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Comparative experiment on the numerical solutions of Hammerstein integral equation arising from chemical phenomenon

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ABSTRACT

In this paper, efficient numerical techniques have been proposed to solve nonlinear Hammerstein integral equation arising from chemical phenomenon. The following integral equation forms the basis for the conductor like screening model for real solvent which appeared in chemical phenomenon. Our aim is to solve the Hammerstein nonlinear integral equation

$$\mu_S(\sigma) = -RT \ln\left[\int P_S(\sigma') \exp(-\frac{E_{int}(\sigma,\sigma') - \mu_S(\sigma')}{RT}) d\sigma'\right]$$

where R is the gas constant, T is the temperature and the term $E_{int}(\sigma,\sigma')$ denotes the interaction energy expression for the segments with screening charge density σ and σ' respectively, the molecular interaction in solvent is $P_S(\sigma)$ and the chemical potential of the surface segments is described by $\mu_S(\sigma)$ which is to be determined. This COSMO-RS integral equation has been solved by Bernstein collocation method, Haar wavelet method, and Sinc collocation method. These methods reduce the integral equation to nonlinear system of algebraic equations and then this algebraic system has been solved numerically by Newton's method. Comparison has been done for these methods. Illustrative examples have been discussed to demonstrate the validity and applicability of Bernstein collocation method, Haar wavelet method and Sinc collocation method.

1. Introduction

Conductor like screening model for real solvent (COSMO-RS) [1] is a quantum chemistry based equilibrium thermodynamics method with the purpose of predicting chemical potential μ in liquids. It processes the screening charge density σ on the surface of molecules to calculate the chemical potential μ of each species in solution. As an initial step a quantum chemical COSMO calculation for all molecules is performed and the results (e.g. screening change density) are stored in a database. In a separate step COSMO-RS uses the stored COSMO results to calculate the chemical potential of the molecules in a liquid solvent or mixture. The resulting chemical potentials are the basis for other thermodynamic equilibrium properties such as activity co-efficients, solubility, partition co-efficients, vapor pressure and free energy of solvation. The method was developed to provide a general prediction method with no need for system specific adjustment.

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Due to use of σ from COSMO calculation, COSMO-RS does not require functional group parameters. Quantum chemical effects like group–group interaction, mesomeric effects and inductive effects also are incorporated into COSMO-RS by this approach.

The COSMO-RS method was first published in 1995 by A. Klamt [1]. A refined version of COSMO-RS was published in 1998 [2] and is the basis for new developments and reimplementations [3–6]. Within the basic formulation of COSMO-RS, interaction terms depend on the screening charge density σ. Each molecule and mixture can be represented by the histogram $P(\sigma)$, the so called σ-profile. The σ-profile of a mixture is the weighted sum of the profiles of all its components. Using the interaction energy $E_{int}(\sigma, \sigma')$ and the σ-profile of the solvent $P(\sigma')$, the chemical potential $\mu_S(\sigma)$ of a surface piece with screening charge σ is determined as [6]

$$\mu_S(\sigma) = -RT \ln \left[\int P_S(\sigma') \exp\left(-\frac{E_{int}(\sigma, \sigma') - \mu_S(\sigma')}{RT} \right) d\sigma' \right] \tag{1}$$

where R is the gas constant, T is the temperature and the term $E_{int}(\sigma, \sigma')$ denotes the interaction energy expression for the segments with screening charge density σ and σ' respectively, the molecular interaction in solvent is $P_S(\sigma)$ and the chemical potential of the surface segments is described by $\mu_S(\sigma)$ which is to be determined. The domain of integration is determined by the characteristics of the σ-profile.

We can rewrite Eq. (1) as

$$-\frac{\mu_S(\sigma)}{RT} = \ln \left[\int_a^b K(\sigma, \sigma') \exp\left(\frac{\mu_S(\sigma')}{RT} \right) d\sigma' \right]$$

where $K(\sigma, \sigma') = P_S(\sigma')\Omega(\sigma, \sigma')$ and $\Omega(\sigma, \sigma') = \exp\{-\frac{E_{int}(\sigma, \sigma')}{RT}\}$.

Now, by substituting $y(\sigma) = \exp\left(-\frac{\mu_S(\sigma)}{RT}\right)$, we have

$$y(\sigma) = \int_a^b K(\sigma, \sigma') \left(y(\sigma')\right)^{-1} d\sigma'. \tag{2}$$

Eq. (2) is nothing but the well known nonlinear Hammerstein integral equation.

The general form of nonlinear Hammerstein integral equation is given as [7]

$$y(x) = g(x) + \int_a^b K(x, t)F(t, y(t))dt \tag{3}$$

where $K(x, t)$, $g(x)$ and $F(t, y)$ are known functions and $y(x)$ is the unknown function which should be determined.

A computational approach to solve integral equation is an essential work in scientific research. There are available many numerical methods for solving Hammerstein integral equations [7–13]. The learned researchers Dehghan et al. have applied Bernstein polynomial operational matrices for solving age-structured population models [14]. Ritz–Galerkin method with Bernstein polynomial basis [15] has been used for solving heat equation with nonclassic boundary conditions. The authors have applied Bernstein polynomial to solve system of nonlinear Fredholm integral equations [16]. Thomas–Fermi equation [17] has been solved by Sinc collocation method that converges to the solution at an exponential rate. Saadatmandi et al. have solved class of fractional convection–diffusion equation with variable coefficients by Sinc–Legendre collocation method [18]. Haar wavelet method has been applied to solve fractional differential equation by Saha Ray et al. [19,20]. Legendre multiwavelets have been used for solving weakly singular Fredholm integro-differential equations [21]. Some iterative techniques and quadrature formulae [7,8] have been applied to solve Hammerstein integral equations by Saha Ray et al. Also Hammerstein integral equation has been solved by B-spline wavelets [10].

In this present paper, nonlinear Hammerstein integral equations have been solved by Bernstein collocation method, Haar wavelet method, and Sinc collocation method. All the above methods have been applied to solve the integral equations by reducing to system of algebraic equations. From the obtained results, it is quite plausible that the results obtained by Bernstein collocation method converge more rapidly than other two methods.

2. Bernstein collocation method

2.1. Bernstein polynomials and its properties

The general form of the Bernstein polynomials of n-th degree over the interval $[a, b]$ as defined in [22,16] is given by

$$B_{i,n}(x) = \binom{n}{i} \frac{(x-a)^i (b-x)^{n-i}}{(b-a)^n}, \quad i = 0, 1, \ldots, n$$

where $\binom{n}{i} = \frac{n!}{i!(n-i)!}$.