Nature-inspired electrocatalysts and devices for energy conversion

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Electronic Supplementary Information

S1. "Murray"-inspired materials: derivation of their design equations

According to Murray's law, the cube of the diameter of the parent vessel \(d_p\) is equal to the sum of the cubes of the diameters of the daughter vessels \(d_i\), where \(n\) is the number of macro-, meso-, or nano-pores in each particle) at each level of bifurcation:1-3:

\[
d_p^3 = \sum_{i=1}^{n} d_i^3
\]

or, in generalized form

\[
d_p^\alpha = \sum_{i=1}^{n} d_i^\alpha
\]

where \(\alpha\) is proposed to be equal to 2 for mass or ionic transfer, and 3 for laminar flow.4

To obtain a relationship between the macro- and meso-pores of the catalyst, a generalized form of Murray’s law is applied, with \(\alpha = 2\):

\[
d_{macro}^2 = \sum_{i=1}^{n} d_{meso,i}^2 \text{ or } d_{macro}^2 = \sum_{i=1}^{n} d_{meso,i}^2
\]

where \(d_{macro}\) and \(d_{meso}\) are the diameters of macro- and meso-pores, respectively. The exchange surface area of the macropores is ignored, since it is negligible compared to the total surface area of the material that contains a large number of meso and micropores as well.4

To connect meso- to micro-pores, the exchange surface area from mesopores and micropores, along with the mass loss ratio \(M_{loss}\), cannot be ignored; the latter is proposed to be \(M_{loss} = (S_{macro})/(S_{macro} + S_{meso} + S_{micro}) \ll 1\) (where \(S_{macro}\), \(S_{meso}\) and \(S_{micro}\) are the specific surface areas of macro-, meso-, and micro-pores, respectively). By applying the law of mass conservation, we obtain:
\[ \dot{m}_p - M_{\text{loss}} \cdot \dot{m}_p = \sum_{i}^{n} m_i \]  

[S4]

where \( \dot{m}_p \) and \( \dot{m}_i \) are the mass flows through parent and daughter vessels, respectively. By applying Fick’s law, the above equation [S4] is deduced to:

\[ d_{\text{meso}}^2 = \frac{1}{1 - M_{\text{loss}}} \sum_{i}^{n} d_{\text{micro}}^2 \]  

[S5]

References


