UNIVERSITI TEKNOLOGI MARA

TECHNICAL REPORT

THE PERFORMANCE TEST OF IMPLICIT BACKWARD DIFFERENTIATION FORMULA ON ROBERTSON'S CHEMICAL REACTION MODEL

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IN THE NAME OF ALLAH, THE MOST GRACIOUS, THE MOST MERCIFUL

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ABSTRACT

Robertson's chemical reaction model is a famous finding by H.H. Robertson in 1966 related to kinetic reaction of chemical reactants. It describes chemical reaction with three main reactants involved which are reactant A, B and C. The reaction rates involved are three different values and largely different from each other. The model proposed is a system of three non-linear equations and it is widely known as a stiff problem. Numerical experiment of implicit Backward Differentiation Formula (BDF) method are adopted computationally to explain the performance of the method in solving stiff problem. The result shows performance of the method in term of computational time and number of iteration used.

1 INTRODUCTION

1.1 Research Backgroud

Chemical reaction may varies based on the reactant used and the condition given during the reaction. The reaction take place due to the kinetic energy that react towards the changing condition or surrounding. The energy of the kinetic will transform into another form of energy such as heat or light energy which can be observed by the researcher. How fast the reaction took place describe the efficiency rate of the reaction. Remodeling a problem using mathematical notations or equations has become one of the basic step in solving the problem. In 1966, H. H. Robertson wrote an article majoring in chemical engineering which stressed on stiff equations. Robertson gave a test example for stiff methods which is a systems of three non-linear ordinary differential equations describing the kinetics of an autocatalytic reaction. According to Gobbert (1996), the models are made to see the depletion and the generation of chemical reactants that are involved. Edsberg (1974) explained that the system proposed by Robertson is stiff. It can be seen through the variation of the Jacobian eigenvalues along the solution trajectory.

Stiff differential equation is a special case of differential equation where it needs special treatment from the technique used to solve it. It is said from the definition of stiff differential equation that it needs extremely small step size for a certain method as it is numerically unstable when using big step size. Technique of solving such special case evolved over time. For instance, they simplify former technique, introduce alternative approach or help solving different nature of problems like stiff problem. Numerical techniques are techniques that calculate the approximated solutions, given the solutions are approaching the exact solutions. These techniques have their own characteristics too whether it is implicit or explicit.