Dead zone for hydrogenation of propylene reaction carried out on commercial catalyst pellets.

M. Szukiewicz [(1)], E. Chmiel-Szukiewicz [(1)], K.Kaczmarski[(1)], A. Szałek[(1)]

[(1)] *Rzeszow University of Technology, Faculty of Chemistry, al. Powstańców Warszawy 6, 35-959 Rzeszów, Poland*

1. Introduction – In the process engineering field, diffusion and reaction problems appear mainly in the processes of heterogeneous catalysis and biochemical processes . In models used for description of such processes, a nonlinear generation term is commonly applied. Mathematical foundations of diffusion-reaction processes (they are also valid for biochemical processes) were presented by Aris [1] in his classical work. A description of typical phenomena occurring in the catalyst pellet will be skipped as a well-known. Aris claimed that, as a result of reaction course and diffusional resistances, in the pellet can be formed zones without reactants and where the reaction does not take place. In literature this zone is usually called "dead zone" for chemical heterogeneous processes or "dead core" for biochemical processes. The dead zone appears in a central part of a pellet if intrinsic diffusion is much slower than reaction rate. As a consequence efficiency of process decreases.

2. Experimental - Catalytic micro-reactor (the Microactivity Effi reactor, PID Eng&Tech, Spain**)** of diameter 9 mm equipped with hydrogen generator, thermocouple for measurement of catalyst temperature inside the bed, mass-flow meters was used for investigations. Gas chromatograph equipped with TCD was used for analysis of reaction mixture. In the reactor was carried out hydrogenation of propylene. As a hydrogenation catalyst the KUB-3 catalyst (the main components of the catalyst are Ni, NiO, and Al2O3.) manufactured by INS, Puławy, Poland was chosen. Catalyst form: pellets with diameter 4-6 mm. Experiments were carried out at temperature range 30-100°C under pressure 1.2×10^{5}Pa.

3. Results and Discussion - On the basis of experiments carried out the following kinetic equation was developed:

$$r = 0.014\, p_P^{0.48}\, e^{-26940}/_{R\cdot T}$$

The kinetic equation suggest that inside the catalyst pellet a dead zone can be formed. The aim of the work is the presentation developed by us simple and effective method to determine the impact of operating conditions on the dead zone formation as well as to evaluate a volume of the dead zone and its impact on process effectivity. The method is based on numerical simulations employed modified shooting method [2]. Calculation were performed using commercial CAS-type program Maple®. The obtained results indicate that dead zone fills 10-40% of the catalyst pellets and can significantly impact on productivity of the catalytic process.

4. Conclusions - On the basis of the results presented the following conclusions can be drawn: (i) the method presented can help to evaluate size of the dead zone and as a consequence help to improve catalyst form or process productivity; (ii) the knowledge on origination of dead zone is still insufficient from practical point of view;

Acknowledgments - The financial support of the National Science Centre, Poland (Project 2015/17/B/ST8/03369) is gratefully acknowledged.

5. References

[1] R Aris. The Mathematical Theory of Diffusion and Reaction in Permeable Catalysts. Vol I. The Theory of the Steady State. Oxford, Clarendon Press, 1975.

[2] M. Szukiewicz, *Braz. Journal of Chem. Eng*., **34(**03), pp. 873 – 883.