Supporting Information for

Ozonolysis of Quinoline and Quinoline Derivatives in a Corning Low Flow Reactor

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S1. Mean residence time

The residence time distribution (RTD) curves were fitted to the modified Gaussian curve through Origin 8 as below.

\[ f(x) = y_0 + \frac{t_0}{A} \exp \left( \frac{1}{2} \left( \frac{w}{t_0} \right)^2 - \frac{x-x_c}{t_0} \right) \int_{-\infty}^{\infty} \exp \left( -\frac{y^2}{2} \right) dy \]

Here, \( z = \frac{x-x_c}{w/t_0} \), \( y_0 \) is offset, \( A \) is amplitude, \( x_c \) is center, \( w \) is width of curve, and \( t_0 \) is modification factor. After deconvolution, the whole system from the bypass curve using MATLAB code, FFT (fast Fourier transform) and iFFT (inverse fast Fourier transform), the function of \( E(t) \) was obtained for the reactor.\(^1\)

The mean residence time and Péclet number were obtained using \( \tau_L = \int_0^\infty tE(t) dt \) and

\[ \frac{\sigma^2}{\tau_L} = \frac{2}{Pe} - \frac{2}{Pe^2} (1-e^{-Pe}) \], respectively. Here, \( \sigma \) is the variance of the tracer calculated by

\[ \sigma^2 = \int_0^\infty (t-\tau_L)^2 E(t) dt . \]
Fig. S1. Residence time distributions after normalization (a) for $Q_l = 0.05$ ml/min and $Q_g = 4$ ml/min in eight Corning LFR and (b) for $Q_l = 0.1$ ml/min and $Q_g = 4$ ml/min in one Corning LFR.

Table S1. Mean residence time, Péclet number, and liquid hold-up for $Q_l = 0.05$ ml/min and $Q_g = 4$ ml/min in eight Corning LFR and for $Q_l = 0.1$ ml/min and $Q_g = 4$ ml/min in one Corning LFR

<table>
<thead>
<tr>
<th>Liquid Flow Rate (ml/min)</th>
<th>Number of LFR</th>
<th>Mean Residence Time ($\tau_L$, min)</th>
<th>Péclet Number ($Pe$)</th>
<th>Liquid Hold-up ($\phi$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>8</td>
<td>34.9</td>
<td>94.3</td>
<td>0.37</td>
</tr>
<tr>
<td>0.1</td>
<td>1</td>
<td>2.9</td>
<td>26.7</td>
<td>0.65</td>
</tr>
</tbody>
</table>

S2. Calculation of conversion and yield

The conversion of quinolines was calculated from the ozonolysis product by the equation,

\[
\text{Conversion (\%)} = \frac{\text{Initial Conc. of Quinolines } (C_{q,in}) - \text{Conc. of Quinolines after Ozonolysis } (C_{q,out})}{\text{Initial Conc. of Quinolines } (C_{q,in})} \times 100
\]

Also, the yield of pyridine-2,3-dicarboxylic acid was calculated after oxidative work-up using the equation,
$$\text{Yield (\%)} = \frac{\text{Conc. of Pyridine-2,3-dicarboxylic acid after Work-up (C_{acid})}}{\text{Initial Conc. of Quinolines (C_{in})}} \times 100$$

S3. Yield to pyridine-2, 3-dicarboxylic acid after oxidative work-up at 70 °C as a function of reaction time

![Graph showing yield as a function of reaction time](image)

S4. Overall mass transfer coefficient

The overall mass transfer coefficient was obtained by measuring the concentration of bicarbonate ions ($HCO_3^-$) with in situ Fourier-Transform infrared spectroscopy (FT-IR) using one Corning LFR plate. The bicarbonate was the product of the reaction between carbon dioxide and aqueous $N$-methyl diethanolamine (0.2 M).

$$R_3N + CO_2 + H_2O \leftrightarrow R_3NH^+ + HCO_3^-$$

The liquid flow rate was 0.05 or 0.1 ml/min with the gas flow rate of 4 ml/min as used in ozonolysis. At steady-state, the peak height at 1361 cm$^{-1}$ which was for bicarbonate ions was recorded. The overall mass transfer coefficient was obtained from the molar flow rate of bicarbonate ions, the concentration difference of carbon dioxide between in the gas phase in the
gas phase and in the bulk liquid, and mole ratio concentration gradient of carbon dioxide in the

gas phase.\textsuperscript{2}

<table>
<thead>
<tr>
<th>Liquid Flow Rate (ml/min)</th>
<th>Peak Height (1361 cm\textsuperscript{-1})</th>
<th>Absorptance</th>
<th>Mean Residence Time (τ\textsubscript{L}, s)</th>
<th>Overall Mass Transfer Coefficient (s\textsuperscript{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.0125</td>
<td>0.084</td>
<td>393.0</td>
<td>0.02</td>
</tr>
<tr>
<td>0.1</td>
<td>0.0186</td>
<td>0.250</td>
<td>175.2</td>
<td>0.074</td>
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</tbody>
</table>