MODEL OF THE CO CATALITIC CONVERSION PROCESS

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This paper presents a three-level modelling approach to the catalytic carbon monoxide oxidation in a temperature range between 400 K – 800 K. The first level involves the description of the chemical kinetics for the exothermic reactions on the catalyst surface. The second level models the thermal and hydrodynamic processes in the boundary diffusion layer. Finally, the third modelling level focuses on the representation of the hydrodynamic and thermal properties for the bulk multi-component gas flow at various gas velocity and temperature range. The initial state of the reaction was steadied and the time dependence of the components predicted by the model were analysed.

The oxidation reaction of CO to CO_2 with molecular oxygen represents an industrially important reaction system whose description involves multiple phenomena despite its simple kinetic mechanism (Bykov et al., 2005). The reaction takes place during deactivation of industrial waste as described by Arash E. (2012). The same reaction in automobile exhaust gas conversion unit was studied by Dvorak R. (2010). Oxidation of carbon monoxide takes place in several stages through either Ili–Ridil or Lengmoore-Hanshelwood mechanism. In this work, a multi-level mathematical model of catalytic conversion has been developed as initially suggested by Ved et al. (2011). The model considers both the case where oxygen, carbon monoxide and carbon dioxide make up the gaseous mixture and the case where the reactive mixture is mixed with a neutral medium.

The general form of the oxidation mechanism is as follows:

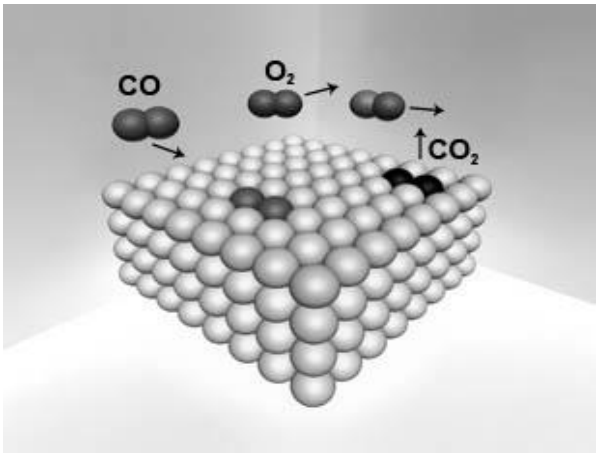

Fig. 1 – The general form of the oxidation mechanism