Supplementary information

1. Preparation of organic and aqueous phase for the synthesis of poly (DVB-co-VBC-co-styrene) resin (Ps.VBC)

The volume and mass of the components in the organic phase for the synthesis of 15 g of Ps.VBC resin were calculated as follows:

**Divinylbenzene (DVB)**

DVB (C$_{10}$H$_{10}$), molecular weight = 130.20 g/mol  
Density = 0.921 g/mL  
Percentage composition = 12%  
Mass of DVB $= \frac{12}{100} \times 15 = 1.8$ g, volume $= \frac{1.8}{0.921} = 1.95$ mL

**Vinylbenzyl chloride (VBC)**

VBC (C$_{9}$H$_{9}$Cl), molecular weight = 152.62 g/mol  
Density = 1.074 g/mL  
Percentage composition = 25%  
Mass of VBC $= \frac{25}{100} \times 15 = 3.75$ g, volume $= \frac{3.75}{1.074} = 3.5$ mL

**Styrene**

Styrene (C$_{8}$H$_{8}$), MW = 104.15 g/mol  
Density = 0.909 g/mL  
Percentage composition = 63%  
Mass of styrene $= \frac{63}{100} \times 15 = 9.45$ g, volume $= \frac{9.45}{0.909} = 10.39$ mL

**AIBN and 2-ethylhexanol**

The total mass of the co-monomers $= 1.8 + 3.75 + 9.45 = 15$ g  
The total volume of the co-monomers $= 1.96 + 3.5 + 10.39 = 15.84$ mL  
The mass of AIBN stabiliser added was 0.15 g (%1 by weight of the co-monomers and the volume of 2-ethylhexanol (porogen) used was 15.84 mL (1/1 by volume ratio of the co-monomers).

**Volume of aqueous phase**

The total volume of organic phase used for the suspension polymerisation was 31.68 mL.  
But the volume ratio of organic to aqueous phase was chosen to be 1:20; hence, the volume of aqueous phase employed was 634 mL.

2. Theoretical composition of Ps.VBC resin

**DVB (C$_{10}$H$_{10}$)**

Molecular weight = 130.20 g/mol  
Percentage composition = 12%  
Mass of DVB $= \frac{12}{100} \times 130.20 = 15.6$ g

**VBC (C$_{9}$H$_{9}$Cl)**

Molecular weight = 152.62 g/mol  
Percentage composition = 25%  
Mass of VBC $= \frac{25}{100} \times 152.62 = 38.155$ g
Styrene (C\textsubscript{8}H\textsubscript{8})
Molecular weight = 104.15 g/mol
Percentage composition = 63%
Mass of styrene = \( \frac{63}{100} \times 104.15 \) = 65.611 g
Total mass = DVB + VBC + styrene
= 15.624 + 38.155 + 65.611 = 119.39 g

The elemental composition of Ps.VBC resin was calculated as follows:

\[
\text{%C} = \frac{(12\% \times \text{mass of C in DVB}) + (25\% \times \text{mass of C in VBC}) + (63\% \times \text{mass of C in styrene})}{\text{Total mass}} \times 100
\]

\[
\text{%C} = \frac{0.12 (10 \times 12) + 0.25 \times (9 \times 12) + 0.63 (8 \times 12)}{119.39} \times 100
\]

C = 85.3%

\[
\text{%H} = \frac{(12\% \times \text{mass of H in DVB}) + (25\% \times \text{mass of H in VBC}) + (63\% \times \text{mass of H in styrene})}{\text{Total mass}} \times 100
\]

\[
\text{%H} = \frac{0.12 (10 \times 1) + 0.25 \times (9 \times 1) + 0.63 (8 \times 1)}{119.39} \times 100
\]

H = 7.11%

\[
\text{%Cl} = \frac{(12\% \times \text{mass of Cl in DVB}) + (25\% \times \text{mass of Cl in VBC}) + (63\% \times \text{mass of Cl in styrene})}{\text{Total mass}} \times 100
\]

\[
\text{%Cl} = \frac{0.12 (0) + 0.25 \times (1 \times 35.45) + 0.63 (0)}{119.39} \times 100
\]

Cl = 7.42%

3. The volume of AMP required for the amination of 35 g Ps.VBC resin
As shown in (2.), the percentage composition of Cl in Ps.VBC was found to be 7.42% (7.2 g per 100 g resin). Hence, the moles of Cl in 100 g of the resin equals to:

\[
\frac{7.42}{35.35} = 0.209 \text{ moles/100 g resin}
\]

Therefore, the moles of Cl in 35 g of resin = 0.07315 moles/35 g

The amination of Ps.VBC resin with AMP was carried out in the mole ratio of 1:4 resin to APM, thus, the volume of AMP used was calculated as follows:

Moles of AMP = 0.07315 × 4 = 0.2926 moles
Mass of AMP = moles × MW = 0.2926 × 108.143 = 31.643 g
Volume of AMP = \( \frac{\text{mass}}{\text{density}} \) = \( \frac{31.643}{1.04} \) = 30.4 mL

4. Loading of Ps.AMP resin with Mo(VI) complex
12% DVB (C\textsubscript{9}H\textsubscript{9}Cl), MW = 130.20 g/mol
25% Ps.AMP (C\textsubscript{15}H\textsubscript{16}N\textsubscript{2}), MW = 224.34 g/mol
63% styrene (C\textsubscript{8}H\textsubscript{8}), MW = 104.15 g/mol

Total mass = (0.12 × 130.20) + (0.25 × 224.34) + (0.63 × 104.15) = 137.32 g

(12\% \times \text{mass of C in DVB}) + (25\% \times \text{mass of C in Ps.AMP}) + (63\% \times \text{mass of C in styrene})

\[
\text{%C} = \frac{(0.12 \times 130.20) + (0.25 \times 224.34) + (0.63 \times 104.15)}{137.32} \times 100
\]
\[
\%C = \frac{0.12 (10 \times 12) + 0.25 \times (15 \times 12) + 0.63 (8 \times 12)}{137.32} \times 100
\]

\[
C = 87.3\%
\]

\[
\%H = \frac{(12\% \times \text{mass of H in DVB}) + (25\% \times \text{mass of H in Ps.AMP}) + (63\% \times \text{mass of H in styrene})}{\text{Total mass}} \times 100
\]

\[
\%H = \frac{0.12 (10 \times 1) + 0.25 \times (16 \times 1) + 0.63 (8 \times 1)}{137.32} \times 100
\]

\[
H = 7.45\%
\]

\[
\%N = \frac{(12\% \times \text{mass of N in DVB}) + (25\% \times \text{mass of N in Ps.AMP}) + (63\% \times \text{mass of N in styrene})}{\text{Total mass}} \times 100
\]

\[
\%N = \frac{0.12 (0) + 0.25 \times (2 \times 14) + 0.63 (0)}{137.32} \times 100
\]

\[
N = 5.1\%
\]

Therefore, 100 g of Ps.AMP contains 5.1 g N.

The moles of N in 100 g of Ps.AMP = \( \frac{\text{mass}}{\text{MW}} \)

\[
= \frac{5.1}{2 \times 14} = 0.182 \text{ moles/100 g}
\]

Hence, 35 g of the resin will have 0.0637 moles.

But the loading of Ps.AMP resin with Mo was carried out in the mole ratio of resin to Mo 1:2. Therefore, the corresponding moles of Mo used were 0.1274 moles.

The equivalent mass of MoO_2(acac)_2 employed for the Mo loading was calculated as follows:

\[
\text{MoO}_2(\text{acac})_2, \text{MW} = 326.15 \text{ g}
\]

\[
\text{Mass of MoO}_2(\text{acac})_2 = 0.1274 \times 326.15 = 41.55 \text{ g}
\]

5. Experimental set-up for suspension polymerisation

The set-up consists of 1 L jacketed glass baffled reactor, equipped with a condenser, double impeller, digital thermocouple, mechanical stirrer and water bath.
Experimental set-up for suspension polymerisation

6. Catalyst characterisation
FTIR spectrum of Ps.AMP.Mo catalyst
SEM image of Ps.AMP.Mo catalyst