

## Reduced General Dispersion Model in Cylindrical Coordinates and Isotope Transient Kinetic Analysis in Laminar Flow

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**Abstract :** This abstract discusses a method that reduces the general dispersion model in cylindrical coordinates to a second order linear ordinary differential equation with constant coefficients so that it can be utilized to conduct kinetic studies in packed bed tubular catalytic reactors at a broad range of Reynolds numbers. The model was tested by  $^{13}\text{CO}$  isotope transient tracing of the CO adsorption of Boudouard reaction in a differential reactor at an average Reynolds number of 0.2 over Pd-Al<sub>2</sub>O<sub>3</sub> catalyst. Detailed experimental results have provided evidence for the validity of the theoretical framing of the model and the estimated parameters are consistent with the literature. The solution of the general dispersion model requires the knowledge of the radial distribution of axial velocity. This is not always known. Hence, up until now, the implementation of the dispersion model has been largely restricted to the plug-flow regime. But, ideal plug-flow is impossible to achieve and flow regimes approximating plug-flow leave much room for debate as to the validity of the results. The reduction of the general dispersion model transpires as a result of the application of a factorization theorem. Factorization theorem is derived from the observation that a cross section of a catalytic bed consists of a solid phase across which the reaction takes place and a void or porous phase across which no significant measure of reaction occurs. The disparity in flow and the heterogeneity of the catalytic bed cause the concentration of reacting compounds to fluctuate radially. These variabilities signify the existence of radial positions at which the radial gradient of concentration is zero. Succinctly, factorization theorem states that a concentration function of axial and radial coordinates in a catalytic bed is factorable as the product of the mean radial cup-mixing function and a contingent dimensionless function. The concentration of adsorbed compounds are also factorable since they are piecewise continuous functions and suffer the same variability but in the reverse order of the concentration of mobile phase compounds. Factorability is a property of packed beds which transforms the general dispersion model to an equation in terms of the measurable mean radial cup-mixing concentration of the mobile phase compounds and mean cross-sectional concentration of adsorbed species. The reduced model does not require the knowledge of the radial distribution of the axial velocity. Instead, it is characterized by new transport parameters so denoted by  $\Omega_c$ ,  $\Omega_a$ ,  $\Omega_r$ , and which are respectively denominated convection coefficient cofactor, axial dispersion coefficient cofactor, and radial dispersion coefficient cofactor. These cofactors adjust the dispersion equation as compensation for the unavailability of the radial distribution of the axial velocity. Together with the rest of the kinetic parameters they can be determined from experimental data via an optimization procedure. Our data showed that the estimated parameters  $\Omega_c$ ,  $\Omega_a$ ,  $\Omega_r$ , are monotonically correlated with the Reynolds number. This is expected to be the case based on the theoretical construct of the model. Computer generated simulations of methanation reaction on nickel provide additional support for the utility of the newly conceptualized dispersion model.

**Keywords :** factorization, general dispersion model, isotope transient kinetic, partial differential equations

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