International Communications in Heat and Mass Transfer 37 (2010) 125–130

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Using bubble functions in the multi-scale finite element modeling of the convection–diffusion–reaction equation ☆

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ARTICLE INFO

Available online 17 October 2009

Keywords:
Convection–diffusion–reaction equation
Bubble functions
Finite elements
Multi-scale
Transport processes

ABSTRACT

The Convection–diffusion–reaction (CDR) equation shows multi-scale behaviour in cases where it represents convection or reaction dominated transport processes. Bubble function enriched finite elements are used to generate stable and accurate solutions for this equation. To validate the approach, the numerical results obtained for a benchmark problem are compared with their corresponding analytical solution for both exponential and propagation regimes.

1. Introduction

The general mathematical model incorporating different types of transport phenomena is expressed as the CDR equation. In general, however, the solution of this equation cannot be assumed to be globally smooth. In particular, if the field variables vary rapidly within thin layers adjacent to domain boundaries, or internal layers, sharp gradients are produced and standard numerical schemes lead to inaccurate and unstable results. Almost all of such situations can be regarded as multi-scale phenomena in which both fine and coarse scale variations of field variables need to be taken into account in the numerical solution of the CDR equation. Theoretically, any basically sound scheme should generate accurate numerical results if sufficiently refined computational grids are used. In practice, however, such an approach will not be computationally cost effective.

These complications can be resolved using variational multi-scale methods [1,2]. The multi-scale approach can be applied to situations where traditional methods can only be used in conjunction with very fine discretizations. Therefore this technique offers a general method for the modeling of transport problems with multi-scale behaviour. Amongst such problems turbulent flow, convection–diffusion processes and flow in porous media can be considered. In all of these problems, the simultaneous representation of all of the governing physical phenomena requires very high levels of mesh refinement or artificial smoothing, otherwise the fine scale information is ignored resulting in the generation of unstable and inaccurate [3] solutions. In the variational multi-scale method, the field unknown (T) is divided into two parts as $T=T_1+T_b$, where T_b represents the fine scale variations of T and may be derived analytically whilst T_1, the coarse scale variations of T, is approximated using standard polynomial finite element discretizations. To generate practical multi-scale schemes the bubble enhanced trial functions can be used in a finite element context. Bubble functions are, typically, high order polynomials which vanish on the element boundaries [4–7]. A systematic approach to derive bubble functions is the residual free bubble (RFB) method [8–11]. In this method, the governing differential equation is solved within each element subject to homogeneous boundary conditions.

The behaviour of the CDR equation has mainly been studied under exponential regimes [12–17]. To study the CDR equation in both exponential and propagation regimes Hauke [18] has developed a sub-grid scale model based on a time-scale parameter, originally defined and formulated by Hughes [1].

In this paper the bubble functions are used for multi-scale finite element modeling of CDR equation in both exponential and propagation regimes for a relatively wide range of Peclet and Damköhler numbers. In multi-dimensional problems the analytical solution of the CDR equation can represent major difficulties. To overcome such problems a semi-discrete method is developed in which the solution of the PDE is replaced by the analytical solution of ordinary differential equations [19]. In this technique the exact solutions obtained from the ODE is expanded using the Taylor series and the multi-dimensional bubble functions are derived by tensor products of one-dimensional functions. The resulting functions are polynomial bubble functions which, for example, have been used to model the flow in porous media by Parvazinia et al. [19].

The method of incorporating bubble functions with Lagrangian shape functions using both semi-discrete and the static condensation methods are explained in the solution of the CDR equation.

☆ Communicated by J.W. Rose and A. Briggs.

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doi:10.1016/j.icheatmasstransfer.2009.09.007

Nomenclature

D_a	Damköhler number
f	a given source term
h	a characteristic length (e.g. width of the domain)
k	diffusion (conduction) coefficient
l	characteristic element length
Pe	Peclet number
s	a source/sink term ($s>0$ represents production and $s<0$ stands for dissipation)
T	the field unknown
T_1	a reference value of the field variable
v	velocity vector
W_i	linear weight function
$\overline{x}$	position vector in the selected coordinate system

Greek symbols

ψ_i	linear shape function

Superscript

*	represents the dimensionless variables

2. Governing equations

The steady state convection–diffusion–reaction equation in domain $\Omega\subset R^d$ can be written as

$$v\cdot\nabla T - k\nabla\cdot\nabla T - sT = f. \quad (1)$$

Using the following dimensionless relations

$$\begin{cases} T^* = \dfrac{T}{T_1} \\ \overline{x}^* = \dfrac{\overline{x}}{h} \end{cases}. \quad (2)$$

The general governing equation is written in a dimensionless form as

$$\nabla T^* - \frac{1}{Pe}\nabla\cdot\nabla T^* - D_a T^* = f^*. \quad (3)$$

In which f^* is the dimensionless source term, Pe is the Peclet number and D_a is the Damköhler number, respectively, defined as

$$\begin{cases} Pe = \dfrac{vh}{k} \\ D_a = \dfrac{sh}{v} \\ f^* = \dfrac{h}{T_1 v} f \end{cases}. \quad (4)$$

It is assumed that Pe is equal in both directions. A similar assumption is made for Da (see Fig. 1). In a two-dimensional system (x^*, y^*) Eq. (3) can be written as

$$\left(\frac{\partial T^*}{\partial x^*} + \frac{\partial T^*}{\partial y^*}\right) - \frac{1}{Pe}\left(\frac{\partial^2 T^*}{\partial x^{*2}} + \frac{\partial^2 T^*}{\partial y^{*2}}\right) - DaT^* = f^*. \quad (5)$$

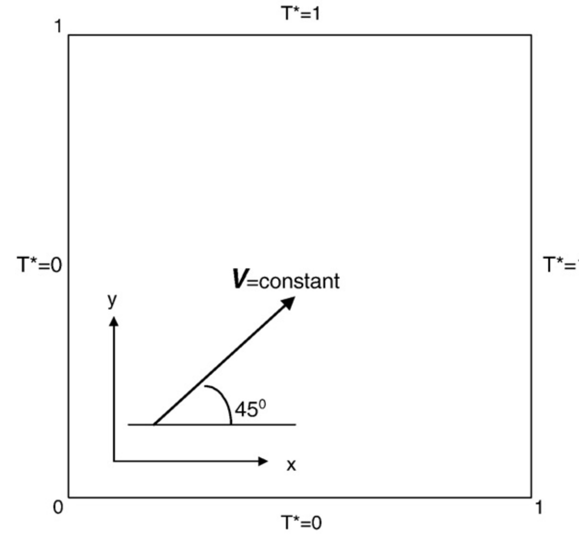

Fig. 1. Domain and the boundary conditions for the exponential regime.

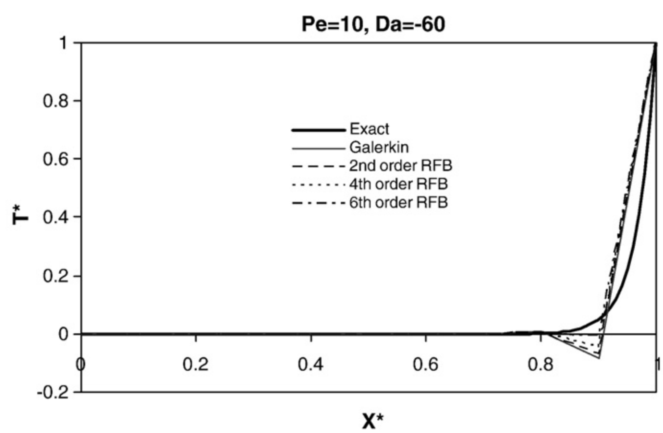

Fig. 2. Results for $Pe=10$ and $D_a=-60$ at $y^*=0.5$ — exponential regime.

Corresponding dimensionless boundary conditions for the rectangular domain are:

a) Dissipation (see Fig. 1):

$$\begin{aligned} &T^* = 0 \quad \text{for } y^* = 0, 0\le x^*\le 1 \text{ and } x^* = 0, 0\le y^* < 1 \\ &T^* = 1 \quad \text{for } x^* = 1, 0\le y^* < 1 \text{ and } y^* = 1, 0\le x^*\le 1. \end{aligned} \quad (6)$$

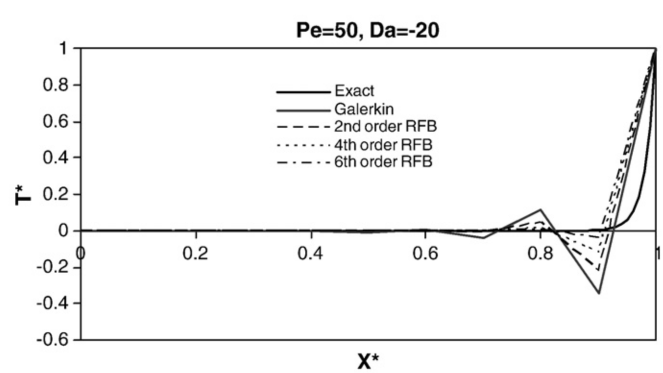

Fig. 3. Results for $Pe=50$ and $D_a=-20$ at $y^*=0.5$ — exponential regime.