

**MODELLING GLOBAL ATMOSPHERIC CHEMISTRY
WITH THE FACSIMILE/CHEKMAT PACKAGE ***

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1. INTRODUCTION

The increasing emission into the atmosphere of substances such as NO and hydrocarbons, combined with the observed increases in the concentrations of trace gases such as ozone, NO_x and methane, necessitate the study of the chemistry of the global atmosphere. Models of the chemistry of the atmosphere such as the two-dimensional global tropospheric model described here link equations of atmospheric transport and diffusion with those describing chemical reactions. The problem of the routine solution of the resulting sets of differential equations from this type of problem has stimulated the production of a program which solves the discretised equations accurately in a routine manner.

2. THE CHEKMAT PROGRAM

2.1 HISTORICAL BACKGROUND

The computer program used in our modelling, CHEKMAT, has been developed at Harwell since 1968. This was when Gear [12] first popularised a method, now known as the Backward Difference Formula (BDF) method, for solving sets of ordinary differential equations (ODEs) which have a property, known as stiffness, common in ODEs arising from chemical kinetics. CHEKMAT was derived as an acronym from CHEmical Kinetics

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