THE POWER SERIES METHOD IN THE EFFECTIVENESS FACTOR CALCULATIONS

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Abstract—In the present paper, exact analytical solutions are obtained for nonlinear ordinary differential equations which appear in complex diffusion-reaction processes. A technique based on the power series method is used. Numerical results were computed for a number of cases which correspond to boundary value problems available in the literature. Additionally, new numerical results were generated for several important cases.

 ${\it Keywords}$ — Diffusion and reaction; power series method.

I. INTRODUCTION

In the present work the exact analytical solutions are presented for a set of non-linear boundary value problems which arise in the analysis of steady diffusionreaction processes. Several investigators have treated the heat and mass transport in catalysis pellets. Particular emphasis has been directed to the determination of the isothermal effectiveness factor. Early studies have been compiled by Gonzo and Gottifredi (1982). These authors predicted the mentioned factor under nonisothermal conditions usually met in most chemical reactor design calculations, using a perturbation technique. More recently Villa (2000) presented a practical approach for a non classical numerical analysis of the solution of boundary value problems for high non-linear second order differential equations. These problems arise from energy and mass balance equations for non isothermal steady diffusion-reaction processes.

The class of described problems, leading to the solution of high non-linear second order differential equations, is the source of considerable theoretical and practical difficulties. It is the purpose of the present paper to demonstrate that an approach based on the power series method is a very effective tool for the solutions of the mentioned problems. The power series method is an old tool to solve ordinary differential equations. A wide open literature is available on this topic. In the last century several methods of finding exact and approximate solutions have been developed with the appearance of new problems in several disciplines. The finitedifference method and the variational methods have been extensively applied to solve problems in engineering. The finite element method gained an immense popularity among applied mathematicians and engineers. Nevertheless, the old technique of power series solutions has been ignored in the solutions of some boundary and/or eigenvalue problems which involve ordinary non-linear differential equations. Filipich *et al.* (2004), with a properly systematisation, applied it in various difficult problems. For instance, they succeeded in the application of this technique to strongly non-linear dynamical systems.

In the present paper, the potential usefulness of the largely ignored power series methods for solving nonlinear ordinary differential equations which appear in the complex diffusion-reaction processes, is demonstrated. A simple, computationally efficient and very accurate analytical approach has been developed for the determination of the values of the nondimensional concentration u, the gradient u and the effectiveness factor η , for different values of the characteristic parameters which correspond to relevant steady diffusion - reaction processes. The obtained algorithm is very general and it is attractive regarding its versatility in handling different values of the reaction order, the Thiele's modulus and other specific parameters.

Close agreement with results presented by previous investigators is demonstrated for several particular cases. Additionally, new numerical results were generated for several important cases, including those with experimental values for the parameters involved in the models of some industrial chemical reactions.

II. THEORETICAL CONCEPTS.

A. Introduction.

The process of diffusion-reaction in catalytic porous media is a matter of great interest in chemical reactor design. A great number of relevant cases are included in the following general boundary value problem:

$$\frac{d^2u(x)}{dx^2} + F(x, u, u') = 0, \qquad \forall x \in (a, b)$$
 (1)

$$c_1 u(a) + c_2 u'(a) = A,$$
 (2)

$$c_3 u(b) + c_4 u'(b) = B,$$
 (3)

where $c_i \in \Re$ where \Re denotes the set of real number, i=1,2,...,4; $a,b,A,B \in \Re$ and the function F is continuous on $[a,b] \times (-\infty,\infty) \times (-\infty,\infty)$.

The problem of existence and uniqueness of solution for initial value problems has extensively been investigated and a detailed analysis has been published. It is well known that in contrast the boundary value problems have several solutions or even no solution. This