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Application of the meshless generalised RKPM to the transient advection-diffusion-reaction equation

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ABSTRACT

A variety of physical problems may be expressed using the advection–diffusion-reaction (ADR) equation that encompasses transport processes into a porous or nonporous material. Finding a theoretical solution to the ADR equation is difficult with time-dependent nonlinear coefficients, complicated geometries, general initial value and/or boundary conditions. In this paper a meshless model is developed by adapting the generalised reproducing kernel particle method to the strong and weak integral forms of ADR equation. Moreover, mixed–type boundary conditions are directly enforced via generalising the corrected collocation method. The model is validated using existing analytical solutions and shown to be both accurate and efficient.

1. Introduction

The continuity equation can be used to describe transport of quantities such as mass, energy and momentum. It is normally a homogenous partial differential equation (PDE) of second order but can also be, more generally, a non-homogeneous PDE with a source term. The source term allows expression of the transport of quantities that may not necessarily be conserved as they can be generated or consumed in a reaction. A variety of physical problems in engineering and science may be expressed using the general form of the continuity equation; the advection-diffusion-reaction (ADR) equation is a good and practical example. The ADR equation covers the general case of the transport phenomenon including heat transfer and transport of mass and chemicals into a porous or a nonporous media. As a point of interest for researchers in the field of concrete durability, the transport of moisture [1–3], CO_2 [1] and chloride ions [2,3] into concrete can be described by this equation. Carbonation or chloride contamination in concrete may result in the corrosion of steel reinforcement that affects the performance and the expected service life of reinforced concrete structures.

Finding a theoretical solution of the ADR equation becomes difficult when the problem has time-dependent and nonlinear coefficients, 2D or 3D domain with complicated geometry, and general initial value and/or boundary conditions (BCs). Numerical simulation is the only feasible way to solve such problems [4]. The Variational approach and the weighted residual method (WRM) are two distinct numerical procedures for deriving approximations of the governing equation and the associated BCs [5,6]. The finite difference method (FDM), the finite element method (FEM), the finite volume method (FVM) and the boundary element method (BEM) are among the commonly used variants of WRMs for solving the ADR equation. All these methods are based on local interpolation schemes and need mesh for modelling the problem [7]. There exist various review papers on summary and comparison of some commonly used finite difference and finite element methods for solving the advection-diffusion (AD) and ADR equations [8,9]. The FDM as a traditional strong formal numerical method has deficiency in dealing with complicated geometry [4] or using non-uniform particle distribution [10]. The FDM also shows lack of accuracy in solving hyperbolic PDEs such as those obtained in advection-dominated problems [7]. The FEM has been successfully established and conveniently applied to a variety of problems in engineering. Nevertheless, it has drawbacks in solving nonlinear diffusion problems with non-homogeneous coefficients because of unavoidable mesh sensitivity and time costs of adaptive mesh generation [4].

During the last three decades, considerable efforts have been devoted to develop mesh free (MFree) methods to overcome cost of the mesh generation, connectivity, dependency and sensitivity problems in mesh-based methods [11]. So far, various meshless

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methods have been introduced in the literature and there exist review papers on summary and comparison of some commonly used meshless methods [12,13]. Lucy [14] and Gingold and Monaghan [15] introduced one of the first MFree methods, the smoothed particle hydrodynamics (SPH), based on kernel approximations. SPH suffers from a lack of consistency that can lead to poor accuracy and tensile instability. The latter is as a result of combination of an Eulerian kernel with a Lagrangian formulation and it can be avoided by substituting a Lagrangian kernel that is preferable in modelling solids and computational costs [16]. Liu et al. introduced the meshless reproducing kernel particle method (RKPM) that provides certain degree of consistency for the finite integral approximation [17]. The RKPM solution and its derivatives can have any desired order of continuity by adopting a window function with adjustable order of continuity [17,18]. RKPM not only maintains the free Lagrange concept as the most attractive feature of the SPH method, but also restores the first order completeness and improves the approximation near boundaries by introducing a continuous correction function to the original kernel function of the SPH approach [16,17].

Some meshless methods have been successfully applied to diffusion and AD equations. To give some examples, one can refer to the solution of unsteady-state heat conduction problem with the SPH method [19], 2D and 3D heat conduction using the element free Galerkin method (EFGM) [20], and also the solution of the AD equation using the finite point method (FPM) [21], the meshless local Petrov-Galerkin method (MLPG) [22] and the radial basis functions (RBF) [7]. Moreover, Liu and Chen [23] applied the RKPM to the steady-state AD equation. Hashemian and Shodja [24] later solved the unsteady Burgers' equation, as a special case of AD equation. The RKPM was also recently used to improve the performance of the triangular B-splines for solving PDEs [25].

Despite the given merits, the enforcement of BCs in MFree methods is usually a source of difficulty because the corresponding shape functions do not necessarily hold the Kronecker delta property [17,26–28]. To remedy this, a variety of methods have been introduced; these are classified into two main groups [29]: methods based on a modification of the weak form such as the Lagrange multiplier method [30], the penalty method [31,32] and the Nitsche's method [33,34], and methods that can be interpreted as a modification of interpolation shape functions [26,35]. Wagner and Liu [27] proposed the corrected collocation method that fully restores the convergence rate decrease as a result of using the invalid traditional collocation method. Wu and Plesha [28] showed that the corrected collocation method is identical to the generally accepted reduced Lagrange multipliers method.

Shodja and Hashemian [36] generalised the corrected collocation method to enforce the gradient type of constraints; they presented the gradient RKPM by incorporating first-order derivatives in the reproduction formula [36,37]. The idea was further extended in [38] that resulted in the formulation of MLS in a way that the derivatives of the field variable with any desired order are incorporated in the formulation; the generalised RKPM was introduced as discretised form of the generalised MLS. Nodal enforcement of derivative-type BCs is the significant advantage of the gradient/generalised RKPM over the conventional RKPM in which the enforcement of such BCs can be cumbersome and inaccurate [36–38].

Previous numerical studies on ADR equation generally solved the problem in weak form and enforced mixed-type BCs (if considered) either implicitly through weak formulation or indirectly using techniques such as the penalty method or the Lagrange multipliers. In this paper the transient ADR equation is formulated in both strong and weak forms and is solved numerically by applying the Bubnov-Galerkin WRM. A new implementation of the meshless generalised RKPM with a continuous Lagrangian kernel is considered for spatial discretisation of the weighted integrals. This method not only holds the key features of the conventional RKPM (such as p-refinement), but also incorporates derivatives of the field variable (up to any desired order) as independent degrees of freedom (DOFs). In this study, the latter feature is utilised to precisely enforce any mixed-type BC or its special cases (*i.e.* natural and essential BCs) in a direct manner. Furthermore, sensitivity analyses to the influencing parameters such as Peclet number, surface diffusivity and reaction rates are undertaken to provide insight to the nature of the problem.

The outline of the paper is as follows. In next section, the general n-dimensional formulation of the unsteady ADR equation and its associated BCs is presented. The generalised RKPM that is utilised for spatial discretisation is briefly reviewed in Section 3. The numerical solution of the governing equation in both strong and weak forms is explained in Section 4 and the proposed procedure for direct enforcement of different types of BCs is detailed in Section 5. A number of numerical examples are given in Section 6 to verify the accuracy and illustrate the capabilities of the new technique, while Section 7 concludes the paper.

2. General formulation

The unsteady advection-diffusion-reaction equation, as the most general mass transport equation, can be expressed in the form of the general continuity equation as:

$$A(\phi) = \alpha_\phi \frac{\partial \phi}{\partial t} + \nabla.\mathbf{q} - Q_\phi = 0, \tag{1}$$

where ϕ is the field variable, α_ϕ is the potential coefficient, t is the time of exposure, $\mathbf{q}$ is the flux vector, and finally Q_ϕ is the source term indicating the rate for consumption or production of the field variable in the corresponding reactions. In general, flux of the field variable is the combination of diffusive and advective fluxes as the main mechanisms for the transport phenomenon; thereby, the flux vector can be written as:

$$\mathbf{q} = -\mathbf{D}_\phi \nabla\phi + \boldsymbol{\beta}\phi, \tag{2}$$

where $\mathbf{D}_\phi$ is the matrix of diffusion coefficients and $\boldsymbol{\beta}$ is the vector of advective velocities in different dimensions of the general n-dimensional space. For example, $\mathbf{D}_\phi$ and $\boldsymbol{\beta}$, in two dimensional Cartesian coordinates, are:

$$\mathbf{D}_\phi = \begin{bmatrix} D_{\phi x} & 0 \\ 0 & D_{\phi y} \end{bmatrix}; \quad \boldsymbol{\beta} = \begin{Bmatrix} \beta_x \\ \beta_y \end{Bmatrix}. \tag{3}$$

By back substitution of Eq. (2) for flux expression into governing Eq. (1) and expanding the advection term, one obtains:

$$A(\phi) = \alpha_\phi \frac{\partial \phi}{\partial t} - \nabla.(\mathbf{D}_\phi \nabla\phi) + (\nabla\phi).\boldsymbol{\beta} + (\nabla.\boldsymbol{\beta})\phi - Q_\phi = 0. \tag{4}$$

The first possible BC of this problem is the essential BC as the set of prescribed values ($\bar{\phi}$) for the field variable on Γ_ϕ. The second possible BC is the set of prescribed flux ($\bar{q}_n$) for the normal flux of the field variable (q_n) on Γ_q. The possible BCs of this problem are thus expressed by:

$$B(\phi) = \begin{Bmatrix} \phi - \bar{\phi} = 0 & : \Gamma_\phi \\ q_n - \bar{q}_n = 0 & : \Gamma_q \end{Bmatrix}. \tag{5}$$

The normal flux of the field variable is equal to $\mathbf{q}.\mathbf{n}$ where $\mathbf{n}$ is the unit normal vector of Γ_q. The flux BC is obtainable by equalising the flux of the field variable at the surface of the material with that in the surface boundary layer (SBL) surrounding the material. The flux BC has been commonly expressed by the following equation:

$$-(\mathbf{D}_\phi \nabla\phi).\mathbf{n} = \vartheta_{sn}(\phi_s - \phi), \tag{6}$$