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Stabilized finite element discretization applied to an operator-splitting method of population balance equations

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A B S T R A C T

An operator-splitting method is applied to transform the population balance equation into two subproblems: a transient transport problem with pure advection and a time-dependent convection–diffusion problem. For discretizing the two subproblems the discontinuous Galerkin method and the streamline upwind Petrov–Galerkin method combined with a backward Euler scheme in time are considered. Standard energy arguments lead to error estimates with a lower bound on the time step length. The stabilization vanishes in the time-continuous limit case. For this reason, we follow a new technique proposed by John and Novo for transient convection–diffusion–reaction equations and extend it to the case of population balance equations. We also compare numerically the streamline upwind Petrov–Galerkin method and the local projection stabilization method.

1. Introduction

Many chemical processes, including polymerization, crystallization, cloud formation, and cell dynamics can be described by population balance equations. Hence, their simulation is required in various applications. A special example is the precipitation process which involves chemical reactions in a flow field. Such processes are modeled by a population balance system [14], consisting of the Navier–Stokes equations for describing the flow field, convection–diffusion problems for describing the chemical reactions, and transport equations for the particle size distribution (PSD). The set of these equations is strongly coupled. Hence, inaccuracies in the concentration of one species directly affects the concentration of all other species. In addition to the coupling of these equations, the main difficulty in simulation is that the PSD depends not only on space and time but also on the properties of particles referred to as internal or property coordinates. Consequently, the dimension of the equation of the PSD is higher than the dimensions of the other equations in the system.

In order to overcome the curse of dimensionality associated with the equation of PSD, we proposed in [1] an operator-splitting scheme. The operator-splitting method reduces the original problem with respect to internal and external directions into a transient transport problem with pure advection and a time-dependent convection–diffusion problem. In applications, most of the problems are convection-dominated and the solution obtained by standard finite element methods exhibit

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nonphysical oscillations. In this case, stabilization techniques are required in order to get physically sound numerical approximations. In [1], the local projection stabilization (LPS) method has been used to stabilize the space discretization combined with a discontinuous Galerkin (dG) method in the internal coordinate to get the error estimates of the two-step method.

The choice of stabilization parameters plays a critical role in the success of the stabilized methods. The standard techniques to get error estimates for residual based stabilization methods for unsteady convection–diffusion–reaction problems lead to lower bounds on the time step length. The stabilization vanishes in the time-continuous limit. This time step restriction does not appear when stabilization methods like LPS [1,2] are used. Recently in [12], John and Novo presented a new technique for the case of time-independent coefficients which allows to get the same error estimates without time step restriction. In this paper, we show that this technique can be extended to the case of population balance equations.

Stabilized finite element methods for time-dependent convection–diffusion–reaction problems have been investigated by many authors. The stability property of consistent stabilization methods in the small time step limit have been discussed in [3,10]. The approach in these studies was to discretize the time-dependent problem in space first and the stabilization is introduced in the semi-discrete problem by using residuals of the time-dependent partial differential equation. Then the stabilization parameters are chosen for the semi-discrete problem. The stabilized semi-discrete problem is then discretized in time by a suitable time-stepping scheme. This procedure results in stabilization parameters that depend only on the mesh width in space since the temporal discretization is performed after the choice of the stabilization parameters. The stability and convergence properties of the SUPG method in space combined with the backward Euler method, the Crank–Nicolson scheme or the second order backward differentiation formula in time for transient transport problem have been studied in [4]. Error bounds in the L^2-norm and in the norm of material derivative are obtained under regularity conditions on the data and the stabilization parameters depend only on the mesh size in space. For non-smooth data the bounds are valid if the stabilization parameters are chosen in dependence of the length of the time step. Numerical studies of the different stabilization techniques and a comparison including SUPG method can be found in [7,17].

On the other hand, if the stabilization parameters are chosen after discretizing the problem in space and time, see [12, 13], then, the stabilization parameters will depend on the time step length. A detailed study of SUPG methods for transient convection–diffusion–reactions equation has been given in [12]. It is shown in the first part of the paper that a finite element discretization in space combined with a backward Euler scheme in time leads to two different choices of stabilization parameters, both depending on the length of the time step. Stability and error estimates are obtained for both choices of stabilization parameters. It is also observed that the stabilization parameters tend to zero as the time step length approaches zero. Furthermore, a special problem where velocity field and reaction do not depend on time has been considered in the second part of the paper. The stabilization parameters are chosen similar to that in the steady-state case. Under certain regularity of the solution, the second part of [12] extended the analysis of [4] and derived error estimates for the L^2-norm and the norm of the material derivative with the standard order of convergence. Moreover, an error estimates in the norm of the streamline derivative has been established. The analysis has also been extended to the fully discrete case where backward Euler and Crank–Nicolson methods are used for time discretization. Numerical studies presented in [12,13] show that this approach leads to solutions which contain nonphysical oscillations for small time steps compared with the approach from [3,10].

Other results concerning the analysis of stabilized finite element methods for time-dependent convection–diffusion–reaction equations can be found in the literature. We refer to [7,17] which consider different stabilizing techniques including SUPG. Symmetric stabilization in space combined with the θ-scheme and the second order backward differentiation formula have been considered in [5]. The analysis of discontinuous Galerkin (dG) in time combined with local projection stabilization (LPS) in space has been studied in [2] and in space and time in [9].

The second subproblem in our splitting method is a transport problem with pure advection, so one suitable choice is to approximate it by the discontinuous Galerkin (dG) finite element method [1]. The dG method was first introduced for the neutron transport problem in [19] and then analyzed in [16]. The theoretical analysis of the dG method for scalar hyperbolic equations can be found in [15] and for the space–time dG finite element method in [9]. For an introduction to dG method we refer to [6].

The main focus of the paper consists in deriving error estimates for operator-splitting methods of population balance equations in which the stabilization parameters do not depend on the length of the time step. In particular, we combine the SUPG method in space with the dG method in internal coordinate. For time discretization, a backward Euler time stepping scheme is used. Under certain regularity of the solution, we extend the analysis of [12] to the two-step method of population balance equations and derive error estimates without a lower bound on the time step length. Furthermore, we compare the numerical results with the results obtained by LPS method in space [1].

The remainder of this paper is organized as follows: Section 2 introduces the problem under consideration and the operator-splitting scheme. The SUPG method in space and dG in internal coordinate are introduced in Section 3. In Section 4, the two subproblems are discretized in time using the backward Euler time-stepping scheme. We derive stability estimates for the two-step method and error estimates are given for two different choices of stabilization parameters. Furthermore, error estimates in which the stabilization parameters are independent of the time step length are given. Section 5 presents the combination of LPS in space and dG in internal coordinate. Numerical results illustrating the theory are reported in Section 6 and some conclusions are given in Section 7.