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Supplementary Material

Microwave-promoted continuous flow synthesis of thermoplastic polyurethane-silver nanocomposites and their antimicrobial performance

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Estimation of fluid temperature at the microwave heating zone

The temperature of the fluid at the outlet was experimentally measured via an FO sensor installed 11 cm away from the MW irradiated zone. Since heat loss occurs as soon as the fluid flows out of the irradiated cavity, the temperature of the fluid at the point immediately outside the MW-heated zone is necessary. Since the fluid is majorly composed of the solvent, properties of DMF were used in the calculations. Hence, following assumptions were made:

- A forced convective heat transfer occurs from the fluid to the tube to the surrounding air.
- A fully-developed laminar flow and convection with uniform surface heat flux exists • within the cylindrical PTFE tube, thus the Nusselt-number will be constant i.e., 4.36 (Incropera & DeWitt' correlation ¹).

To find the convective heat transfer coefficient, hi, for DMF, the following definition of Nusselt number is used:

$$N_u = \frac{hi \, di}{\lambda_f} \qquad hi = \frac{N_u \, di}{\lambda_f} \tag{1}$$

The rate of heat transfer (dQ) can be calculated as:

$$dQ = K_o \pi d_o (T_{measured} - RT)(dl)$$

$$K_{o} = \left[\frac{1 \, d_{o}}{h_{i} d_{i}} + \frac{d_{o}}{\lambda_{f}} ln \frac{d_{o}}{d_{i}} + \frac{1}{h_{0}}\right]^{-1}$$
(3)

Where, K_o is given as:

And the heat balance equation is given as:

$$T_{estimated} = T_{measured} + \frac{dQ}{\dot{m} C_p}$$

Parameters and Properties used in calculations:

Parameter/Property	Value (unit)
Distance of FO from the cavity (dl)	0.11 m
Outer diameter of the tube (do)	0.00318 m
Inner diameter of the tube (di)	0.002 m
Room Temperature (RT)	298 K (24.85°C)
Temperature measure by FO ($^{T_{measured}}$)	313.15 K (40°C)
Thermal Conductivity of DMF at 313.15 K ($^{\lambda}f$)	$0.1836 \text{ W/m}^2 \text{K}$
Convective heat transfer coefficient of DMF at 313.15 K (hi)	$400.248 \text{ W/m}^2 \text{K}$
Natural convection heat transfer coefficient of air at 298 K (ho)	$10 \text{ W/m}^2 \text{K}$
Density of DMF	944 kg/m ³
Volumetric Flow Rate	2 mL/min
Mass Flow Rate (\dot{m})	0.0314666667 g/s
Heat Capacity (C _p) of DMF at 313.15K	2.0916678 J/gK

All thermal properties for DMF were obtained from Shokouhi et al.²

The fluid temperature immediately outside the MW-irradiated zone was estimated to be 42.5 °C when the measured temperature was 40 °C.

(2)

(4)



Figure S1 UV-vis spectra of samples prepared at RT by dissolving (A) AgNO₃ in DMF at concentrations (i) 0.2 mg/mL, (ii) 0.1 mg/mL, and (iii) 0.05 mg/mL, recorded at regular time intervals, and (B) AgNO₃ in DMSO at concentration 0.2 mg/mL recorded after 30 minutes.

Investigation of AgNPs production in DMF and DMSO at RT

To study the production of AgNPs at room temperature, a measured amount of AgNO3 (3mg) was dissolved in different volumes of DMF at RT to prepare samples having precursor concentrations (0.2 mg/mL, 0.1 mg/mL, 0.05 mg/mL). UV-vis spectra were recorded at regular time intervals. Similarly, a solution of AgNO₃ in DMSO was prepared to have the highest concentration, i.e. 0.2 mg/mL at RT, and UV-vis spectra were recorded after 30 minutes to ensure no particle production. The results are given in **Figure S1**.



Figure S2 (A) Temperature profile of DMF at different MW powers (30, 40, 50, 60, 70W) and (B) UV-vis spectra and (C) color change of samples prepared by dissolving AgNO₃ in DMF heated at different MW powers (30, 40, 50, 60, 70, 80, 90, 100, 110W) in the MW-promoted continuous flow system (single syringe). [Constant Parameters - AgNO₃ conc. 0.2 mg/mL, FR: 1 mL/min, Pressure: 20 psi].



Figure S4 TEM micrographs of NC-8 obtained at different magnifications.



Figure S5 Steps of solvent casting method: (A) collected product, (B) sample cast in petri dish, (C) sample coated the bottom of the dish, (D) washed and solidified final product.



Figure S6 Experimental set-up of conventionally-heated flow system (CHFS).



Figure S7 (A) UV-vis spectra and (B) DLS spectra showing the size distribution of the sample prepared via MW-heated Batch system (MWB-3) at 70 °C [PU concentration 26.6 mg/mL and AgNO3 concentration 0.1 mg/mL.]



Figure S8 Graphical illustration of antibacterial test performed as per JIS Z2801:2010 protocol to gauge the antibacterial performance of PU-Ag NCs.



Figure S9 (A) Variable Angle Spectroscopic Ellipsometry Data and (B) Optical Constant Depth Profile (651.5 nm) of NC-8.

References:

1. Incropera, F. P.; DeWitt, D. P.; Bergman, T. L.; Lavine, A. S., *Fundamentals of heat and mass transfer*. Wiley New York: 1996; Vol. 6.

2. Shokouhi, M.; Jalili, A.; HOSSEINI, J. M., Thermophysical properties of some physical and chemical solvents at atmospheric pressure. **2013**.