



HAL
open science

SWCNT functionalised with poly(vinyltriazole): a method to determine the optimal stoichiometry through adsorption kinetics and isotherms

Leshan Usgodaarachchi, Eleftheria Zelou, Nicolas Battaglini, Samia Zrig, Benoît Piro, Bérengère Lebental

► To cite this version:

Leshan Usgodaarachchi, Eleftheria Zelou, Nicolas Battaglini, Samia Zrig, Benoît Piro, et al.. SWCNT functionalised with poly(vinyltriazole): a method to determine the optimal stoichiometry through adsorption kinetics and isotherms. 2024 Spring Meeting of the European Materials Research Society (E-MRS), May 2024, Strasbourg, France. 393, 2020, 10.1016/j.jhazmat.2020.122383 . hal-04605905

HAL Id: hal-04605905

<https://hal.science/hal-04605905v1>

Submitted on 8 Jun 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

SWCNT functionalised with poly(vinyltriazole): a method to determine the optimal stoichiometry through adsorption kinetics and isotherms

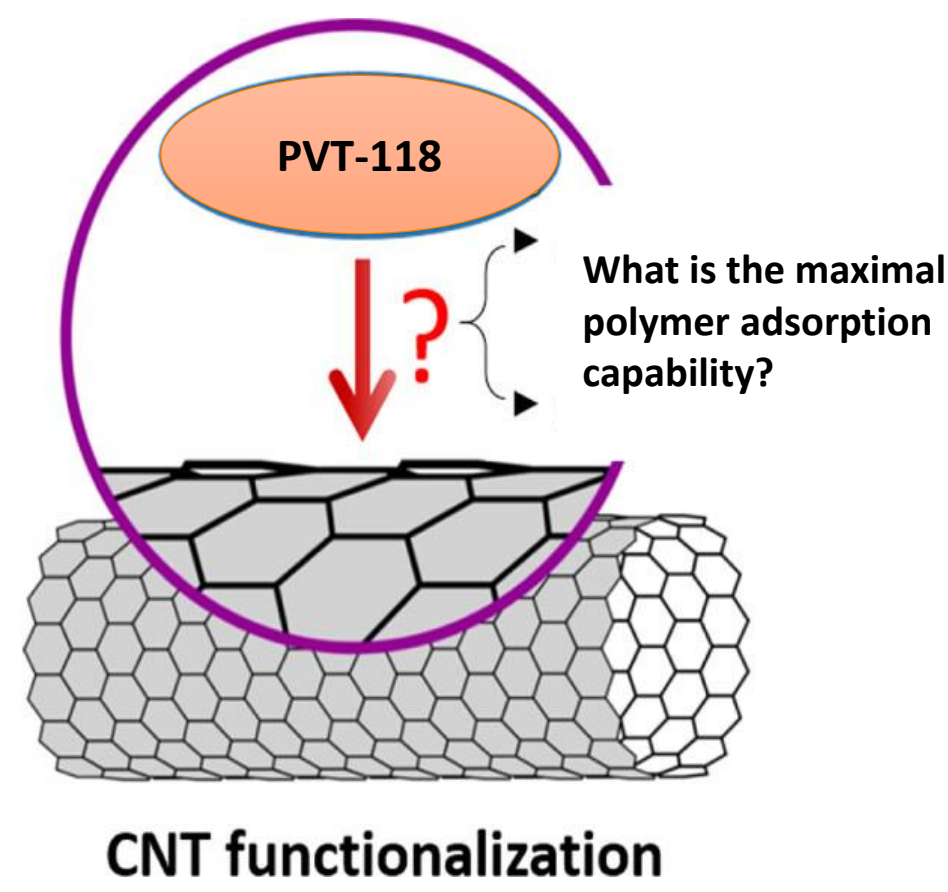
Leshan Usgodaarachchi^{1,2}, Eleftheria Zelou², Nicolas Battaglini², Samia Zrig², Benoit Piro², Bérengère Lebental^{1,*}

¹ IMSE (Laboratoire Instrumentation, Modélisation, Simulation Et Experimentation) - Université Gustave Eiffel

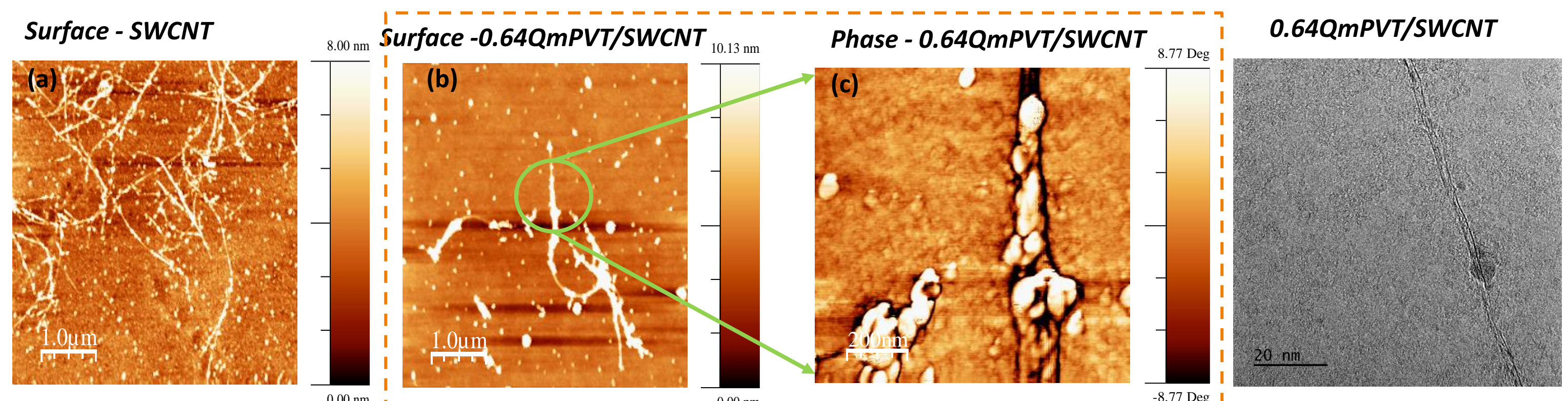
² ITODYS (Interfaces – Traitement – Organisation et Dynamique des Systèmes) – Université Paris Cité

1. Why the study of Polymer:SWCNT stoichiometry is important for optoelectronic applications?

- Excess of polymer compared to the available CNT binding sites leads:
 - Polymer aggregation by intermolecular coiling
 - Low electrical performance due to high contact resistance
- Excess of SWCNT leads to free binding sites
 - Lack of sensitivity
 - Lack of selectivity

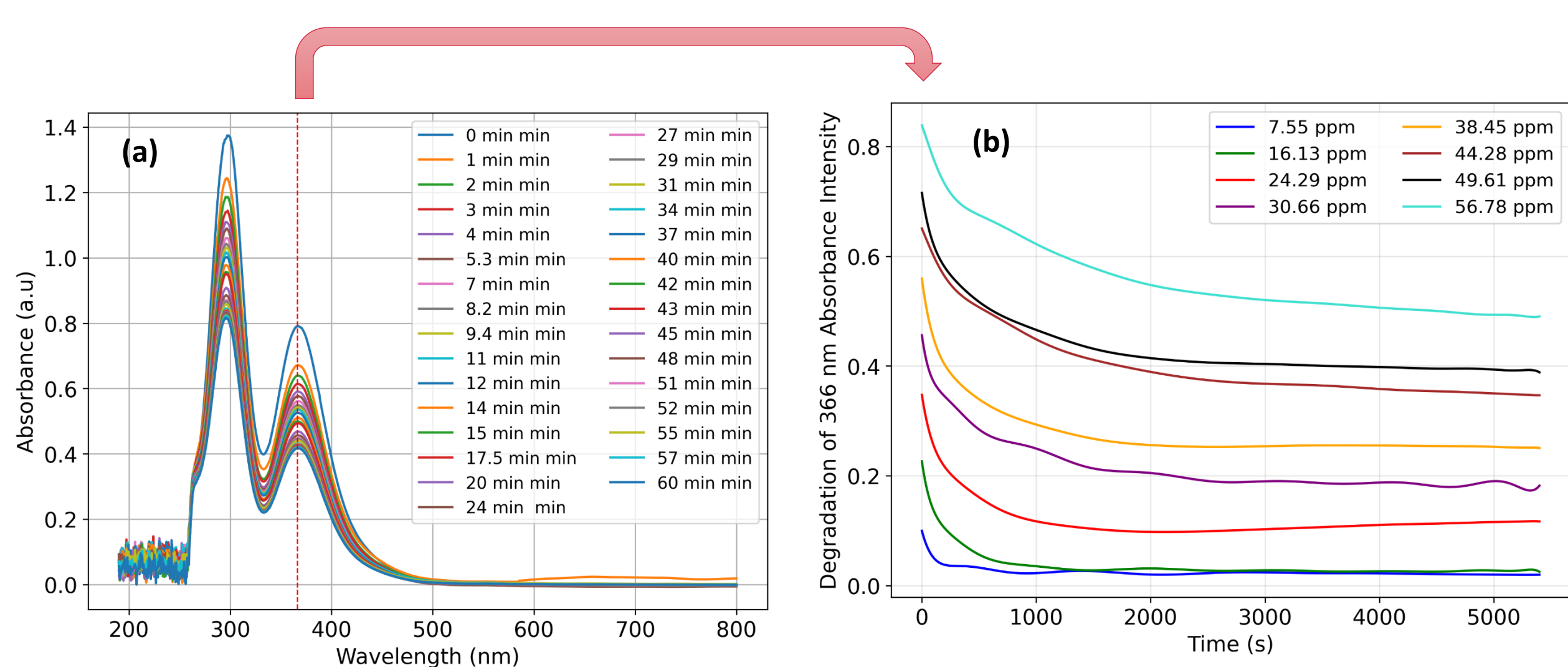


2. 1 Surface Morphology



- TEM diameter of SWCNT is 0.60 nm
- TEM diameter of 0.64QmPVT/SWCNT is 2.79 nm

2.2. Evolution of Absorbance as a function of time

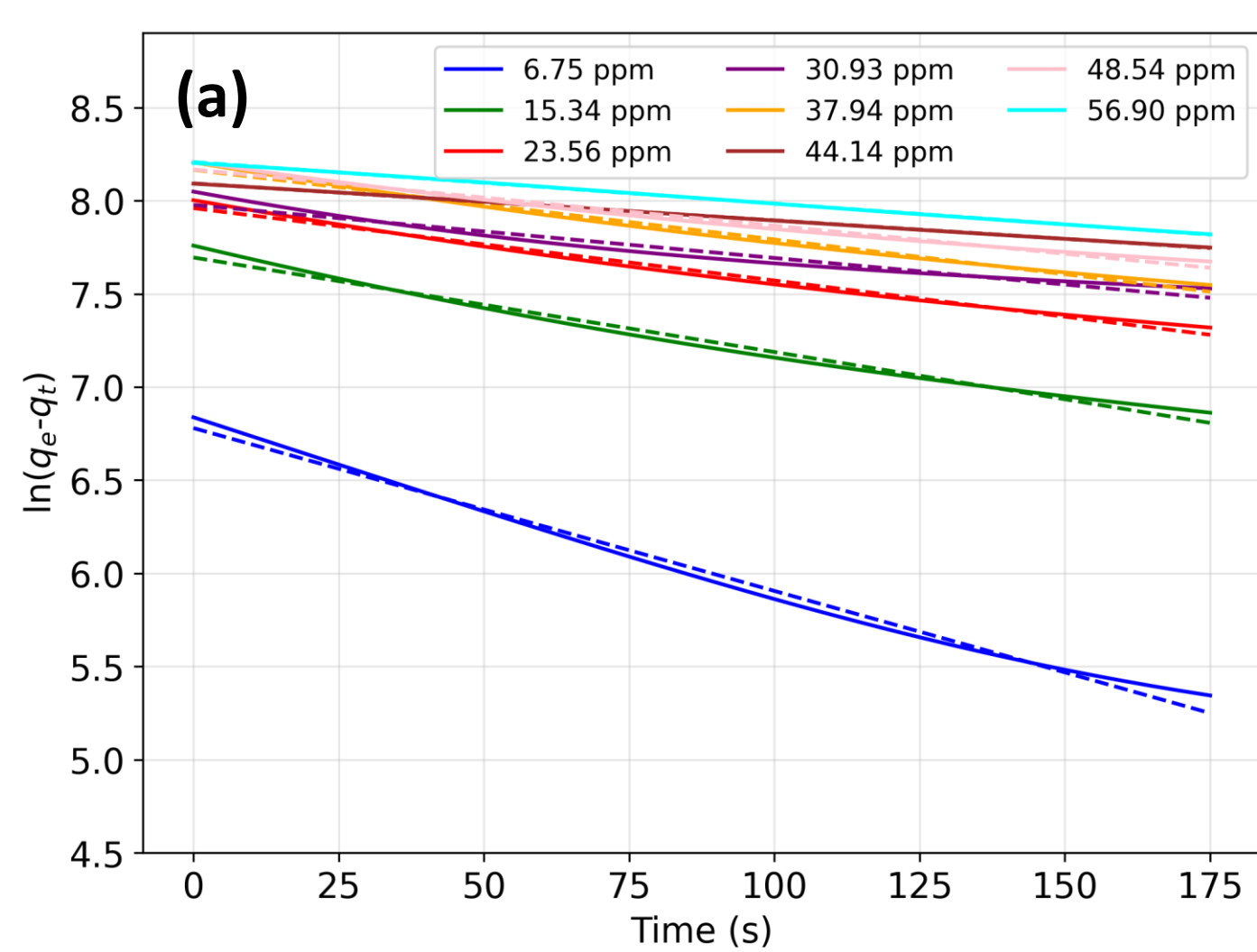


- Absorption spectra of PVT-118 (a) show two peaks at 295 nm (assigned to the poly(vinyl) chain) and 366 nm (assigned to the triazole groups)
- 366 nm peak is a good marker because PVT-118 interacts with SWCNT through the triazole groups by π -stacking

2.3 Kinetics models for understanding the dynamics

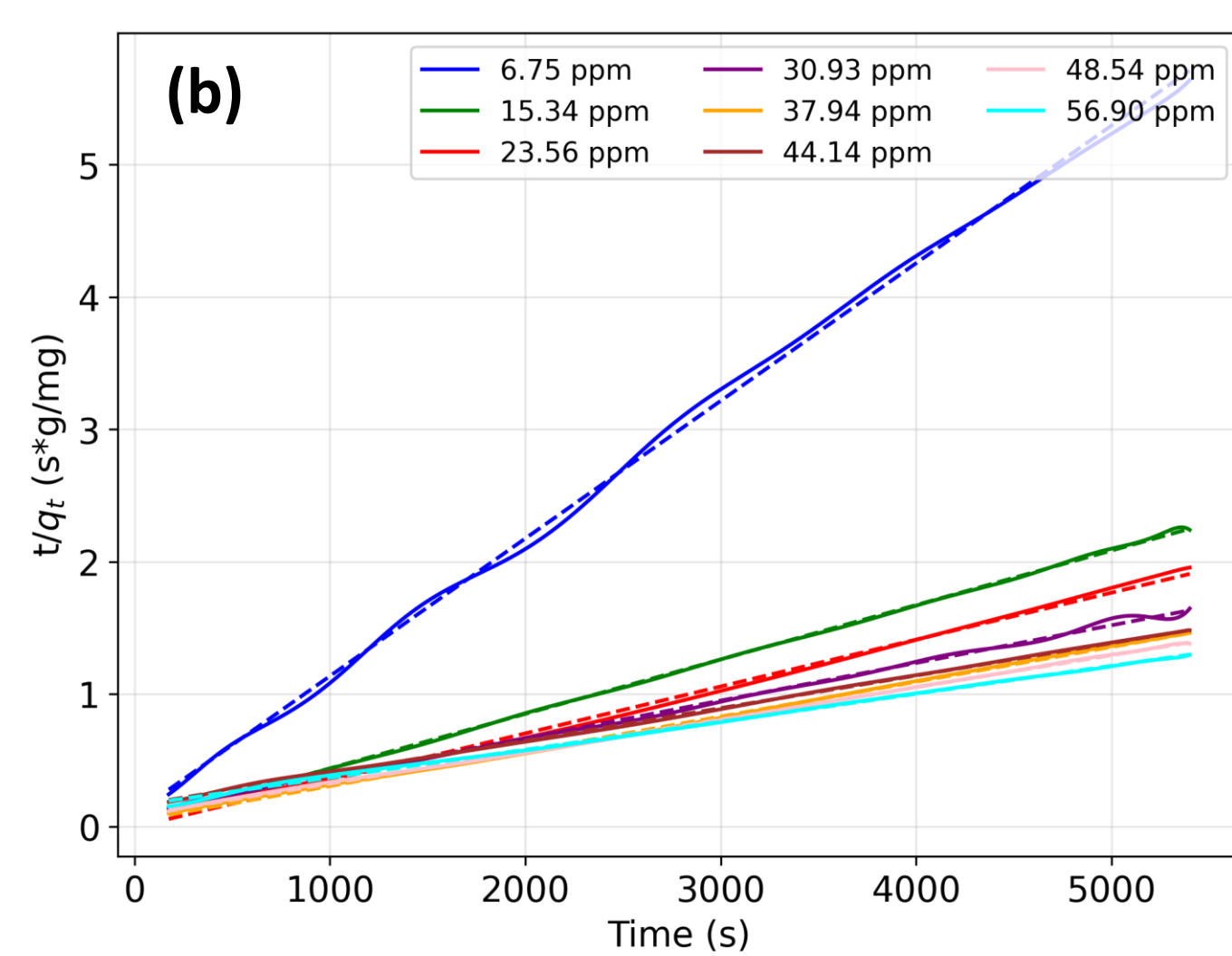
Pseudo-first-order kinetics model

$$\ln(q_e - q_t) = \ln q_e - k_1 t$$



Pseudo-second-order kinetics model

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \left(\frac{1}{q_e}\right) t$$

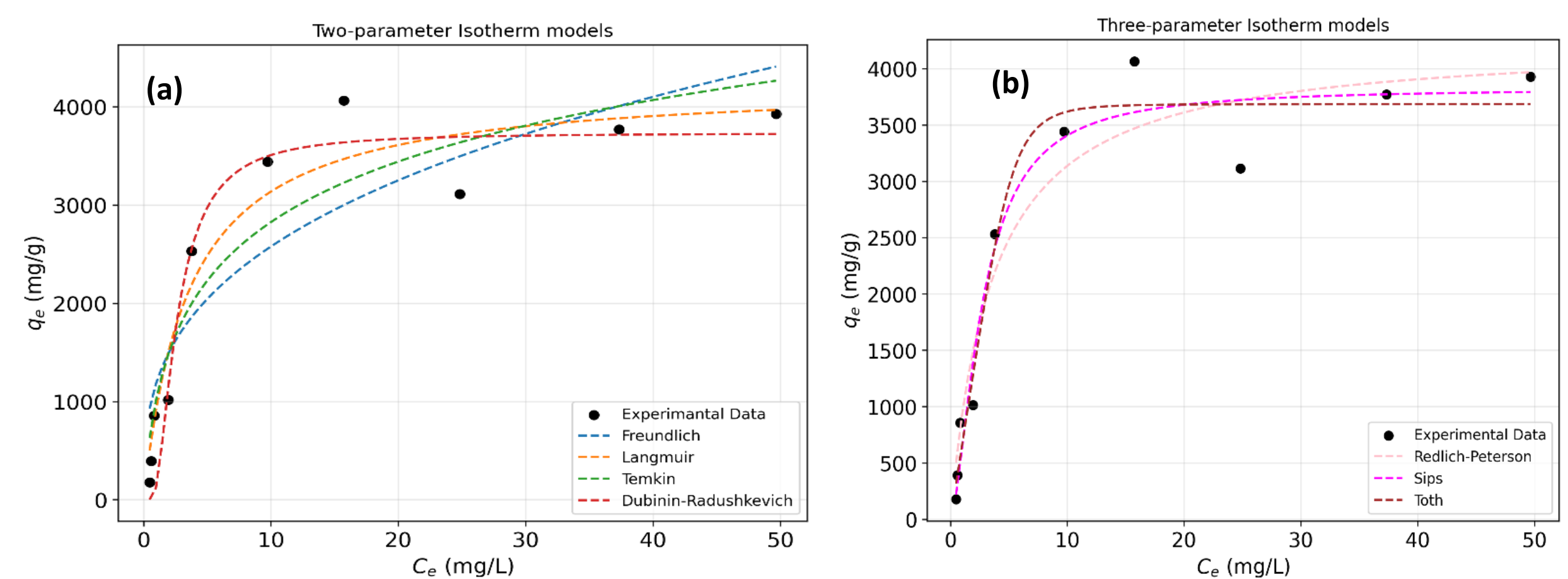


- q_e - mass of polymer at equilibrium per unit mass of SWCNT ($mg.g^{-1}$)
- q_t - mass of polymer at time t per unit mass of SWCNT ($mg.g^{-1}$)
- k_1 - first-order adsorption rate constant (s^{-1})
- k_2 - second-order adsorption rate constant ($g.mg^{-1}.s^{-1}$)
- t - time (s)
- C_0 - Initial concentration (mg/L)
- C_t - Concentration at time t (mg/L)
- m - mass of the adsorbent (g)
- V - Volume of the dynamic system (L)

$$q_t = \frac{(C_0 - C_t)}{m} V$$

- Before 175s, 1st-order kinetics \rightarrow process governed by availability of free binding sites
- After 175s, 2nd-order kinetics \rightarrow process governed by rarity of binding sites

2.4 Isotherm Models for understanding the surface coverage



Name of the Isotherm model	Name of the parameter	Value	R ²	MAPE
Freundlich	$K_f (mg/g)$	1191	0.82	76%
Langmuir	$q_m (mg/g)$	4324	0.94	35%
Temkin	$K_{Te} (Lg^{-1})$	2.1	0.89	48%
Dubinin-Radushkevich	$q_m (mg/g)$	3733	0.93	34%
Redlich-Peterson	$K_R (L/g)$	1195	0.94	35%
Sips	$q_m (mg/g)$	3828	0.96	16%
Toth	$q_m (mg/g)$	3684	0.96	18%

MAPE – Mean absolute percentage error

- The calculated C_e values for the plot isotherms were covered by first order and second order kinetic part

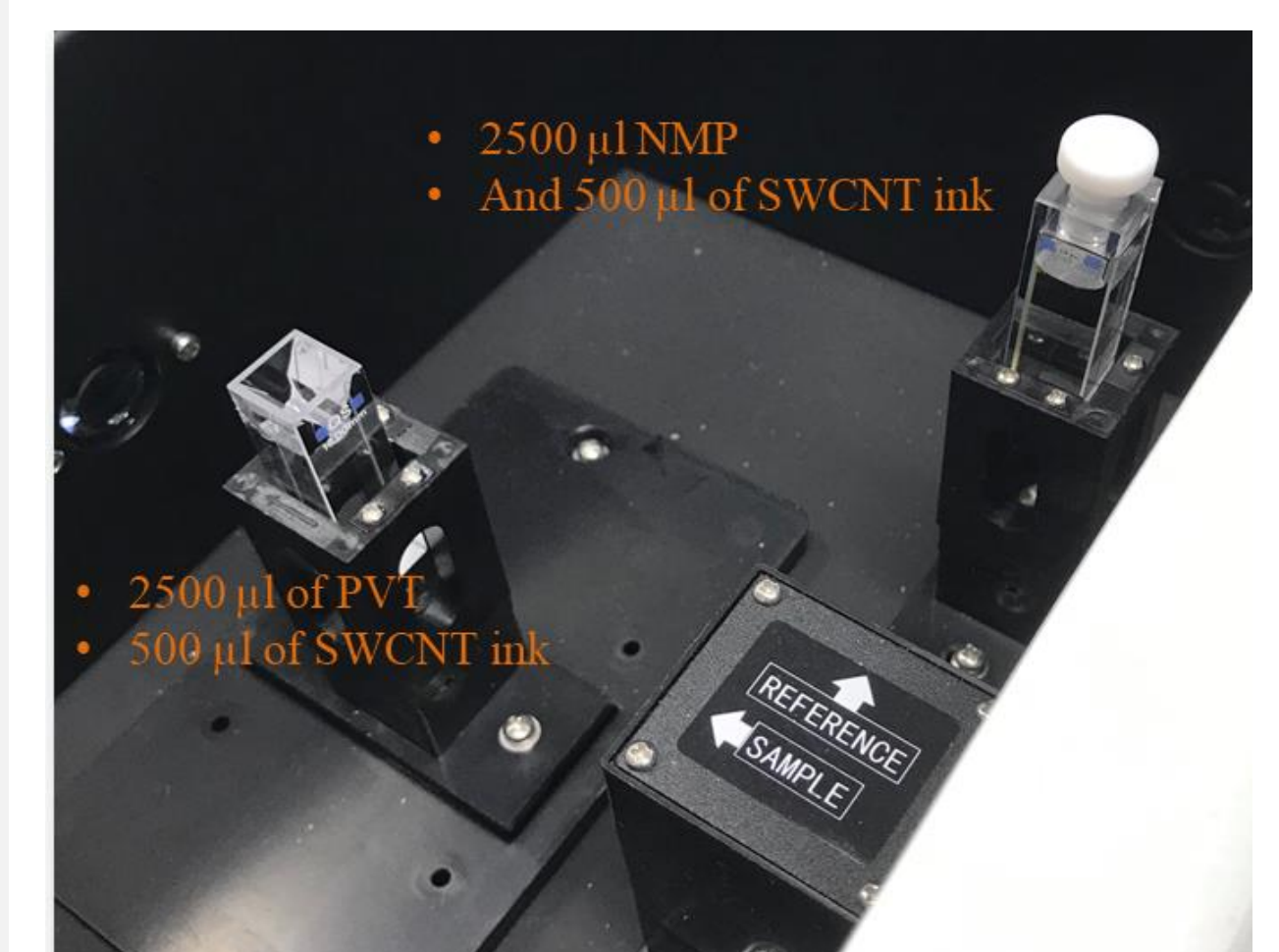
$$q_e = \frac{(C_0 - C_e)}{m} V$$

q_e - Equilibrium adsorption capacity (mg/g)
 C_e - Equilibrium concentration (mg/L)

- Maximum surface coverage obtained from the Toth isotherm model (Q_m) is 3684.5 mg/g

3. UV-Vis spectrophotometer based Methodology for adsorption Kinetics and Isotherm analysis on solution phase SWCNT ink

- 1st step - Automatic Zero calibration with NMP (solvent) in both cuvette
- 2nd step - Reference cuvette with the NMP (2500 μ l) + SWCNT ink (500 μ l)
- 3rd step - Sample cuvette filled with the PVT polymer (2500 μ l) + SWCNT ink (500 μ l) and run the kinetics studies



4. Conclusion

- PVT-118 and SWCNT functionalization demonstrated by mix order kinetics
- Multilayer adsorption process follow the Toth Isotherm model
- The calculated Maximum surface coverage (Q_m) by the Toth Isotherm model is 3684.5 mg/g

5. Acknowledgment

The authors acknowledge support from the European Union for HS4U project under Grant Agreement N°101069937 and for the project LOTUS under Grant Agreement N° 820881. LOTUS is also financed by the Indian Government, Ministry of Science and Technology

6. Bibliography

Al-Ghouti, M. A., & Da'ana, D. A. (2020). Guidelines for the use and interpretation of adsorption isotherm models: A review. Journal of Hazardous Materials, 393, 122383. <https://doi.org/10.1016/j.jhazmat.2020.122383>