AI accelerated micro-kinetic modelling in heterogeneous catalysis: an application of physically enhanced ANNs to CFD simulations of industrial packed-bed reactors

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Highlights

- First application of physically enhanced neural networks for heterogeneous catalysis
- Retain full mechanistic detail (accuracy > 99.9 %) with artificial neural networks
- Simulation 120 fold speed-up of lab-scale simulation
- CFD simulations of industrial packed-bed reactors in 9 h with 32 cores (2.3 GHz)

1. Introduction

The comprehension of the interactions between the catalytic mechanism and transport phenomena in heterogeneous reactors is a crucial task[1]. In this context, numerical simulations have gained more and more importance. However, solving micro-kinetics consumes 70%-90% of the computational resources[2]. Surrogate modelling has been an integral method to overcome this drawback. However, conventional techniques, e.g. splines, are limited to small problems or are prone of reducing the level of mechanistic detail. In recent years, machine learning (ML) algorithms received increasing attention[3-5]. With their great flexibility in design, e.g. embedding chemical and physical knowledge[3] and their capability of generalizing complex problems, artificial neural nets (ANNs) are the most promising ML algorithms for surrogate modelling[4]. To the author's knowledge, ANNs have not been employed in CFD catalytic modelling. In this work, we examine the application within a 2D-packed-bed reactor, obtaining a 120-fold speed-up of the micro-kinetic simulation. This enables industrial scale CFD simulations of catalytic reactors, which we show-case in an example simulation.

2. Methods

In this work, we include ANNs as surrogates of the detailed microkinetic chemistry in reactive CFD simulations carried out with the *catalyticFOAM*[6] framework. We assess the performance on a gas-solid packed-bed reactor under water-gas shift conditions. A multi-region approach has been adopted, hence solving diffusion-reaction in the solid phase in addition to the description of the fluid flow in the gas phase. The chemical kinetics is described by the UBI-QEP based mechanism proposed by MAESTRI *et al*.[7]. As surrogate, a physics enhanced ANN[4] is chosen and applied to the steady-state isothermal simulation of the reactor.

3. Results and discussion

Figure 1A-B show the comparison between the CO map in a fixed bed reactor filled with 10 mm diameter spherical pellets. Given that an excellent qualitative agreement is achieved, the axial CO conversion (χ_{CO}) is analyzed in Figure 1C. In particular, it is shown the comparison of χ_{CO} predicted with and without ANN: CO is converted between 10 and 30 cm after the reactor inlet and in this length a maximum error of 0.5 % is detected with the surrogate model, highlighting an excellent quantitative agreement. Figure 1D shows the simulation speed-up as a function of the simulation iteration towards the steady state. As reported, ANN are able to significantly reduce the computational time by not solving the micro-kinetic scheme on the fly. Consequently, the CFD simulation is accelerated by ~120 times.

The obtained accuracy and speed-up enables the coupling of micro-kinetic models and transport phenomena in the simulation of industrial size packed-bed reactors. Figure 2 shows the CO map in a 3D fixed bed reactor with in total 45 million cells (54 % pellets). The simulation is run using the same inlet composition as in the previous simulation (Figure 1).

With a pre-solution of the flow field (~ 3 h), the isothermal simulation requires around 6 h computational time until convergences on 32 CPUs (Intel® Xeon® Platinum/2.3 GHz).

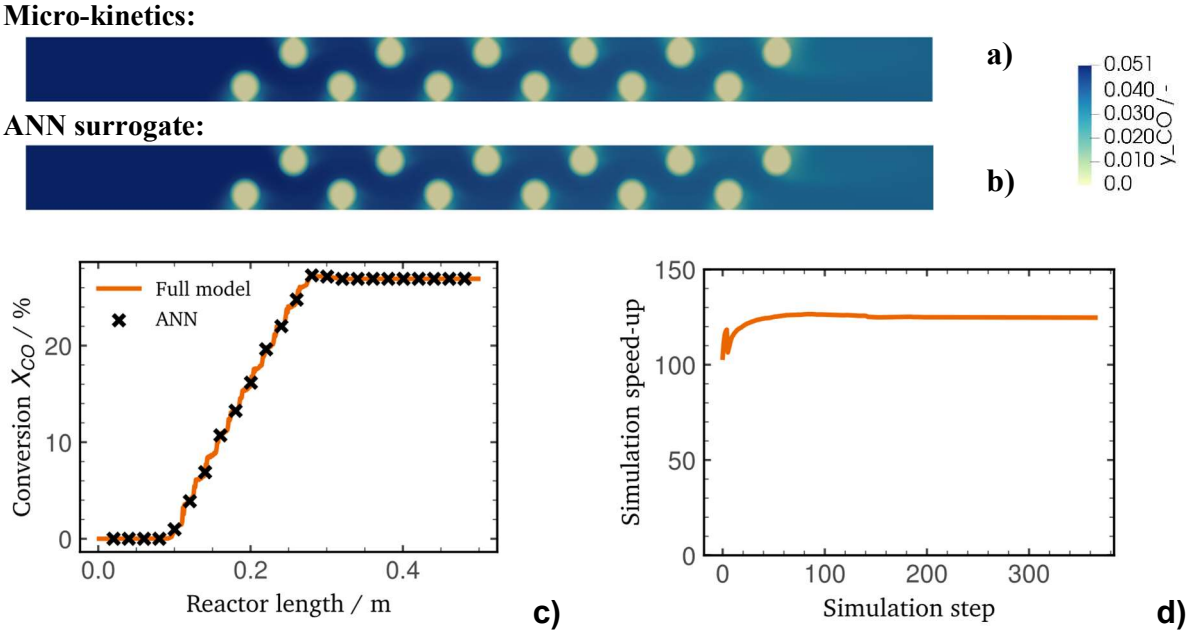

Figure 1: Comparative study of ANNs against the full micro-kinetic model: (a) CO map without ANN. (b) CO map with ANN (c) Axial conversion of CO (d) Simulation speed-up against simulation iteration.

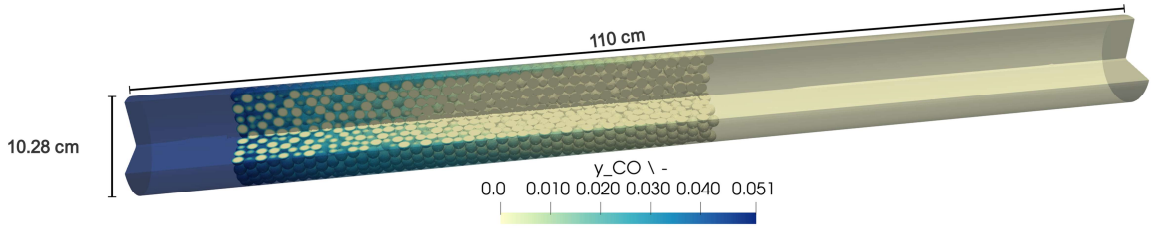

Figure 2: Mass fraction y_{CO} map of a industrial scale water-gas shift fixed bed reactor simulation. The catalytic bed has a length of 50 cm and consists of around 2400 pellets with a diameter of 1.27 cm.

4. Conclusions

ML models are widely used in chemical reaction engineering, but not yet implemented for the most demanding heterogeneous reactor simulations (CFD). In this work, we enable the community to harness the full potential of these methods, by means of OpenFoam framework. Employing physically enhanced ANNs, the total simulation of a packed-bed is speed up by 120, maintaining high accuracy (< 0.5 %). This is paving the way for industrial scale reactor simulations with full mechanistic details coupled with transport phenomena. To show case the potential, we performed a 45 million cell simulation of a 110 cm long reactor (50 cm bed length), which converged in 9 h on 32 cores (2.3 GHz).

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Keywords
reactive CFD; packed-bed; artificial intelligence; artificial neural networks