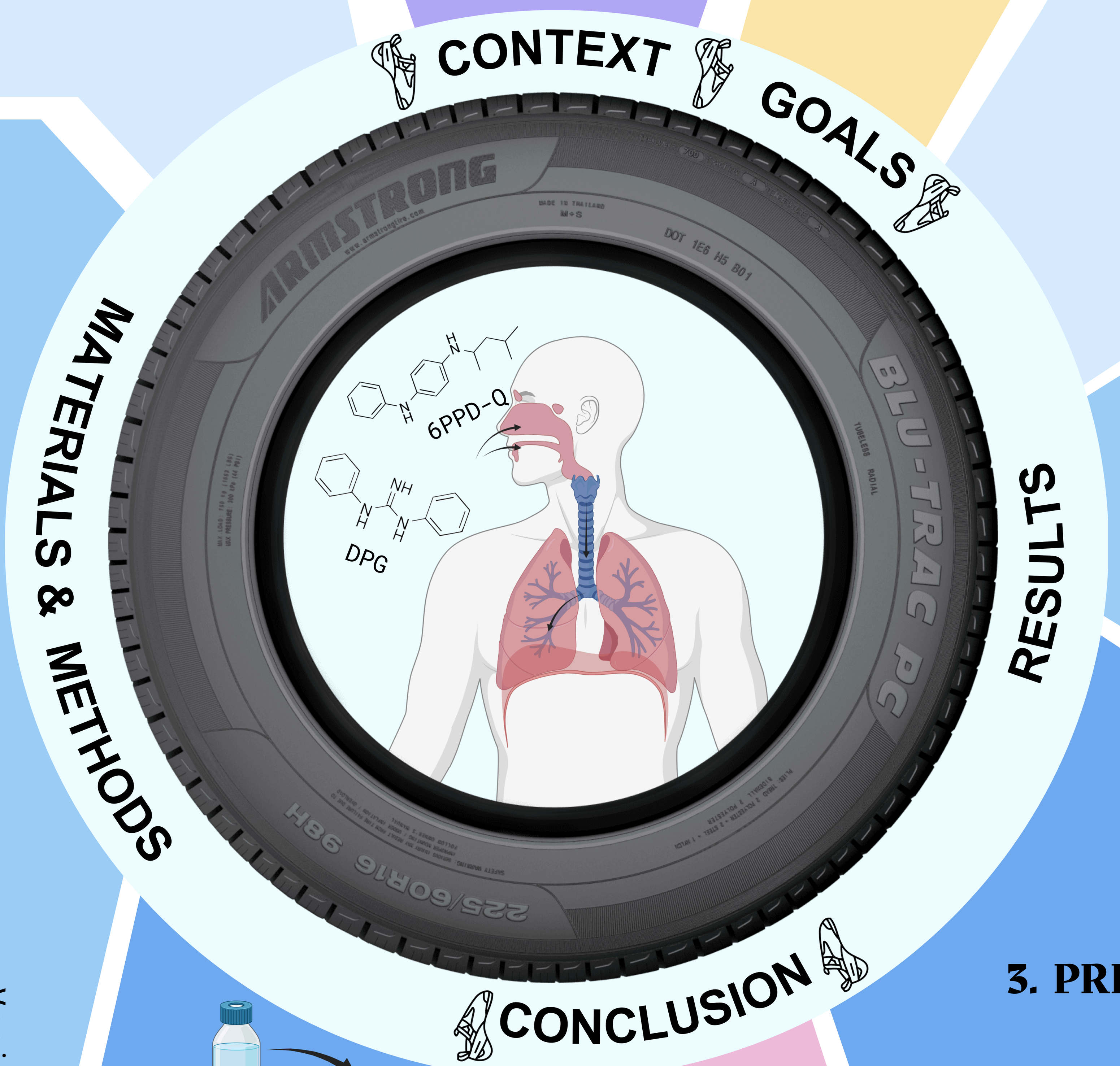
Plastics and rubber often contain chemical additives that can leach into the environment, especially from tire-wear. Among these, 1,3-diphenylguanidine (DPG) and 6PPD-quinone (6PPD-Q) are increasingly detected in air, dust, and human biological samples, yet their behavior following inhalation remains poorly understood. Building on previous studies that successfully simulated inhalation exposure to plastic additives using vaping-based systems, this project aims to generate and characterize aerosols containing newly selected substances. The results will support the design of a safe, controlled toxicokinetic study in human participants.




This study aims to select suitable substances for experimental testing and to answer the following questions:

- **Can aerosolizable exposure solutions be formulated for selected plastic additives using a vaping-based delivery system?**
- **Can these solutions reliably produce aerosols at concentrations relevant for controlled human toxicokinetic studies?**




## MATERIALS & METHODS

### 1. CHOICE OF SUBSTANCES

From a list of substances of tire additives and phthalates, relevant physicochemical properties were collected and analyzed, including boiling point, flash point, decomposition temperature and water solubility.
Five key criteria were used to select the final substances for the study:

1. Boiling point < heating temperature of the ADS
2. Availability in deuterated form
3. Regulatory approval in Switzerland and EU
4. Solubility in vegetable glycerin (VG)
5. Reasonable cost

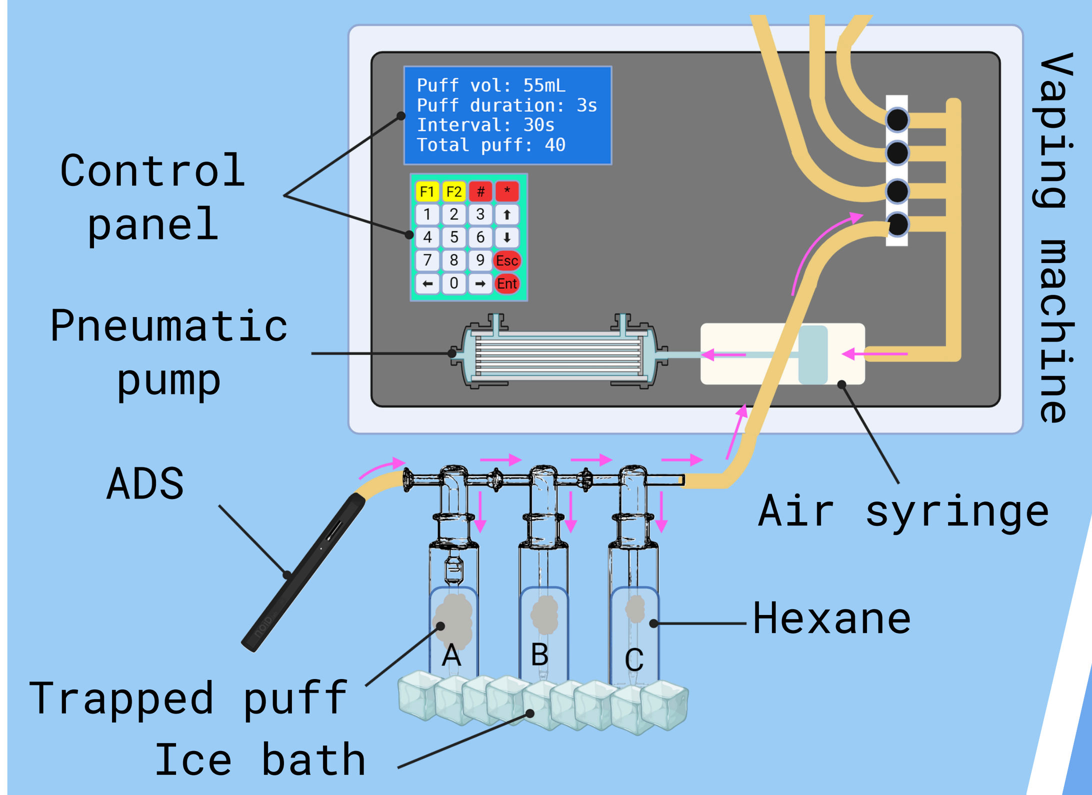
### 2. AEROSOL GENERATION AND QUANTIFICATION

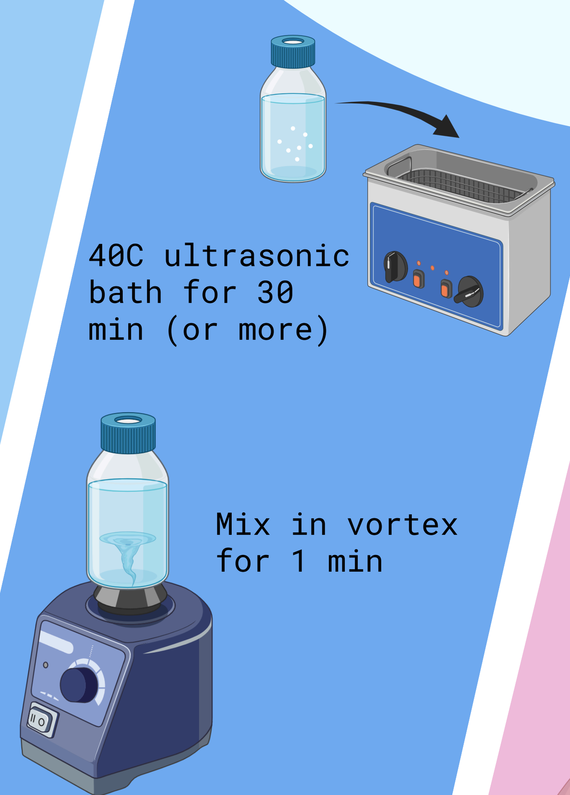
- Preparation of exposure solution with a concentration of 1.94mg DPG/mL 50/50 PG/VG
- Generation of aerosols using 2 ADS
- Quantification of DPG in the hexane with the trapped puffs, the hexane used to rinse the tubes connecting the impingers and the remaining exposure solution in the ADS using GC-MS/MS analysis
- Calculate aerosolization yield of each ADS

$$\text{Aero. yield} = \frac{M^{exp}_{aer}}{M^{theo}_{aer}} = \frac{M^{exp}_{aer}}{M^{i}_{tank} - M^{f}_{tank}}$$

- Calculate theoretical inhaled concentration by human participants

$$\text{Inhaled DPG concentration} = \frac{M^{exp}_{aer}}{40 \times V_{tidal}} \times 50\%$$




### 3. PREPARATION OF EXPOSURE SOLUTION

- **Target concentration** was defined based on literature data, selecting the highest indoor air value detected in the lower respiratory tract fraction of a bouldering hall
- **Aerosolization medium** was an 80/20 VG/water mix, replacing PG with water to reduce respiratory irritation, while maintaining sufficient solubility
- **Inhalation assumption**: 50% of inhaled particles were assumed to reach the lower lungs
- **Concentration calculation** was based on target air levels, tidal value, puff count, aerosolization yield and VG volume in the device tank
- **Yield assumption**: the lowest observed yield (3%) from DPG aersolization testes with NoidLab devices was used for conservative estimation
- **Preparation method** involved serial dilution due to balance sensitivity limits, using vortex and ultrasonic bath for dissolution, followed by dilution with water to reach the final 80/20 ratio

## RESULTS

### 1. CHOICE OF SUBSTANCES

DPG and 6PPD-Q were chosen based on their properties and for their environmental relevance, known toxicity to aquatic organisms, growing concern regarding potential human inhalation exposure and absence of OEL values.

**DPG** is a vulcanization accelerator, it enhances elastic properties of rubber

**6PPD-Q** improves durability, prevents cracking and prolongs life of rubber

### 2. AEROSOL GENERATION AND QUANTIFICATION

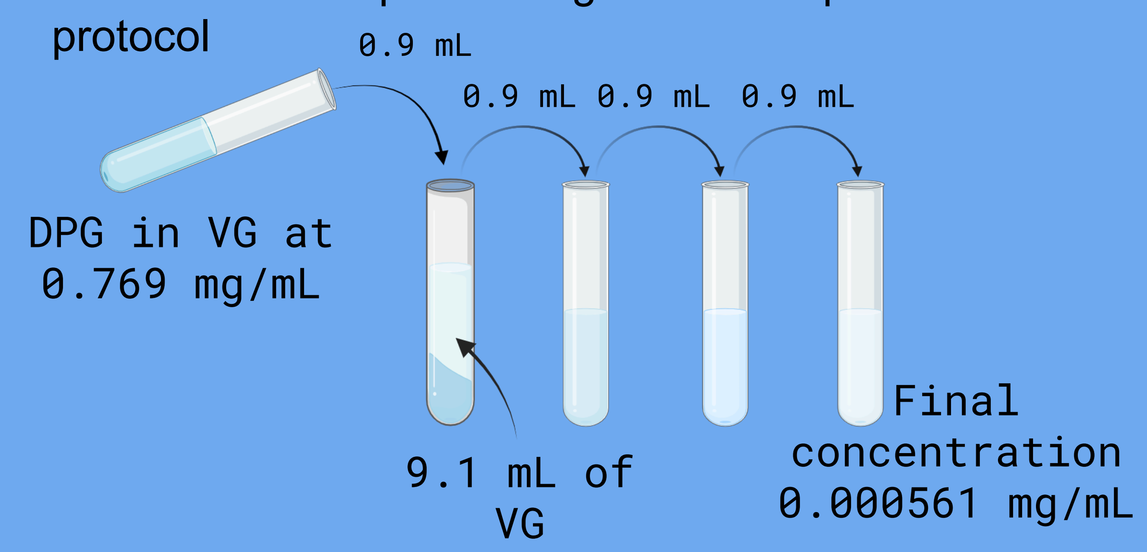
DPG was successfully aerosolized by both ADSs.

| | ADS 1 | ADS 2 |
|---|---|---|
| Aero. yield | 0.03% | 0.05% |
| Inhaled DPG concentration [mg/m3] | 0.00763 | 0.01150 |

### 3. PREPARATION OF EXPOSURE SOLUTION

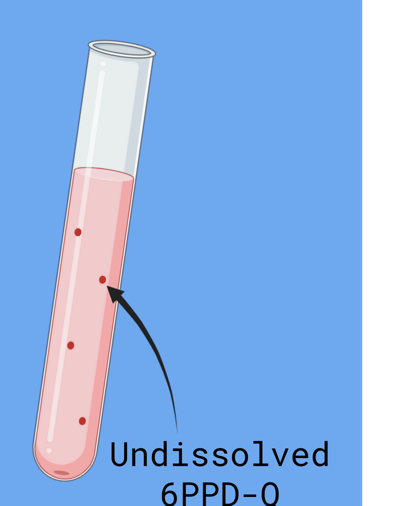
#### DPG

- The required concentration of DPG in the VG fraction was calculated to be 0.000561 mg/mL
- A complete dissolution in the final 80/20 VG/water mixture was achieved implementing a three-step serial dilution protocol

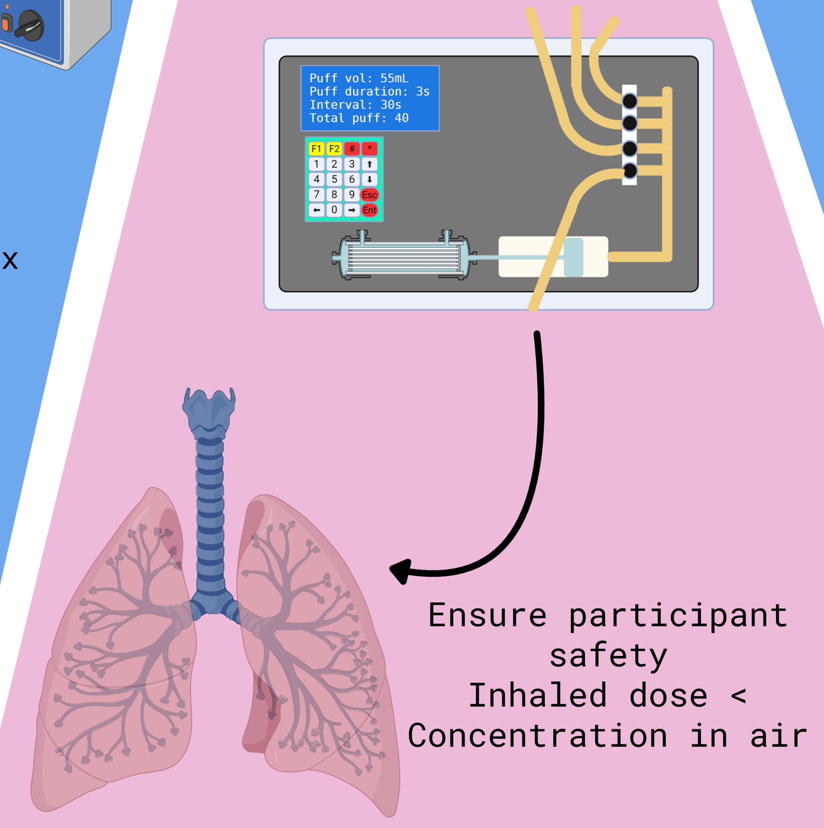



#### 6PPD-Q

- The required concentration of 6PPD-Q in the VG fraction was calculated to be 0.000106 mg/mL
- Dissolution was attempted using heating and vortexing, but the compound did not fully dissolve, even after increasing temperature and VG volume
- The process was interrupted due to a shortage of VG
- Future steps: the sample was stored for future dilutions and toxicological tests




## CONCLUSION




- The project showed that the vaping-based system can simuate inhalation of tire-derived additives
- DPG was succesfully aerosolized and measured
- 6PPD-Q was tested for dissolution in VG, but solubility in VG/water is still unclear. Its aerosolization with the vaping machine hasn't been tested yet
- Next steps include measuring aerosol particle size to assess lung deposition.
- This work supports future toxicology studies on airborne micropollutants