Chapter 4
MATLAB® Commands and Numerical Methods

ABSTRACT

The chapter presents numerical methods and corresponding MATLAB® commands based on these methods and designed to solve problems that arise in science and technology. The explicated methods, along with the developed live script programs, are the most popular and frequently used in solving many actual problems, in particular, in performing and processing solutions to ODEs, BVPs, and PDEs. Topics of the chapter include solving linear equations, interpolation and extrapolation, solving nonlinear equation with one unknown, integration, differentiation, and fitting by polynomials. Various applications are provided throughout the chapter and at its end; they illustrate how to fit, interpolate and extrapolate the electric resistance-temperature data, determine specific volume from the P(V,T) equation of state, calculate integral of the gas fugacity, obtain derivative representing the linear coefficient of thermal expansion, as well as another actual problems.

4.1. INTRODUCTION

Engineering and laboratory practice require usage of a variety of math operations such as interpolation, extrapolation, solution of algebraic equations, integration, differentiation, fitting. These operations are used in solving DE and/or presenting their results. Various numerical methods are used to apply these operations in computers (see e.g. Otto & Denier, 2005; Hoffman, Hoffman, & Frankel, 2001; Hamming,1986;). Among them are the Gaussian elimination method for solving system of linear equations, the bisection and secant methods for solving a nonlinear equation with one variable, the method of polynomial inter/extrapolation of data, the Simpson and trapezoidal integration methods, the finite differences method for calculating the derivative, and the least square method for polynomial data fitting. Along with the presented methods, the corresponding MATLAB® commands are provided. All methods and available commands are explained with examples that solve actual engineering problems. In separate section of the chapter, applications are given that demonstrate the use of the methods in solving the following problems:

DOI: 10.4018/978-1-6684-6850-0.ch004

- fitting and inter/extrapolation of electrical resistance versus temperature data;
- finding the specific volume of gas by the numerical solution of the nonlinear Redlich-Kwong equation;
- Numerical calculation of the integral representing the fugacity coefficient of a real gas;
- Determining the linear and volumetric thermal expansion coefficients of an isotropic material by numerical differentiaton of the measured temperature-length values.

So, general information about the numerical methods, the corresponding MATLAB® functions, and the appropriate applications are given below.

4.2. SOLVING SYSTEM OF LINEAR EQUATIONS

An equation with n unknowns x is called a linear equation: $a_1x_1+a_2x_2+\ldots a_nx_n=b$. The m of these equations is a system of linear equations:

$$\left.\begin{array}{l} a_{11} + a_{12}x_2 + \ldots a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots a_{2n}x_n = b_2 \\ \ldots \\ a_{m1}x_1 + a_{m2}x_2 + \ldots a_{mn}x_n = b_n \end{array}\right\} \tag{4.1}$$

System (4.1) can be written in matrix form as $\boldsymbol{Ax=B}$ (Chapter 2.3.1 and 2.6.4), where $\boldsymbol{A}$ and $\boldsymbol{B}$ are an nxm matrix and a column-vector (they contain the coefficients a_{ij} and b_i, respectively), and $\boldsymbol{x}$ is a column vector the unknowns x_i that can be determined using left dividing as $\boldsymbol{x=A\backslash B}$. Here it is assumed here that the matrix $\boldsymbol{A}$ is square, i.e. $n=m$.

Solution a linear equation system by the left division are based on the Gauss elimination method, in which two adjacent equations (beginning from the first one) subtract one from the other in such a way that each new equation has one fewer unknowns, so that the last equation has only one unknown x_n that can be calculated. Then this value is substituted back into the previous equation to obtain x_{n-1} and so on until the first equation. In matrix form this procedure is represented as:

$$\begin{bmatrix} a_{11} + a_{12} + \ldots a_{1n} \\ 0 \;+\; a_{22}' + \ldots a_{2n}' \\ \ldots \\ 0 \;+\; 0 + \ldots a_{nn}' \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \ldots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2' \\ \ldots \\ b_n' \end{bmatrix} \tag{4.2}$$