

Supplementary Material for

**Effect of TiO₂ on Ru/ZrO₂ Catalysts in the Catalytic Wet
Air Oxidation of Isothiazolone**

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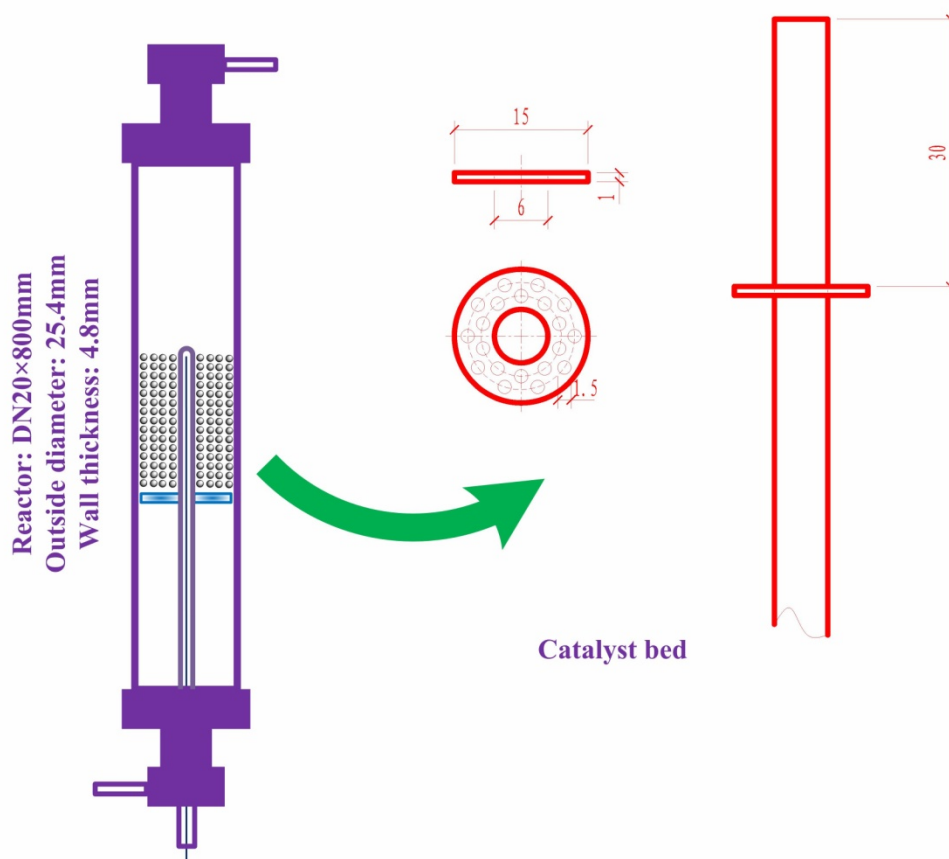
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Summary: This file contains 4 pages, including 3 figures.

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S1. Characteristics of the reactor



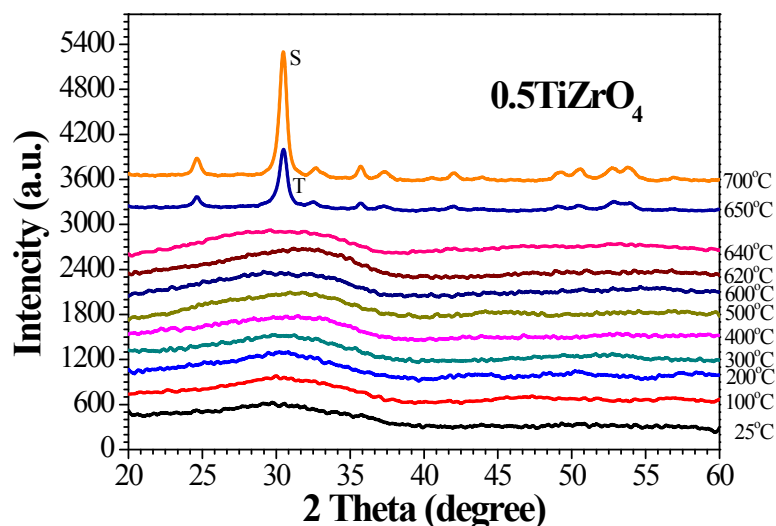
S-Fig. 1. The exact characteristics of the reactor and the catalyst bed.

S2. In-situ XRD of the 0.5TiZrO_4 support

The in-situ X-ray diffraction (XRD) spectra of the 0.5TiZrO_4 support were obtained using an X'Pert PRO instrument produced by PANalytical, which were collected under the ambient air conditions and a heating rate of $10\text{ }^\circ\text{C}\cdot\text{min}^{-1}$.

The phase changes of freshly precipitated hydrous 0.5TiZrO_4 were monitored using in-situ X-ray diffractometry; the results are presented in S-Fig. 2. As shown in S-Fig. 2, the amorphous hydrous 0.5TiZrO_4 transformed to the tetragonal phase and the Srilankite phase (S) at 650°C and 700°C in air, respectively. The peak at

$2\theta=30.5^\circ$ corresponds to the (111) reflection of the Srilankite phase. Note that the Srilankite phase is difficult to distinguish from tetragonal ZrO_2 . However, the peak intensity of the Srilankite phase (5398 a.u.) is larger than that of the tetragonal phase (4049 a.u.).



S-Fig. 2. In-situ XRD pattern of the $0.5TiZrO_4$ support.

S3. Intermediate products analyses

For the $Ru/0.2TiZrO_4$ catalyst, the difference between isothiazolone conversion and TOC removal is 17.4%, which indicates that some intermediates are produced during the CWAO treatment process for isothiazolone. The treated effluent was analyzed by GC-MS, GC, IC and NMR, and the results are presented in S-Fig. 3. As shown in S-Fig. 3, there were ten types of intermediates.

As shown in S-Fig. 3 (D), 1H NMR ($CDCl_3$, 400 MHz) δ 6.22 (d, $J=13.5$ Hz, 1H) and 7.4 (d, $J=13.5$ Hz, 1H) were attributed to an ethylenic bond H, and δ 2.07 was a methyl H connected to N. ^{13}C NMR ($CDCl_3$, 400 MHz) δ 167.48 was a carbonyl C,

