

## Real-Scale Numerical Simulation of Subcritical Gas-Liquid Two-Phase Flow in a Wastewater Treatment Apparatus

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### Introduction

Catalytic Wet Air Oxidation (CWAO)[1] is a wastewater purification technology utilized in chemical plants. In the CWAO process, harmful and refractory organic compounds are oxidatively decomposed into harmless products. This technology is considered promising for wastewater treatment due to its significant reduction in CO<sub>2</sub> emissions compared to incineration methods, and it achieves energy savings through the reuse of the reaction heat.

However, wastewater treatment apparatus utilizing CWAO operates under high-temperature and high-pressure conditions, making experimental observation of the internal flow difficult. Since understanding the flows inside the wastewater treatment apparatus, especially interactions between the gas-liquid two-phase flow and the solid catalyst, is crucial for improving reaction efficiency, numerical simulations were conducted to obtain comprehensive insights into these phenomena.

### Numerical Simulation

Numerical simulations of the gas-liquid two-phase flow were performed considering the actual scale of the apparatus. The apparatus has a height scale of 10 m and a processing amount of 400 m<sup>3</sup>/day, operating under extreme conditions of 240 °C and 7.5 MPa. Under these conditions, the gas-liquid two-phase flow inside the apparatus is in a subcritical state. Therefore, the physical properties of fluids in the subcritical state undergo significant changes, resulting in drastic changes in the gas-liquid two-phase flow inside the apparatus. The thermophysical properties of both gas and liquid phases were determined using the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)[2], which provides fluid properties over a wide range of temperature and pressure conditions. A one-fluid approximation was applied to the gas-liquid two-phase flow, and the compressible Navier-Stokes equations were computed using Large Eddy Simulation (LES). The catalyst layer was approximated as a porous medium.

### Results

Figure 1 shows the distribution of liquid volume fraction in a vertical cross-section passing through the center of the apparatus. Only the upper part of the apparatus is shown. Several characteristic structures are observed within the catalyst layer, including not only gas-liquid mixed regions but also liquid-rich regions. The liquid-rich regions are vertically distributed throughout the catalyst layer, and similar to the salt fingers, the liquid slowly descends in these regions. The gas-liquid mixture flows upward between the liquid-rich regions. Above the catalyst layer, the gas and liquid phases separate to form stratified layers. This stratification, called gravitational segregation, is attributed to changes in liquid viscosity under operating conditions and the large spatial scale of the apparatus. Such gas-liquid stratification is observed at several locations within the apparatus. The results suggest that improving reaction efficiency requires eliminating the gravitational segregation occurring within the apparatus.

### References

- [1] NIPPON SHOKUBAI CO., LTD., Wastewater Treatment Catalysts for Catalytic Wet Air Oxidation (CWAO), <https://www.shokubai.co.jp/en/products/detail/waste-water/>. (accessed 2025-08-19)
- [2] NIST, Reference Fluid Thermodynamic and Transport Properties Database (REFPROP), <https://www.nist.gov/srd/refprop>. (accessed 2025-08-19)

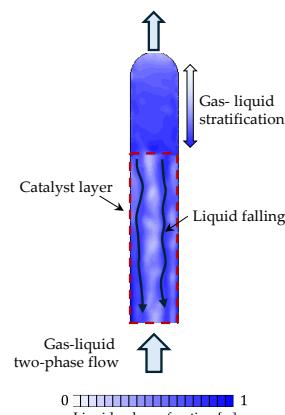


Figure 1 Distribution of liquid volume fraction in a vertical cross-section