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The moment method for one-dimensional dynamic reactor models with axial dispersion

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ABSTRACT

A polynomial approximation method for calculating state profiles for plug-flow reactors is extended to one-dimensional reactor models that include axial dispersion. The method is based on the conservation of reactor state profile moments along the spatial dimension. The moments are then transformed analytically into a polynomial approximation at each timestep. The boundary conditions of the parabolic partial differential equation are given special attention. It is shown that the Danckwerts boundary conditions are an appropriate set of boundary conditions for flow problems with axial dispersion in closed-closed geometries. A significant feature of the present method is that boundary conditions of the partial differential equation model to be solved are implicitly satisfied via the moment transformation, while the polynomial profile in the numerical approximation does not have to satisfy the boundary conditions exactly. The method is tested in two cases: startup of a tubular reactor and fixed-bed adsorber involving axial dispersion.

1. Introduction

Alopaeus, Laavi, and Aittamaa (2008) presented a solution method based on the conservation of moments for dynamic plug-flow reactor models. This paper describes a generalization of the moment method for models involving axial dispersion. An important application of these models are chemical reactor models, and the mathematical model for axially dispersed reactors is featured in all well-known chemical reaction engineering textbooks, for example Fogler (1999). Axial dispersion is usually accounted for by adding a 2nd order, diffusion-type term to the model equations describing temporal and spatial variations of the concentration of a property or the temperature. Due to the 2nd order term, the type of the partial differential equation changes from hyperbolic to parabolic, and the specification of boundary conditions must be given special attention. The general mathematical expression for convection and diffusion with a source term is not only applicable in chemical engineering, but also in environmental and biological modeling, for example pollutant transport in river beds (Pimpunchat, Sweatman, Wake, Triampo, & Parshotam, 2009) or transport in underground reservoirs (Golz, 2003).

The method presented in this paper may be used as an alternative to the commonly used collocation and finite difference/finite volume methods or when an analytical solution is not available. Even when analytical solutions exist, they are usually limited to linear source terms, and their evaluation can be tedious (Liao & Shiau, 2000; Li, 2008; Zheng & Gu, 1996). However, analytical solutions still serve an important role as reference solutions for the verification of numerical methods such as the one presented in this paper.

The moment method belongs to the class of weighted residual methods (WRMs), together with the orthogonal collocation/orthogonal collocation on finite elements (OCFEs) and the Galerkin methods (Finlayson, 1972; Villadsen & Michelsen, 1978). In the moment method, the state profiles within an element are approximated by polynomials of desired degree (although there are some numerical limitations to the degree of the polynomials, see below). A moment transformation is carried out for the profiles that result in a linear expression between the moments and the polynomial coefficients: $[A](w) = (m)$. The polynomial coefficients at any given time can be calculated by simple matrix inversion. In theory and application the moment method is very similar to the Galerkin method, since both methods aim to make the trial function orthogonal to a complete set of functions. The Galerkin method forms the basis for the finite element and the moving finite element methods (MFEMs) (Carmo Coimbra, Sereno, & Rodrigues, 2001; Sereno, Rodrigues, & Villadsen, 1991; Sereno, Rodrigues, & Villadsen, 1992). In the Galerkin method, usually linear or quadratic trial functions are used, but in principle polynomials of any degree are possible (Sereno et al., 1991).

The idea behind the moment method is that the state profiles are approximated with polynomials that do not have to meet

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Nomenclature

$[A]$	linear operator between polynomial coefficients and distribution moments
b	parameter in the packed-bed adsorber case
$(b)^T$	row vector that transforms the moments into the convective-dispersive part of the integral in Eq. (7)
$[BC]$	transformation matrix between the moments and the numerical boundary conditions
c	concentration ($\mathrm{mol\,m^{-3}}$)
C	dimensionless concentration
C^*	modified dimensionless concentration in the packed-bed adsorber case
C_p	heat capacity ($\mathrm{J\,kg^{-1}\,K^{-1}}$)
Da	Damköhler number
G	result of numerical integration (quadrature)
$(Inlet)$	vector containing inlet boundary condition in 1st element, zero elsewhere
j	jth moment
$[J^j]$	diagonal matrix with elements (1.7)
k	reaction rate constant ($\mathrm{m^3\,mol^{-1}\,s^{-1}}$, $\mathrm{m^6\,mol^{-2}\,s^{-1}}$)
K_d	packed-bed adsorber parameter
$[K^i]$	diagonal matrix with elements (1.10)
L	reactor length (m)
m	moment of a distribution
$[N]$	matrix with $N_{1,1} = 1$, identically zero elsewhere
NE	number of elements
NVAR	number of variables
NQ	number of quadrature points
Pe	Péclet number
R	numerical boundary value
R_d	Retardation factor
S	general source term, dimensional in Eq. (1), otherwise dimensionless
(S)	vector of source terms at the quadrature points
t	time (s)
T	temperature (K)
u	velocity ($\mathrm{m\,s^{-1}}$)
w	polynomial coefficient
$(w)^T$	vector of quadrature weights
z	axial coordinate (m)
(z_c)	vector of quadrature points
$[Z]$	transformation matrix between polynomial coefficients and polynomial values at quadrature points
$[Z_{out}]$	transformation matrix between polynomial coefficients and polynomial values at the outflow boundary
$[Z_d]$	transformation matrix between polynomial coefficients and polynomial derivative values at quadrature points
$[Z_d^{out}]$	transformation matrix between polynomial coefficients and polynomial derivative values at the outflow boundary
$[Z_d^{in}]$	transformation matrix between polynomial coefficients and polynomial derivative values at the inflow boundary
$[*]$	matrix
$(*)$	column matrix

Greek symbols

α	order of reaction
β	parameter in the packed-bed adsorber case
δ	Kronecker delta
θ	dimensionless time
θ^*	modified dimensionless time in the packed-bed adsorber case
ρ	density ($\mathrm{kg\,m^{-3}}$)
ξ	dimensionless axial coordinate
Ψ	concentration of a property (usually $\mathrm{kg\,m^{-3}}$, $\mathrm{mol\,m^{-3}}$, $\mathrm{J\,m^{-3}}$)
ψ	dimensionless concentration of a property
ζ	dimensionless axial coordinate

Subscripts and superscripts

0	initial value, boundary value
e	index of element
i	ith element
$init$	initial condition of the adsorber in the adsorber case
j	jth moment
L	with respect to overall reactor length
ref	reference value
$\hat{}$	value calculated from polynomial

the boundary conditions exactly; it suffices that the boundary conditions are met approximately (Alopaeus et al., 2008) (in the Galerkin method, this holds for boundary conditions that involve 1st derivatives, Finlayson, 1980). This feature distinguishes the moment method from other common polynomial approximation methods, especially the orthogonal collocation methods. The way of specifying the boundary conditions in the moment method is to some extent similar to the Galerkin method, but in the moment method boundary conditions are specified at all element boundaries, whereas in the Galerkin method boundary conditions are only needed at the domain boundaries. This may be a disadvantage when strict continuity of the profiles is required, but has also advantages when the profiles have discontinuities due to physical reasons, e.g. in distillation columns at the feed location (Roininen & Alopaeus, 2010).

Actually, the boundary conditions in the moment method can be regarded as the flux through the boundary as in the finite volume method, rather than a continuity condition, as in the orthogonal collocation method. When the approximating polynomials are chosen as 0th degree polynomials, the moment method is reduced to the finite volume method with 1st order upwind discretization.

When comparing the computational time, the OCFE method is usually the fastest since it requires the least amount of operations at a time step. The moment and Galerkin methods require approximately the same amount of operations, since in both methods nonlinear integrals (quadrature) need to be evaluated. The drawback of the OCFE method is, however, that the boundary conditions at the endpoints and the element boundaries appear as algebraic equations that have to be satisfied during time integration (Finlayson, 1980).

An important question that arises in conjunction with axial dispersion models is that of the appropriate boundary conditions. The Danckwerts boundary conditions for flow systems with axial dispersion and reaction, named after a famous paper by Danckwerts (1953), have been scrutinized for now more than a half of a century. Although the Danckwerts boundary conditions are widely established, they are still questioned by many researchers. A number of papers dealing with the issue have been published since the original paper appeared (e.g. Bischoff, 1961; Deckwer & Mählmann, 1976; Golz & Dorroh, 2001; Golz, 2003; Lee, Wang, & Newell, 1998; Salmi & Romanainen, 1995; Wehner & Wilhelm, 1956). Parulekar and Ramkrishna (1984a,b,c) analyzed systematically different types of open and closed boundary conditions in transient systems with appended semi-infinite fore and aft sections to the reactor using