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Effects of Jacobi polynomials on the numerical solution of the pellet equation using the orthogonal collocation, Galerkin, tau and least squares methods

Jannike Solsvik*, Hugo A. Jakobsen

Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), N-7491 Trondheim, Norway

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ABSTRACT

A number of different numerical techniques in the family of weighted residual methods; the orthogonal collocation, Galerkin, tau and least squares (LSQ) methods, are used within the spectral framework to solve a linear reaction–diffusion pellet problem with slab and spherical geometries. The node points are in this work taken as the roots of orthogonal polynomials in the Jacobi family. Two Jacobi polynomial parameters, α and β, can be used to tune the distribution of the roots within the domain. The objective of this paper is thus to investigate the influence of the node point distribution within the domain adopting the weighted residual methods mentioned above. Moreover, the results obtained with the different weighted residual methods are compared to examine whether the numerical approaches show the same sensitivity to the node point distribution. The notifying findings are as follows:

(i) Considering the condition number of the coefficient matrices, the different weighted residual methods do not show the same sensitivity to the roots of the polynomials in the Jacobi family. On the other hand, the simulated error obtained adopting the Galerkin, tau and orthogonal collocation methods for different α, β-combinations differ insignificantly. The condition number of the LSQ coefficient matrix is relatively large compared to the other numerical methods, hence preventing the simulation error to approach the machine accuracy.
(ii) The Legendre polynomial, i.e., $\alpha = \beta = 0$, is a very robust Jacobi polynomial giving on average the lowest condition number of the coefficient matrices and the polynomial also give among the best behaviors of the error as a function of polynomial order. This polynomial gives good results for small and large gradients within both slab and spherical pellet geometries.
(iii) Adopting the Legendre polynomial, the Galerkin and tau methods obtain favorable lower condition numbers than the orthogonal collocation and LSQ methods.

1. Introduction

The node points are the set of points in a given domain where the dependent variable values are approximated. In general, the choice of the location of the node points are optional, but adopting the roots of some orthogonal polynomial; referred to as collocation points, gives particularly accurate solutions for the methods of weighted residual (MWR). The focus of this paper is to investigate the effect of the collocation point distribution in a specified domain using the roots of the Jacobi orthogonal polynomials whose distributions can be tuned by two parameters, α and β. For this study different methods in the family of the MWR (Finlayson & Scriven, 1966) have been applied to solve a linear pellet problem: the orthogonal collocation method (Finlayson, 1987; Rice & Do, 1995; Villadsen, 1970; Villadsen & Michelsen, 1978; Villadsen & Stewart, 1967), the Galerkin and tau methods (Fish & Belytschko, 2007; Fletcher, 1984; Oran & Boris, 1987; Reddy & Gartling, 2010), and the least squares (LSQ) method (Bo-nan, 1998; Dorao, 2006).

Solution of reactor model equations is still challenging due to stability, accuracy and CPU-time requirements. The MWR techniques have the potential of providing sufficient accuracy with less computational expenses; but perhaps with longer model implementation time, than the finite difference and finite volume methods commonly adopted in chemical reactor engineering. The methods in the family of MWR

* Corresponding author. Tel.: +47 73594030; fax: +47 73594080.
E-mail addresses: jannike.solsvik@chemeng.ntnu.no (J. Solsvik), hugo.jakobsen@chemeng.ntnu.no (H.A. Jakobsen).

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Nomenclature

$\mathbf{A}$	coefficient matrix
$\mathcal{A}$	LSQ inner product defined by Eqs. (17a) and (17b)
$\mathcal{B}$	linear boundary operator
$\mathbf{b}$	source term of algebraic system defined by Eq. (44)
$\mathbf{g}$	source term in Eqs. (9) and (10)
c	concentration
C^0	continuous function
Collocation I	tau method boundary condition treatment
Collocation II	Galerkin method boundary condition treatment
D	diffusion coefficient
$f(x)$	solution function
f_P	trial solution
$\mathcal{F}$	LSQ source terms in Eqs. (16), (17c) and (17d)
$J_p^{\alpha,\beta}(x)$	Jacobi polynomials
J	non-dimensionalized dependent variable
k	reaction rate coefficient
L	characteristic pellet dimension
$\mathcal{L}$	linear operator
N	number of node/collocation points
P	polynomial order
r	reaction rate
$\mathbb{R}$	real number
R	residual
U	non-dimensionalized concentration
$\mathbf{v}$	perturbation function in variational statement (14)
$W_{iq} = W(x_{iq})$	quadrature weight
$w(x)$	weighting function in Eq. (23)
x	coordinate
x_i	node/collocation point
$x_{i,n}^{\alpha,\beta}$	roots of Jacobi polynomials
X	function space

Greek letters

α, β	parameters of Jacobi polynomial
α_j	basis coefficients
$\ell_{Pj}(x)$	Lagrange coefficient polynomials of degree P
$\Gamma = \partial\,\Omega$	boundary
$\mathcal{J}$	functional
κ	condition number
δ	Dirac delta
λ	eigenvalue
Ω	domain
$\partial\Omega$	boundary of Ω
ϕ	Thiele modulus
φ_{Pj}	basis function
ϵ	perturbation variable in variational statement (14)
ψ	weighting function
ξ	non-dimensionalized length

Subscript

ana	analytical solution
i	index indicating a collocation point or node point
iq	index indicating a quadrature point
j	index indicating a collocation point or node point
k	index associated with the weighting function
P	polynomial order
p	polynomial order
q	polynomial order
num	numerical solution
min	minimum
s	pellet surface