Weierstraß-Institut

für Angewandte Analysis und Stochastik

An operator-splitting heterogeneous finite element method for population balance equations: Stability and convergence

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Abstract

   We present a heterogeneous finite element approximation of the solution of a population balance equation, which depends both the physical and internal property coordinates. The operator-splitting method is employed to split the high-dimensional population balance equation into two low-dimensional equations, and discretize the low-dimensional equations separately. In particular, we discretize the physical and internal spaces with the standard Galerkin and Streamline Upwind Petrov Galerkin (SUPG) finite elements, respectively. It is demonstrated that the discrete form of the operator-split population balance equation is equivalent to the discrete form of the standard equation up to a perturbation term of order τ^2 in the backward Euler scheme, where τ is a time step. Further, the stability and error estimates have been derived for the heterogeneous finite element discretization scheme applied to the population balance equation. It is shown that a slightly more regularity, *i.e*, the mixed partial derivatives of the solution has to be bounded, is necessary for the solution of the population balance equation with the operator-splitting finite element method. Numerical results are presented to demonstrate the accuracy of the numerical scheme.

1. Introduction. The numerical simulation of population balance equations (PBEs) is highly demanded in many industrial applications such as crystallization, polymerization etc, see for example [3, 19, 20]. In this paper, we present a heterogeneous finite element method for a $(d+s)$-dimensional population balance equation of the following type. A population balance equation describing the particle size distribution f in a population balance system (PBS) of a crystallization process can be defined as:

$$
\begin{aligned}
\frac{\partial f}{\partial t} - \varepsilon \Delta_x f + \mathbf{u} \cdot \nabla_x f + \mathbf{g} \cdot \nabla_\ell f &= \mathscr{S} && \text{in } (0,T] \times \Omega, \\
f(t,x,\ell) &= 0 && \text{on } (0,T] \times \partial\Omega, \\
f(0,x,\ell) &= f_0(x,\ell) && \text{in } \Omega.
\end{aligned}
\tag{1}
$$

Here, the computational domain Ω is the Cartesian product of the physical space (X-direction) domain $\Omega_X \subset \mathbb{R}^d$, $d = 2,3$ and the internal property coordinate (L-direction) domain $\Omega_L \subset \mathbb{R}^s$, $s = 1,2$, *i.e.*, $\Omega := (\Omega_X \times \Omega_L) \subset \mathbb{R}^{d+s}$ with a polyhedral boundary $\partial\Omega$. Further, the fluid transport velocity $\mathbf{u}(t,x)$ and the growth rate $\mathbf{g}(t,x)$ are given $d-$ and $s-$dimensional vector functions, respectively, $\varepsilon > 0$ is a constant diffusion coefficient in Ω_X, f_0 is a given initial distribution of f, and T is a given final computational time. The source term $\mathscr{S}$ may be considered as terms arising from the aggregation and breakage. For simplicity, we use the homogeneous Dirichlet boundary condition and assume $\mathscr{S} \in C^0(0,T;L^2(\Omega_L))$. Further, in order to reduce the technicalities as much as possible, we assumed that the fluid transport velocity

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$\mathbf{u}(t, x)$ is divergence free,

$$\nabla_x \cdot \mathbf{u} = 0. \tag{1.2}$$

Since we are interested in crystallization process, often the growth rate $\mathbf{g}(t, x)$ in crystallization process is assumed to be independent of the particle size $\ell \in \Omega_L$. Therefore, we naturally have the property

$$\nabla_\ell \cdot \mathbf{g}(t, x) = 0. \tag{1.3}$$

One of the main challenges in the finite element solution of high-dimensional PBEs of type (1.1) is to discretize it spatially with the standard finite elements, especially the spatial discretization of 4D and 5D PBEs. Further, developing a fully-practical numerical scheme to solve coupled multidimensional PBSs with a standard numerical method is still challenging, since the dimension of PBEs will be higher than the dimension of all other equations in PBSs [11]. Thus, in order to develop a fully-practical numerical scheme for PBSs an efficient and robust numerical method is needed for high-dimensional PBEs.

Several numerical methods, method of moments and its variants, discretization methods, finite difference, least square method, spectral and finite element methods, have been proposed and used to solve PBEs by several authors, see for example [13, 14, 15, 16, 18, 19, 20] and the references therein for an overview. However, most of these methods are restricted to PBEs, which depend only the internal property coordinates. Due to higher-dimensions and strong coupling with the system of partial differential equations in PBS, solving PBE with standard numerical methods will be very expensive. A mixed Euler-Lagrange method based on operator-splitting has been presented in [4] for PBEs, which depend both the physical and internal coordinates. In the Euler-Lagrange method, the authors first split the PBE into a system of non-homogeneous hyperbolic and ordinary differential equations using the operator-splitting method. Then, the authors applied the total variation diminishing (TVD) scheme for the hyperbolic equations. The operator-splitting approach has also been employed for Fokker-Planck equation in computations of multidimensional polymeric fluid systems in [5, 12]. A rigorous numerical analysis of operator-splitting method for the Fokker-Planck equation has been presented in [12]. In general, to solve a multidimensional system the operator-splitting method can be applied to the high-dimensional equations in the system to split it into a set of low-dimensional equations, and the low-dimensional equations can be solved separately. The operator-splitting method has produced a large number of literature, and it is mainly used for solving multidimensional conservation laws and multiscale, multiphysics problems, see [6, 7, 9, 21] for an overview.

The main goal of this paper is to present a numerical analysis of the operator-splitting Galerkin-SUPG finite element method for the population balance equation. In particular, we split the $(d + s)$-dimensional population balance equation (1.1) into $d-$ and $s-$dimensional equations, and solve the $d-$ and s-dimensional equations separately with the standard Galerkin and Streamline Upwind Petrov Galerkin (SUPG) finite element methods, respectively.

The paper is organized as follows. In Section 2, we briefly discuss the standard discrete and algebraic form of the population balance equation. Then, we present the operator-splitting methods for the population balance equation in Section 3. After that, in Section 4, stability and a priori error estimates of the operator-splitting finite element method applied to the population balance equation are presented. Finally, we present the numerical results in Section 5.

2. Preliminaries. Let $\Omega := \Omega_X \times \Omega_L \subset \mathbb{R}^{d+s}$ be a bounded domain. Assume that the particle size distribution function $f(t, x, \ell)$ in (1.1) is measurable, *i.e.*,

$$\int_0^T \int_{\Omega_X \times \Omega_L} |f(t, x, \ell)| d(x, \ell) < \infty$$

then, due to Fubini's theorem we have

$$\int_0^T \int_{\Omega_X \times \Omega_L} f(t, x, \ell) \, d(x, \ell) = \int_0^T \int_{\Omega_X} \left(\int_{\Omega_L} f(t, x, \ell) d\ell \right) dx$$

$$= \int_0^T \int_{\Omega_L} \left(\int_{\Omega_X} f(t, x, \ell) dx \right) d\ell.$$

Moreover, if $f(t, x, \ell) = g(t, x)h(t, \ell)$, then we have

$$\int_0^T \int_{\Omega_X \times \Omega_L} g(t, x)h(t, \ell) \, d(x, \ell) = \int_0^T \int_{\Omega_X} g(t, x) \, dx \left(\int_{\Omega_L} h(t, \ell) \, d\ell \right).$$

2.1. Finite element spaces for operator-splitting method. Let $H^{m_1}(\Omega_X)$ and $H^{m_2}(\Omega_L)$ be the usual Sobolev spaces with the weak derivatives of order m_1 and m_2, respectively. Then, we define

$$H^{m_1}(\Omega_X) \otimes H^{m_2}(\Omega_L) := \left(H^{m_1}(\Omega_X; H^{m_2}(\Omega_L)) \right) \cap \left(H^{m_1}(\Omega_L; H^{m_2}(\Omega_X)) \right), \quad (2.1)$$

and denote it as $H^{m_1, m_2}(\Omega)$. For each integer $m_1 \geq 0$ and $m_2 \geq 0$, the associated norm of a function $u \in H^{m_1}(\Omega_X; H^{m_2}(\Omega_L))$ can be defined as

$$\|u\|^2_{H^{m_1}(\Omega_X; H^{m_2}(\Omega_L))} := \sum_{|\beta| \leq m_2, \, |\alpha| \leq m_1} \|\partial_\ell^\beta \partial_x^\alpha u\|^2_{L^2(\Omega)}.$$

Hence, the associated norm for a function $f \in H^{m_1, m_2}(\Omega)$ can be defined as

$$\|f\|^2_{H^{m_1, m_2}(\Omega)} := \sum_{|\beta| \leq m, \, |\alpha| \leq m} \|\partial_\ell^\beta \partial_x^\alpha f\|^2_{L^2(\Omega)},$$

where $m = \min\{m_1, m_2\}$. Further, the seminorm can be defined as

$$|f|^2_{m_1, m_2} := \sum_{|\beta| = m, \, |\alpha| = m} \|\partial_\ell^\beta \partial_x^\alpha f\|^2_{L^2(\Omega)}.$$

Note that when $m_1 = 0$ or $m_2 = 0$ we get

$$L^2(\Omega) := H^{m_1, 0}(\Omega) \equiv H^{0, m_2}(\Omega).$$

Further, the space $H^{m,m}(\Omega)$ is slightly more regular than the usual Sobolev space $H^m(\Omega)$, *i.e.*, the mixed partial derivatives of functions from the space $H^{m,m}(\Omega)$ are bounded. This additional regularity is necessary in the analysis of operator-splitting finite element method.

Now, let $V_0 := H_0^1(\Omega_X)$ and $Q_0 := H_0^1(\Omega_L)$ be the usual Sobolev spaces, whose function values are zero on their respective boundaries. Let $\mathcal{T}_h$ and $\mathcal{S}_h$ be the triangulation of Ω_X and Ω_L, respectively. Suppose $V_{h,0} \subset V_0$ and $Q_{h,0} \subset Q_0$ are conforming finite element (finite dimensional) spaces. We denote the diameter of the cells $K' \in \mathcal{T}_h$

and $K \in \mathcal{S}_h$ by $h_{K'}$ and h_K, respectively. Further, the global mesh size in each domain is defined as $h_x := \max\{h_{K'} \ : \ K' \in \mathcal{T}_h\}$ and $h_\ell := \max\{h_K \ : \ K \in \mathcal{S}_h\}$, respectively, and the global mesh size h in Ω is defined as $h := \max\{h_x, \ h_\ell\}$. Let $\phi_h := \phi_i(x)$, $i = 1, 2, ..., \mathcal{M}$, and $\psi_h := \psi_k(\ell)$, $k = 1, 2, ..., \mathcal{N}$, be the basis functions of $V_{h,0}$ and $Q_{h,0}$, respectively, $i.e.$,

$$V_{h,0} = \mathrm{span}\{\phi_i(x)\}, \qquad Q_{h,0} = \mathrm{span}\{\psi_k(\ell)\}. \tag{2.2}$$

Then, using (2.1) we define the discrete finite element space $W_{h,0} \subset V_0 \otimes Q_0$ such that

$$W_{h,0} = \{\xi_h : \ \xi_h = \sum_j^{\mathcal{M}} \sum_k^{\mathcal{N}} \xi_{j,k} \phi_j(x) \psi_k(\ell); \quad \xi_{j,k} \in \mathbb{R}.$$

Also, the finite element functions are defined as follows

$$
\begin{aligned}
f_h &= \sum_j^{\mathcal{M}} \sum_k^{\mathcal{N}} f_{j,k} \phi_j \psi_k, & v_h &= \sum_i^{\mathcal{M}} \sum_m^{\mathcal{N}} \phi_i \psi_m, \\
\nabla_x f_h &= \sum_j^{\mathcal{M}} \sum_k^{\mathcal{N}} f_{j,k} (\nabla_x \phi_j) \psi_k, & \nabla_x v_h &= \sum_i^{\mathcal{M}} \sum_m^{\mathcal{N}} (\nabla_x \phi_i) \psi_m, \qquad (2.3) \\
\nabla_\ell f_h &= \sum_j^{\mathcal{M}} \sum_k^{\mathcal{N}} f_{j,k} \phi_j (\nabla_\ell \psi_k), & \nabla_\ell v_h &= \sum_i^{\mathcal{M}} \sum_m^{\mathcal{N}} \phi_i (\nabla_\ell \psi_m).
\end{aligned}
$$

Further, for all $K' \in \mathcal{T}_h$ and $K \in \mathcal{S}_h$, we define the mesh-dependent norm

$$\|v_h\|_{0,K',K}^2 := \int_K \int_{K'} v_h^2, \quad \|v_h\|_{1,1,K',K}^2 := \int_K \int_{K'} (\partial_\ell \partial_x v_h)^2 \,.$$

2.2. Galerkin and SUPG stabilized discretization. It is well known that the standard Galerkin discretization of convection diffusion equations is not stable for small diffusion coefficients (in comparison with convection), and induce spurious oscillations in the solution. In the considered problem (1.1), even if we assume ϵ is sufficiently large, still the standard Galerkin discretization induce spurious oscillations due to the absents of the diffusion in the $L-$direction. One possibility to circumvent the instability and suppress spurious oscillations is to use the SUPG method. SUPG is one of the most popular stabilization methods for finite element discretization, and it adds artificial diffusion along the streamlines of the solution, see for example [2, 10] and the references there in. Since we assumed that ϵ is sufficiently large, it is sufficient to stabilize the equation (1.1) only in the $L-$direction. Therefore, we use the standard Galerkin and the consistent SUPG stabilized discretizations in the X-and L-directions, respectively. Since we use different discretizations in different directions, we call it as a heterogeneous discretization method. Applying the heterogeneous discretization, the semi-discrete form of the (1.1) reads:

For a given $f_h(0) = f_{h,0}$, find $f_h(t) \in W_{h,0}$ such that for all $t \in (0, T]$

$$\left(\frac{\partial f_h}{\partial t}, v_h\right) + a_{LS}(f_h, v_h) + a_{LT}\left(\frac{\partial f_h}{\partial t}, v_h\right) = (\mathcal{S}, v_h) + F_S(\mathcal{S}, v_h), \quad v_h \in W_{h,0}, \ (2.4)$$

where

$$a_{LS}(f_h, v_h) := \int_\Omega \left(\epsilon \nabla_x f_h \cdot \nabla_x v_h + \mathbf{u}_h \cdot \nabla_x f_h \, v_h + \mathbf{g}_h \cdot \nabla_\ell f_h \, v_h \right)$$

$$+ \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathbf{g}_h \cdot \nabla_\ell f_h, \mathbf{g}_h \cdot \nabla_\ell v_h \right)_K,$$

$$a_{LT}(f_h, v_h) := \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(f_h, \ \mathbf{g}_h \cdot \nabla_\ell v_h \right)_K,$$

$$F_S(\mathcal{S}, v_h) := \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathcal{S}, \ \mathbf{g}_h \cdot \nabla_\ell v_h \right)_K.$$

Here, $f_{h,0} \in W_{h,0}$ is a L^2-projection of the initial value f_0 onto $W_{h,0}$. Further, $(\cdot, \cdot)_K$ denotes the L^2-inner product in the mesh cell $K \in \mathcal{S}_h$, and $\{\delta_K\}$ are the local stabilization parameters which have to be chosen appropriately.

LEMMA 2.1 (Coercivity of $a_{LS}(\cdot, \cdot)$). *Let the discrete form of the assumptions (1.2) and (1.3) be satisfied. Then, the bilinear form associated with the heterogeneous discretization satisfies*

$$a_{LS}(f_h, f_h) \geq |||f_h|||^2, \tag{2.5}$$

where the mesh-dependent heterogeneous norm

$$|||f_h|||^2 := \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \left(\epsilon \|\nabla_x f_h\|_{K',K}^2 + \delta_K \|\mathbf{g}_h \cdot \nabla_\ell f_h\|_{K',K}^2 \right) \tag{2.6}$$

Proof.

$$a_{LS}(f_h, f_h) = \int_{\Omega_L} \int_{\Omega_X} \left(\epsilon \nabla_x f_h \cdot \nabla_x f_h + \frac{1}{2} \mathbf{u}_h \cdot \nabla_x f_h^2 \right) + \frac{1}{2} \int_{\Omega_X} \int_{\Omega_L} \mathbf{g}_h \cdot \nabla_\ell f_h^2$$

$$+ \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \int_K \mathbf{g}_h \cdot \nabla_\ell f_h \, \mathbf{g}_h \cdot \nabla_\ell f_h,$$

$$= \int_{\Omega_L} \int_{\Omega_X} \left(\epsilon \nabla_x f_h \cdot \nabla_x f_h - \frac{1}{2} \nabla_x \cdot \mathbf{u}_h f_h^2 \right) - \frac{1}{2} \int_{\Omega_X} \int_{\Omega_L} \nabla_\ell \cdot \mathbf{g}_h f_h^2$$

$$+ \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \int_K (\mathbf{g}_h \cdot \nabla_\ell f_h)^2,$$

$$\geq \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \left(\epsilon \|\nabla_x f_h\|_{0,K',K}^2 + \delta_K \|\mathbf{g}_h \cdot \nabla_\ell f_h\|_{0,K',K}^2 \right).$$

□

2.3. Temporal discretization. Let $0 = t^0 < t^1 < \cdots < t^N = T$ be a decomposition of the considered time interval $[0, T]$. Let us denote $\tau = \tau^n = t^n - t^{n-1}$, $1 \leq n \leq N$, be an uniform time step, and denote f_h^n be the approximation of $f(t^n)$ in $W_{h,0}$. Further, we denoted the one step finite difference operator

$$\bar{\partial} f_h^n = \frac{f_h^n - f_h^{n-1}}{\tau}.$$

After applying the backward Euler time discretization in (2.4), the heterogeneous discrete form of (1.1) can be written as:

For given $\mathcal{S}^n$, $f_h^0 = f_{h,0}$, find $f_h^n \in W_{h,0}$ in the time interval (t^{n-1}, t^n) such that $\forall\, v_h \in W_{h,0}$

$$\left(\bar{\partial} f_h^n,\ v_h\right) + a_{LS}(f_h^n, v_h) + a_{LT}\left(\bar{\partial} f_h^n, v_h\right) = (\mathcal{S}^n, v_h) + F_S(\mathcal{S}^n, v_h). \qquad (2.7)$$

2.4. Algebraic form. Using the definition of finite element functions (2.3), the algebraic form of the discrete equation (2.7) can be written as

$$(M + M^S + \tau A + \tau A^S)f^n = \tau F^n + \tau F^{S,n} + (M + M^S)f^{n-1}, \qquad (2.8)$$

where, the mass, stiffness and stabilization matrices are defined as follows:

$$M := M_X \otimes M_L, \ \ A := A_X \otimes M_L + M_X \otimes A_L,$$
$$M^S := M_X \otimes S_L, \ \ A^S := M_X \otimes G_L. \qquad (2.9)$$

Here,

$$A_X := \int_{\Omega_X} \nabla_x \phi_j \cdot \nabla_x \phi_i + \int_{\Omega_X} \phi_j\, \mathbf{u}_h \cdot \nabla_x \phi_i, \qquad M_X := \int_{\Omega_X} \phi_j \phi_i,$$

$$A_L := \int_{\Omega_L} \psi_m\, \mathbf{g}_h \cdot \nabla_\ell \psi_k, \qquad\qquad M_L := \int_{\Omega_L} \psi_m \psi_k,$$

$$S_L := \sum_{K \in \mathcal{S}_h} \delta_K \left(\psi_k,\ \mathbf{g}_h \cdot \nabla_\ell \psi_m\right)_K, \qquad F^n := \int_{\Omega} f^n v_h$$

$$G_L := \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathbf{g}_h \cdot \nabla_\ell \psi_k,\ \mathbf{g}_h \cdot \nabla_\ell \psi_m\right)_K$$

$$F^{S,n} := \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(f^n, \mathbf{g}_h \cdot \nabla_\ell v_h\right)_K$$

$$(2.10)$$

and the tensor of matrices is defined as follows:

$$M := M_X \otimes M_L = \begin{bmatrix} M_{1,1} & \cdot & \cdot & \cdot & M_{1,\mathcal{M}} \\ & \cdot & & & \cdot \\ \cdot & & \cdot & & \cdot \\ \cdot & & & \cdot & \cdot \\ M_{\mathcal{M},1} & \cdot & \cdot & \cdot & M_{\mathcal{M},\mathcal{M}} \end{bmatrix},$$

where the order of the matrix M will be $\mathcal{M}\mathcal{N} \times \mathcal{M}\mathcal{N}$. Here, the order of the block matrix $M_{i,j}$, $1 \le i, j \le \mathcal{M}$, will be $\mathcal{N} \times \mathcal{N}$, and is defined by

$$M_{i,j} := \int_{\Omega_X} \phi_i \phi_j \int_{\Omega_L} \psi_k \psi_\ell, \qquad 1 \le k, l \le \mathcal{N}.$$

Solving an algebraic system of size $\mathcal{M}\mathcal{N} \times \mathcal{M}\mathcal{N}$ in each time step is itself very expensive. Moreover, when the PBE is coupled with a system of partial differential equations in a population balance system, this large system has to be solved repeatedly several times in each time step to linearize the system of equations. This, requires enormous computing power. To overcome this challenge, in the next Section, we present a two-step operator-splitting scheme for the population balance equation (1.1).

3. Operator-splitting finite element method. The operators Δ_x, ∇_x and ∇_ℓ in the population balance equation (1.1) are the decomposition of unmixed partial derivatives of the Cartesian coordinates x and ℓ, respectively. Thus, we can take advantage of the decomposition, and discretize the equation (1.1) in space with $d-$and $s-$dimensional finite elements instead of $(d+s)$-dimensional finite elements. Using the Lie's operator-splitting method, see for *e.g.*, [9], the first-order operator-split equations of (1.1) can be written as

Step 1 (L-direction)
Find $\hat{f}$ for all $x \in \Omega_X$ such that

$$
\begin{aligned}
\frac{\partial \hat{f}}{\partial t} + \mathbf{g} \cdot \nabla_\ell \hat{f} &= \mathcal{S} && \text{in } (0, T] \times \Omega_L, \\
\hat{f}(t, x, \ell) &= 0 && \text{in } (0, T] \times \partial\Omega_L, \\
\hat{f}(0, x, \ell) &= f_0(x, \ell)
\end{aligned}
\tag{3.1}
$$

by considering x as a parameter.
Step 2 (X-direction)
Find $\tilde{f}$ for all $\ell \in \Omega_L$ such that

$$
\begin{aligned}
\frac{\partial \tilde{f}}{\partial t} - \epsilon\Delta_x \tilde{f} + \mathbf{u} \cdot \nabla_x \tilde{f} &= 0 && \text{in } (0, T] \times \Omega_X, \\
\tilde{f}(t, x, \ell) &= 0 && \text{in } (0, T] \times \partial\Omega_X, \\
\tilde{f}(0, x, \ell) &= \hat{f}(T, x, \ell),
\end{aligned}
\tag{3.2}
$$

by considering ℓ as a parameter. Note that the L-direction equation (3.1) has to be solved only for inner point $x \in \Omega_X$ due to the Dirichlet boundary condition. However, if we consider non-Dirichlet boundary conditions, then the equation (3.1) has to be solved for all boundary points $x \in \partial\Omega_X$ also. Similar arguments hold for the X-direction equation (3.2).

Next, to derive the discrete forms of the operator-split equations (3.1) and (3.2), we define

$$
\hat{f}_h^n := \sum_l^{\mathcal{N}} \hat{f}_{j,l}^n \psi_l, \qquad \tilde{f}_h^n := \sum_j^{\mathcal{M}} \tilde{f}_{j,l}^n \phi_j
$$

as the finite element functions for the equations (3.1) and (3.2), respectively. Further, to obtain the global solution from these finite element functions, we use the definition

$$
f_h^n = \sum_j^{\mathcal{M}} \sum_k^{\mathcal{N}} \tilde{f}_{j,k} \phi_j \psi_k.
$$

As discussed before, the X-direction equation (3.2) is a standard convection-diffusion equation, and with sufficiently large ϵ in comparison to $|\mathbf{u}|$, it can be solved with the standard Galerkin method. However, the L-direction equation (3.1) is a pure advection equation and a stabilization method has to be used since the standard Galerkin method induce spurious oscillations in the solution. After applying the SUPG in (3.1)

and the standard Galerkin in (3.2), the discrete form of operator-split equations (3.1) and (3.2) in the time interval (t^{n-1}, t^n) with $f_h^0 = f_0$ read:

Step 1 (L-direction):
For a given $\mathcal{S}^n$ and $\hat{f}_h^{n-1} = f_h^n$, find $\hat{f}_h^n \in Q_{h,0}$, for all $x \in \Omega_X$ by considering x as a parameter such that $\forall \, \psi_h \in Q_{h,0}$

$$\left(\bar{\partial}\hat{f}_h^n, \psi_h\right)_\ell + a_S(\hat{f}_h^n, \psi_h) + a_T\left(\bar{\partial}\hat{f}_h^n, \psi_h\right) = (\mathcal{S}^n, \psi_h)_\ell + F_S^L(\mathcal{S}^n, \psi_h), \qquad (3.3)$$

where

$$a_S(f_h, \psi_h) := \int_{\Omega_L} \mathbf{g}_h \cdot \nabla_\ell f_h \, \psi_h + \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathbf{g}_h \cdot \nabla_\ell f_h, \, \mathbf{g}_h \cdot \nabla_\ell \psi_h\right)_K,$$

$$a_T(f_h, \psi_h) := \sum_{K \in \mathcal{S}_h} \delta_K \left(f_h, \, \mathbf{g}_h \cdot \nabla_\ell \psi_h\right)_K,$$

$$F_S^L(\mathcal{S}, \psi_h) := \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathcal{S}, \, \mathbf{g}_h \cdot \nabla_\ell \psi_h\right)_K.$$

Step 2 (X-direction):
For a given $\tilde{f}_h^{n-1} = \hat{f}_h^n$, find $\tilde{f}_h^n \in V_{h,0}$, for all $\ell \in \Omega_L$ by considering ℓ as a parameter such that $\forall \, \phi_h \in V_{h,0}$

$$\left(\bar{\partial}\tilde{f}_h^n, \phi_h\right)_x + a_X(\tilde{f}_h^n, \phi_h) = 0, \qquad (3.4)$$

where

$$a_X(\tilde{f}_h, \phi_h) := \int_{\Omega_X} \epsilon \nabla_x \tilde{f}_h \cdot \nabla_x \phi_h \; + \; \int_{\Omega_X} \mathbf{u}_h \cdot \nabla_x \tilde{f}_h \, \phi_h.$$

Here, $(\cdot, \cdot)_\ell$ and $(\cdot, \cdot)_x$ in the equations (3.3) and (3.4) denote the L^2-inner products in Ω_L and Ω_X, respectively. From computational point of view, the main challenge in solving the two-step operator-split equations (3.3) and (3.4) is the communication of the solution $\hat{f}_h^n$ from the Step 1 to the right hand side of the Step 2 and vice versa. To overcome this challenge, efficient algorithms have been proposed in [8]. In the next section, we address the consistency error, stability and the convergence of the operator-splitting finite element scheme for the equations (3.3) and (3.4).

4. Analysis of operator-splitting finite element method. To obtain the stability and *a priori* error estimates for the operator-split equations (3.3) and (3.4), we first derive the equivalent one-step operator-split discrete form of the operator-split equations (3.3) and (3.4).

LEMMA 4.1 (Consistency). *The equivalent one-step operator-split discrete form of the operator-split equations* (3.3) *and* (3.4) *is*

$$\left(\bar{\partial}f_h^n, v_h\right) + a_{LS}(f_h^n, v_h) + a_{LT}\left(\bar{\partial}f_h^n, v_h\right) + a_{OS}(f_h^n, v_h) = (\mathcal{S}^n, v_h) + F_S(\mathcal{S}^n, v_h) \quad (4.1)$$

where the consistency error due to the operator-splitting is given by

$$a_{OS}(f_h^n,\ v_h) = \tau \int_\Omega \epsilon \mathbf{g}_h \cdot \nabla_\ell(\nabla_x f_h^n)\ \nabla_x v_h + \tau \int_\Omega \mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x f_h^n)\ v_h$$

$$+\tau \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\epsilon \mathbf{g}_h \cdot \nabla_\ell(\nabla_x f_h^n),\ \mathbf{g}_h \cdot \nabla_\ell(\nabla_x v_h)\right)_K$$

$$+\tau \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x f_h^n),\ \mathbf{g}_h \cdot \nabla_\ell v_h\right)_K \tag{4.2}$$

$$+\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\epsilon \nabla_x f_h, \mathbf{g}_h \cdot \nabla_\ell(\nabla_x v_h)\right)_K$$

$$+\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathbf{u}_h \cdot \nabla_x f_h,\ \mathbf{g}_h \cdot \nabla_\ell v_h\right)_K.$$

Proof. The algebraic form of the L-direction equation (3.3) can be written as

$$\left(M_L + S_L + \tau(A_L + G_L)\right) \hat{f}_h^n = \tau(F_L^n + F_L^{S,n}) + (M_L + S_L)f_h^{n-1}, \tag{4.3}$$

where

$$F_L^n := \int_{\Omega_L} \mathcal{S}^n \psi_h, \qquad F_L^{S,n} = \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathcal{S}^n, \mathbf{g}_h \cdot \nabla \psi_h\right)_K$$

Here, the matrices S_L, G_L and $F_L^{S,n}$ belong to the SUPG stabilization terms. Next, the algebraic form of the X-direction equation (3.4) can be written as

$$\left(M_X + \tau A_X\right) f_h^n = M_X \hat{f}_h^n. \tag{4.4}$$

Now, multiply (4.3) by $M_X \otimes \mathbb{I}$, and (4.4) by $\mathbb{I} \otimes (M_L + \tau A_L + S_L + \tau G_L)$, we get

$$\left((M_X \otimes M_L) + \tau(M_X \otimes A_L) + (M_X \otimes S_L) + \tau(M_X \otimes G_L)\right) \hat{f}^n$$
$$= \tau(M_X \otimes F_L^n) + \tau(M_X \otimes F_L^{S,n}) + \left((M_X \otimes M_L) + (M_X \otimes S_L)\right) f_h^{n-1}$$

and

$$\Big((M_X \otimes M_L) + \tau \left\{(A_X \otimes M_L) + (M_X \otimes A_L)\right\} + (\tau)^2(A_X \otimes A_L)$$
$$+ (M_X \otimes S_L) + \tau \left\{(A_X \otimes S_L) + (M_X \otimes G_L)\right\} + (\tau)^2(A_X \otimes G_L)\Big) f_h^n$$
$$= \left((M_X \otimes M_L) + \tau(M_X \otimes A_L) + (M_X \otimes S_L) + \tau(M_X \otimes G_L)\right) \hat{f}_h^n,$$

respectively. Equating, the above equations, we get

$$\Big((M_X \otimes M_L) + \tau((A_X \otimes M_L) + (M_X \otimes A_L)) + (M_X \otimes S_L) + \tau(M_X \otimes G_L)$$
$$+\tau(A_X \otimes S_L) + (\tau)^2((A_X \otimes A_L) + (A_X \otimes G_L))\Big) f_h^n$$
$$= \tau(M_X \otimes F_L^n) + \tau(M_X \otimes F_L^{S,n}) + \left\{(M_X \otimes M_L) + (M_X \otimes S_L)\right\} f_h^{n-1}.$$

Using the definitions (2.9) in the above equation, we get

$$\Big(M + \tau A + M^S + \tau A^S$$
$$+ \tau(A_X \otimes S_L) + (\tau)^2(A_X \otimes A_L) + (\tau)^2(A_X \otimes G_L)\Big) f_h^n \tag{4.5}$$
$$= \tau(M_X \otimes F_L^n) + \tau(M_X \otimes F_L^{S,n}) + (M + M^S)f_h^{n-1}.$$

For the cross terms resulting from the operator-splitting we have

$$(A_X \otimes S_L)f^n = \int_{\Omega_X} \sum_{K \in S_h} \delta_K \int_K (\epsilon \nabla_x \phi_j \nabla_x \phi_i + \mathbf{u}_h \cdot \nabla_x \phi_j \phi_i) \mathbf{g}_h \cdot \nabla_\ell \psi_m \psi_k$$

and for each K over Ω_X, we have

$$\int_K \epsilon f_{j,k}^n \nabla_x \phi_j \nabla_x \phi_i \, \mathbf{g}_h \cdot \nabla_\ell \psi_m \psi_k \ + \ f_{j,k}^n \mathbf{u}_h \cdot \nabla_x \phi_j \phi_i \, \mathbf{g}_h \cdot \nabla_\ell \psi_m \psi_k$$

$$= \int_K \epsilon f_{j,k}^n \mathbf{g}_h \cdot \nabla_\ell (\nabla_x \phi_i \psi_m) \nabla_x \phi_j \psi_k \ + \ f_{j,k}^n \mathbf{g}_h \cdot \nabla_\ell (\phi_i \psi_m) \mathbf{u}_h \cdot \nabla_x \phi_j \psi_k$$

$$= \int_K \epsilon \nabla_x f_h \, \mathbf{g}_h \cdot \nabla_\ell (\nabla_x v_h) \ + \ \mathbf{u}_h \cdot \nabla_x f_h \, \mathbf{g}_h \cdot \nabla_\ell v_h.$$

Further, the $A_X \otimes A_L$ term, we have

$$(A_X \otimes A_L)f_h^n$$

$$= \int_\Omega \epsilon f_{j,k}^n \nabla_x \phi_j \nabla_x \phi_i \, \mathbf{g}_h \cdot \nabla_\ell \psi_k \psi_m \ + \ f_{j,k}^n \mathbf{u}_h \cdot \nabla_x \phi_j \phi_i \, \mathbf{g}_h \cdot \nabla_\ell \psi_k \psi_m$$

$$= \int_\Omega \epsilon \mathbf{g}_h \cdot \nabla_\ell (f_{j,k}^n \nabla_x \phi_j \psi_k) \, \nabla_x v_h \ + \ \mathbf{g}_h \cdot \nabla_\ell (\mathbf{u}_h \cdot (f_{j,k}^n \nabla_x \phi_j) \psi_k) \, v_h$$

$$= \int_\Omega \epsilon \mathbf{g}_h \cdot \nabla_\ell (\nabla_x f_h^n) \, \nabla_x v_h \ + \ \mathbf{g}_h \cdot \nabla_\ell (\mathbf{u}_h \cdot \nabla_x f_h^n) \, v_h.$$

Similarly, for each K over Ω_X in the cross term $A_X \otimes G_L$, we have $(A_X \otimes G_L)f_h^n$

$$\int_K \epsilon f_{j,k}^n \nabla_x \phi_j \nabla_x \phi_i \, \mathbf{g}_h \cdot \nabla_\ell \psi_k \mathbf{g}_h \cdot \nabla_\ell \psi_m \ + \ f_{j,k}^n \mathbf{u}_h \cdot \nabla_x \phi_j \phi_i \, \mathbf{g}_h \cdot \nabla \psi_k \mathbf{g}_h \cdot \nabla_\ell \psi_m$$

$$= \int_K \epsilon f_{j,k}^n \mathbf{g}_h \cdot \nabla_\ell (\nabla_x \phi_j \psi_k) \, \mathbf{g}_h \cdot \nabla_\ell (\nabla \phi_i \psi_m) \ + \ f_{j,k}^n \mathbf{g}_h \cdot \nabla_\ell (\mathbf{u}_h \cdot \nabla_x \phi_j \psi_k) \, \mathbf{g}_h \cdot \nabla_\ell (\phi_i \psi_m)$$

$$= \int_K \epsilon \mathbf{g}_h \cdot \nabla_\ell (\nabla_x f_h^n) \, \mathbf{g}_h \cdot \nabla_\ell (\nabla_x v_h) \ + \ \mathbf{g}_h \cdot \nabla_\ell (\mathbf{u}_h \cdot \nabla_x f_h^n) \, \mathbf{g}_h \cdot \nabla_\ell v_h.$$

Next, we show that the source term $M_x \otimes F_L^n = F^n$. Each equation in the algebraic system (4.5) is obtained by applying summation to the ansatz indices j and k on both sides of the system. Therefore, the source term in the algebraic system (4.5) becomes

$$M_x \otimes F_L^n = \int_{\Omega_X \times \Omega_L} \sum_i^{\mathcal{M}} \sum_j^{\mathcal{M}} \sum_m^{\mathcal{N}} \mathcal{S}^n \phi_i \phi_j \psi_m.$$

Thus, the right hand side vector, $rhs_{i,m}$, $i = 1, \ldots, \mathcal{M}$, $m = 1, \ldots, \mathcal{N}$, can be written as

$$rhs_{i,m} = \int_{\Omega_X \times \Omega_L} \sum_j^{\mathcal{M}} \mathcal{S}^n \phi_i \phi_j \psi_m = \int_{\Omega_X \times \Omega_L} \mathcal{S}^n \phi_i \psi_m \sum_j^{\mathcal{M}} \phi_j$$

$$= \int_{\Omega_X \times \Omega_L} \mathcal{S}^n \phi_i \psi_m,$$

which is the source term in the algebraic system (2.8). Thus, we have $M_x \otimes F_L^n = F^n$. Similar argument holds for $M_x \otimes F_L^{S,n} = F^{S,n}$. Hence, the statement of the Lemma. □

Note that the discrete bilinear form (4.1) of the two-step operator-split equations is not same as the original discrete form (2.7). The difference is the consistency error due to the operator-splitting method. Nevertheless, the cross terms are of order τ^2 in the backward Euler time discretization.

LEMMA 4.2. *Let the discrete form of the assumptions* (1.2) *and* (1.3) *be satisfied. Then,* $\forall\ v_h \in W_{h,0}$, *we have*

$$\int_\Omega \mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x v_h)v_h = 0, \quad \int_{\Omega_X} \sum_{K\in\mathcal{S}_h} \delta_K \left(\mathbf{u}_h \cdot \nabla_x v_h,\ \mathbf{g}_h \cdot \nabla_\ell v_h\right)_K = 0,$$

$$\int_{\Omega_X} \sum_{K\in\mathcal{S}_h} \delta_K \left(\mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x v_h^n),\ \mathbf{g}_h \cdot \nabla_\ell v_h\right)_K = 0.$$

Proof. We use the definitions of the finite element spaces (2.2) to show this property. In particular, we repeatedly use the properties that the basis functions of $V_{h,0}$ and $Q_{h,0}$ are independent of $\ell \in \Omega_L$ and $x \in \Omega_X$, respectively.

$$\int_\Omega \mathbf{g}_h \nabla_\ell(\mathbf{u}_h \cdot \nabla_x v_h)v_h$$

$$= \int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial}{\partial \ell_q}\left(\mathbf{u}_{p,h}\frac{\partial v_h}{\partial x_p}\right)v_h = \int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial}{\partial \ell_q}\left(\mathbf{u}_{p,h}\frac{\partial(\phi_h\psi_h)}{\partial x_p}\right)\phi_h\psi_h$$

$$= \int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q}\psi_h\ \mathbf{u}_{p,h}\frac{\partial \phi_h}{\partial x_p}\phi_h = \frac{1}{4}\int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial \psi_h^2}{\partial \ell_q}\ \mathbf{u}_{p,h}\frac{\partial \phi_h^2}{\partial x_p}$$

$$= \frac{1}{4}\int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial}{\partial \ell_q}\left(\mathbf{u}_{p,h}\frac{\partial \phi_h^2}{\partial x_p}\psi_h^2\right) = \frac{1}{4}\int_\Omega \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial}{\partial \ell_q}\left(\mathbf{u}_{p,h}\frac{\partial(\phi_h\psi_h)^2}{\partial x_p}\right)$$

$$= \frac{1}{4}\int_\Omega \mathbf{g}_h \cdot \nabla_\ell\left(\mathbf{u}_h \cdot \nabla_x v_h^2\right) = -\frac{1}{4}\int_\Omega \nabla_\ell \cdot \mathbf{g}_h\left(\mathbf{u}_h \cdot \nabla_x v_h^2\right) = 0.$$

Next we have,

$$\int_{\Omega_X} \sum_{K\in\mathcal{S}_h} \delta_K \mathbf{u}_h \cdot \nabla_x v_h\ \mathbf{g}_h \cdot \nabla_\ell v_h = \sum_{K'\in\mathcal{T}_h} \int_{K'} \sum_{K\in\mathcal{S}_h} \int_K \delta_K \mathbf{u}_h \cdot \nabla_x v_h\ \mathbf{g}_h \cdot \nabla_\ell v_h.$$

and for each $K \in \mathcal{S}_h$, we have

$$\int_K \delta_K \mathbf{u}_h \cdot \nabla_x v_h\ \mathbf{g}_h \cdot \nabla_\ell v_h$$

$$= \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h}\frac{\partial \phi_h}{\partial x_p}\psi_h\ \mathbf{g}_{q,h}\frac{\partial \psi_h}{\partial \ell_q}\phi_h = \frac{1}{4}\int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h}\frac{\partial \phi_h^2}{\partial x_p}\ \mathbf{g}_{q,h}\frac{\partial \psi_h^2}{\partial \ell_q}$$

$$= \frac{1}{4}\int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h}\frac{\partial}{\partial \ell_q}\left(\mathbf{u}_{p,h}\frac{\partial \phi_h^2}{\partial x_p}\psi_h^2\right) = \frac{1}{4}\int_K \delta_K \mathbf{g}_h \cdot \nabla_\ell\left(\mathbf{u}_h \cdot \nabla_x v_h^2\right)$$

$$= -\frac{1}{4}\int_K \delta_K \nabla_\ell \cdot \mathbf{g}_h\left(\mathbf{u}_h \cdot \nabla_x v_h^2\right) = 0.$$

Finally, we have

$$\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \int_K \delta_K \mathbf{g}_h \cdot \nabla_\ell (\mathbf{u}_h \cdot \nabla_x v_h) \, \mathbf{g}_h \cdot \nabla_\ell v_h$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{g}_{q,h} \frac{\partial}{\partial \ell_q} \left(\mathbf{u}_{p,h} \frac{\partial \phi_h}{\partial x_p} \psi_h \right) \, \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q} \phi_h$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h} \frac{\partial \phi_h}{\partial x_p} \phi_h \, \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q} \, \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q}$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \frac{1}{2} \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h} \frac{\partial \phi_h^2}{\partial x_p} \, \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q} \, \mathbf{g}_{q,h} \frac{\partial \psi_h}{\partial \ell_q}$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \frac{1}{2} \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h} \frac{\partial}{\partial x_p} \left(\phi_h^2 \frac{\partial \psi_h}{\partial \ell_q} \frac{\partial \psi_h}{\partial \ell_q} \right) \, \mathbf{g}_{q,h} \, \mathbf{g}_{q,h}$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \frac{1}{2} \int_K \delta_K \sum_{p=1}^d \sum_{q=1}^s \mathbf{u}_{p,h} \frac{\partial}{\partial x_p} \left(\frac{\partial v_h}{\partial \ell_q} \frac{\partial v_h}{\partial \ell_q} \right) \, \mathbf{g}_{q,h} \, \mathbf{g}_{q,h}$$

$$= \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \frac{1}{2} \int_K \delta_K |\mathbf{g}_h|^2 \mathbf{u}_h \cdot \nabla_x (\nabla_\ell v_h \nabla_\ell v_h)$$

$$= -\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \frac{1}{2} \int_K \delta_K |\mathbf{g}_h|^2 \nabla_x \cdot \mathbf{u}_h (\nabla_\ell v_h \nabla_\ell v_h) = 0.$$

☐

LEMMA 4.3 (Coercivity of $a_{OS}(\cdot, \cdot)$). *Let the discrete form of the assumptions (1.2) and (1.3) be satisfied. Then, the bilinear form $a_{OS}(\cdot, \cdot)$ associated with the operator-splitting method satisfies*

$$a_{OS}(f_h^n, f_h^n) \geq \tau \|| f_h^n \||_{OS}^2 \tag{4.6}$$

with

$$\||f_h^n\||_{OS}^2 = \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \delta_K \left(\epsilon \| \mathbf{g}_h \cdot \nabla_\ell (\nabla_x f_h^n) \|_{1,1,K',K}^2 \right)$$

Proof. Using the definitions of the finite element spaces $V_{h,0}$ and $Q_{h,0}$, and the estimates in Lemma 4.2 in $a_{OS}(f_h^n, f_h^n)$, we get

$$a_{OS}(f_h^n, f_h^n) \geq \frac{\tau}{2} \int_\Omega \epsilon \mathbf{g}_h \cdot \nabla_\ell ((\nabla_x f_h^n)^2) + \frac{1}{2} \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \int_K \delta_K \epsilon \mathbf{g}_h \cdot \nabla_\ell ((\nabla_x f_h^n)^2)$$

$$+ \tau \int_{\Omega_X} \epsilon \sum_{K \in \mathcal{S}_h} \int_K \delta_K \mathbf{g}_h \cdot \nabla_\ell (\nabla_x u_h^n) \mathbf{g}_h \cdot \nabla_\ell (\nabla_x f_h^n)$$

$$= \tau \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \delta_K \left(\epsilon \| \mathbf{g}_h \cdot \nabla_\ell (\nabla_x f_h^n) \|^2 \right).$$

☐

4.1. Stability of the operator-split finite element discretization. The stability of the operator-split discrete equation (4.1) is studied in this section. In the stability analysis, we use the following discrete form of the Grownwall's lemma.

LEMMA 4.4 (Discrete Grownwall's lemma). *Assume that* w_n, $n \geq 0$, *satisfies*

$$w^N \leq \alpha^n + \sum_{n=1}^{N} \beta^n w^n, \quad for \ n \geq 0,$$

where α_n *is a non-decreasing and* $\beta_n \geq 0$. *Then, we have*

$$w^N \leq \alpha^n \exp\left\{\sum_{n=1}^{N} \beta^n\right\}.$$

The proof is rather technical, see for example [22].

LEMMA 4.5 (Stability). *For given* $T > 0$, *let* $\tau = T/N$, $N \geq 1$, *be an uniform time step. Then, for* $f_h^N \in W_{h,0}$ *with the additional condition*

$$\delta \leq \frac{\tau}{2}, \quad where \ \delta = \max\{\delta_K\}, \ \forall \ K \ \in \mathcal{S}_h, \tag{4.7}$$

we have the following stability estimate

$$\|f_h^N\|^2 + \tau \sum_{n=1}^{N} |||f_h^n|||^2 + 2\tau^2 \sum_{n=1}^{N} |||f_h^n|||_{OS}^2$$

$$\leq \left\{\|f_h^0\|^2 + \tau(1+\tau)\sum_{n=1}^{N} \|\mathcal{S}^n\|^2\right\} \exp(T),$$

for $1 \leq N \leq N_T$.

Proof. Consider the operator-split discrete equation (4.1), and set $v_h = f_h^n$ to get

$$\left(f_h^n - f_h^{n-1}, \ f_h^n\right) + \tau \ a_{LS}(f_h^n, \ f_h^n) + \tau \ a_{OS}(f_h^n, \ f_h^n)$$
$$= \tau(\mathcal{S}_1^n, \ f_h^n) + \tau F_S(\mathcal{S}_2^n, f_h^n) - a_{LT}\left(f_h^n - u_h^{n-1}, f_h^n\right), \tag{4.8}$$

where $\mathcal{S}_1 = \mathcal{S}_2 = \mathcal{S}$. To use the stability estimate later in the error estimate, we used different notations for source terms in the right hand side of (4.8). Now, Applying the identity 2a(a-b)=a^2 - b^2 + (a - b)^2 for the first term, and using the Lemmas 2.1 and 4.3 for the bilinear forms $a_{LS}(f_h^n, \ f_h^n)$ and $a_{OS}(f_h^n, \ f_h^n)$ in (4.8), we get

$$\|f_h^n\|^2 + \|f_h^n - f_h^{n-1}\|^2 + 2\tau|||f_h^n|||^2 + 2\tau^2|||f_h^n|||_{OS}^2 \ \leq \ \|f_h^{n-1}\|^2 + 2|\tau(\mathcal{S}_1^n, f_h^n)|$$

$$+ 2\tau \left|\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathcal{S}_2^n, \ \mathbf{g}_h \cdot \nabla_\ell f_h^n\right)_K\right| + 2\left|\int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(f_h^n - f_h^{n-1}, \ \mathbf{g}_h \cdot \nabla_\ell f_h^n\right)_K\right|$$

Applying the Cauchy-Schwarz inequality and Young's inequality to the right hand side terms, we get

$$2|\tau(\mathcal{S}_1^n, f_h^n)| \leq \tau\|\mathcal{S}_1^n\|^2 + \tau\|f_h^n\|^2, \tag{4.9}$$

$$2\tau \left| \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\mathcal{S}_2^n, \ \mathbf{g}_h \cdot \nabla_\ell f_h^n\right)_K \right|$$

$$\leq 2\tau\delta\|\mathcal{S}_2^n\|^2 + \sum_{K \in \mathcal{S}_h} \sum_{K' \in \mathcal{T}_h} \frac{\tau\delta_K}{2}\|\mathbf{g}_h \cdot \nabla_\ell f_h^n\|_{0,K',K}^2 \qquad (4.10)$$

and

$$2\left| \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(f_h^n - f_h^{n-1}, \ \mathbf{g}_h \cdot \nabla_\ell f_h^n\right)_K \right|$$

$$\leq \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \left(\frac{2\delta_K}{\tau} \left\|f_h^n - f_h^{n-1}\right\|_{0,K',K}^2 + \frac{\tau\delta_K}{2} \left\|\mathbf{g}_h \cdot \nabla_\ell f_h^n\right\|_{0,K',K}^2 \right)$$

$$\leq \frac{2\delta}{\tau} \left\|f_h^n - f_h^{n-1}\right\|^2 + \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \frac{\tau\delta_K}{2} \left\|\mathbf{g}_h \cdot \nabla_\ell f_h^n\right\|_{0,K',K}^2 \qquad (4.11)$$

Using these bounds, we get

$$\|f_h^n\|^2 + \tau\||f_h^n\||^2 + 2\tau^2\||f_h^n\||_{OS}^2 \ \leq \ \|f_h^{n-1}\|^2 + \tau\|f_h^n\|^2 + \tau\left(\|\mathcal{S}_1^n\|^2 + 2\delta\|\mathcal{S}_2^n\|^2\right)$$

Now, summing over $n = 1, \ldots, N$, we get

$$\|f_h^n\|^2 + \tau\sum_{n=1}^N \||f_h^n\||^2 + 2\tau^2\sum_{n=1}^N \||f_h^n\||_{OS}^2$$

$$\leq \ \left\{ \|u_h^0\|^2 + \tau\sum_{n=1}^N \left(\|\mathcal{S}_1^n\|^2 + 2\delta\|\mathcal{S}_2^n\|^2\right) \right\} + \sum_{n=1}^N \tau\|f_h^n\|^2. \qquad (4.12)$$

With the additional condition (4.7), by applying the discrete form of Grownwall's lemma 4.4, and using the fact that $\mathcal{S}_1 = \mathcal{S}_2 = \mathcal{S}$, we get the statement of the lemma.
□

4.2. A priori error estimates. To derive the error estimate for the solution of the operator-split finite element discretization (4.1), let us introduce the following approximation properties, (cf. Theorem 4.8.12 and Corollary 4.8.15 in [1]).

(A1) Approximation property of $V_{h,0}$: We assume that there exist an interpolation operator $I_X \in \mathcal{L}(H^r(\Omega_X) \cap H_0^1(\Omega_X); V_{h,0})$ such that

$$\|I_X u\|_{H^s(\Omega_X)} \leq C|u|_{H^s(\Omega_X)}, \quad 1 \leq s \leq r, \qquad (4.13)$$

$$\|u - I_X u\|_{L^2(\Omega_X)} + h_x\|u - I_X u\|_{H^1(\Omega_X)} \leq Ch_x^s|u|_{H^s(\Omega_X)}, \quad 1 \leq s \leq r. \qquad (4.14)$$

(A2) Approximation property of $Q_{h,0}$: There exist an interpolation operator $I_L \in \mathcal{L}(H^r(\Omega_L) \cap H_0^1(\Omega_L); Q_{h,0})$ such that

$$\|I_L u\|_{H^s(\Omega_L)} \leq C|u|_{H^s(\Omega_L)}, \quad 1 \leq s \leq r, \qquad (4.15)$$

$$\|u - I_L u\|_{L^2(\Omega_L)} + h_\ell\|u - I_L u\|_{H^1(\Omega_L)} \leq Ch_\ell^s|u|_{H^s(\Omega_L)} \quad 1 \leq s \leq r. \qquad (4.16)$$

Here, $\mathcal{L}(X;Y)$ denotes the set of linear and continuous mappings from X to Y. Now, we define a projection operator $I_h \in \mathcal{L}(H^{r,r}(\Omega) \cap (V_0 \otimes Q_0), W_{h,0})$ as

$$I_h : I_X I_L = I_L I_X.$$

The error analysis of (4.1) starts by decomposition of the error into two parts in which one measures the interpolation error and the other measures the difference of the interpolation and the discrete solution.

$$e_h^n := f(t^n) - f_h^n = (f(t^n) - I_h f(t^n)) + (I_h f(t^n) - f_h^n) =: \eta^n + \xi^n.$$

The interpolation error η^n can be estimated using the approximation properties of the finite element spaces. For the error $\xi^n \in W_{h,0}$, apply $\xi^n = f(t^n) - f_h^n - \eta^n$ and $v_h = \xi^n$ in (4.1) to obtain

$$
\begin{aligned}
\left(\bar{\partial}\xi^n,\ \xi^n\right) &+ a_{LS}(\xi^n,\ \xi^n) + a_{LT}\left(\bar{\partial}\xi^n, \xi^n\right) + a_{OS}(\xi^n,\ \xi^n) \\
&= \left(\bar{\partial}f(t^n), \xi^n\right) + a_{LS}(f(t^n),\ \xi^n) + a_{LT}\left(\bar{\partial}f(t^n), \xi^n\right) \\
&\quad + a_{OS}(f(t^n),\ \xi^n) - (\mathcal{S}^n,\ \xi^n) - F_S(\mathcal{S}^n, \xi^n) \\
&\quad - \left(\bar{\partial}\eta^n,\ \xi^n\right) - a_{LS}(\eta^n,\ \xi^n) - a_{LT}\left(\bar{\partial}\eta^n, \xi^n\right) - a_{OS}(\eta^n,\ \xi^n)
\end{aligned}
\tag{4.17}
$$

where the source terms arise from the terms containing f_h^n and f_h^{n-1} due to (4.1). Thus, we have

$$
\begin{aligned}
\left(\xi^n - \xi^{n-1}, \xi^n\right) &+ \tau a_{LS}(\xi^n, \xi^n) + \tau a_{OS}(\xi^n, \xi^n) \\
&= \tau(E_1^n, \xi^n) + \tau \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K(E_2^n,\ \mathbf{g}_h \cdot \nabla_\ell \xi^n)_K \\
&\quad + \tau(E_3^n, \nabla_x \xi^n) + \tau \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K(E_4^n,\ \mathbf{g}_h \cdot \nabla_\ell \nabla_x \xi^n)_K,
\end{aligned}
\tag{4.18}
$$

where

$$
\begin{aligned}
E_1^n &:= K_1^n + \bar{\partial}f(t^n) - \frac{\partial f(t^n)}{\partial t} \\
E_2^n &:= K_1^n - \mathbf{u}_h \cdot \nabla_x f(t^n) \\
E_3^n &:= -\epsilon \nabla_x \eta^n - \tau \epsilon \mathbf{g}_h \cdot \nabla_\ell(\nabla_x \eta^n) - \tau \epsilon \mathbf{g}_h \cdot \nabla_\ell(\nabla_x f(t^n)) \\
E_4^n &:= E_3^n - \epsilon \nabla_x f(t^n) \\
K_1^n &:= -\bar{\partial}\eta^n - \mathbf{u}_h \cdot \nabla_x \eta^n - \mathbf{g}_h \cdot \nabla_\ell \eta^n - \tau \mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x \eta^n) \\
&\quad - \tau \mathbf{g}_h \cdot \nabla_\ell(\mathbf{u}_h \cdot \nabla_x f(t^n))
\end{aligned}
$$

When we take $\mathcal{S}_1^n = E_1^n$ and $\mathcal{S}_2^n = E_2^n$, the error equation (4.18) contains only the additional terms E_3 and E_4 in comparison with the operator-split discrete form (4.8) used in the stability estimate. Therefore, the estimate for the error equation will be similar as in the Lemma 4.5. Thus, to use the Lemma 4.5, we first derive the estimates for E_3 and E_4 terms. Using the Cauchy-Schwarz inequality and Young's inequality, we get

$$
|(E_3^n, \nabla_x \xi^n)| \leq \frac{1}{2\epsilon}\|E_3^n\|^2 + \frac{\epsilon}{2}\|\nabla_x \xi^n\|^2
\tag{4.19}
$$

and

$$\left| \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K (E_4^n, \ \mathbf{g}_h \cdot \nabla_\ell \nabla_x \xi^n)_K \right|$$

$$= \left| \int_{\Omega_X} \sum_{K \in \mathcal{S}_h} \delta_K \left(\frac{1}{(\epsilon)^{1/2}} E_4^n, \ (\epsilon)^{1/2} \mathbf{g}_h \cdot \nabla_\ell \nabla_x \xi^n \right)_K \right|$$

$$\leq \frac{\delta}{\epsilon} \|E_4^n\|^2 + \epsilon \sum_{K' \in \mathcal{T}_h} \sum_{K \in \mathcal{S}_h} \delta_K \|\mathbf{g}_h \cdot \nabla_\ell \nabla_x \xi^n\|^2 \qquad (4.20)$$

Using the estimates (4.9), (4.10), (4.19) and (4.20) for the bilinear terms in the right hand side of the error equation (4.18), and applying the Lemma 4.5, we get

$$\|\xi^N\|^2 + \tau \sum_{n=1}^N |||\xi^n|||^2 + \tau C_\tau \sum_{n=1}^N |||\xi^n|||^2_{OS} \leq \exp(T) \left\{ \|\xi^0\|^2 \right.$$

$$\left. + \sum_{n=1}^N \left\{ \tau \left(\|E_1^n\|^2 + 2\delta \|E_2^n\|^2 \right) + \frac{\tau}{\epsilon} \left(\|E_3^n\|^2 + 2\delta \|E_4^n\|^2 \right) \right\} \right\}, \qquad (4.21)$$

where $C_\tau = 2(\tau - 1)$. Now, we derive the bounds for the terms E_1^n and E_2^n. For the term E_1^n, we have

$$\|E_1^n\|^2 \leq \|K_1^n\|^2 + \left\| \bar{\partial} f(t^n) - \frac{\partial f(t^n)}{\partial t} \right\|^2.$$

Applying the Taylor's theorem with remainder in integral form and using the supremum of $\mathbf{u}$ and $\mathbf{g}$, we get

$$\|E_1^n\|^2 \leq \|K_1^n\|^2 + C\tau \int_{t^{n-1}}^{t^n} \left\| \frac{\partial^2 f(t)}{\partial t^2} \right\|^2,$$

where

$$\|K_1^n\|^2 \leq \frac{1}{\tau} \int_{t^{n-1}}^{t^n} \left\| \frac{\partial \eta}{\partial t} \right\|^2 + |\mathbf{u}|^2 \|\nabla_x \eta^n\|^2 + |\mathbf{g}|^2 \|\nabla_\ell \eta^n\|^2$$

$$+ \tau |\mathbf{u}|^2 |\mathbf{g}|^2 \|\nabla_\ell \nabla_x \eta^n\|^2 + \tau |\mathbf{u}|^2 |\mathbf{g}|^2 \|\nabla_\ell \nabla_x f(t^n)\|^2$$

Here, $|\mathbf{u}|^2 = \|\mathbf{u}\|^2_{L^\infty(0,T;\Omega_X)}$ and $|\mathbf{g}|^2 = \|\mathbf{g}\|^2_{L^\infty(0,T;\Omega_X)}$. Next by applying the triangular inequality to E_2, E_3 and E_4 terms, we get

$$\|E_2^n\|^2 \leq \|K_1^n\|^2 + |\mathbf{u}|^2 \|\nabla_x f(t^n)\|^2,$$
$$\|E_3^n\|^2 \leq \epsilon \|\nabla_x \eta^n\|^2 + \tau \epsilon |\mathbf{g}|^2 \|\nabla_\ell \nabla_x \eta^n\|^2 + \tau \epsilon |\mathbf{g}|^2 \|\nabla_\ell \nabla_x f(t^n)\|^2,$$
$$\|E_4^n\|^2 \leq \|E_3^n\|^2 + \epsilon \|\nabla_x f(t^n)\|^2.$$

Using all these bounds, we get

$$\|\xi^N\|^2 + \tau \sum_{n=1}^{N} |||\xi^n|||^2 + \tau C_\tau \sum_{n=1}^{N} |||\xi^n|||^2_{OS}$$

$$\leq \exp(T) \left\{ \|\xi^0\|^2 + \sum_{n=1}^{N} \left[C_\delta \left\|\frac{\partial \eta}{\partial t}\right\|^2 + \tau^2(1 + |\mathbf{u}|^2)\|\nabla_x f(t^n)\|^2 \right. \right. \tag{4.22}$$

$$+ \tau^2 C_\delta^{\mathbf{g}} |\mathbf{g}|^2 \left(\|\nabla_\ell \nabla_x f(t^n)\|^2 + \|\nabla_\ell \nabla_x \eta^n\|^2 \right)$$

$$\left. \left. + \tau C_\delta^{\mathbf{g}} \|\nabla_x \eta^n\|^2 + \tau C_\delta |\mathbf{g}|^2 \|\nabla_\ell \eta^n\|^2 + C\tau^2 \left\|\frac{\partial^2 f(t)}{\partial t^2}\right\|^2 \right] \right\},$$

where $C_\delta = 1 + 2\delta$ and $C_\delta^{\mathbf{g}} = 1 + \tau + C_\delta |\mathbf{u}|^2$. Next, we derive bounds for the terms containing η, the interpolation error. For these terms, We have the following bounds:

$$\|\eta\| = \|f - I_X I_L f\| \leq \|f - I_X f\| + \|I_X f - I_X I_L f\|$$

$$= \left(\int_{\Omega_L} \|f - I_X f\|^2_{L^2(\Omega_X)}\right)^{\frac{1}{2}} + \left(\int_{\Omega_X} \|I_X f - I_L I_X f\|^2_{L^2(\Omega_L)}\right)^{\frac{1}{2}}$$

$$\leq C_1 h_x^r \left(\int_{\Omega_L} |f|^2_{H^r(\Omega_X)}\right)^{\frac{1}{2}} + C_2 h_\ell^s \left(\int_{\Omega_X} \|I_X f\|^2_{H^s(\Omega_L)}\right)^{\frac{1}{2}}$$

$$\leq C_1 h_x^r \left(\int_{\Omega_L} |f|^2_{H^r(\Omega_X)}\right)^{\frac{1}{2}} + C_2 h_\ell^s \left(\int_{\Omega_X} |f|^2_{H^s(\Omega_L)}\right)^{\frac{1}{2}} \tag{4.23}$$

$$\left\|\frac{\partial \eta}{\partial t}\right\| \leq C_1 h_x^r \left(\int_{\Omega_L} \left|\frac{\partial f}{\partial t}\right|^2_{H^r(\Omega_X)}\right)^{\frac{1}{2}} + C_2 h_\ell^s \left(\int_{\Omega_X} \left|\frac{\partial f}{\partial t}\right|^2_{H^s(\Omega_L)}\right)^{\frac{1}{2}} \tag{4.24}$$

$$\|\nabla_x \eta\| \leq \|\nabla_x f - \nabla_x I_X f\| + \|\nabla_x I_X f - I_L \nabla_x I_X f\|$$

$$\leq C_1 h_x^r \left(\int_{\Omega_L} |f|^2_{H^{r+1}(\Omega_X)}\right)^{\frac{1}{2}} + C_2 h_\ell^s \left(\int_{\Omega_X} \|I_X f\|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}}$$

$$\leq C_1 h_x^r \left(\int_{\Omega_L} |f|^2_{H^{r+1}(\Omega_X)}\right)^{\frac{1}{2}} + C_2 h_\ell^s \left(\int_{\Omega_X} |f|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}} \tag{4.25}$$

$$\|\nabla_\ell \eta\| \leq \|\nabla_\ell f - \nabla_\ell I_L f\| + \|\nabla_\ell I_L f - I_X \nabla_\ell I_L f\|$$

$$\leq C_1 h_\ell^s \left(\int_{\Omega_X} |f|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}} + C_2 h_x^r \left(\int_{\Omega_L} \|I_L f\|^2_{H^{r+1}(\Omega_X)}\right)^{\frac{1}{2}}$$

$$\leq C_1 h_\ell^s \left(\int_{\Omega_X} |f|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}} + C_2 h_x^r \left(\int_{\Omega_L} |f|^2_{H^{s+1}(\Omega_X)}\right)^{\frac{1}{2}} \tag{4.26}$$

$$\|\nabla_\ell \nabla_x \eta\| \leq \|\nabla_\ell \nabla_x f - \nabla_\ell I_L \nabla_x f\| + \|\nabla_x \nabla_\ell I_L f - I_X \nabla_x \nabla_\ell I_\ell f\|$$

$$\leq C_1 h_\ell^s \left(\int_{\Omega_X} |\nabla_x f|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}} + C_2 h_x^r \left(\int_{\Omega_L} \|\nabla_\ell I_L f\|^2_{H^{r+1}(\Omega_X)}\right)^{\frac{1}{2}}$$

$$\leq C_1 h_\ell^s \left(\int_{\Omega_X} |\nabla_x f|^2_{H^{s+1}(\Omega_L)}\right)^{\frac{1}{2}} + C_2 h_x^r \left(\int_{\Omega_L} \|\nabla_\ell f\|^2_{H^{r+1}(\Omega_X)}\right)^{\frac{1}{2}} \tag{4.27}$$

Substituting these estimates (4.23)-(4.27) in (4.22), we get

$$\|f^N - f_h^N\|_{L^\infty(0,T;L^2(\Omega))}^2 + \tau \sum_{n=1}^N \||f^N - f_h^N|\|^2$$

$$+ \tau C_\tau \sum_{n=1}^N \||f^N - f_h^N|\|_{OS}^2 \le h^k(C_1 h + C_2) + C_3 \tau^2,$$

where the constants C_1 C_2 and C_3 depend on f, $\frac{\partial f}{\partial t}$ $\frac{\partial^2 f}{\partial t^2}$, $\mathbf{u}$ and $\mathbf{g}$. Further, it should be noted that the mixed partial derivatives of the solution, *i.e.,*, $\nabla_\ell \nabla_x f(t^n)$, has to be bounded in the estimate (4.22) of the operator splitting discretization. It is the reason we use the $H^{1,1}(\Omega)$ space instead of $H^1(\Omega)$ spaces.

5. Numerical results. To validate the operator-splitting heterogeneous finite element scheme, we consider the equation (1.1) in $\Omega_X = (0,1)^2$ and $\Omega_L = (0,1)$. Further, we have chosen $\epsilon = 1$, $\mathbf{u} = (0,0)$, $\mathbf{g} = 1$ and $T = 1$. The right-hand side $\mathcal{S}$ is chosen such that

$$f(t,x,\ell) = e^{-0.1t} \sin(\pi x_1) \cos(\pi x_2) \cos(\pi \ell)$$

is the solution of (1.1) with the above data. For this configuration, the operator split population balance equations (3.1) and (3.2) will reduce to a time dependent diffusion and a pure advection equations, respectively. Further, to evaluate the numerical errors, we define

$$L^\infty(L^2) := \sup_{t^n \in (0,T]} \|f(t^n, x, \ell) - f_h(t^n, x, \ell)\|_{L^2(\Omega)}$$

$$L^2(L^2) := \left(\int_0^T \|f - f_h\|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}}$$

where the L^2−error at the time t^n is evaluated by

$$\|f^n - f_h^n\|_{L^2(\Omega)}^2 = \int_{\Omega_X \times \Omega_L} (f^n - f_h^n)^2 \, d(x, \ell) = \int_{\Omega_X} \left(\int_{\Omega_L} (f^n - f_h^n)^2 \, d\ell \right) dx$$

$$= \sum_{K' \in \mathcal{T}_h} \sum_{m=1}^{N\_XQP} w_m^x \int_{\Omega_L} (f(t^n, q_m, \ell) - f_h(t^n, q_m, \ell))^2 \, d\ell$$

$$= \sum_{K' \in \mathcal{T}_h} \sum_{m=1}^{N\_XQP} w_m^x \sum_{K \in \mathcal{S}_h} \sum_{l=1}^{N\_LQP} w_l^\ell \left(f(t^n, q_m, \ell_l) - f_h(t^n, q_m, \ell_l) \right)^2.$$

Here, w_m^x, q_m, N_XQP and w_l^ℓ, ℓ_l, N_LQP are the Gaussian quadrature data (weights, points, number of points) in K' and K, respectively.

At level 1, the initial grid of Ω_X contains four quadrilaterals, whereas the initial grid of Ω_L contains two line segments. The higher grid levels of Ω_X and Ω_L are obtained by successively refining their respective initial grids uniformly. In this numerical study, we used (*i*) Q_1/P_1, (*ii*) Q_2/P_2, *i.e.*, linear and quadratic finite element pairs. The computational results obtained with the Galerkin/Galerkin and Galerkin/SUPG discretizations are presented in Figure 5.1. For Q_1/P_1, the numerical errors obtained in both the Galerkin/Galerkin and Galerkin/SUPG are similar. For the Q_2/P_2 finite element pair, the error and the order of convergence obtained with the Galerkin/SUPG are slightly better than the Galerkin/Galerkin case. Nevertheless, in all cases the optimal order of convergence is obtained.
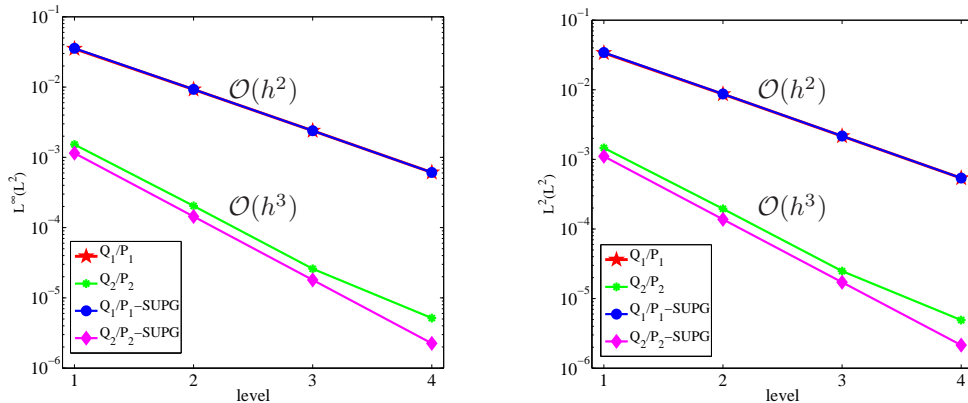
FIG. 5.1. *Numerical errors in $L^\infty(L^2)$ and $L^2(L^2)$ norms for the 2D+1D test example.*

6. Summary. We have presented a novel operator-splitting finite element method for high-dimensional population balance equations, which depend on both physical and internal property coordinates. The application of the operator-splitting method alleviates the "curse of dimensionality" associated with the solution of a population balance equation in a population balance system. Applying the operator-splitting method, we split the population balance equation into two low-dimensional equations, where the first equation depends only the physical space and the second equation depends only the internal space. This splitting facilitates to use different discretizations in physical and internal spaces, and therefore we used the standard Galerkin and the Streamline Upwind Petrov Galerkin (SUPG) finite element discretizations for physical and internal spaces, respectively. For this heterogeneous finite element scheme we were able to estimate the operator-splitting error and prove stability for the heterogeneous finite element discretization of the population balance equation. In the error estimate, it is shown that a slightly more regularity, *i.e.*, mixed partial derivative of the solution should be bounded, is required to apply the operator-splitting finite element method. Moreover, the numerical results were presented for a test problem with know smooth solution. The optimal order of convergences were obtained for first and second order approximations.

REFERENCES

[1] S. C. BRENNER, L. R. SCOTT, *The Mathematical Theory of Finite Element Methods* , Third ed., Springer, 2008.

[2] E. BURMAN, *Consistent SUPG-method for transient transport problems: Stability and convergence*, Comput. Methods in Appl. Mech. and Engrg., 199 (2010), pp. 1114-1123.

[3] I.T. CAMERON AND F.Y. WANG AND C.D. IMMANUEL AND F. STEPANEK, *Process systems modelling and applications in granulation: a review*, Chem. Engrg. Sci., 60 (2005), pp. 3723-3750.

[4] F. B. CAMPOS AND P. L. C. LAGE, *A numerical method for solving the transient multidimensional population balance equation using an Euler-Lagrange formulation*, Chem. Engrg. Sci., 58 (2003), pp. 2725-2744.

[5] C. CHAUVIÈRE AND A. LOZINSKI, *Simulation of dilute polymer solutions using a FokkerPlanck equation*, Computers and Fluids, 33 (2004), pp. 687–696.

[6] E. J. DEAN AND R. GLOWINSKI, *An operator-splitting approach to multilevel methods*, Applied

Math. Letters, 15 (2002), pp. 505–511.

[7]   J. Douglas, *Alternating direction methods for three space variables*, Numer. Math, 4 (1962), pp. 41–63.

[8]   S. Ganesan and L. Tobiska, *Implementation of an operator-splitting finite element method for high-dimensional parabolic problems*, (in preparation), (2010).

[9]   R. Glowinski, E. J. Dean, G. Guidoboni, D. H. Peaceman and H. H. Rachford, *Applications of operator-splitting methods to the direct numerical simulation of particulate and free-surface flows and to the numerical solution of the two-dimensional elliptic Monge-Ampère equation*, Japan J. Indust. Appl. Math., 25 (2008), pp. 1–63.

[10] V. John, and J. Novo, *Error Analysis of the SUPG Finite Element Discretization of Evolutionary Convection-Diffusion-Reaction Equations*, WIAS Preprint No. 1494, (2010).

[11] V. John, M. Roland, T. Mitkova, K. Sundmacher, L. Tobiska and A. Voigt, *Simulations of population balance systems with one internal coordinate using finite element methods*, Chem. Engrg. Sci., 64 (2009), pp. 733-741.

[12] D. J. Knezevic and E. Süli, *A heterogeneous alternating-direction method for a micro-macro dilute polymeric fluid model*, ESAIM: M2AN, 43 (2009), pp. 1117-1156.

[13] V. Kulikov, H. Briesen, R. Grosch, A. Yang, L. von Wedel and W. Marquardt, *Modular dynamic simulation for integrated particulate processes by means of tool integration*, Chem. Engrg. Sci., 60 (2005), pp. 2069-2083.

[14] V. Kulikov, H. Briesen and W. Marquardt, *A framework for the simulation of mass crystallization considering the effect of fluid dynamics*, Chem. Engrg. Sci., 45 (2006), pp. 886-899.

[15] D. Marchisio and R. Fox, *Solution of population balance equations using the direct quadrature method of moments*, J. Aero. Sci., 36 (2005), pp. 43-73.

[16] M. N. Nandanwara and S. Kumar, *A new discretization of space for the solution of multi-dimensional population balance equations: Simultaneous breakup and aggregation of particles*, Chem. Engrg. Sci., 63 (2008), pp. 3988-3997.

[17] H.-G. Roos, M. Stynes and L. Tobiska, *Robust Numerical Methods for Singularly Perturbed Differential Equations*, Second ed., Springer Berlin Heidelberg, 2008.

[18] D. L. Marchisio and R. O. Fox *Solution of population balance equations using the direct quadrature method of moments*, J. Aero. Sci., 36 (2005), pp. 43-73.

[19] D. Ramkrishna , *Population Balances, Theory and Applications to Particulate Systems in Engineering*, Academic Press, San Diego, 2000.

[20] D. Ramkrishna and Alan W. Mahoney, *Population balance modeling. Promise for the future*, Chem. Engrg. Sci., 57 (2002), pp. 595-606.

[21] G. Strang, *On the construction and comparison of difference schemes*, SIAM J. Num. Anal., 5 (1968), pp. 506–517.

[22] V. Thomee, *Galerkin Finite Element Methods for Parabolic Problems*, Second ed., Springer, Berlin Heidelberg, 2006.