*Supplementary Materials*

# Effect of Catalyst Inlet Flow Field Distribution Characteristics on Outlet NO Concentration Distribution in SCR Denitration Reactor Based on Monte Carlo Method

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## 1. Multi-Scale Numerical Simulation Analysis of Catalysts

The catalyst is placed in the main part of the SCR denitration reaction system. The type and structure of the catalyst directly affect the denitration efficiency. In the numerical simulation, the reasonable setting of the catalyst is the guarantee for the accurate simulation of the SCR denitration reaction system. In this section, the commercial computational fluid dynamics software ANSYS fluent is used to simulate the honeycomb SCR denitration catalyst and compare the flow and chemical reaction processes at the meso scale and macro scale.

### 1.1. Establishment of Fine and Macro Models of Catalysts

The catalyst meso model is established according to the actual honeycomb channel of the catalyst in literature [1]. As shown in Figure S1, the honeycomb catalyst model has $5 \times 5 = 25$ square channels with opening size of 6 mm, wall thickness of 1 mm and length of honeycomb catalyst of 50 mm. In the meso dimension, the wall area of the catalyst is a porous medium model, the outer surface, inlet and outlet parts of the catalyst are set as walls, and the inner surface of the catalyst part is set as interior. The honeycomb channel area, inlet and outlet are ordinary flow models. The macro model simplifies the actual structures such as honeycomb channel and catalyst wall into porous media, as shown in Figure S2. The turbulence in the model is realizable k-ε Turbulence model description. The porosity of catalyst wall is 42.3%, and the average particle size in porous medium is $1 \times 10^{-6}$ m [1] According to Formula (6) and Formula (7) in literature [2], the viscous resistance coefficient is $1.264 \times 10^{15}$ m$^{-2}$, inertia resistance coefficient is 502,541 m$^{-1}$.
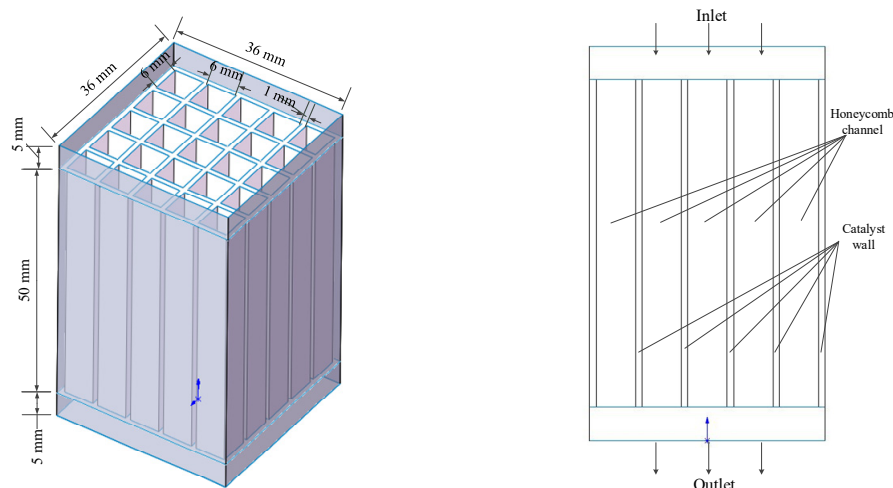
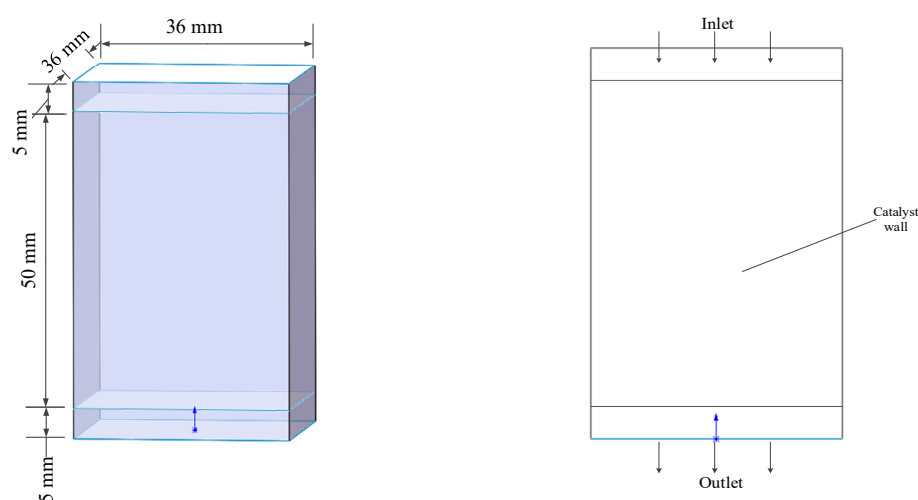**Figure S1.** Structure of catalyst meso model.



**Figure S2.** Structure of catalyst macro model.

The inlet boundary conditions of the catalyst model are set as follows: the inlet velocity is 0.417 m/s; the inlet temperature range is 553–593 K; the components of inlet flue gas are 0.04% NO, 0.05% $NH_3$, 5% $O_2$, 8% $H_2O$ and others are $N_2$. It is ensured that the experimental conditions of this simulation are the same as those in literature [1].

### 1.2. Experimental Verification

Under five different temperature conditions, the simulation results of the catalyst meso and macro models are compared with the experimental results in literature [1], as shown in Figure S3. It is evident from the figure that the maximum error between the meso numerical simulation and the experimental value is 14.5%, which is within the acceptable range. The maximum error between macro numerical simulation and experimental value is 6.5%, which shows that macro numerical simulation can accurately simulate the denitration process, and the error of macro numerical simulation is smaller than that of meso simulation.
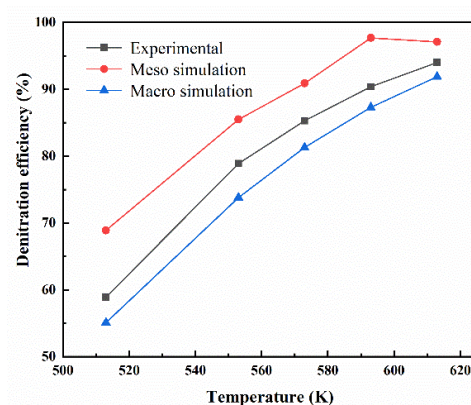
**Figure S3.** Comparison between numerical simulation results and experimental results based on [1].

### 1.3. Comparison of Catalyst Meso Simulation and Macro Simulation

The meso and macro numerical simulation results at 553 K are compared. Figure. S4 is the comparison diagram of meso simulation and macro simulation velocity of catalyst, and Figure. S5 is the comparison diagram of NO concentration. It is evident from the figure that there is almost no change in the velocity field in the macro numerical simulation results, while in the meso numerical simulation results, when the air flow variable cross-section enters the honeycomb channel, the velocity will change. The trend of NO concentration distribution in the meso and macro simulation results is consistent, and the NO concentration gradually decreases from top to bottom in the axial direction of the catalyst. The difference is that the NO concentration distribution in the meso numerical simulation results is wavy, and the NO concentration distribution in the meso numerical simulation results is inverted trapezoid. This is because when the air flow enters the honeycomb channel, the velocity near the catalyst wall is small and the chemical reaction time is relatively long, so the NO concentration is small at this place, which is the case at each catalyst wall, and a wavy concentration distribution is formed from the; When the gas flow enters the overall porous medium, the velocity near the overall four walls of the catalyst is small, and the chemical reaction time is relatively long, resulting in a small NO concentration, thus forming an inverted trapezoidal concentration distribution.
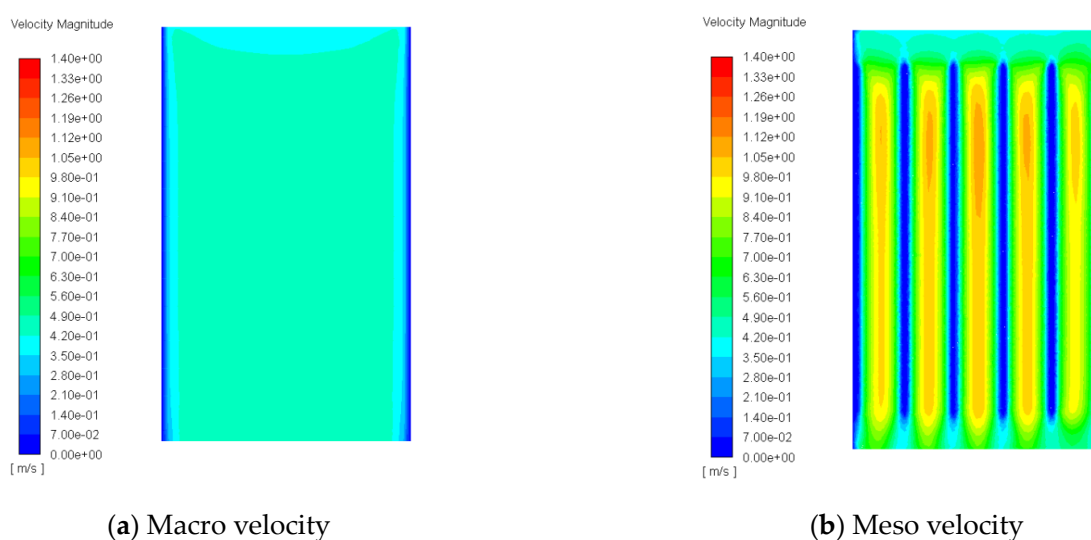


(**a**) Macro velocity          (**b**) Meso velocity

**Figure S4.** Comparison of meso (**b**) and macro (**a**) simulation velocity of catalyst.

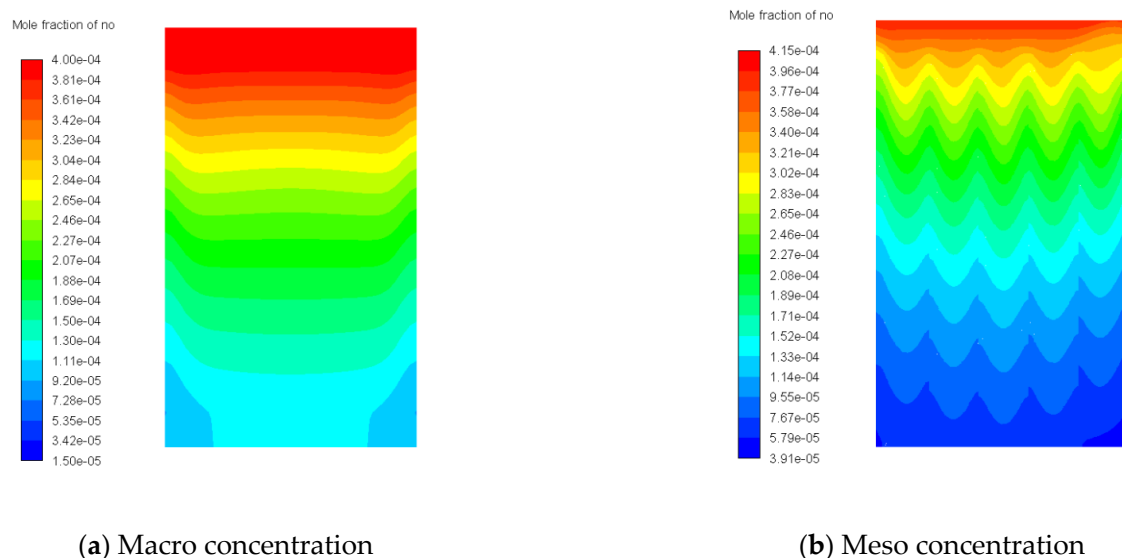(**a**) Macro concentration　　　　　　　　　(**b**) Meso concentration

**Figure S5.** Comparison of meso (**b**) and macro (**a**) simulation NO concentration of catalyst.

In order to further explore the similarities and differences between meso simulation and macro simulation of catalyst, the nonuniform inlet velocity of catalyst was set. As shown in Figure S6, the inlet velocity of catalyst is linearly distributed, and the average velocity is 0.417 m/s.
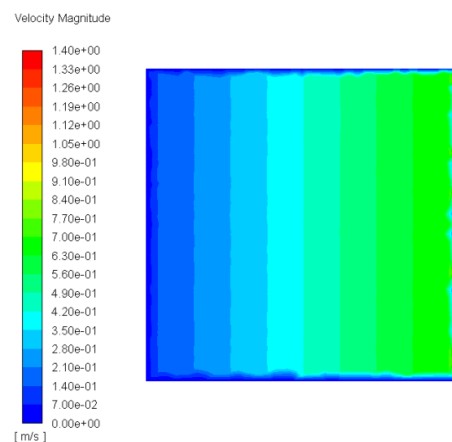


**Figure S6.** Nonuniform velocity inlet distribution.

Under the conditions of nonuniform velocity inlet and 553K temperature, the numerical simulation results are shown in Figure S7 and Figure S8. It is evident that distribution trends of velocity field and concentration field of macro numerical simulation and meso numerical simulation are consistent. When the gas flow enters the catalyst layer, the velocity distribution is still nonuniform, the NO concentration gradually decreases from top to bottom in the axial direction of the catalyst, and the NO concentration is larger in the part with high velocity.
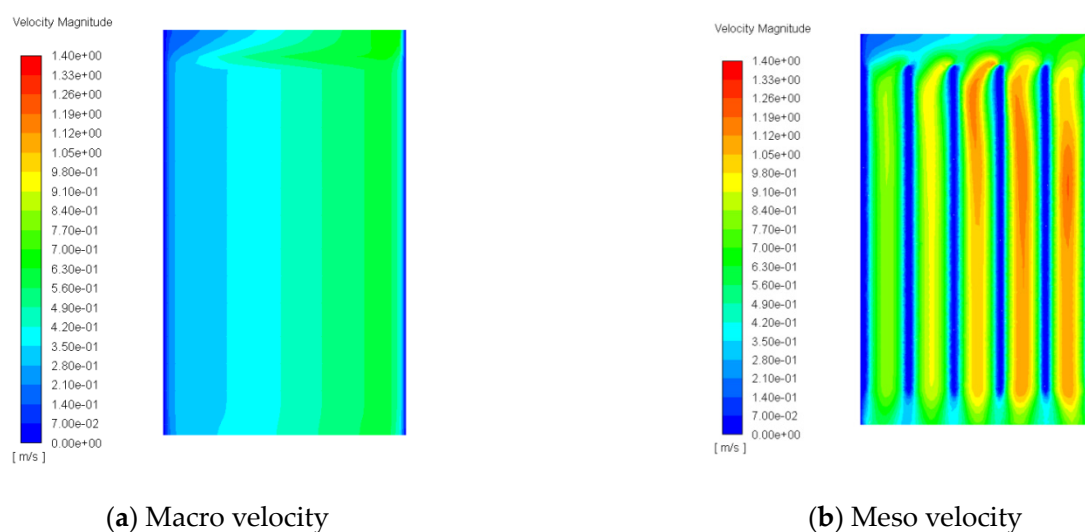
(**a**) Macro velocity



(**b**) Meso velocity

**Figure S7.** Comparison of meso (**b**) and macro (**a**) simulated velocity of catalyst under nonuniform inlet conditions.



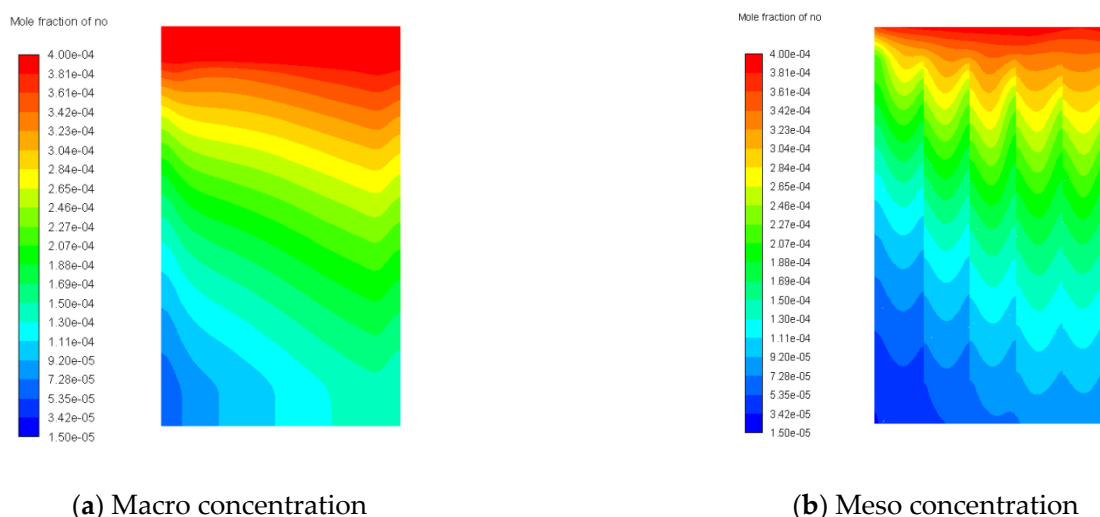(**a**) Macro concentration



(**b**) Meso concentration

**Figure S8.** Comparison of meso (**b**) and macro (**a**) simulated NO concentration of catalyst under nonuniform inlet conditions.

Through the above comparative analysis, it is evident that the distribution trend of NO concentration in macro simulation and meso simulation is consistent, and compared with the experimental values, the results of macro simulation and meso simulation can meet the calculation accuracy. With a small size of 36 mm × 36 mm × 60 mm, the number of meso grids of the catalyst is 38 times that of the macro grid. If the honeycomb shaped catalyst bed is constructed and meshed according to the entity, a large number of grid bodies will be generated, which will greatly increase the calculation cost. Therefore, in the numerical simulation, it is preferred to reasonably simplify the catalyst and treat the catalyst as a porous medium area. Porous media model is widely used, and the flow pressure drop is determined by the content input by the momentum equation of porous media. Using this model, the heat conduction problem of media can also be described. Therefore, the catalyst part of this study adopts macro scale numerical simulation.

# Reference

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2. Wang, L.; Qian, F.; Zhu, J.; Huang, N.; Xu, B.; Wu, H. Multi-scale simulation of flow characteristics in selective catalytic reduction honeycomb catalyst. *Chin. J. Process. Eng.* **2020**, *20(2)*, 134–140. https://doi.org/10.12034/j.issn.1009-606X.219172.