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EVALUATION OF MASS TRANSFER COEFFICIENTS FOR LAMINAR FLOW IN MONOLITHIC REACTORS WITH CATALYTIC WALLS

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Monolithic reactors have a wide application in chemical engineering, both for pollution control and in production processes. Their greatest advantages are the very limited pressure drop and the large geometric surface/volume ratio, that is interesting in case of fast catalytic reactions. They can be modelled using a simplified one-dimensional lumped approach, provided the heat and mass transfer coefficients are available; as the flow is usually laminar, due to the small size of the channels, these coefficients can be evaluated solving the correspondent two- or three-dimensional problem, and calculating the Sh and Nu number.

Many data are available in the literature on Nu value in compact heat exchangers; a complete analogy with the Graetz-Nusselt problem for heat transfer in a duct with constant wall temperature has been usually assumed in order to evaluate the Sherwood number, but it has been shown that the boundary conditions in the actual cases may be different and can significantly modify the mass transfer coefficient, if a reaction occurs on the catalytic wall.

Previous works have shown the dependence of Sh on the Damkohler number in case of a first order reaction occurring at the wall; different geometries were investigated but only in isothermal conditions. In this work exothermal reactions will be investigated, and orders of reaction both lower and higher than one will be considered. The analysis will be limited to the case of cylindrical channels, with constant density fluid and hydrodynamically developed flow. The thermal conductivity of the solid support has been neglected (that is reasonable for ceramic monoliths).

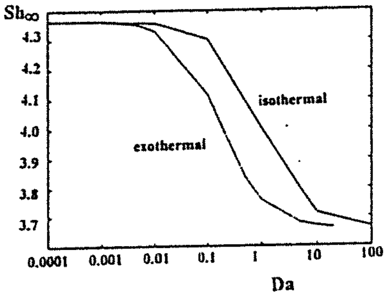

Fig. 1 - Sh_∞ vs. Da for isothermal (—) and exothermal (- - -) first order reaction.

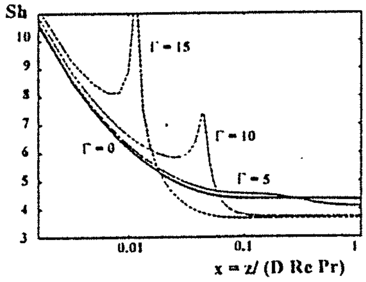

Fig. 2 - Local Sh for different Γ. First order reaction; Da= 0.05; δ=1; Le=1.

The two-dimensional system has been solved using the orthogonal collocation method along the radial direction and a standard Gear method along the axial one. The local and asymptotic Sherwood and Nusselt numbers have been evaluated as a function of Damkohler, dimensionless adiabatic temperature rise (δ) and activation energy (Γ). The influence of the Lewis number (Sc/Pr) has also been evidenced. For non-first order kinetics the dependence of Sh on axial coordinates is more complex, even for isothermal conditions, and a non-monotone behaviour can be observed. The influence of the exothermicity is significant especially for intermediate Damkohler numbers, and cause the asymptotic Sh to decrease (see Fig. 1). The dimensionless activation energy is the parameter having the strongest effect on the variation of the Sherwood number with the axial coordinate; at relatively low value of Da, spikes can be observed, that indicate the occurrence of ignition and transition from kinetic to mass-transfer control (see Fig. 2).

The results obtained have evidenced that in some cases the mass transfer coefficients can be affected significantly by the presence of the exothermal reaction. It must be pointed out that the use of the asymptotic value of Sh is not generally acceptable as the reaction is often complete before the asymptotic conditions are reached.