Project presentation

Mass Transfer Innovation Project

Group-3

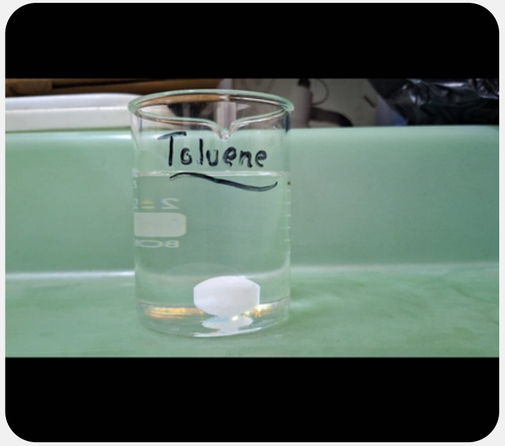
Origin of the creative idea

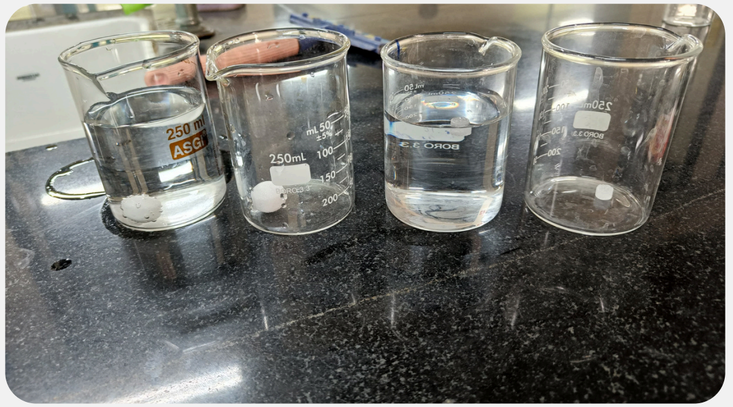
Our creative idea was to take a topic from theory—the diffusion of a solid ball into a solvent—and turn it into something that's easy to see and understand. By combining **recorded videos** of actual experiments with **MATLAB simulations**, we made a simple and visual way to compare what happens in reality with what the formulas say should happen.

We hope that this approach can be **shown to future batches** as a helpful tool. Instead of just reading about mass transfer and diffusivity in textbooks, they can watch it happen and then compare it with a computer model.
This makes learning more interactive, clear, and interesting, and can help others understand the concept just like it helped us.

Experimental Setup

- Number of Beakers: 6
  - Each beaker contained a different medium.
- Ball sizes were measured using a circular gauge.
- Naphthalene ball size(Average): 16.33 mm (vertical), 19.13 mm (horizontal)
- Camphor ball size(Average): 5.95 mm (vertical), 9.00 mm (horizontal)
- Solvents for Naphthalene Balls:
  - MIBK (Methyl isobutyl ketone)
  - Toluene(Rectified)
  - Decane
- Solvents for Camphor Balls:
  - Ethanol
  - Water
  - Air (open beaker for sublimation observation)
- Recording Method:
  - 3 Smartphones were used to record the dissolution/sublimation process from top and side angles, enabling accurate tracking of mass transfer over time.





Project Development Process

01

We first chose solvents that showed reasonable solubility for both camphor and naphthalene balls, ensuring they would be suitable for the dissolution process.

02

We video-taped the dissolution process to accurately track the rate of mass transfer over time.

03

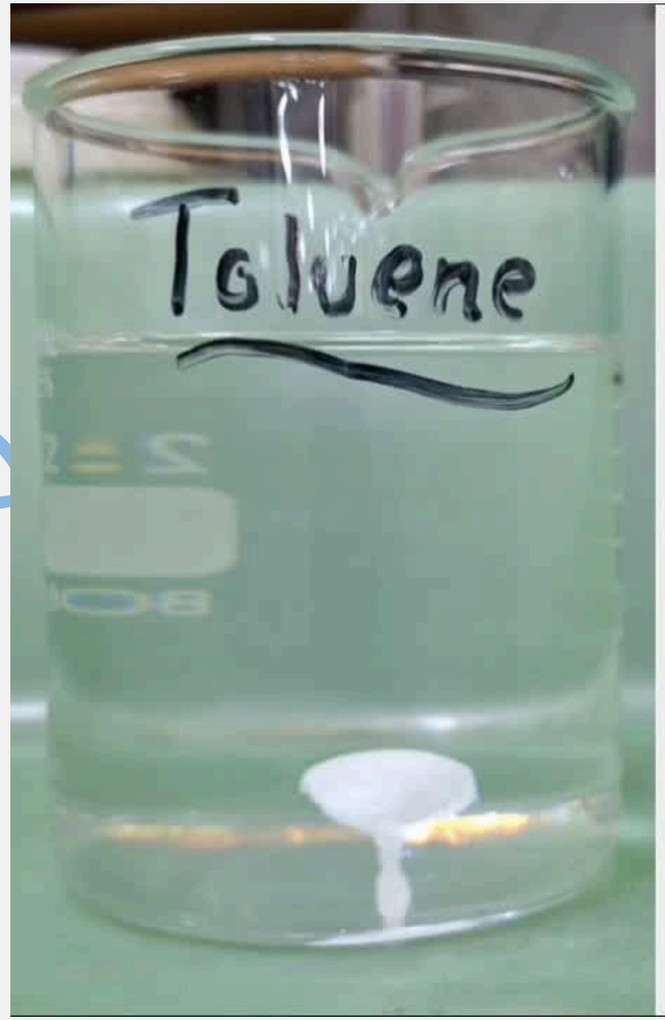
Using theoretical Dab values available online, we coded a simulation to model the mass transfer process and predict expected outcomes.

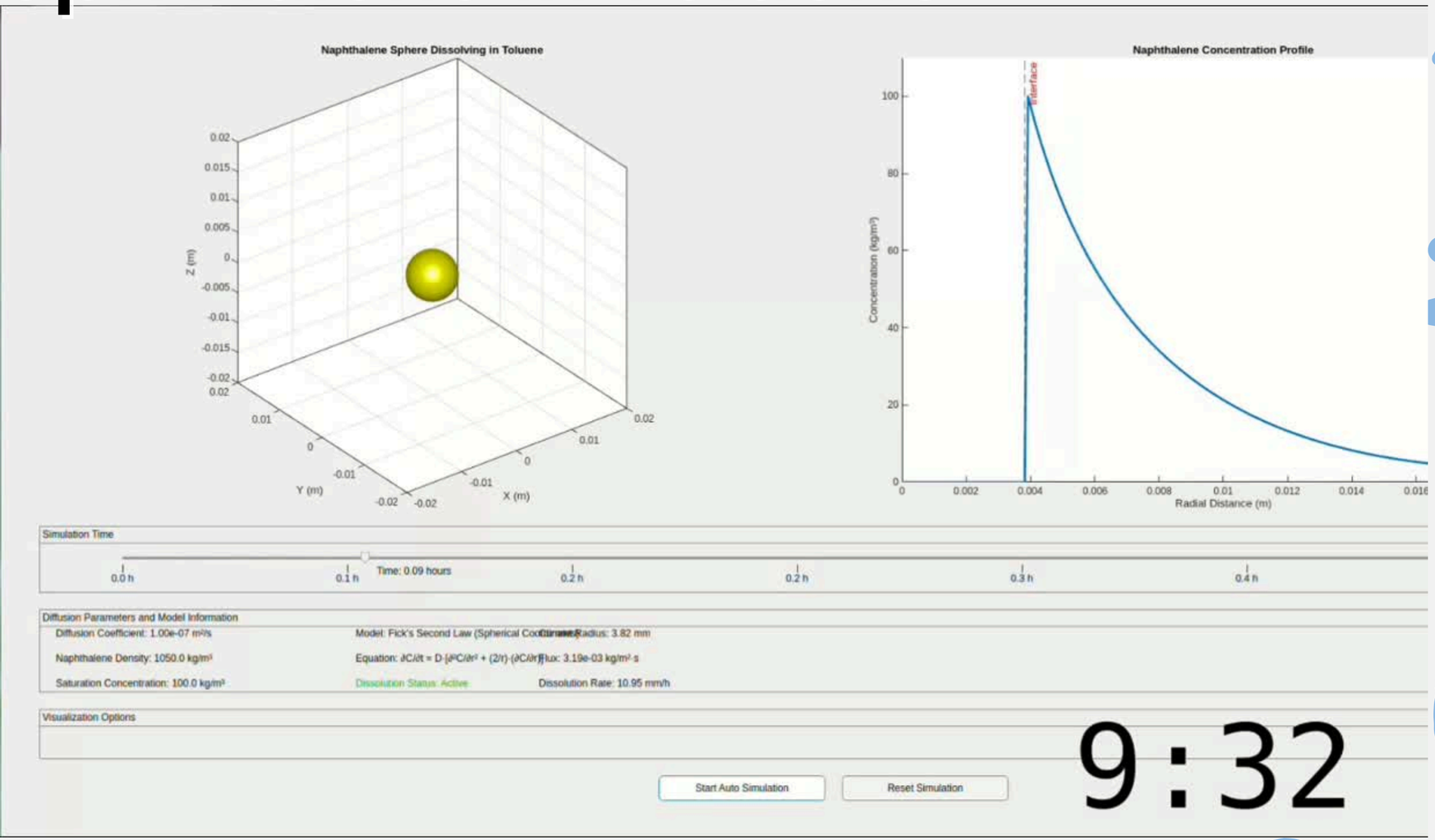
04

Finally, we compared our experimental results with the simulation to validate the accuracy of our findings and check if the observed dissolution rates aligned with the theoretical models.

OBSERVATIONS

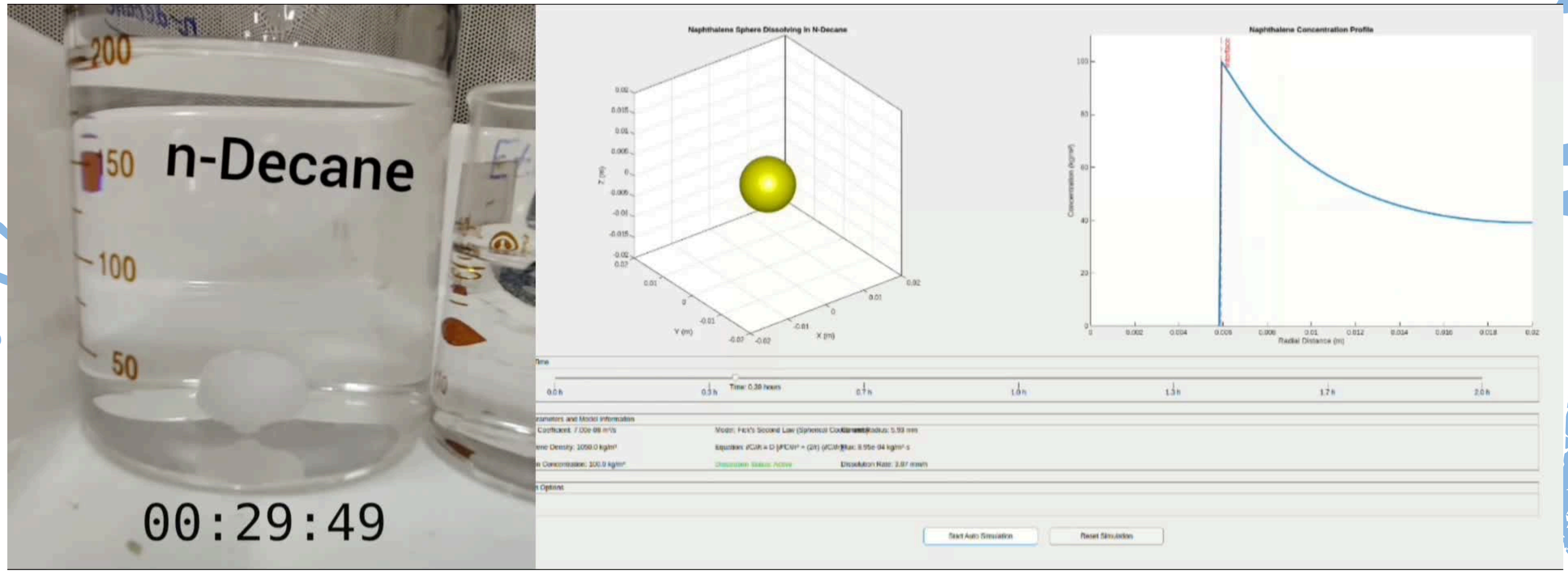
Naphthalene in Toluene





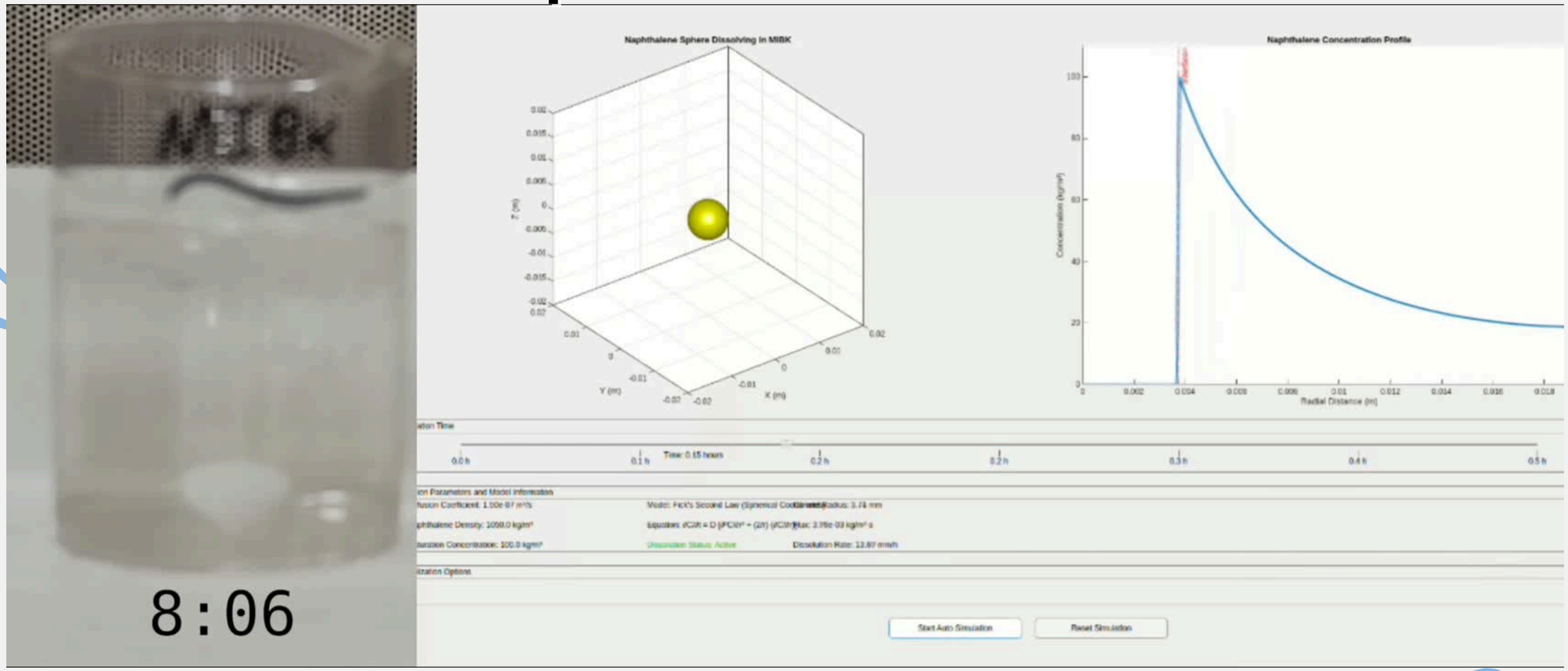
Speed up by 80x

Naphthalene in n-Decane



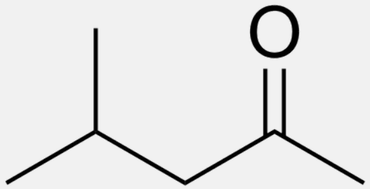
Speed up by 250x

Naphthalene in MIBK



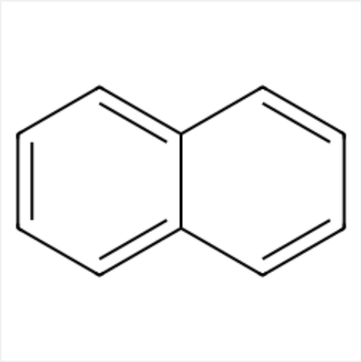
Speed up by 50x

Possible Explanations

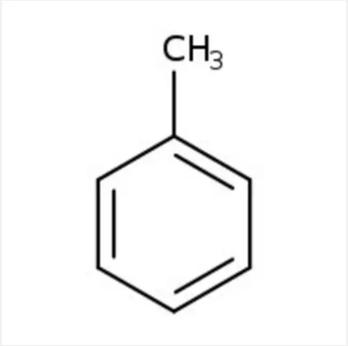


MIBK
(Polar)

Fastest

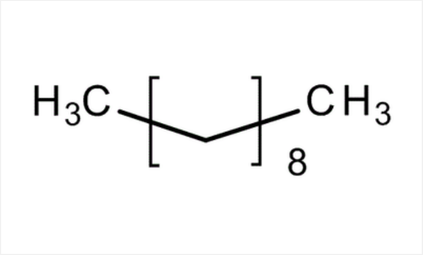


Naphthalene
(Non-Polar)



Toluene
(Slightly Polar)

Slower



n-Decane
(Non-Polar)

Slowest

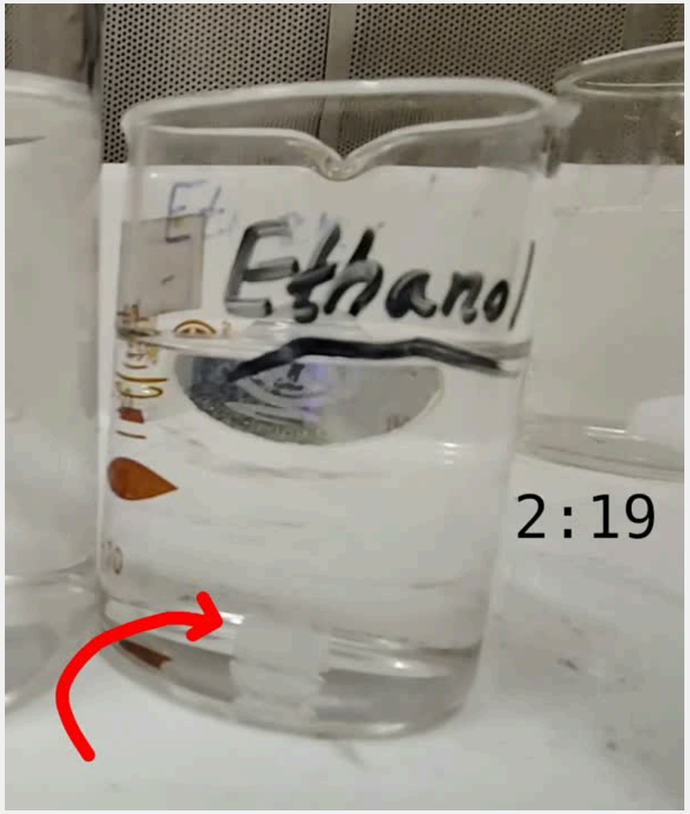
Generally, non-polar compounds should be soluble in non-polar compounds. Then why slowest in n-decane?

Case of n-Decane

N-decane is a relatively large and linear hydrocarbon. No pi-electrons => no pi-pi stabilisation. It dissolves faster in toluene due to this pi-pi interaction.

n-Decane has a higher viscosity (~0.92 cP at 25°C) compared to toluene (~0.59 cP) and MIBK (~0.66 cP). Higher viscosity can impede molecular diffusion, slowing down the dissolution process.

Camphor in Ethanol



Speed up by 30x

- **Simulation ?**

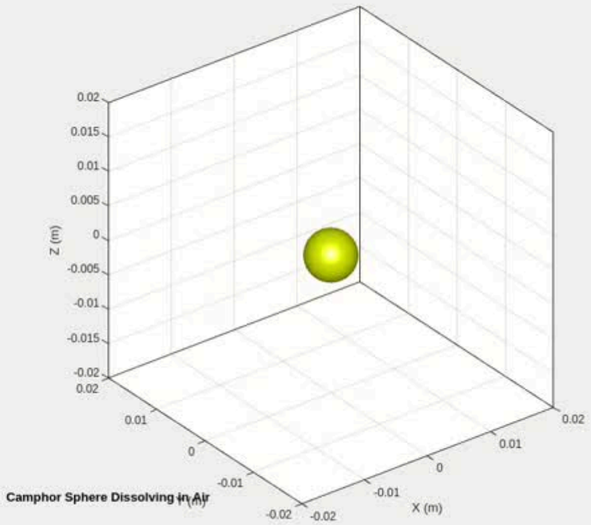
We ran into a very fundamental problem of numerical instability while simulating this case.
Will be discussed later in the slides.

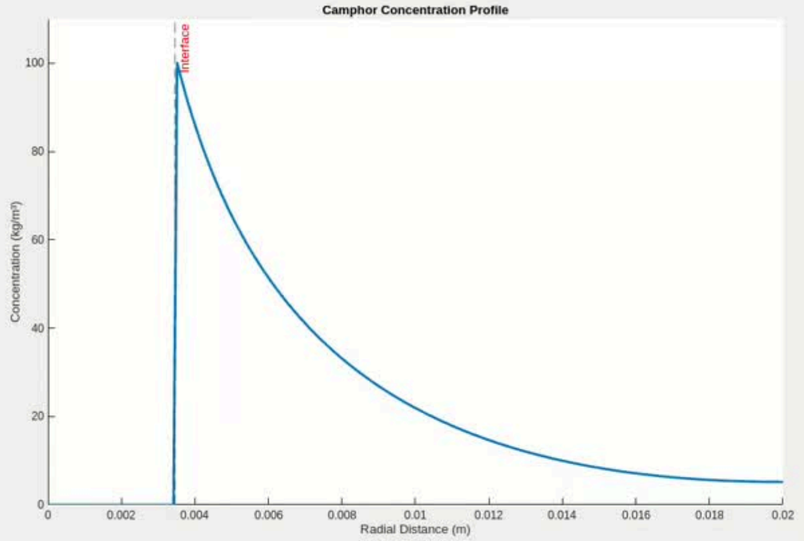
Camphor in Water and Air

We were unable to effectively record the dissolution and sublimation of camphor in water and air, respectively, because both processes occur at extremely slow rates under ambient conditions.

So we just took the readings of the camphor in water and air for 2-3 days and simulated the process based upon that.

Camphor in Air





Simulation Time

0.0 h | 8.0 h | Time: 11.52 hours | 16.0 h | 24.0 h | 32.0 h | 40.0 h | 48.0 h

Diffusion Parameters and Model Information

Diffusion Coefficient: 1.00e-09 m²/s | Model: Fick's Second Law (Spherical Coordinates) | Radius: 3.47 mm

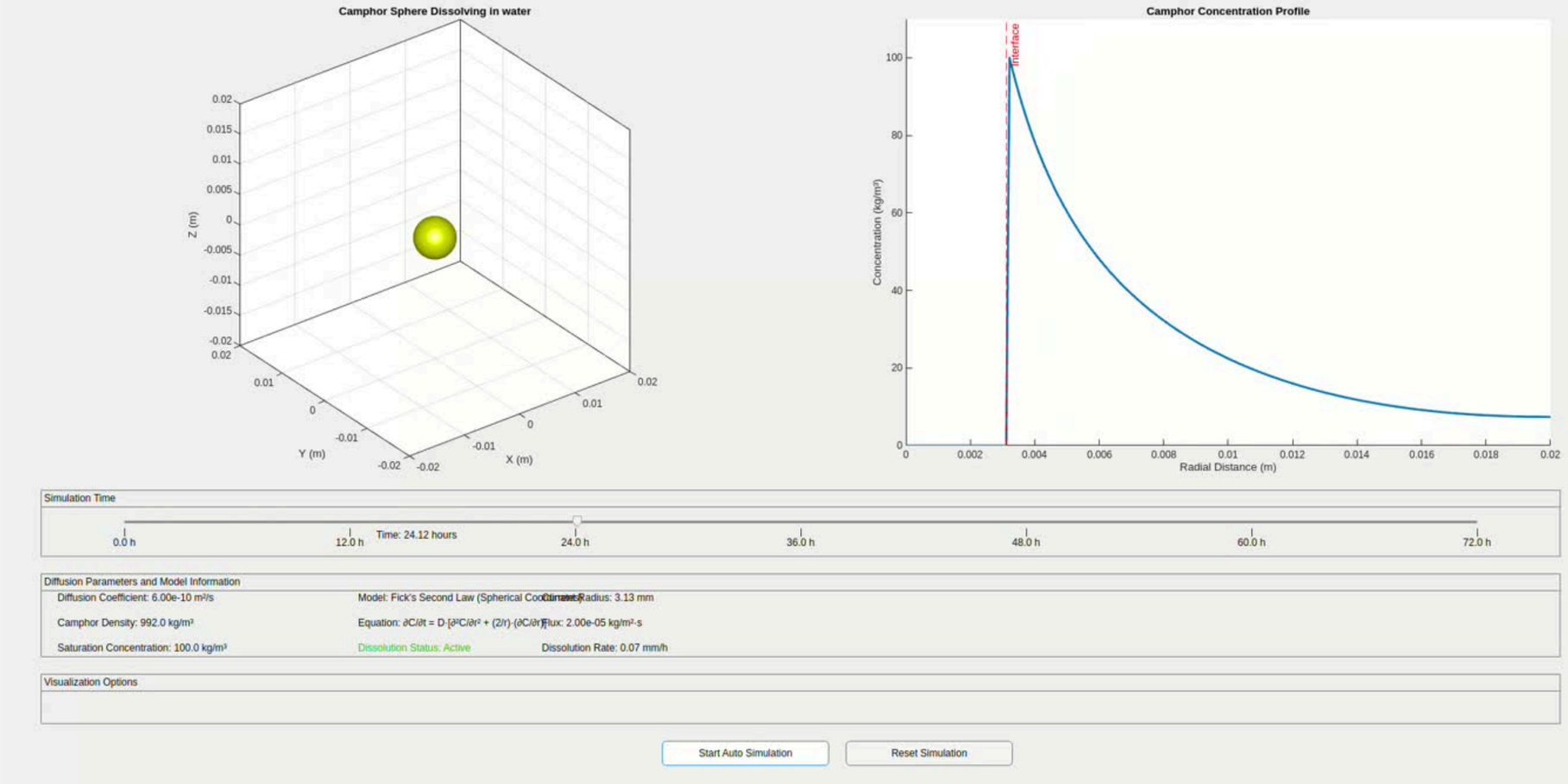
Camphor Density: 992.0 kg/m³ | Equation: $\partial C/\partial t = D\cdot[\partial^2 C/\partial r^2 + (2/r)\cdot(\partial C/\partial r)]$ | Flux: 3.20e-05 kg/m²·s

Saturation Concentration: 100.0 kg/m³ | Dissolution Status: Active | Dissolution Rate: 0.12 mm/h

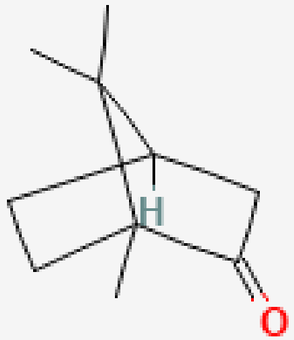
Visualization Options

Start Auto Simulation | Reset Simulation

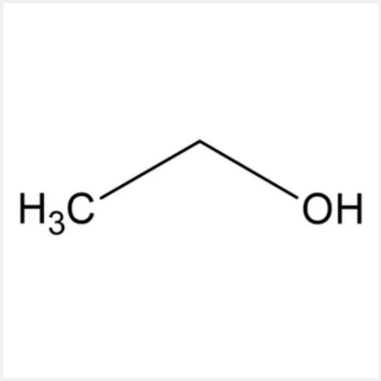
Camphor in Water



Possible Explanations

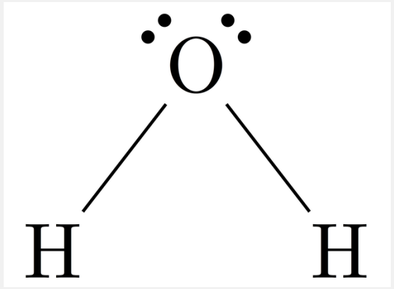


Camphor
(Polar)



Ethanol
(Polar)

Very Fast



Water
(Polar)

Very Slow

Both Ethanol and Water are polar compounds, then why so much difference in solvation time?

Case of Water and Ethanol

Ethanol is a polar solvent but also has a nonpolar ethyl group. This amphiphilic nature enables it to dissolve both polar and nonpolar substances. Camphor, with its nonpolar hydrocarbon framework and polar carbonyl group, is well accommodated by ethanol's solvent properties.

Whereas water is strongly repelled by the hydrophobic organic part of camphor.

Simulation of Fick’s Law

Built a numerical solver of Fick’s 2nd law in spherical coordinates and check whether its predicted radius–vs.–time curve matches our experiments text

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right)$$

Fick’s Law in Spherical Coordinate

Assumptions

1. **Spherical Symmetry** – We took the **horizontal and vertical diameters** of Napthalene and Camphor balls, then using **surface area comparison assumed an equivalent Sphere.**

$$V_{\text{cyl}} = \frac{4}{3}\pi R_{\text{eq}}^3 \quad \Longrightarrow \quad R_{\text{eq}} = \left(\frac{3\,V_{\text{cyl}}}{4\pi}\right)^{1/3}.$$

2. **Constant Physical Properties**

3. **No Convection or Bulk Flow**

Challenges Faced

Due to **stability issues in explicit method.** We needed to choose our “dt” very carefully.

$$\Delta t \leq \frac{\Delta r^2}{2\,D}$$

$$N_{\text{steps}} = \frac{t_{\max}}{\Delta t}$$

Due to which when we simulated the dissolution of **camphor in ethanol** , we needed our **“dt “ to be very less** which raised storage issues due to which we couldn’t simulate it

Further , we can use **implicit methods** to further optimize our approach and tackle **these stability issues .**

Comparison Results

1. **Naphthalene Dissolution**: Toluene dissolved naphthalene fastest due to π-π stacking and low viscosity (~0.59 cP); MIBK was intermediate; n-decane was slowest due to high viscosity (~0.92 cP).
2. **Camphor in Ethanol**: Camphor dissolved rapidly in ethanol, as its amphiphilic hydroxyl and ethyl groups stabilize camphor's polar and nonpolar parts.
3. **Camphor in Water**: Camphor showed minimal dissolution in water, whose hydrogen-bonding network repels camphor's hydrophobic regions.
4. **Camphor Sublimation**: Camphor sublimated gradually in air, with mass loss driven by vapor pressure and gaseous diffusion.

Conclusion

- Viscosity Over Polarity: n-Decane’s high viscosity (~0.92 cP) slowed naphthalene dissolution despite polarity matching, outweighing solubility predictions.
- π-π Stacking Boost: Toluene’s π-π interactions with naphthalene accelerated dissolution, creating a fast pathway out of the solid phase.
- Ethanol’s Amphiphilic Advantage: Ethanol rapidly dissolved camphor by stabilizing both its polar carbonyl and nonpolar hydrocarbon parts, unlike water’s negligible effect.

- **Dissolution Rankings: Naphthalene dissolved fastest in MIBK, moderately in Toluene, slowest in n-decane; camphor was fastest in ethanol, negligible in water, and gradually sublimated in air**.

Thank you very much!

Group-3