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An adaptive moving grid method for solving convection dominated transport equations in chemical engineering

R. Kelling[a,*], J. Bickel[a], U. Nieken[a], P.A. Zegeling[b]

[a] Institute of Chemical Process Engineering, Boeblinger Str. 78, 70199 Stuttgart, Germany
[b] Department of Mathematics, P.O. Box 80010, 3508 TA Utrecht, The Netherlands

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ABSTRACT

Convection dominated processes in chemical engineering are frequently accompanied by steep propagating fronts. Numerical simulation of corresponding models with uniform fixed grids requires an excessive amount of grid points along the expected range of the front movement. In this contribution the implementation of an efficient adaptive grid method is presented and applied to two relevant spatially one-dimensional cases, the chlorination stage of the Deacon process and oxygen storage processes in a three-way catalyst. The algorithm exhibits a high accuracy with a much lower number of grid points and a therefore reduced computational effort as opposed to a fixed grid simulation. The present work demonstrates that the algorithm allows for a robust, simple, and fast implementation of the adaptive grid method in common simulation tools and, together with adequate supplementary material, aims to make the method readily accessible to the interested reader.

1. Introduction

Many convection dominated processes in chemical engineering, especially industrial scale applications, are characterized by the formation of steep moving fronts (Eigenberger et al., 2007). A well-known example is the propagation of a thermal and a reaction front during an endothermic or exothermic reaction in a tubular packed bed. Traveling fronts are common phenomena in adsorption columns, ion exchangers, regenerative heat exchangers, or membrane reactors.

The numerical simulation of steep moving fronts or shock fronts with adequate accuracy in time and space is computationally expensive. Many adaptive methods are available to rearrange the grid points according to the local errors of the partial differential equations describing such systems. This allows reducing the number of grid points and therefore the number of equations and the computational cost. Desirable requirements for such methods are a straightforward and easy adaptation of the adaptive grid to the actual physical problem and a fast implementation of the algorithm in common simulation tools. The method has to find high local gradients automatically without an a priori specification of their temporal position, using general grid defining parameters. In this paper we present such a technique using the adaptive grid method as developed in Zegeling (2007) and van Dam and Zegeling (2010) for two typical, spatially one-dimensional models of chemical engineering applications. The models are solved on a moving grid by established simulation tools (MATLAB©, DIANA (Krasnyk et al., 2006)) which provide efficient and robust solvers.

In Section 2 we classify the presented adaptive grid method and describe the main steps of implementation for a general model. In Section 3 the adaptive grid is used to simulate the chlorination stage of the Deacon process. Here, chlorine is stored in a fixed bed leading to a decrease of the total gas flow. The resulting steep fronts make it difficult to carry out an accurate and efficient numerical simulation of this process with uniform grids. In Section 4 we analyze traveling fronts during oxygen storage in a three-way catalyst. Both models are used to provide practical implementation remarks and investigate the performance of the adaptive grid method.

2. Adaptive grid method

In this section we classify the presented adaptive method and describe the algorithmic structure corresponding to its key ingredients: discretization and transformation of the balance equations, the grid defining equation with corresponding parameters, and the monitor function. Although the method handles problems in more than one dimension (Zegeling, 2007; Zegeling et al., 2005; Zegeling

* Corresponding author. Tel.: +49 711 685 85247.
E-mail addresses: rene.kelling@icvt.uni-stuttgart.de, kelling.rene@googlemail.com (R. Kelling).

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Notation

Latin letters

A	reactor cross-section area
B	left hand side matrix of grid equation
c	concentration
c_p	specific heat capacity
D	coefficient of dispersion
E_A	activation temperature
Δh_r	heat of reaction
k^∞	rate constant
L	reactor length
$\dot{m}$	mass flow
MW	molar mass
n	number of grid points
OSC	oxygen storage capacity
OSL	oxygen storage level
p	partial pressure
q	quality of a solution
ROL	relative oxygen level
r	reaction rate per unit of reactor volume
s	steepness of a front
s	right hand side vector of grid equation
t	time
T	temperature
TWC	three-way catalyst
u	states
v_R	velocity of reaction front
w	mass fraction
x	spatial coordinate

Greek letters

α	monitor regularizing parameter
ϵ	volume fraction gas phase
θ	transformed time
λ	axial heat conduction
ν	transformed states
ξ	uniform computational coordinate
σ	spatial smoothing parameter
ρ	density
τ	time smoothing parameter
ω	monitor function

Superscripts

G	gas
S	solid

Subscripts

0	initial
i	index for each grid point
in	inlet
s	index for each state
exh	exhaust

and Kok, 2004), we focus on one-dimensional models for a better understanding of the basic principle.

2.1. Classification of the method

In combination with the method of lines, the discretization in space is carried out using an adaptive grid while the solution in time is obtained with an appropriate solver for the resulting differential-algebraic equation system (DAE). Regarding the implementation of the adaptive grid, different strategies can be applied (Huang and Russel, 2011). To locally increase the grid resolution, mesh cells can be divided into smaller cells by adding grid points (h-refinement). This method is disadvantageous if the number of DAEs has to be fixed for the simulation process (as is the case in several numerical tools). During the so-called r-refinement, which is used in the presented method, the grid nodes are moved to increase local resolution and the number of grid points remains constant. Besides, static and dynamic regridding is distinguished. In static regridding the grid adapts after each time step whereas in the here considered dynamic regridding the adaption is made during each step, which is powerful for traveling fronts and results in larger time steps (Nowak et al., 1996). The presented adaptive method applies a monitor based grid definition equation, using features of the underlying balance equations (physical states) and mesh quality measures. The method is described in the following.

2.2. Discretization and transformation of balance equations

In order to model chemical engineering processes, balance equations (1) for each model state u (e.g. temperature or concentrations) together with corresponding initial conditions (2) can be derived. In the resulting system of partial differential equations (PDEs) the right hand side f does, in general, depend on a function of the states, the time t, the spatial coordinate x and spatial derivatives of the states.

$$\frac{\partial u}{\partial t} = f(u, t, x), \tag{1}$$

$$u(x, t = 0) = u_o(x). \tag{2}$$

In the present case, the PDEs describing the systems considered are parabolic PDEs, consisting of an accumulation term $a(u, t, x)$, a convective term $b(u, t, x)$, a dispersion term $c(u, t, x)$, and a nonlinear reaction source term $d(u, t, x)$:

$$a(u, t, x)\frac{\partial u}{\partial t} = -b(u, t, x)\frac{\partial u}{\partial x} + \frac{\partial}{\partial x}\left(c(u, t, x)\frac{\partial u}{\partial x}\right) + d(u, t, x). \tag{3}$$

To numerically approximate the solution of the resulting PDE system, the spatially dependent variable is discretized along n grid points x_i in the method of lines approach:

$$x = (x_1 = 0, \ldots, x_i, \ldots, x_n = L)^T. \tag{4}$$

Due to the underlying physical processes, steep moving fronts of some states such as temperature and concentration fronts may arise. Consequently, a uniform fixed distribution of the grid points x_i is highly inefficient regarding the computational cost to resolve these fronts. Thus, we apply a technique that is based on a minimization of a so-called mesh-energy integral (Zegeling and Kok, 2004) which distributes the grid points in an adaptive and more efficient way. An additional adaptive grid PDE, describing the movement of the grid, is resulting from this minimization.

The implementation of the adaptive grid is carried out through a coordinate transformation depicted in Fig. 1. The physical (real) solution $u(x, t)$, including 'steep' fronts, is now considered along a non-uniform adaptive coordinate $x(t)$. Through the transformation, this solution is mapped to a computational uniform coordinate system (ξ, θ). Here the solution $\nu(\xi, \theta)$ becomes 'milder'. The balance equations are now considered along this computational coordinate and are therefore easier to solve. To be more precise, the regular transformation (5)–(6) maps the 'steep' solution of the state $u(x, t)$ to a 'mild' computational function $\nu(\xi, \theta)$.

$$\Phi : (x, t) \to (\xi, \theta) \tag{5}$$

$$t(\xi, \theta) = \theta \tag{6}$$