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Using Moving Finite Elements Method to solve Population Balance Equations comprising breakage terms

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Abstract

This paper introduces a Moving Finite Elements Method (MFEM) based on cubic Hermite polynomial local approximations to handle Population Balance Equations (PBE) modeling breakage phenomena. The adequacy and performance of the MFEM framework are tested in two case studies involving breakage: a benchmark problem with known analytical solution and the hydrolysis of starch. Both examples emphasize the stability and accuracy of MFEM in handling PBE models, thus proving its suitability for this kind of problem.

Keywords: Moving Finite Elements, Population Balance Equation, Breakage.

1. Introduction

Particulate and emulsion systems have always been present in nature and in chemical and biological processes. Many of the recently developed products also correspond to good examples of dispersed multiphase systems and this led to a growing interest on the development of models for these particulate systems characterized by both a continuous and a dispersed phase. The population balance models (PBE), based on the extensity density balance

regarding the particles, enable to describe their behavior in a particular surrounding environment.
The numerical approaches employed to solve PBE models fall into two main strategies: i. solution representation by global/local basis function approximations, encompassing all finite element schemes; ii. Discretized Population Balance (DPB) methods, based on the concept of pivot. For a detailed analysis of DPB methods see [1]. In recent years Finite Elements methods became quite appealing to handle PBE models, since they provide a general framework [2]. The literature on the application of adaptive grid strategies to PBE models is scarce, although these schemes are remarkably promising since some PBE models develop moving fronts and sharp dynamics caused by the initial distribution. Most of the adaptive techniques applied to PBE are based on DPB methods, exploiting the moving pivot concept introduced by Kumar and Ramkrishna [3] (see for instance the work of Attarakih *et al*. [4]). Mahoney and Ramkrishna [5] presented an approach based on the combination of a Galerkin-finite elements scheme with the method of characteristics to capture the motion of pivots. Tsang and Rao [6] presented a Moving Finite Elements explicit approach based on linear approximations to handle PBE models. In this work a general Moving Finite Elements approach based on cubic Hermite polynomial approximations and the Method of Lines to handle PBE models comprising breakage terms are used.

2. Moving Finite Elements Method formulation

The MFEM, firstly proposed by Miller and Miller [7], stands on the minimization of the residuals all over the domain $\Omega=[0,\ t^f]$**Error! Objects cannot be created from editing field codes.**$[0,\ V]$, where t^f is the maximum integration time and V the limit of the spatial domain. A general PBE model is represented as:

$$n_t = \ell\left(n, n_v, \int n\,\mathrm{d}v, v, t\right) \tag{1.a}$$

$$n(0,t) = \beta\left(n, n_v, \int n\,\mathrm{d}v, v, t\right) \tag{1.b}$$

$$n(v,0) = f(v) \tag{1.c}$$

where $n(v,t)$ represents the density of particles with v dimension at time t, n_t stands for its time derivative, n_v for its spatial derivative, $\ell(\bullet)$ is an operator comprising differential, integral and non-linear transformations of $n(v,t)$, $\beta(\bullet)$ is the boundary condition, and $f(v)$ the initial particle size distribution (PSD). The global residuals, $r(\bullet)$, can be calculated by:

$$r(\bullet) = n_t - \ell\left(n, n_v, \int n\,\mathrm{d}v, v, t\right) \tag{2}$$

which are approximated by using a global polynomial approximation to represent the particles density. In this paper, cubic Hermite polynomials are employed [8]:

$$n = \sum_{k=1}^{N} \sum_{i=1}^{4} a_{k,i}(t) H_i\left[u, h_k(t)\right] \tag{3}$$

where $a_{k,i}(t)$ stands for the time dependent coefficients, $H_i[\bullet]$ for the cubic Hermite polynomials, $u=(v-s_{k-1})/(s_k-s_{k-1})$ for a scaled spatial variable, $h_k(t)=s_k(t)-s_{k-1}(t)$ for the size of kth finite element, $s_k(t)$ for kth node position and N for the number of finite elements. The minimization of the square norm of the residuals with respect to time derivatives of coefficients $a_{k,i}(t)$ and node velocities, here represented as $\dot{s}_j$, leads to the basic equations of the method, with $k \in \{1, \cdots, N\}$:

$$\int_{s_{k-1}}^{s_k} R_k \frac{\partial R_k}{\partial \dot{a}_{i,k}} dh_k + \int_{s_k}^{s_{k+1}} R_{k+1} \frac{\partial R_{k+1}}{\partial \dot{a}_{i,k}} dh_{k+1} = 0 \qquad i \in \{1, \cdots, 4\} \tag{4.a}$$

$$\int_{s_{k-1}}^{s_k} R_k \frac{\partial R_k}{\partial \dot{s}_j} dh_k + \int_{s_k}^{s_{k+1}} R_{k+1} \frac{\partial R_{k+1}}{\partial \dot{s}_j} dh_{k+1} = 0 \qquad j \in \{0, \cdots, N\} \tag{4.b}$$

where R_k stands for the approximation of $r(\bullet)$ in the kth finite element. To avoid node coalescence a penalty term is added to the square residuals objective function. Therefore, equation (4.b) is replaced by equation (5) with ε standing for the internodal force:

$$\int_{s_{k-1}}^{s_k} R_k \frac{\partial R_k}{\partial \dot{s}_j} dh_k + \int_{s_k}^{s_{k+1}} R_{k+1} \frac{\partial R_{k+1}}{\partial \dot{s}_j} dh_{k+1} + \varepsilon\left(2\dot{s}_j - \dot{s}_{j-1} - \dot{s}_{j+1}\right) = 0 \tag{5}$$
$$k \in \{1, \cdots, N\}, j \in \{0, \cdots, N\}$$

Equations (4.a) and (5) coupled with the relations arising from the discretization of the boundary conditions lead to the Differential Algebraic Equations (DAE) system to be solved. The solver used, which is based on BDF methods, enables one to exploit the jacobian sparsity in order to increase the computational efficiency. The structure of the differential component of the jacobian has the form of a diagonal band matrix of width 9, and the algebraic component is an upper triangular full matrix due to integral terms that represent the breakage phenomena. Both components are computed numerically. In the solver the relative tolerance was set to 10^{-6} and the absolute tolerance to 10^{-9}. The integral

terms involved in Equations (4.a) and (5) are calculated by Gaussian Quadrature (GQ) based on 8 collocation points, two of them located at the nodes.

3. Application of MFEM to PBE models involving breakage terms

In this section the framework derived in Section 2 is applied to PBE models describing physical processes involving some extent of breakage – division of the particles into smaller size entities. Case 1 intends to evaluate the accuracy of the approach in dealing with a benchmark problem with analytical solution available. Case 2 aims at submitting the method to a more challenging problem, and handling simultaneously the model describing the wheat starch hydrolysis, of interest to the food industry.

3.1. Case 1 – Ziff's fragmentation model

This model was proposed by Ziff and McGrady [9], and is commonly used as a benchmark problem for numerical strategies handling breakage terms, since its analytical solution is available:

$$\frac{\partial n(v,t)}{\partial t} = -S(v)n(v,t) + \int_{v}^{+\infty} \rho(v,v')S(v')n(v',t)\,\mathrm{d}v' \tag{6.a}$$

$$\rho(v,v') = 2/v',\ S(v) = v,\quad v \in \left[10^{-5};5\right],\ t \in [0;2] \tag{6.b}$$

$$n(v,0) = \exp(-v) \tag{6.c}$$

where $n(v,t)$ is the PSD, $\rho(v,v')$ is the breakage function and $S(v)$ the breakage rate kernel. Figure 1 highlights the accuracy and stability of the MFEM approach based on a non-regular initial grid, particularly on the zones of smaller particles. As time elapses, at the zones of larger particles the approach is less accurate as a result of the approximation of the upper limit of the integral. One may see that the nodes tend to move to the zone where the gradients of the solution are higher. However, due to the stabilization introduced by the integral term and the smoothness of the solution, its motion is slow. The results, particularly the numerical solution accuracy, allow us to state that the MFEM is suitable for solving PBE models involving breakage terms.

3.2. Case 2 – Hydrolysis of wheat starch model

The model describing the hydrolysis of wheat starch was proposed by Chang *et al.* [10] aiming at studying the effect of the hydrolysis phenomenon on the Falling Number measurement. In this problem $n(v,t)$ represents the molecular

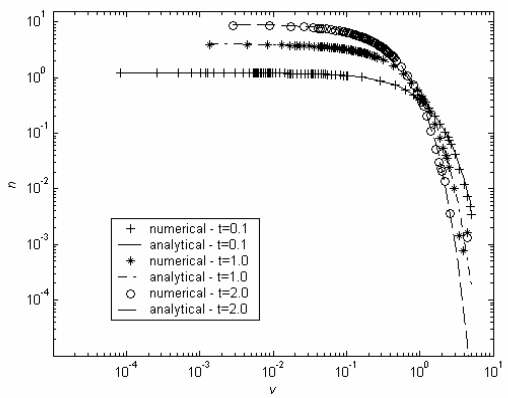

Figure 1 – Fragmentation model: comparison of analytical *vs.* numerical solution.

weight distribution (MWD) of starch, and v stands for the molecular weight, yielding the model:

$$\frac{\partial n(v,t)}{\partial t} = -r(T,t)n(v,t) + \int_{v}^{+\infty} 2\sigma(v,v')r(T,t)n(v',t)\,\mathrm{d}v' \tag{10.a}$$

$$r(T,t) = C_0\left[1-\exp\left(-k_g t\right)\right]k_0 \exp\left(-E_a/(RT)\right) n_0\, e\exp\left[-k_d \exp\left(-E_d/(RT)\right)t\right] \tag{10.b}$$

$$n(v,0) = \left[\frac{z^z}{M_n \Gamma(z)}\right]\left(\frac{v}{M_n}\right)^z \exp\left(\frac{-zv}{M_n}\right),\ z = \frac{M_n}{M_w - M_n} \tag{10.c}$$

$$\sigma(v,v') = 1/v', \qquad v \in \left[4\times10^2;1.5\times10^7\right],\ t \in [0;350] \tag{10.d}$$

where $r(T,t)$ is the temperature dependent depolymerization reaction rate and $\sigma(v,v')$ the partition function that describes the probability of breaking starch chain of mass fraction *v'* into a mass fraction *v*, which is described in this case by a uniform function. It was considered that the temperature remains constant, T = 298.50 K, and the parameters are listed in the work of Chang *et al*. [10].
One may see in Figure 2 that the starch chain breaks as the time evolves producing lower molecular weight chains. Such a behavior is remarkably fast until the steady state is reached, around 350 s. However, MFEM presents stable solutions for the all domain and captures the solution magnitudes quite accurately.

4. Conclusions

This paper presents a moving finite grid strategy for the solution of PBE models, particularly those including breakage terms. The numerical approach –

Moving Finite Elements Method – provides a general framework to deal with evolutive Partial Differential Equations, from which PBE models are good examples. The MFEM formulation presented is based on local cubic Hermite polynomials and the Method of Lines. Its application to a benchmark problem allowed us to evaluate its accuracy and stability, which is indeed remarkable. The ability of the numerical approach to handle problems that involve changes of large magnitude was successfully tested using an example from the food industry. Based on the results achieved, MFEM is a good choice for handling general PBE models because of the generality it provides and the ability to deal with complex dynamics such as moving fronts, common when breakage phenomena are present or the initial distribution is complex.

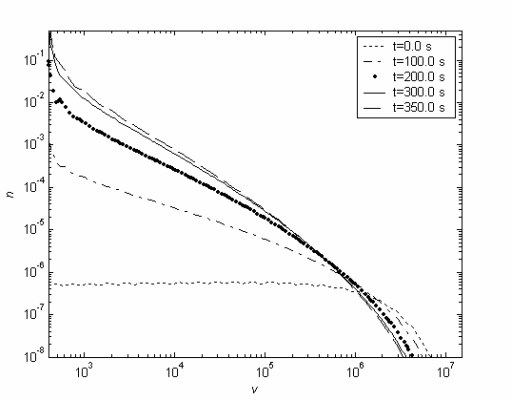

Figure 2 – Numerical solution of the hydrolysis of wheat starch model at particular instants.

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