A SECOND ORDER PROJECTION-BASED TIME-SPLITTING SCHEME FOR COMPUTING CHEMICALLY REACTING FLOWS

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Abstract. The computation of velocity field, pressure, temperature distribution and mass fraction functions that are coupled in a nonlinear PDE describing chemically reacting flows is a challenging task since computational resources are limited. Implicit solution ansatzes of the coupled quantities require a vast amount of storage capacities that is lacking on normal workstations to resolve complex flow structures. The present paper proposes and analyzes a $2nd$ order time-splitting scheme that leads to a significant reduction of computational work and is appropriate to parallelization strategies in solving approximates in each iteration step. Optimal convergence results justify the accuracy of the splitting approach.

Key words. Chemically reacting flows, Boussinesq model, incompressible Navier-Stokes equations, convergence analysis, projection methods, splitting methods, Chorin scheme, Van Kan scheme, parallelization.

AMS subject classifications. 35Q35, 65M12, 76D05, 76V05.

1 Introduction. The study of chemically reacting fluid flows is the subject of many engineering sciences: the observation and prediction of future flow phenomena is basic for people working in these areas to optimize involved reaction processes. For example, complex flow structures arising in chemical vapor deposition (CVD) reactors need to be understood to design an optimized apparatus that ensures an improved manufacturing of semiconductors. In typical construction processes, there can be more than thirty important chemical species undergoing more than fifty reactions, see [1, 6, 9, 14].

Computer modeling of these complex flows can greatly aid in the understanding, design and optimization of engineering procedures. Moreover, it is particularly attractive for applications where involved chemicals are expensive and/or toxic, like e.g. Arsine. However, the numerical modeling of ongoing relevant processes is a challenging task for existing computer resources, since standard discretization strategies lead to very large (algebraic) nonlinear problems that can only be solved on huge parallel machines, see [14].

This motivates to develop new, less expensive algorithms that can be implemented even on workstations, and give reasonably accurate solutions. A first step in this direction has been made in [13], where a first order time-splitting scheme has been proposed and analyzed. This scheme is based on the projection method of Chorin, see [2, 3], to reduce the computational effort. In particular, this scheme is appropriate for parallelization strategies, since the computation of iterates will be accomplished in a decoupled manner. — In the present work, we focus on a higher order projection-based time-splitting scheme that inherits the advantages of the first order projection-based time-splitting scheme of [13].

We start with the presentation of the system of equations that describes the dynamics of the chemically reacting flow. They are derived from the the conservation principles for impulse, mass and energy. If we consider a bounded domain $\Omega \subset \mathrm{R}^d$, $d = 2,3$ where the

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reactive flow is in and observe its behavior over a period of time $[0, t_{M+1}]$, the dynamics is described by the system of equations

$$
\begin{aligned}
&u_t - Pr\Delta u + (u\cdot\nabla)u + \nabla p = f_0(T),\\
&\mathrm{div} u = 0,\\
&T_t - \Delta T + (u\cdot\nabla)T = -\sum_{i=1}^{N} h_i W_i\big(\{Y_i\}_{i=1}^N, T\big),\\
&Y_{i,t} - \frac{1}{Le}\Delta Y_i + (u\cdot\nabla)Y_i = W_i\big(\{Y_i\}_{i=1}^N, T\big), \qquad i = 1,\dots,N.
\end{aligned}
\tag{1}
$$

Here, the motion of the fluid flow is described by a solenoidal velocity field $u = u(x,t)$ and a pressure function $p = p(x,t)$ moving around chemicals (species) that are represented by mass fractions Y_i, for $1 \le i \le N$. The mass conservation principle leads to the identities

$$
0 \le Y_i \le 1, \qquad \text{and} \qquad \sum_{i=1}^{N} Y_i = 1, \qquad \sum_{i=1}^{N} W_i = 0, \qquad \forall\, x \in \Omega,\ t \ge 0,
$$

with W_i the net production/removal rates of the species indicated by i. The reaction of the chemicals produces heat and thus affects the temperature $T = T(x,t)$. The changing temperature then affects the flow through buoyancy effects, as we employ the Boussinesq model. — In the presented model, Pr is the Prandl number, Le the Lewis number that scale the diffusive and the convective character of the equations. Throughout this work, they will be set equal to 1.

For simplicity, we suppose the following initial and boundary value data for the problem under consideration,

$$
\begin{aligned}
&u\big|_{\partial\Omega} = 0, \qquad T\big|_{\partial\Omega} = 0, \qquad Y_i\big|_{\partial\Omega} = 0, \qquad \text{for } 1 \le i \le N,\\
&u(0) = u_0 \in \mathbf{J}_1 \cap \mathbf{H}^2, \qquad T(0) = T_0 \in H_0^1 \cap H^2, \qquad Y_i(0) = Y_i^0 \in H_0^1 \cap H^2.
\end{aligned}
\tag{2}
$$

The chemical reactions between the diverse species are described by means of the so-called Arrhenius model in which the W_i take the form

$$
W_i\big(\{Y_i\}_{i=1}^N, T\big) = \sum_{j=1}^{m_i} A_j e^{-E_j/R_0 T} \prod_{k=1}^{N} C_j^{\nu_{j,k}},
\tag{3}
$$

with A_j the frequency factors, E_j the activation energies, R_0 the universal gas constant, and C_i the concentrations, i.e., the mass fraction Y_i divided by the molecular weight, and the $\nu_{j,k}$ are nonegative integers, where at least one of $\nu_{j,k}$ for $k = 1,\dots,N$, is nonzero for each j. The h_i is the enthalpy of species i divided by its molecular weight, i.e., a measure of the amount of heat contained in species i.

In the subsequent analysis, we abstract from the specific form of the change of mass fractions, and make the following assumptions:

1. The W_i are smooth functions, $W_i \in C^2(0, t_{M+1}; \prod_{i=1}^{N+1} L^2)$. In particular, there exists a constant $C > 0$, s.t.
$$\big|W_i(\cdot,\cdot)\big| + \big|DW_i(\cdot,\cdot)\big| + \big|D^2 W_i(\cdot,\cdot)\big| \leq C, \qquad 1 \leq i \leq N.$$
2. The mass conservation implies the relation
$$\sum_{i=1}^{N} W_i\big(\{Y_i\}_{i=1}^N, T\big) = 0, \qquad \forall\ \big(\{Y_i\}_{i=1}^N, T\big) \in [0,1]^N \times [0,\infty).$$

Note that these requirements are satisfied for (3), in particular. — The well-posedness of (1), (2) has been shown in [8, 16], and the analysis has been extended in [11] to practically more relevant boundary conditions. For further discussions, especially on the chemical background, we refer to [10, 11].

Owing to the huge computational amount that is necessary to compute iterates from an implicit time-discretization scheme, accurate splitting-based discretization methods are particular attractive to significantly reduce the computational effort. In [13], a new algorithm is proposed and analyzed that combines first order accuracy of the iterates with low computational cost of the algorithm. This scheme is also suitable for parallelization strategies, since we can compute velocity and pressure independently from the temperature, and iterates of the mass fractions. Moreover, velocity and pressure iterates are calculated by means of Chorin's projection method, see [2, 3].

From [13], we know that a slight implicit/explicit shifting of certain phenomena in (1) is possible, without a loss of accuracy in a *first order* approximation setting. In the present paper, we will follow a corresponding idea to compute the iterates of velocity field, pressure, temperature and mass fraction functions, based on a splitting ansatz to keep the computational costs at a comparable size, but (hopefully) with an improved order of accuracy. To be specific, the numerical algorithm is as follows, for a time-step $k = t_{m+1} - t_m$:

Given approximations $\big\{\tilde{u}^{m-1}, \tilde{u}^m, u^{m-1}, u^m, p^{m-1}, p^m, T^{m-1}, T^m, \{Y_i^{m-1}\}_{i=1}^N, \{Y_i^m\}_{i=1}^N\big\}$ of velocity, pressure, temperature and mass fraction functions, evaluated at time $t = t_{m-1}$ or $t = t_m$, determine $\big\{\tilde{u}^{m+1}, u^{m+1}, p^{m+1}, T^{m+1},\ \{Y_i^{m+1}\}_{i=1}^N\big\}$ as the solution of the following system, for a parameter $\beta > \frac{1}{2}$,

1. Start with initial guesses $u^0 = u_0$, $T^0 = T_0$, $Y_i^0 = Y_{i,0}$, $1 \leq i \leq N$, and $\|p^0 - p(0)\|_1 \leq Ck$. Then, for $m \geq 0$, perform the following steps determine the iterates.
2. Find $\tilde{u}^{m+1}$ that solves
$$\begin{aligned} &\frac{1}{k}\big\{\tilde{u}^{m+1} - u^m\big\} - \frac{1}{2}\Delta\big\{\tilde{u}^{m+1} + \tilde{u}^m\big\} \\ &+ \tilde{\mathcal{N}}_1\big(\{\tilde{u}^{m-\ell}\}_{\ell=0}^1, \{\tilde{u}^{m+1-\ell}\}_{\ell=0}^1\big) + (\frac{3}{2} - \beta)\nabla p^m + (\beta - \frac{1}{2})\nabla p^{m-1} \\ &= f_0(\frac{3}{2}T^m - \frac{1}{2}T^{m-1}). \end{aligned} \tag{4}$$

3. Determine $\{u^{m+1}, p^{m+1}\}$ that solves the system

$$
\begin{aligned}
&\frac{1}{k}\{u^{m+1} - \tilde{u}^{m+1}\} + \beta\nabla\{p^{m+1} - p^m\} = 0, \\
&\mathrm{div} u^{m+1} = 0, \qquad u^{m+1}\big|_{\partial\Omega}\cdot n = 0.
\end{aligned} \tag{5}
$$

4. Compute T^{m+1} that is the solution of

$$
\begin{aligned}
&\frac{1}{k}\{T^{m+1} - T^m\} - \frac{1}{2}\Delta\{T^{m+1} + T^m\} + \tilde{\mathcal{N}}_2(\{\tilde{u}^{m-\ell}\}_{\ell=0}^1, \{T^{m+1-\ell}\}_{\ell=0}^1) \\
&\quad = -\sum_{i=1}^N h_i W_i\big(\frac{3}{2}\{Y_i^m\}_{i=1}^N - \frac{1}{2}\{Y_i^{m-1}\}_{i=1}^N, \overline{T}^{m+1/2}\big).
\end{aligned} \tag{6}
$$

5. The N-tuple $Y^{m+1} := \{Y_i^{m+1}\}_{i=1}^N$ is governed by

$$
\begin{aligned}
&\frac{1}{k}\{Y_i^{m+1} - Y_i^m\} - \frac{1}{2}\Delta\{Y_i^{m+1} + Y_i^m\} + \tilde{\mathcal{N}}_3(\{\tilde{u}^{m-\ell}\}_{\ell=0}^1, \{Y_i^{m+1-\ell}\}_{\ell=0}^1) \\
&\quad = W_i\big(\{\overline{Y}_i^{m+1/2}\}_{i=1}^N, \frac{3}{2}T^m - \frac{1}{2}T^{m-1}\}\big).
\end{aligned} \tag{7}
$$

Remark 1.1 *In the presentation of the scheme, we have chosen $m = 0$ to be the initial value of the iteration, although $\{u^{-1}, T^{-1}, Y^{-1}\}$ is not given. Therefore, we can modify the algorithm in the first step, $m = 0$, by shifting the convective term to an implicit, stabilized form, as it can be found in [17],*

$$(\overline{\tilde{u}}^{1/2} \cdot \nabla)\overline{\tilde{u}}^{1/2} + \frac{1}{2}(\mathrm{div}\overline{\tilde{u}}^{1/2})\overline{\tilde{u}}^{1/2}.$$

For $m = 0$, we set $\beta = 0$ to suppress the second pressure term in the momentum equation. As we know from [12], this again does not cause any theoretical problem. — To preserve second order of convergence, the right hand side of (4) has to be replaced by $f_0(\overline{T}^{1/2})$, and correspondingly the right hand sides of (6) and (7) by their implicit forms. This amounts to a coupling of the total system (4) through (7) in the first step. — For theoretical purposes, we can assume $\{u^{-1}, T^{-1}, Y^{-1}\}$ to be given and to satisfy

$$
\begin{aligned}
&\|u^{-1} - u(-k)\| + \|T^{-1} - T(-k)\| + \sum_{i=1}^N \|Y_i^{-1} - Y_i(-k)\| + k\|p^{-1} - p(-k)\|_1 \\
&\quad + \sqrt{k}\Big\{\|u^{-1} - u(-k)\|_1 + \|T^{-1} - T(-k)\|_1 + \sum_{i=1}^N \|Y_i^{-1} - Y_i(-k)\|_1\Big\} \le Ck^2,
\end{aligned} \tag{8}
$$

additionally to the requirements for the iterates that are indicated by $m = 0$ and are mentioned above. This is to avoid taking into account a modification of the involved operators in our algorithm. However, we emphasize that this modification does not affect the general character of the subsequent analysis in a decisive way.

In our formulation, the nonlinear mappings $\tilde{\mathcal{N}}_j(\cdot,\cdot)$, for $j = 1, 2, 3$, stand for a second order discretization of the nonlinear term, with the possibility of varying explicit or implicit discretizations in the leading first part. The first part has to be in $\mathbf{J}_0$ to assure the stability of the convective term, $\tilde{\mathcal{N}}_j(\cdot,\cdot) = \mathcal{N}_j(P_{\mathbf{J}_0}\cdot,\cdot)$. — For the purpose of this presentation, we set

$$\tilde{\mathcal{N}}(\cdot,\cdot) = \tilde{\mathcal{N}}_j(\cdot,\cdot) \qquad j = 1, 2, 3,$$

with

$$\mathcal{N}\big(\{\phi^{m-\ell}\}_{\ell=0}^{1}, \{\psi^{m+1-\ell}\}_{\ell=0}^{1}\big) = \big[\{\frac{3}{2}\phi^m - \frac{1}{2}\phi^{m-1}\}\cdot\nabla\big]\overline{\psi}^{m+1/2}, \tag{9}$$

for $\overline{\psi}^{m+1/2} = \frac{1}{2}\{\psi^{m+1} + \psi^m\}$. — The application of this mapping in the algorithm allows for the possibility to compute iterates in each iteration cycle *in parallel*.

This scheme is designed, using Van Kan's projection idea [18]. Van Kan's projection method has originally been introduced to compute the velocity field and the pressure function of the incompressible Navier-Stokes equations in a decoupled manner. Note, that (5) can be reformulated as a Laplace-Neumann problem for the pressure difference,

$$-\Delta d_t p^{m+1} = -\frac{1}{\beta k^2}\mathrm{div}\tilde{u}^{m+1}, \qquad \partial_n d_t p^{m+1}\big|_{\partial\Omega} = 0,$$

followed by an algebraic update

$$u^{m+1} = \tilde{u}^{m+1} - \beta k^2 \nabla d_t p^{m+1}.$$

This decoupling of velocity and pressure iterates is the main reason for the wide-spread use of projection methods in computational fluid flow codes.
From the analysis that is performed in [12], it is known that Van Kan's scheme is of $2nd$ order accuracy, provided initial data and the given right hand side $f = f(x,t)$ of the incompressible Navier-Stokes equations (see system (16) below) satisfy a nonlocal compatibility condition, that gives rise to improved regularity properties of the actual solution. We refer to [5] for a detailed discussion on this matter. In fact, computations that are presented in [12] show a reduction of the order of convergence in general applications from second to first order; numerical techniques have been developed in [12] to overcome this loss of accuracy for flow situations where the compatibility condition is not satisfied (*multi-component schemes*, *stretched time-grids* during the initial time interval $[0,1]$).

In order to avoid a too technical presentation, we apply Van Kan's original scheme to the algorithm (4) through (7), and refer to [12] for the mentioned stabilization techniques that allow the application of modified versions of Van Kan's method to general flows, i.e., flows that do not satisfy the compatibility condition. Therefore, we assume the actual flow $t \mapsto \big\{u(t), p(t), T(t), \{Y_i(t)\}_{i=1}^N\big\}$ to satisfy the following uniform (in time) bounds:

Postulate B: There exists a constant $C > 0$ for a time $t_{M+1} = \mathcal{O}(1)$, such that the solution $\{u, p, T, Y\}$ in (1) satisfies the following uniform bound,

$$\sup_{(0,t_{M+1}]} \Big\{ \|\nabla p_t\| + \|\Delta u_t\| + \|\Delta T_t\| + \sum_{i=1}^{N} \|\Delta Y_{i,t}\| \Big\} \leq C.$$

Remark 1.2 *We stress the fact that the assumptions made in Postulate B with respect to $\{u,p\}$ are essential for our analysis, and its validity cannot be checked a-priori for general applications. This is due to the nonlocal character of the initial compatibility condition that has to be satisfied, see [5] on this matter. In contrast to this, the assumptions made for $\{T, \{Y_i\}_{i=1}^N\}$ are only technical to simplify the study, and can be omitted in a more involved analysis, by taking into account a certain damping behavior. We refer to [7] and [12] for further details in this topic.*

As we know from the analysis of the incompressible Navier-Stokes equations, we need some technical assumptions regarding the regularity of the given problem data. In the following, we often refer to the spaces

$$\mathbf{J}_0 = \Big\{ v \in \mathbf{L}^2, \ \mathrm{div} v = 0 \text{ and } v\big|_{\partial\Omega} \cdot n = 0, \ \text{weakly} \Big\},$$

and

$$\mathbf{J}_1 = \Big\{ v \in \mathbf{H}_0^1, \ \mathrm{div} v = 0 \Big\}.$$

Now, in order to assure the existence of strong solutions, we make the following basic assumptions for our analysis, compare [5],

- *condition (A1), concerning the regularity of the domain:* The unique solution $u \in \mathbf{J}_1$ of the stationary, incompressible Stokes problem with homogeneous boundary data of Dirichlet-type (with the Stokes operator $A \equiv -P_{\mathbf{J}_0}\Delta$) is already in $\mathbf{J}_1 \cap \mathbf{H}^2$, provided the right-hand side enjoys $f \in \mathbf{L}^2$, and satisfies the following stability result,

$$\|u\|_2 \leq C\|Au\|.$$

- *condition (A2), concerning the regularity of the given data:* We suppose the following degrees of regularity for the given data $\{u_0, T_0, \{Y_i^0\}_{i=1}^N\}$,

$$u_0, T_0, \{Y_i^0\}_{i=1}^N \in \mathbf{H}_0^1 \cap \mathbf{H}^2.$$

  The given function f_0 is supposed to be affine.

- *condition (A3), concerning the existence of a strong solution:* Given $t_{M+1} > 0$, suppose that there exists a strong solution $\{u, p, T, \{Y_i\}_{i=1}^N\} \in L^\infty(0, t_{M+1}; \mathcal{X})$, with the space $\mathcal{X}$ defined below.

Note that the existence of a strong solution can only be verified locally in time, with the length of the time interval $[0, t_{M+1}]$ depending on the parameters of the given problem.

Subsequently, we will make use of the following notation: let $L^2(\Omega)$, $H^r(\Omega)$, and $H_0^r(\Omega)$, r an integer be the standard Lebesgue and Sobolev spaces, see [4] for details. These spaces are endowed with the standard scalar products and their induced norms $\|\cdot\|_r$. Further, $H^{-r}(\Omega)$ is the space that is dual to $H^r(\Omega) \cap H_0^1(\Omega)$. $L_0^2(\Omega)$ is the subspace of $L^2(\Omega)$ consisting of functions with vanishing spatial average, which is isomorphic to $L^2(\Omega)/\mathrm{R}$. The spaces of vector-valued functions will be indicated with boldface letters, for instance $\mathbf{H}_0^1 \equiv \left(H_0^1\right)^d$, for $d = 2, 3$.
Due to the evolutionary character of the problem, let $L^p(0, t_{M+1}; X)$ be the space of functions $\phi = \phi(x,t)$ s.t. holds: the map $t \mapsto \|\phi(t)\|_X^p$, $t \in [0, t_{M+1}]$ is measurable almost everywhere, and $\int_0^{t_{M+1}} \|\phi(s)\|_X^p \, ds < \infty$, for $1 \leq q < \infty$ and X a Banach space. For the case $p = \infty$, we require the property $\sup_{0 \leq s \leq t_{M+1}} \|\phi(s)\|_X < \infty$ to be satisfied. Correspondingly, we define $C(0, t_{M+1}; X)$ to be the space of functions $\phi = \phi(x,t)$, s.t. the map $t \mapsto \|\phi(t)\|_X$ is continuous, for all $t \in [0, t_{M+1}]$, and $\max_{0 \leq s \leq t_{M+1}} \|\phi(s)\|_X < \infty$. — In the following, we make frequent use of the difference quotient defined by $d_t\phi^{m+1} := \frac{1}{k}\{\phi^{m+1} - \phi^m\}$. Further, we employ the spaces $\ell^p(0, t_{M+1}; X)$, for $1 \leq p < \infty$, which is the space of functions $\{\phi^{m+1}\}_{m=0}^M$, with bounded norm $\left(k \sum_{m=0}^M \|\phi^{m+1}\|_X^p\right)^{1/p}$, for the time-step $k = t_{m+1} - t_m$. For the case $p = \infty$, functions $\{\phi^{m+1}\}_{m=0}^M$ need to satisfy $\max_{0 \leq m \leq M} \|\phi^{m+1}\|_X < \infty$. Finally, we employ the notations $\tau(s) \equiv \min\{1, s\}$ and $\tau_{m+1} \equiv \min\{1, t_{m+1}\}$. In the following, we make frequent use of a shorthand notation for algebraic combinations of subsequent iterates, $\overline{\phi}^{m+1/2} := \frac{1}{2}\{\phi^{m+1} + \phi^m\}$, and $\overline{\overline{\phi}}^m := \frac{1}{2}\{\overline{\phi}^{m+1/2} + \overline{\phi}^{m-1/2}\}$.

The analysis of the splitting scheme (4) through (7) is split in several steps, each of it dealing with different error effects that arise from the violation of the implicit coupling of the involved quantities. We refer to section 2 for a presentation of the diverse auxiliary problems that are devoted to the investigation of the different error impacts. We have to quantify the effects of the projection scheme approach as well as those of the decoupling of the remaining equations. We mention, that the subsequent study heavily relies on results that have been obtained for the Van Kan scheme, see [12], applied to the incompressible Stokes equations. A summary and extension of these results to the incompressible Navier-Stokes equations will be given in section 3.

The analysis of scheme (4) through (7) is split in an investigation of its stability and approximation properties. The following shorthand notation will be used throughout the work: Given the quadruple $\{a_i^{m+1}\}_{i=1}^4 \in \mathcal{X}$ with

$$\mathcal{X} := \left(\mathbf{H_0^1} \cap \mathbf{H^2}\right) \times H^1/\mathrm{R} \times \left(H_0^1 \cap H^2\right) \times \prod_{i=1}^N \left(H_0^1 \cap H^2\right).$$

We then say that

1. the quadruple $\{a_i^{m+1}\}_{i=1}^4 \in \mathcal{X}$ satisfies *Property (P1)*, provided the following a-priori statements are satisfied, for $i \in \{1,3,4\}$,

$$\max_{1\le m\le M}\Big\{\|d_t a_i^{m+1}\|_1 + \|d_t^2 a_i^{m+1}\| + \|\Delta \overline{a}_i^{m+1/2}\| + \|\Delta d_t \overline{a}_i^{m+1/2}\| + \|\nabla d_t \overline{a}_2^{m+1/2}\|\Big\}$$
$$+ \Big(k\sum_{m=1}^{M}\|\nabla d_t^2 \overline{a}_i^{m+1/2}\|^2\Big)^{1/2} + \Big(k^2\sum_{m=1}^{M}\|\nabla d_t^2 \overline{a}_2^{m+1/2}\|^2\Big)^{1/2} \le C\big(1+\log\frac{1}{k}\big).$$

2. The quadruple $\{a_i^{m+1}\}_{i=1}^4 \in \mathcal{X}$ satisfies *Property* $(P2)_\ell$, for $\ell = 0,1$, if the following approximation properties are satisfied:

$$\max_{1\le m\le M}\Big\{\tau_{m-1/2}^{\ell/2}\|u(t_{m+1/2}) - \overline{a}_1^{m+1/2}\| + \|T(t_{m+1/2}) - \overline{a}_3^{m+1/2}\| + \|Y(t_{m+1/2}) - \overline{a}_4^{m+1/2}\|$$
$$+ k\Big(\|u(t_{m+1/2}) - \overline{\overline{a}}_1^{m}\|_1 + \tau_{m-1/2}^{\ell/2}\|p(t_{m+1/2}) - \overline{\overline{a}}_2^{m}\|$$
$$+ \|T(t_{m+1/2}) - \overline{\overline{a}}_3^{m}\|_1 + \|Y(t_{m+1/2}) - \overline{\overline{a}}_4^{m}\|_1\Big)\Big\} \le Ck^2\big(1+\log\frac{1}{k}\big),$$

where, here and in the following, $Y := \{Y_i\}_{i=1}^N$ and $Y^{m+1} := \{Y_i^{m+1}\}_{i=1}^N$. — We are now in a position to formulate the main result that states optimal convergence behavior for the solution of (4) through (7).

Theorem 1.1 *Let the initial pressure function $p^0 \in H^1/\mathrm{R}$ satisfy the bound $\|p^0 - p(0)\|_1 \le Ck$. Further, suppose the basic assumptions (A1), (A2), (A3) to be valid and additionally Postulate B. Then, the solution $\{u^{m+1}, p^{m+1}, T^{m+1}, Y^{m+1}\} \in \mathcal{X}$ of scheme (4) through (7) with its modification for the case $m = 0$ given in Remark 1.1 satisfies property $(P2)_1$, for a sufficiently small time-step $k \le k_0(t_{M+1})$.*

As we already know from [13], the character of the time-splitting scheme (4) through (7) as a projection method is the reason for slightly suboptimal convergence results for gradients of temperature distribution and gradients of mass fraction functions. The same phenomenon can be observed for the present scheme.

Corollary 1.1 *Suppose the conditions of Theorem 1.1 to be valid. Then, the approximates $\{T^{m+1}, \{Y_i^{m+1}\}_{i=1}^N\}$ satisfy the improved estimates*

1. *in two space dimensions (i.e., $d = 2$), for all $\gamma > 0$, and $\lim_{\gamma\to 0} C_\gamma = \infty$:*

$$\max_{1\le m\le M}\sqrt{\tau_{m+1}}\Big\{\|T(t_{m+1/2}) - \overline{\overline{a}}_3^{m}\|_1 + \|Y(t_{m+1/2}) - \overline{\overline{a}}_4^{m}\|_1\Big\} \le C_\gamma k^{2-\gamma},$$

2. *in three space dimensions (i.e., $d = 3$):*

$$\max_{1\le m\le M}\sqrt{\tau_{m+1}}\Big\{\|T(t_{m+1/2}) - \overline{\overline{a}}_3^{m}\|_1 + \|Y(t_{m+1/2}) - \overline{\overline{a}}_4^{m}\|_1\Big\} \le Ck^{3/2}.$$

2 Outline of the Proof of Theorem 1.1. For the understanding of the ongoing error mechanisms in the numerical scheme (4) through (7), we will propose several auxiliary problems in the following that will be the subject of further investigation in the subsequent sections. Each of the presented auxiliary problems is formulated to identify and analyze one of the present error sources that are inherent to the systems (4) through (7). It is our aim to verify the properties (P1) and $(P2)_0$ for each single problem.

In the following formulations, we omit to write down the boundary conditions and the initial data if they coincide with those given for the corresponding quantities in (4) through (7).

1st auxiliary problem: This problem is proposed to study the impact of implicit time-discretization effects.
For the initial data $\{u^0, T^0, Y^0\}$ given in (1), determine iterates $\{u_a^{m+1}, p_a^{m+1}, T_a^{m+1}, Y_a^{m+1}\} \in \mathcal{X}$ successively as the solution of

$$\begin{aligned}
&d_t u_a^{m+1} - \Delta \overline{u}_a^{m+1/2} + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big]\overline{u}_a^{m+1/2} + \nabla \overline{p}_a^{m+1/2} = f_0(\overline{T}_a^{m+1/2}),\\
&\mathrm{div} u_a^{m+1} = 0,\\
&d_t T_a^{m+1} - \Delta \overline{T}_a^{m+1/2} + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big]\overline{T}_a^{m+1/2} = -\sum_{i=1}^{N} h_i W_i\big(\overline{Y}_a^{m+1/2}, \overline{T}_a^{m+1/2}\big),\\
&d_t Y_{a,i}^{m+1} - \Delta \overline{Y}_{a,i}^{m+1/2} + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big]\overline{Y}_{a,i}^{m+1/2} = W_i\big(\overline{Y}_a^{m+1/2}, \overline{T}_a^{m+1/2}\big).
\end{aligned} \tag{10}$$

The result of the investigation is given in Lemma 5.1.

2nd auxiliary problem: In this auxiliary problem, we analyze the explicit coupling of the temperature phenomena in the momentum equation.
For the initial data $\{u^0, \{T^\ell\}_{\ell=-1}^0, Y^0\}$ given in (1) and satisfying the approximation property (8) for $\ell = -1$, determine iterates $\{u_b^{m+1}, p_b^{m+1}, T_b^{m+1}, Y_b^{m+1}\} \in \mathcal{X}$ being the solution of

$$\begin{aligned}
&d_t u_b^{m+1} - \Delta \overline{u}_b^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big]\overline{u}_b^{m+1/2} + \nabla \overline{p}_b^{m+1/2} = f_0\big(\tfrac{3}{2}T_b^m - \tfrac{1}{2}T_b^{m-1}\big),\\
&\mathrm{div} u_b^{m+1} = 0,\\
&d_t T_b^{m+1} - \Delta \overline{T}_b^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big]\overline{T}_b^{m+1/2} = -\sum_{i=1}^{N} h_i W_i\big(\overline{Y}_b^{m+1/2}, \overline{T}_b^{m+1/2}\big),\\
&d_t Y_{b,i}^{m+1} - \Delta \overline{Y}_{b,i}^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big]\overline{Y}_{b,i}^{m+1/2} = W_i\big(\overline{Y}_b^{m+1/2}, \overline{T}_b^{m+1/2}\big).
\end{aligned} \tag{11}$$

We refer to Lemma 5.2 for corresponding statements of convergence and stability.

3rd auxiliary problem: The investigation of the influence of an "explicit treatment" of the convective part is subject to the following auxiliary problem:
For initial data $\{u^\ell, T^\ell, Y^\ell\}_{\ell=-1}^0$ given in (1) and functions satisfying the approximation property (8) for $\ell = -1$, determine iterates $\{u_c^{m+1}, p_c^{m+1}, T_c^{m+1}, Y_c^{m+1}\} \in \mathcal{X}$ that are the

solution of

$$
\begin{aligned}
& d_t u_c^{m+1} - \Delta \overline{u}_c^{m+1/2} + \big[\{\frac{3}{2}u_c^m - \frac{1}{2}u_c^{m-1}\}\cdot\nabla\big]\overline{u}_c^{m+1/2} + \nabla \overline{p}_c^{m+1/2} = f_0(\frac{3}{2}T_c^m - \frac{1}{2}T_c^{m-1}),\\
& \mathrm{div} u_c^{m+1} = 0,\\
& d_t T_c^{m+1} - \Delta \overline{T}_c^{m+1/2} + \big[\{\frac{3}{2}u_c^m - \frac{1}{2}u_c^{m-1}\}\cdot\nabla\big]\overline{T}_c^{m+1/2} = -\sum_{i=1}^N h_i W_i\big(\overline{Y}_c^{m+1/2}, \overline{T}_c^{m+1/2}\big),\\
& d_t Y_{c,i}^{m+1} - \Delta \overline{Y}_{c,i}^{m+1/2} + \big[\{\frac{3}{2}u_c^m - \frac{1}{2}u_c^{m-1}\}\cdot\nabla\big]\overline{Y}_{c,i}^{m+1/2} = W_i\big(\overline{Y}_c^{m+1/2}, \overline{T}_c^{m+1/2}\big).
\end{aligned}
\tag{12}
$$

The results of this analysis are summarized in Lemma 5.3.

4th auxiliary problem: This auxiliary problem deals with the decoupling of the chemical part, i.e., the temperature and the concentrations. — For the initial data $\{u^\ell, T^\ell, Y^\ell\}_{\ell=-1}^0$ given in (1) and values satisfying the approximation property (8) for $\ell = -1$, determine iterates $\{u_d^{m+1}, p_d^{m+1}, T_d^{m+1}, Y_d^{m+1}\} \in \mathcal{X}$ that are the solution of

$$
\begin{aligned}
& d_t u_d^{m+1} - \Delta \overline{u}_d^{m+1/2} + \big[\{\frac{3}{2}u_d^m - \frac{1}{2}u_d^{m-1}\}\cdot\nabla\big]\overline{u}_d^{m+1/2} + \nabla \overline{p}_d^{m+1/2} = f_0(\frac{3}{2}T_d^m - \frac{1}{2}T_d^{m-1}),\\
& \mathrm{div} u_d^{m+1} = 0,\\
& d_t T_d^{m+1} - \Delta \overline{T}_d^{m+1/2} + \big[\{\frac{3}{2}u_d^m - \frac{1}{2}u_d^{m-1}\}\cdot\nabla\big]\overline{T}_d^{m+1/2}\\
& \qquad\qquad = -\sum_{i=1}^N h_i W_i\big(\frac{3}{2}Y_d^m - \frac{1}{2}Y_d^{m-1}, \overline{T}_d^{m+1/2}\big),\\
& d_t Y_{d,i}^{m+1} - \Delta \overline{Y}_{d,i}^{m+1/2} + \big[\{\frac{3}{2}u_d^m - \frac{1}{2}u_d^{m-1}\}\cdot\nabla\big]\overline{Y}_{d,i}^{m+1/2} = W_i\big(\overline{Y}_d^{m+1/2}, \frac{3}{2}T_d^m - \frac{1}{2}T_d^{m-1}\big).
\end{aligned}
\tag{13}
$$

We refer to Lemma 5.4 for a summary of the related analysis.

5th auxiliary problem: In order to study the impact of the projection scheme of the Van Kan scheme, we deal with the following problem:
For the initial data $\{u^\ell, T^\ell, Y^\ell\}_{\ell=-1}^0$ given in (1) and satisfying the approximation property (8) for $\ell = -1$, and p^0,s.t. $\|p^0 - p(0)\|_1 \le Ck$, further for the given iterates $\{T_d^{m+1}, Y_d^{m+1}\}_{m=0}^M$, determine iterates $\{u_e^{m+1}, p_e^{m+1}\} \in \mathbf{H}_0^1(\Omega) \times H^1/\mathrm{R}$ that are the solution of

$$
\begin{aligned}
& d_t u_e^{m+1} - \Delta \overline{u}_e^{m+1/2} + \big[P_{\mathbf{J}_0}\{\frac{3}{2}u_e^m - \frac{1}{2}u_e^{m-1}\}\cdot\nabla\,\big]\overline{u}_e^{m+1/2} + \frac{3}{2}\nabla p_e^m - \frac{1}{2}\nabla p_e^{m-1}\\
& \qquad\qquad = f_0(\frac{3}{2}T_d^m - \frac{1}{2}T_d^{m-1}),\\
& \mathrm{div} u_e^{m+1} - \beta k^2 \Delta d_t p_e^{m+1} = 0, \qquad \partial_n d_t p_e^{m+1}\big|_{\partial\Omega} = 0, \qquad \beta > \frac{1}{2}.
\end{aligned}
\tag{14}
$$

Corresponding statements on the solution behavior will be given in Lemma 5.5.

6th auxiliary problem: We will finally study the recoupling of the "flow part" with the "chemical part".
For the initial data $\{u^\ell, T^\ell, Y^\ell\}_{\ell=-1}^0$ given in (1) and satisfying the approximation property (8) for $\ell=-1$, and p^0,s.t. $\|p^0-p(0)\|_1 \leq Ck$, determine iterates $\{u_f^{m+1}, p_f^{m+1}, T_f^{m+1}, Y_f^{m+1}\} \in \mathcal{X}$ being the solution of

$$
\begin{aligned}
& d_t u_f^{m+1} - \Delta \overline{u}_f^{m+1/2} + \left[P_{\mathbf{J}_0}\{\tfrac{3}{2}u_f^m - \tfrac{1}{2}u_f^{m-1}\}\cdot\nabla\right]\overline{u}_f^{m+1/2} + \frac{3}{2}\nabla p_f^m - \frac{1}{2}\nabla p_f^{m-1} \\
&\qquad\qquad\qquad = f_0\big(\tfrac{3}{2}T_f^m - \tfrac{1}{2}T_f^{m-1}\big), \\
& \mathrm{div} u_f^{m+1} - \beta k^2 \Delta d_t p_f^{m+1} = 0, \qquad \partial_n d_t p_f^{m+1}|_{\partial\Omega} = 0, \qquad \beta > \frac{1}{2}, \\
& d_t T_f^{m+1} - \Delta \overline{T}_f^{m+1/2} + \left[P_{\mathbf{J}_0}\{\tfrac{3}{2}u_f^m - \tfrac{1}{2}u_f^{m-1}\}\cdot\nabla\right]\overline{T}_f^{m+1/2} \\
&\qquad\qquad\qquad = -\sum_{i=1}^N h_i W_i\big(\tfrac{3}{2}Y_f^m - \tfrac{1}{2}Y_{f,i}^{m-1}, \overline{T}_f^{m+1/2}\big), \\
& d_t Y_{f,i}^{m+1} - \Delta \overline{Y}_{f,i}^{m+1/2} + \left[P_{\mathbf{J}_0}\{\tfrac{3}{2}u_f^m - \tfrac{1}{2}u_f^{m-1}\}\cdot\nabla\right]\overline{Y}_{f,i}^{m+1/2} \\
&\qquad\qquad\qquad = W_i\big(\overline{Y}_f^{m+1/2}, \tfrac{3}{2}T_f^m - \tfrac{1}{2}T_f^{m-1}\big).
\end{aligned} \tag{15}
$$

Lemma 5.6 gives a summary of the results of the corresponding analysis.

The combination of the Lemmata 5.1 through 5.6 then provides the proof of Theorem 1.1.

3 The projection method of Van Kan. According to the strategy of Chorin in his projection method, see [2, 3], Van Kan's method decouples the computation of velocity field and pressure function in each iteration step, see [18]. For the latter method, a second order discretization of the arising terms is applied in order to increase the accuracy of the calculated approximation, compared to the Chorin ansatz.
In this section, let us recall the analysis of the Van Kan scheme for the incompressible Navier-Stokes equations,

$$
\begin{aligned}
& u_t - \nu\Delta u + (u\cdot\nabla)u + \nabla p = f, \\
& \mathrm{div} u = 0,
\end{aligned} \tag{16}
$$

together with the initial and boundary data,

$$
u(0) = u_0 \in \mathbf{J}_1 \cap \mathbf{H}^2, \qquad u\big|_{\partial\Omega} = 0. \tag{17}
$$

For the subsequent analysis, we assume $\Omega \subset \mathrm{R}^3$ to be a bounded domain where an incompressible fluid flow with constant viscosity $\nu > 0$ is in, driven by an external force $f = f(x,t) \in C^2(0, t_{M+1}; \mathbf{L}^2)$. — Then, the Van Kan projection method reads as follows,

1. Start with approximate initial guesses $u^0 = u_0$ and $p^0 \approx p(0)$.

2. For $m \geq 0$, find $\tilde{u}^{m+1}$ that solves

$$
\begin{aligned}
&\frac{1}{k}\{\tilde{u}^{m+1} - u^m\} - \nu\Delta\overline{\tilde{u}}^{m+1/2} + [\{\frac{3}{2}u^m - \frac{1}{2}u^{m-1}\} \cdot \nabla)]\overline{\tilde{u}}^{m+1/2} \\
(18) \qquad &\qquad + (\frac{3}{2} - \beta)\nabla p^m + (\beta - \frac{1}{2})\nabla p^{m-1} = \overline{f}^{m+1/2}, \qquad \beta > \frac{1}{2}, \\
&\tilde{u}^{m+1}\big|_{\partial\Omega} = 0.
\end{aligned}
$$

3. Provided with $\tilde{u}^{m+1}$, determine the tuple $\{u^{m+1}, p^{m+1}\}$ as the solution of

$$
\begin{aligned}
(19) \qquad &\frac{1}{k}\{u^{m+1} - \tilde{u}^{m+1}\} + \beta\nabla\{p^{m+1} - p^m\} = 0, \qquad \beta > \frac{1}{2}, \\
&\mathrm{div} u^{m+1} = 0, \qquad u^{m+1}\big|_{\partial\Omega} \cdot n = 0.
\end{aligned}
$$

The latter part can be reformulated as a Laplace-Neumann problem for the pressure difference,

$$
-\Delta d_t p^{m+1} = -\frac{1}{\beta k^2}\mathrm{div}\tilde{u}^{m+1}, \qquad \partial_n d_t p^{m+1}\big|_{\partial\Omega} = 0.
$$

For a corresponding discussion on lacking initial data in the first step (i.e., $m = 0$), we refer to Remark 1.1.
Owing to this reformulation, the algorithm of Van Kan assembles from solving a Burger's type equation for the auxiliary velocity field, followed by a problem for the pressure difference. From these two functions, $u^{m+1} \in \mathbf{J}_0$ can be computed through an algebraic update.

The Van Kan scheme has been analyzed in [12]. The key observation for its analysis is the reformulation as a semi-explicit pressure-correction method: if we shift the index in (19) by -1 and add the resulting identity to the first one in (18), we arrive at

$$
\begin{aligned}
&d_t\tilde{u}^{m+1} - \nu\Delta\overline{\tilde{u}}^{m+1/2} + \big[P_{\mathbf{J}_0}\frac{1}{2}\{3\tilde{u}^m - \tilde{u}^{m-1}\} \cdot \nabla\big]\overline{\tilde{u}}^{m+1/2} \\
&\qquad\qquad + \frac{1}{2}\{3\nabla p^m - \nabla p^{m-1}\} = \overline{f}^{m+1/2}, \\
(20) \qquad &\mathrm{div}\tilde{u}^{m+1} - \beta k^2 \Delta d_t p^{m+1} = 0, \qquad \beta > \frac{1}{2}, \\
&\tilde{u}^{m+1}\big|_{\partial\Omega} = 0, \qquad \partial_n d_t p^{m+1}\big|_{\partial\Omega} = 0, \\
&u^0 = u_0, \qquad \|u^{-1} - u(-k)\| + k\|p^{-1} - p(-k)\|_1 \leq Ck^2.
\end{aligned}
$$

The analysis of this system is made difficult through a series of inherent error sources: in the corresponding investigation, we have to qualify the effects of (implicit/explicit) time-discretization, the explicit evaluation of the leading term in the convective part, and the impact of employing the pressure function in an explicit way in the momentum equation.

Further, the optimal control of the perturbed incompressibility constraint by means of an *evolutionary* term is another major part of the analysis. Note that the evolutionary term also enforces the prescription of accurate initial data for the pressure function. Finally, the prescription of "unphysical" homogeneous data for the boundary data of Neumann type implies a singular perturbation character of the system.

As it turns out from the analysis for the Stokes equations in [12], optimal approximation properties for the Van Kan scheme can only be assured provided the continuous Navier-Stokes flow satisfies certain regularity properties that are given in Postulate $\tilde{B}$, see below. The necessity of this requirement is affirmed through a computational counterexample, given in [12].

The goal of this section is to extend the error and stability analysis for Van Kan's scheme for the Stokes case as it is given in [12] to the Navier-Stokes equations (16). Therefore, we formulate again a postulate to be satisfied by the solution of (16).

Postulate $\tilde{B}$: The solution of the incompressible Navier-Stokes equations (16) satisfies the following a-priori bound,

$$\sup_{(0,t_{M+1}]} \Big\{ \|\Delta u_t\| + \|\nabla p_t\| \Big\} \leq C.$$

The following result has been proven in [12].

Lemma 3.1 *Let $\{\tilde{u}^{m+1}, p^{m+1}\}$ be the solution of the Van Kan scheme in its application for the Stokes equation, with the first step ($m = 0$) modified analogous to Remark 1.1. We assume (A1), (A2) to be satisfied and the exact solution $\{u(t_{m+1}), p(t_{m+1})\}$ to enjoy the properties given in Postulate $\tilde{B}$. Further, suppose the initial iterates to satisfy*

$$\|u(0) - u^0\| + k\|p(0) - p^0\|_1 \leq Ck^2,$$

and take $k < 1$. Then, the following statements hold true, with a constant C that is only depending on the given data of the problem,

$$\max_{1\leq m\leq M} \Big\{ \sqrt{\tau_{m-1/2}}\|u(t_{m+1/2}) - \overline{\overline{\tilde{u}}}^{m+1/2}\| + k\|u(t_{m+1/2}) - \overline{\overline{\tilde{u}}}^{m}\|_1 \Big\}$$
$$+ \Big(k \sum_{m=0}^{M} \|u(t_{m+1/2}) - \overline{\overline{\tilde{u}}}^{m+1/2}\|^2 \Big)^{1/2} \leq Ck^2\big(1 + \log\frac{1}{k}\big),$$
$$\max_{1\leq m\leq M} \Big\{ \sqrt{\tau_{m+1/2}}\|p(t_{m+1/2}) - \overline{\overline{p}}^{m}\| \Big\} \leq Ck\big(1 + \log\frac{1}{k}\big).$$

Remark 3.1 *A corresponding result can also be obtained for the choice $\beta = \frac{1}{2}$, see [12].*

The next result — an extension of Lemma 3.1 to the Navier-Stokes equations (16) — is a basic ingredient for the study of the algorithm (4) through (7), but it is also of its own interest.

Theorem 3.1 *Let $\{\tilde{u}^{m+1}, p^{m+1}\}$ be the solution of the Van Kan scheme (18),(19), with a modification for the first step ($m = 0$) analogous to Remark 1.1. Suppose (A1),(A2),(A3) to be satisfied for the data and solution of system (16), for a given time $t_{M+1} > 0$. Additionally, we assume the exact solution $\{u(t_{m+1}), p(t_{m+1})\}$ to enjoy the properties given in Postulate $\tilde{B}$. Suppose the initial iterates to satisfy*

$$\|u(0) - u^0\| + k\|p(0) - p^0\|_1 \le Ck^2,$$

for $k \le k_0 < 1$, with $k_0 = k_0(t_{M+1})$ sufficiently small. Then, the following statements hold true, with a constant C that is only depending on the given data of the problem,

$$\max_{1\le m\le M}\Big\{\sqrt{\tau_{m-1/2}}\|u(t_{m+1/2}) - \overline{\tilde{u}}^{m+1/2}\| + k\|u(t_{m+1/2}) - \overline{\overline{\tilde{u}}}^{m}\|_1\Big\}$$
$$+ \Big(k\sum_{m=0}^{M}\|u(t_{m+1/2}) - \overline{\tilde{u}}^{m+1/2}\|^2\Big)^{1/2} \le Ck^2\big(1 + \log\frac{1}{k}\big),$$
$$\max_{1\le m\le M}\Big\{\sqrt{\tau_{m+1/2}}\|p(t_{m+1/2}) - \overline{\overline{p}}^{m}\|\Big\} \le Ck\big(1 + \log\frac{1}{k}\big).$$

Proof. The verification of this theorem is split into several steps to benefit from Lemma 3.1.

1st step: The pressure correction formulation of the Stokes equations
Denote by $\{u^{m+1}\}_{m=0}^{M}$ the iterates of a discretized version of (16), as it is given in (11) (for a given right hand side $f = f_0$). Then, they satisfy the properties (P1) — see Lemma 5.2 below. Let now $\{v_\varepsilon^{m+1}, q_\varepsilon^{m+1}\} \in \mathbf{H}_0^1 \times H^1/\mathrm{R}R$ be given as the solution of the following system of equations, by taking $\varepsilon = \mathcal{O}(k^2)$,

$$\begin{aligned} & d_t v_\varepsilon^{m+1} - \Delta\overline{v}_\varepsilon^{m+1/2} + \nabla\overline{q}_\varepsilon^{m+1/2} = \mathcal{F}^{m+1}, \\ & \mathrm{div} v_\varepsilon^{m+1} - \varepsilon\Delta d_t q_\varepsilon^{m+1} = 0, \\ & v_\varepsilon^{m+1}\big|_{\partial\Omega} = 0, \qquad \partial_n d_t q_\varepsilon^{m+1}\big|_{\partial\Omega} = 0, \\ & v_\varepsilon^0 = u_0, \qquad \|q_\varepsilon^0 - p(0)\|_1 \le C\sqrt{\varepsilon}, \end{aligned} \tag{21}$$

with

$$\mathcal{F}^{m+1} \equiv \overline{f}^{m+1/2} - \big[\{\frac{3}{2}u^m - \frac{1}{2}u^{m-1}\}\cdot\nabla\big]\overline{u}^{m+1/2}. \tag{22}$$

The following error estimate has been verified in [12] (see Lemma 7.4 and formula (7.42) there),

$$\begin{aligned} & \max_{0\le m\le M}\sqrt{\tau_{m+1/2}}\Big\{\|u(t_{m+1/2}) - \overline{v}_\varepsilon^{m+1/2}\| + \sqrt{\varepsilon}\big\{\|u(t_{m+1/2}) - \overline{\overline{v}}_\varepsilon^{m}\|_1 \\ & + \|p(t_{m+1/2}) - \overline{\overline{q}}_\varepsilon^{m}\|\big\}\Big\} + \Big(k\sum_{m=0}^{M}\|u(t_{m+1/2}) - \overline{v}_\varepsilon^{m+1/2}\|^2\Big)^{1/2} \le C\varepsilon\big(1 + \log\frac{1}{\varepsilon}\big). \end{aligned} \tag{23}$$

This result is valid, since the right hand side of the first equation in (21) can be controlled through application of the a-priori results (P1) that hold for the iterates $\{u^{m+1}\}_{m=0}^{M}$ (see also Lemma 5.2). In particular, $\mathcal{F}^{m+1}$ and its various discrete time-derivatives can be bounded as follows, using elementary energy arguments, [2]

$$\max_{0\le m\le M}\Big\{\|\mathcal{F}^{m+1}\| + \|d_t\mathcal{F}^{m+1}\|\Big\} + \Big(k\sum_{m=1}^{M}\|d_t^2\mathcal{F}^{m+1}\|^2\Big)^{1/2} \le C.$$

Moreover, this argument allows to take over the following a-priori bounds from the analysis of [12] for the solution $\{v_\varepsilon^{m+1}, q_\varepsilon^{m+1}\}$ of problem (21),

$$\begin{aligned}\max_{1\le m\le M}\Big\{&\|d_t v_\varepsilon^{m+1}\|_1^2 + \|\Delta d_t\overline{v}_\varepsilon^{m+1/2}\|^2 + \|\nabla d_t\overline{q}_\varepsilon^{m+1/2}\|^2 + \|d_t^2 v_\varepsilon^{m+1}\|^2\\ &+ k\sum_{m=1}\|\nabla d_t^2\overline{v}_\varepsilon^{m+1/2}\|^2 + k^2\sum_{m=1}\|\nabla d_t^2\overline{q}_\varepsilon^{m+1/2}\|^2\Big\} \le C\big(1+\log\frac{1}{k}\big).\end{aligned} \tag{24}$$

This inequality is proven in [12], pp. 161, apart from the fourth term. The validity of this result for the fourth term follows now from a corresponding argument that is applied to obtain formula (7.43) in [12].

2nd step: The pressure correction formulation of the Navier-Stokes equations
In order to estimate the difference in the computed iterates $\{u^{m+1}\}_{m=0}^{M}$ that arise from a discretization of (16) which corresponds to the one given in (11) and the iterates of its pressure-corrected version, given by

$$\begin{aligned}&d_t u_\varepsilon^{m+1} - \Delta\overline{u}_\varepsilon^{m+1/2} + \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_\varepsilon^m - \frac{1}{2}u_\varepsilon^{m-1}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m+1/2} + \nabla\overline{p}_\varepsilon^{m+1/2} = \overline{f}^{m+1/2},\\ &\mathrm{div}u_\varepsilon^{m+1} - \varepsilon\Delta d_t p_\varepsilon^{m+1} = 0, \qquad \text{for } \varepsilon = \mathcal{O}(k^2),\\ &u_\varepsilon^{m+1}\big|_{\partial\Omega} = 0, \qquad \partial_n d_t p_\varepsilon^{m+1}\big|_{\partial\Omega} = 0,\\ &u_\varepsilon^0 = u_0, \qquad \|p_\varepsilon^0 - p(0)\|_1 \le C\sqrt{\varepsilon},\end{aligned} \tag{25}$$

it is now sufficient to study the following error equations, with $\xi^{m+1} := u_\varepsilon^{m+1} - v_\varepsilon^{m+1}$, and $\chi^{m+1} := p_\varepsilon^{m+1} - q_\varepsilon^{m+1}$,

$$\begin{aligned}&d_t\xi^{m+1} - \Delta\overline{\xi}^{m+1/2} + \nabla\overline{\chi}^{m+1/2} = \mathcal{G}^{m+1}(u,u_\varepsilon),\\ &\mathrm{div}\xi^{m+1} - \varepsilon\Delta d_t\chi^{m+1} = 0,\\ &\xi^{m+1}\big|_{\partial\Omega} = 0, \qquad \partial_n d_t\chi^{m+1}\big|_{\partial\Omega} = 0,\\ &\xi^0 = 0, \qquad \chi^0 = 0,\end{aligned} \tag{26}$$

with

$$\mathcal{G}^{m+1}(u,u_\varepsilon) := \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u^m - \frac{1}{2}u^{m-1}\}\cdot\nabla\big]\overline{u}^{m+1/2} - \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_\varepsilon^m - \frac{1}{2}u_\varepsilon^{m-1}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m+1/2}. \tag{27}$$

[2]In fact, the logarithmic factor is not necessary here.

This term can be reformulated in terms of errors $\{\xi^{m+\ell}\}_{\ell=-1}^{1}$, and $\{u^{m+\ell} - v_\varepsilon^{m+\ell}\}_{\ell=-1}^{1}$, and the functions $\{u^{m+\ell}\}_{\ell=-1}^{1}$,

$$
\begin{aligned}
\mathcal{G}^{m+1}(u,u_\varepsilon) := & \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3(u^m - v_\varepsilon)^m - (u^{m-1} - v_\varepsilon^{m-1})\big\}\cdot\nabla\Big]\overline{u}^{m+1/2} \\
& - \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3\xi^m - \xi^{m-1}\big\}\cdot\nabla\Big]\overline{u}^{m+1/2} - \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3\xi^m - \xi^{m-1}\big\}\cdot\nabla\Big]\overline{\xi}^{m+1/2} \\
& - \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3\xi^m - \xi^{m-1}\big\}\cdot\nabla\Big](\overline{v}_\varepsilon^{m+1/2} - \overline{u}^{m+1/2}) - \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3v_\varepsilon^m - v_\varepsilon^{m-1}\big\}\cdot\nabla\Big]\overline{\xi}^{m+1/2} \\
& - \frac{1}{2}\Big[\mathrm{P}_{\mathbf{J}_0}\big\{3v_\varepsilon^m - v_\varepsilon^{m-1}\big\}\cdot\nabla\Big](\overline{v}_\varepsilon^{m+1/2} - \overline{u}^{m+1/2}).
\end{aligned}
\tag{28}
$$

The latter step now allows optimal error statements in this context, if we test (26) with $\overline{\xi}^{m+1/2}$ in the first equation,

$$
\begin{aligned}
& d_t\|\xi^{m+1}\|^2 + \|\nabla\overline{\xi}^{m+1/2}\|^2 + \varepsilon d_t\|\nabla\overline{\chi}^{m+1/2}\|^2 \\
& \qquad + \varepsilon k\|\nabla d_t\overline{\chi}^{m+1/2}\|^2 \le C\big|\big(\mathcal{G}^{m+1}(u,u_\varepsilon),\xi^{m+1/2}\big)\big|.
\end{aligned}
\tag{29}
$$

In the following, we make frequent use of the identity

$$
\frac{1}{2}\{3\phi^m - \phi^{m-1}\} = \overline{\phi}^{m+1/2} - \frac{1}{2}k^2 d_t^2\phi^{m+1}.
\tag{30}
$$

This identity shall be used in the first part of the first term of $\mathcal{G}^{m+1}(u,u_\varepsilon)$ to express the error in terms of averaged functions that can be controlled by (23). The arising further term $k^2 d_t^2\{u^{m+1} - v_\varepsilon^{m+1}\}$ can be bounded in $\ell^\infty(0,t_{M+1};\mathbf{L}^2)$ by $Ck^2(1+\log\frac{1}{k})$, with C a constant that only depends on the given data of the problem, owing to (24), and a stability result corresponding to the one given by Lemma 5.3.

The second term in (28) does not involve further difficulties in the subsequent estimate, and the same holds for the third and fourth term. As far as the last term in (28) is concerned, we may again benefit from (30) to reformulate the first part. It can then be controlled by means of the approximation and stability results (23), (24), and Lemma 5.3 at hand. The last but one term in (28) drops out, when we consider the tested form $(\mathcal{G}^{m+1}(u,u_\varepsilon),\overline{\xi}^{m+1/2})$, because of the skew-symmetricity rule. — From these arguments, we end up with

$$
\begin{aligned}
& \|\xi^{M+1}\|^2 + k\sum_{m=1}^{M}\|\nabla\overline{\xi}^{m+1/2}\|^2 + \varepsilon\|\nabla\overline{\chi}^{M+1/2}\|^2 \\
& \qquad + \varepsilon k^2\sum_{m=1}^{M}\|\nabla d_t\overline{\chi}^{m+1/2}\|^2 \le Ck^4\big(1+\log\frac{1}{k}\big).
\end{aligned}
\tag{31}
$$

Second, the verification of the subsequent a-priori results now follows from easy considerations and energy arguments. Note, that we can therefore benefit from the approximation features of $\mathcal{G}^{m+1}(u, u_\varepsilon)$ discussed above.

$$\begin{aligned}\max_{1\le m\le M}\Big\{\|d_t u_\varepsilon^{m+1}\|^2 + \|\Delta d_t \overline{u}_\varepsilon^{m+1/2}\|^2 + \|\nabla d_t \overline{p}_\varepsilon^{m+1/2}\|^2 + \|d_t^2 u_\varepsilon^{m+1}\|^2\Big\}\\ + k\sum_{m=1}^{M}\|\nabla d_t^2 \overline{u}_\varepsilon^{m+1/2}\|^2 + k^2\sum_{m=1}^{M}\|\nabla d_t^2 \overline{p}_\varepsilon^{m+1/2}\|^2 \le C\big(1+\log\frac{1}{k}\big).\end{aligned} \tag{32}$$

We omit the detailed, technical verification of this result.

3rd step: Transition to the projection step of Van Kan
Finally, we have to control the errors caused by the transition from the pressure-correction formulation of the Navier-Stokes equations (25) to the Van Kan scheme (18),(19), as well as the stability of its solution $\{u_{VK}^{m+1}, p_{VK}^{m+1}\}$. For this purpose, we introduce error quantities

$$e^{m+1} := u_\varepsilon^{m+1} - u_{VK}^{m+1}, \qquad \eta^{m+1} := p_\varepsilon^{m+1} - p_{VK}^{m+1}.$$

Then, setting $\varepsilon = \beta k^2$, for $\beta > \frac{1}{2}$, the error identities read as follows, using the abbreviative notation that was introduced in (27),

$$\begin{aligned}& d_t e^{m+1} - \Delta\overline{e}^{m+1/2} + \nabla\overline{\eta}^{m+1/2} = -\mathcal{G}^{m+1}(u_\varepsilon, u_{VK}) + \frac{1}{2}k^2\nabla d_t^2\eta^{m+1} - \frac{1}{2}k^2\nabla d_t^2 p_\varepsilon^{m+1},\\ & \mathrm{div} e^{m+1} - \beta k^2\Delta d_t\eta^{m+1} = 0,\\ & e^{m+1}\big|_{\partial\Omega} = 0, \qquad \partial_n d_t\eta^{m+1}\big|_{\partial\Omega} = 0,\\ & e^0 = 0, \qquad \eta^0 = 0.\end{aligned} \tag{33}$$

In the error identities (33), the term that causes major difficulties is $\frac{1}{2}k^2\nabla d_t^2 p_\varepsilon^{m+1}$. As we know from (32), only an *averaged* version of it can be controlled, and we therefore have to sum over each two subsequent error identities in (33). This strategy, on the other hand, causes difficulties in dealing with $\mathcal{G}^{m+1}(u_\varepsilon, u_{VK})$, since it only carries averaged data of the iteration in the second entries of the related bilinear form. — From this consideration, we verify more local a-priori statements in a first step (part *a)*) to obtain a-priori statements for the solution $\{u_{VK}^{m+1}, p_{VK}^{m+1}\}$ of (18)/(19). Then, in a second step (part *b)*), we benefit from these stability results for $\{u_{VK}^{m+1}, p_{VK}^{m+1}\}$ to handle the error identities (33) in averaged form.

a) If we apply the second equation in (26), we obtain the following stability result from (31),

$$k^3\sum_{m=1}^{M}\|\nabla d_t^2 p_\varepsilon^{m+1}\|^2 \le C\big(1+\log\frac{1}{k}\big). \tag{34}$$

Now, if we test system (33) with $\{\overline{e}^{m+1/2}, \overline{\eta}^{m+1/2}\}$, and observe that the term $\mathcal{G}^{m+1}(u_\varepsilon, u_{VK})$ can be reformulated in the way

$$\begin{aligned}\mathcal{G}^{m+1}(u_\varepsilon, u_{VK}) &:= \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_\varepsilon^m - \frac{1}{2}u_\varepsilon^{m-1}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m+1/2} \\ &\quad - \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}\}\cdot\nabla\big]\overline{u}_{VK}^{m+1/2} \\ &= \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}e^m - \frac{1}{2}e^{m-1}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m+1/2} \\ &\quad - \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}\}\cdot\nabla\big]\overline{e}^{m+1/2},\end{aligned} \tag{35}$$

we obtain the following error estimate, by taking benefit from the stability results (32), (34),

$$\begin{aligned}&\|e^{M+1}\|^2 + k\sum_{m=1}^{M}\|\nabla\overline{e}^{m+1/2}\|^2 + k^2\|\nabla\overline{\eta}^{M+1/2}\|^2 \\ &\quad + k^4\sum_{m=1}^{M}\|\nabla d_t\overline{\eta}^{m+1/2}\|^2 \le Ck^3\big(1+\log\frac{1}{k}\big).\end{aligned} \tag{36}$$

Note, that the limited choice of parameter values for β, $\beta > \frac{1}{2}$, is essential here to absorb the term of the pressure error on the right hand side by the velocity errors on the left hand side. — The estimate (36) is the key result to derive further a-priori bounds for the solution $\big\{u_{VK}^{m+1}, p_{VK}^{m+1}\big\}$ of (18), and its (discrete) time derivatives, using (32),

$$\max_{0\le m\le M}\Big\{\|d_t u_{VK}^{m+1}\| + \|\nabla\overline{p}_{VK}^{m+1/2}\|\Big\} + k\sum_{m=1}^{M}\|\nabla d_t\overline{u}_{VK}^{m+1/2}\|^2 \le C\big(1+\log\frac{1}{k}\big). \tag{37}$$

In order to derive bounds for spatially differentiated forms of u_{VK}^{m+1}, we first have to bound the pressure gradient $\nabla\eta^{m+1}$. This can be accomplished by means of the parallelogram identity, the error result (36), and the second identity in (33),

$$\begin{aligned}\|\nabla\eta^m\|^2 + \|\nabla\eta^{m+1}\|^2 &= \frac{1}{2}\|\nabla\overline{\eta}^{m+1/2}\|^2 + \frac{1}{2}k^2\|\nabla d_t\eta^{m+1}\|^2 \\ &\le Ck\big(1+\log\frac{1}{k}\big) + \frac{1}{\beta^2k^2}\|e^{m+1}\|^2 \le Ck\big(1+\log\frac{1}{k}\big).\end{aligned} \tag{38}$$

It is now an easy task to verify the following bounds, by using standard energy arguments,

$$\max_{0\le m\le M}\Big\{\|\nabla u_{VK}^m\| + \|\Delta\overline{u}_{VK}^{m+1/2}\|\Big\} \le C\big(1+\log\frac{1}{k}\big). \tag{39}$$

We emphasize that a result of the form $\max_{0\le m\le M}\|\nabla d_t u_{VK}^{m+1}\| \le C\big(1+\log\frac{1}{k}\big)$ cannot be obtained, owing to the application of pressure iterates in the momentum equation in (18). The lack of such a result makes it more difficult to handle the nonlinearity in the subsequent error analysis.

b) Let us turn back to the system of error equations (33) in the averaged form

$$d_t\overline{e}^{m+1/2} - \Delta\overline{\overline{e}}^m + \nabla\overline{\overline{\eta}}^m + \overline{\mathcal{G}}^{m+1/2}(u_\varepsilon, u_{VK}) = \frac{1}{2}k^2\nabla d_t^2\overline{\eta}^{m+1/2} - \frac{1}{2}k^2\nabla d_t^2\overline{p}_\varepsilon^{m+1/2}. \tag{40}$$

This identity will now be tested with $\overline{\overline{e}}^m$. Then, in order to treat $\big|\big(\overline{\mathcal{G}}^{m+1/2}(u_\varepsilon, u_{VK}), \overline{\overline{e}}^m\big)\big|$, we recall

$$\begin{aligned}\overline{\mathcal{G}}^{m+1/2}(u_\varepsilon, u_{VK}) &= \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}e^m - \frac{1}{2}e^{m-1}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m+1/2}\\ &- \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}\}\cdot\nabla\big]\overline{e}^{m+1/2}\\ &+ \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}e^{m-1} - \frac{1}{2}e^{m-2}\}\cdot\nabla\big]\overline{u}_\varepsilon^{m-1/2}\\ &- \big[\mathrm{P}_{\mathbf{J}_0}\{\frac{3}{2}u_{VK}^{m-1} - \frac{1}{2}u_{VK}^{m-2}\}\cdot\nabla\big]\overline{e}^{m-1/2} = I + II.\end{aligned} \tag{41}$$

For the first term I, to be tested with $\overline{\overline{e}}^m$, we find the following results, using the abbreviative notation of the trilinear form $b(\phi,\psi,\xi) = \big((\phi\cdot\nabla)\psi, \xi\big)$, and $\hat{b}(\cdot,\cdot,\cdot) := b\big(P_{\mathbf{J}_0}\cdot,\cdot,\cdot\big)$,

$$\begin{aligned}\big|(I, \overline{\overline{e}}^m)\big| &\le \big|\hat{b}(\frac{3}{2}\overline{e}^{m+1/2} - \frac{1}{2}\overline{e}^{m-1/2}, \overline{u}_\varepsilon^{m+1/2}, \overline{\overline{e}}^m)\big|\\ &+ k\big|\hat{b}(\frac{3}{2}e^{m-1} - \frac{1}{2}e^{m-2}, d_t\overline{u}_\varepsilon^{m+1/2}, \overline{\overline{e}}^m)\big|\\ &\le C\Big\{\big\{\|\Delta\overline{u}_\varepsilon^{m+1/2}\|^2 + k^2\|\Delta d_t\overline{u}_\varepsilon^{m+1/2}\|^2\big\}\|\overline{e}^{m+1/2}\|^2\\ &+ k^4\big\{\|d_te^m\|^2 + \|d_te^{m+1}\|^2\big\}\|\Delta\overline{u}_\varepsilon^{m+1/2}\|^2\Big\} + \frac{1}{4}\|\nabla\overline{\overline{e}}^m\|^2\\ &\le C\Big\{k^4(1+\log\frac{1}{k}) + \|\overline{e}^{m+1/2}\|^2\Big\} + \frac{1}{4}\|\nabla\overline{\overline{e}}^m\|^2.\end{aligned} \tag{42}$$

The last inequality is valid, owing to the a-priori bounds (32), (37). — In order to bound the expression $\big|(II, \overline{\overline{e}}^m)\big|$ in an optimal way, we can benefit from the skew-symmetricity rule that holds for the form $\hat{b}(\phi,\cdot,\cdot)$, $\forall\phi\in\mathbf{J}_0$. For

$$\big|(II, \overline{\overline{e}}^m)\big| = \big|\hat{b}(\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}, \overline{e}^{m+1/2}, \overline{\overline{e}}^m) + \hat{b}(\frac{3}{2}u_{VK}^{m-1} - \frac{1}{2}u_{VK}^{m-2}, \overline{e}^{m-1/2}, \overline{\overline{e}}^m)\big|, \tag{43}$$

the following equality is a consequence of the skew-symmetricity rule,

$$\hat{b}(\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}, \overline{e}^{m+1/2}, \overline{\overline{e}}^m) + \hat{b}(\frac{3}{2}u_{VK}^m - \frac{1}{2}u_{VK}^{m-1}, \overline{e}^{m-1/2}, \overline{\overline{e}}^m) = 0. \tag{44}$$

Therefore, we can continue with (43) as follows,

$$
\begin{aligned}
&\leq k\big|\hat{b}(\frac{3}{2}d_t u_{VK}^m - \frac{1}{2}d_t u_{VK}^{m-1}, \overline{e}^m, \overline{e}^{m-1/2})\big| \\
(45)\qquad &= k^2\big|\hat{b}(\frac{3}{2}d_t u_{VK}^m - \frac{1}{2}d_t u_{VK}^{m-1}, \overline{e}^m, d_t\overline{e}^{m+1/2})\big| \\
&\leq Ck^4\Big\{\big\{\|d_t u_{VK}^{m-1}\|\|\nabla d_t u_{VK}^{m-1}\| + \|d_t u_{VK}^m\|\|\nabla d_t u_{VK}^m\|\big\}\|\nabla d_t\overline{e}^{m+1/2}\|^2\Big\} + \frac{1}{4}\|\nabla\overline{e}^m\|^2.
\end{aligned}
$$

We can now collect these results, coming back to inequality (40). Due to (32), (42), (43), (45), (37), and by means of Gronwall's inequality, we find

$$
\begin{aligned}
&\|\overline{e}^{M+1/2}\|^2 + k\sum_{m=1}^{M}\|\nabla\overline{\overline{e}}^m\|^2 + k^2\|\nabla\overline{\overline{\eta}}^M\|^2 + k^4\sum_{m=1}^{M}\|\nabla d_t\overline{\overline{\eta}}^m\|^2 \\
(46)\qquad &\leq Ck^4\big(1+\log\frac{1}{k}\big) + Ck^5\max_{1\leq m\leq M}\|\nabla d_t u^m\|\sum_{1\leq m\leq M}\|\nabla d_t\overline{e}^{m+1/2}\|^2.
\end{aligned}
$$

with $C = C(\beta)$, in particular. Thanks to (36) and (39), we can now bound the terms on the right hand side of the latter equation by $Ck^4(1+\log\frac{1}{k})$. This furnishes the proof. □

4 A priori Analysis of the Chemically Flow Problem. This section is devoted to the presentation of striking a priori bounds for the solution of system (1), (2) as well as to the presentation of energy arguments that will continuously be employed in the following sections. For a verification of existence and uniqueness of solutions, we refer to [8] or [16]. The following theorem is the basis for the derivation of sharp error statements for scheme (4) through (7).

Lemma 4.1 *Assume $\{u(t), p(t), T(t), Y(t)\} \in \mathcal{X}$ to be the solution of (1), (2), satisfying the assumptions (A1),(A2),(A3) and Postulate B. Then, the following a priori statements are satisfied,*

$$
\sup_{(0,t_{M+1}]}\Big\{\|\partial_t^\ell u\|_2 + \|\partial_t^\ell p\|_1 + \|\partial_t^\ell T\|_2 + \sum_{i=1}^{N}\|\partial_t^\ell Y_i\|_2\Big\} \leq C, \qquad \ell = 0,1,
$$

$$
\begin{aligned}
&\sup_{(0,t_{M+1}]}\Big\{\|\partial_t^\ell u\| + \|\partial_t^\ell T\| + \sum_{i=1}^{N}\|\partial_t^\ell Y_i\|\Big\}^2 + \int_0^{t_{M+1}}\Big\{\|\partial_t^\ell u(s)\|_1^2 + \|\partial_t^\ell T(s)\|_1^2\Big\}\,ds \\
&\qquad + \sum_{i=1}^{N}\int_0^{t_{M+1}}\|\partial_t^\ell Y_i(s)\|_1^2\,ds \leq C, \qquad \ell = 1,2,
\end{aligned}
$$

where C is a constant that depends on the given data and geometry of the problem.

Proof. The verification of these results for the case $\ell = 0$ (in the first inequality) and $\ell = 1$ (in the second estimate) has been given in [13]. The extension to the remaining cases $\ell = 1$ (in the first estimate) and $\ell = 2$ (in the first inequality) is straightforward and will be omitted here. □

5 Analysis of the Auxiliary Problems.

5.1 The auxiliary problem (10) The investigation of the implicit time-discretization is based on the strong regularity results for the continuous flow that is supposed to satisfy Postulate B, further on the lipschitz continuity of the mappings f_0 and $\{W_i\}_{i=1}^N$.

The goal of this section is the verification of the following lemma.

Lemma 5.1 *Suppose the basic assumptions (A1), (A2), (A3) to be valid and additionally Postulate B for the solution of (1),(2). Then, the solution* $\{u_a^{m+1}, p_a^{m+1}, T_a^{m+1}, Y_a^{m+1}\} \in \mathcal{X}$ *of scheme (10) satisfies the properties (P1) and* $(P2)_0$*, for sufficiently small time-steps* $k \leq k_0(t_{M+1})$.

Proof. We omit the verification of the statements given in (P1) for the problem, since they can be immediately verified by means of arguments that are analogous to those presented in Lemma 4.1, causing no further difficulties. — In order to verify the property $(P2)_0$, we subtract the equations (1) and (10). In the following, we will make use of the following abbreviative notation,

$$
\begin{aligned}
e^{m+1} &:= u(t_{m+1}) - u_a^{m+1}, \qquad & \eta^{m+1} &:= p(t_{m+1}) - p_a^{m+1},\\
\mathcal{T}^{m+1} &:= T(t_{m+1}) - T_a^{m+1}, \qquad & \mathcal{Y}_i^{m+1} &:= Y(t_{m+1}) - Y_{a,i}^{m+1}.
\end{aligned}
$$

Then, the resulting error equations are as follows,

$$
\begin{aligned}
& d_t e^{m+1} - \Delta \overline{e}^{m+1/2} + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big] \overline{e}^{m+1/2} + \big[\overline{e}^{m+1/2} \cdot \nabla\big] u(t_{m+1/2}) + \nabla \overline{\eta}^{m+1/2} \\
&\quad = r_1^{m+1}(u) + r_2^{m+1}(\Delta u) + r_2^{m+1}(-\nabla p) \\
&\quad + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big] r_2^{m+1}(u) + \big[r_2^{m+1}(u) \cdot \nabla\big] u(t_{m+1/2}) \\
&\quad + f_0\Big(\frac{1}{2}\{T(t_{m+1}) + T(t_m)\} + r_2^{m+1}(T)\Big) - f_0(\overline{T}^{m+1/2}), \\
& \mathrm{div} e^{m+1} = 0, \\
& d_t \mathcal{T}^{m+1} - \Delta \overline{\mathcal{T}}^{m+1/2} + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big] \overline{\mathcal{T}}^{m+1/2} + \big[\overline{e}^{m+1/2} \cdot \nabla\big] T(t_{m+1/2}) \\
&\quad = r_1^{m_1}(T) + r_2^{m+1}(\Delta T) + \big[\overline{u}_a^{m+1/2} \cdot \nabla\big] r_2^{m+1}(T) \\
&\quad + \big[r_2^{m+1}(u) \cdot \nabla\big] T(t_{m+1/2}) + \sum_{i=1}^{M} h_i W_i\big(\overline{Y}_a^{m+1/2}, \overline{T}^{m+1/2}\big), \\
&\quad - \sum_{i=1}^{N} h_i W_i\Big(\{\frac{1}{2}\{Y_i(t_{m+1}) + Y_i(t_m)\} + r_2^{m+1}(Y_i)\}_{i=1}^N, \\
&\quad \frac{1}{2}\{T(t_{m+1}) + T(t_m)\} + r_2^{m+1}(T)\Big)
\end{aligned}
\tag{47}
$$

$$
\begin{aligned}
d_t\mathcal{Y}_i^{m+1} &- \Delta\overline{\mathcal{Y}}_i^{m+1/2} + \big[\overline{u}_a^{m+1/2}\cdot\nabla\big]\overline{\mathcal{Y}}_i^{m+1/2} + \big[\overline{e}^{m+1/2}\cdot\nabla\big]Y_i(t_{m+1/2})\\
&= r_1^{m+1}(Y_i) + r_2^{m+1}(\Delta Y_i) + \big[\overline{u}_a^{m+1/2}\cdot\nabla\big]r_2^{m+1}(Y_i)\\
&+ \big[r_2^{m+1}(u)\cdot\nabla\big]Y_i(t_{m+1/2}) - W_i\big(\overline{Y}_a^{m+1/2},\overline{T}^{m+1/2}\big)\\
&+ W_i\Big(\{\frac{1}{2}\{Y_i(t_{m+1})+Y_i(t_m)\} + r_2^{m+1}(Y_i)\}_{i=1}^N,\\
&\frac{1}{2}\{T(t_{m+1})+T(t_m)\} + r_2^{m+1}(T)\Big),
\end{aligned}
$$

where

$$
\begin{aligned}
r_1^{m+1}(\phi) &:= \frac{1}{k}\int_{t_m}^{t_{m+1}} \beta_m(s)\phi_{ttt}(s)\ ds,\\
r_2^{m+1}(\phi) &:= \frac{1}{k}\int_{t_m}^{t_{m+1}} \big\{\alpha_m-\beta_m\big\}(s)\phi_{tt}(s)\ ds,
\end{aligned}
\tag{48}
$$

for

$$
\begin{aligned}
s &\mapsto \alpha_{m+1}(s) \equiv \frac{1}{12}\big(t_{m+1}-s\big)(s-t_m),\\
s &\mapsto \beta_{m+1}(s) \equiv \frac{1}{2}\min\big\{(t_{m+1}-s)^2,(s-t_m)^2\big\}.
\end{aligned}
\tag{49}
$$

Now, we test the error equations (47) with $\big\{\overline{e}^{m+1/2},\overline{\mathcal{T}}^{m+1/2},\overline{\mathcal{Y}}^{m+1/2}\big\}$. Because of the mapping properties of f_0 and $\{W_i\}_{i=1}^N$, we obtain

$$
\begin{aligned}
d_t\Big\{&\|e^{m+1}\|^2 + \|\mathcal{T}^{m+1}\|^2 + \sum_{i=1}^N\|\mathcal{Y}_i^{m+1}\|^2\Big\}\\
&+\|\nabla\overline{e}^{m+1/2}\|^2 + \|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \sum_{i=1}^N\|\nabla\overline{\mathcal{Y}}_i^{m+1/2}\|^2\\
&\le C\Big\{\|r_1^{m+1}(u)\|_{-1}^2 + \|r_2^{m+1}(T)\|_{-1}^2 + \sum_{i=1}^N\|r_1^{m+1}(Y_i)\|_{-1}^2\\
&+\|u(t_{m+1/2})\|_2^2\Big\{\|r_2^{m+1}(u)\|^2 + \|r_2^{m+1}(T)\|^2 + \sum_{i=1}^N\|r_2^{m+1}(Y_i)\|^2\Big\}\\
&+\|r_2^{m+1}(u)\|^2\Big\{\|u(t_{m+1/2})\|_2^2 + \|T(t_{m+1/2})\|_2^2 + \sum_{i=1}^N\|Y_i(t_{m+1/2})\|_2^2\Big\}\\
&+\|\overline{\mathcal{T}}^{m+1/2}\|^2 + \|r_2^{m+1}(T)\|^2 + \sum_{i=1}^N\big\{\|\overline{\mathcal{Y}}_i^{m+1/2}\|^2 + \|r_2^{m+1}(Y_i)\|^2\big\}\Big\}.
\end{aligned}
\tag{50}
$$

Owing to the regularity of the solution $\{u,T,Y_i\}$ of (1), we can bound the discretization errors as follows,

$$k \sum_{m=1}^{M} \|r_1^{m+1}(\phi)\|_{-1}^2 \le C \frac{1}{k} \sum_{m=1}^{M} \int_{t_m}^{t_{m+1}} \beta_m^2(s)\; ds \int_{t_m}^{t_{m+1}} \|\phi_{ttt}(s)\|_{-1}^2 \; ds \le Ck^4, \tag{51}$$

and

$$k \sum_{m=1}^{M} \|r_2^{m+1}(\phi)\|_1^2 \le C \frac{1}{k} \sum_{m=1}^{M} \int_{t_m}^{t_{m+1}} \{\alpha - \beta_m\}^2(s)\; ds \int_{t_m}^{t_{m+1}} \|\phi_{tt}(s)\|_1^2 \; ds \le Ck^4. \tag{52}$$

Therefore, summing over all iteration steps in (50) verifies property $(P2)_0$. □

5.2 The auxiliary problem (11). We will now focus on the perturbation effect that an explicit treatment of the temperature function in (11) has on the approximation of the solution $\{u_a^{m+1}, p_a^{m+1}, T_a^{m+1}, Y_a^{m+1}\} \in \mathcal{X}$. The proof of the following Lemma is presented in the remainder of this section.

Lemma 5.2 *Suppose the solution of (1),(2) to satisfy the assumptions (A1),(A2),(A3) and Postulate B. Then, the solution $\{u_b^{m+1}, p_b^{m+1}, T_b^{m+1}, Y_b^{m+1}\} \in \mathcal{X}$ of scheme (11) satisfies the properties (P1) and $(P2)_0$, provided the time-step is sufficiently small, $k \le k_0(t_{M+1})$.*

Proof. It is sufficient to compare the difference in the solutions of (10) and (11), since (10) inherits the properties under consideration, see Lemma 5.1. — Again, let us start with the introduction of the error notation,

$$\begin{aligned} e^{m+1} &:= u_a^{m+1} - u_b^{m+1}, & \eta^{m+1} &:= p_a^{m+1} - p_b^{m+1}, \\ \mathcal{T}^{m+1} &:= T_a^{m+1} - T_b^{m+1}, & \mathcal{Y}_i^{m+1} &:= Y_{a,i}^{m+1} - Y_{b,i}^{m+1}. \end{aligned}$$

The error equations are then the following ones,

$$\begin{aligned} &d_t e^{m+1} - \Delta \overline{e}^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big] \overline{e}^{m+1/2} + \big[\overline{e}^{m+1/2} \cdot \nabla\big] \overline{u}_a^{m+1/2} + \nabla \overline{\eta}^{m+1/2} \\ &\qquad = f_0(\overline{T}_a^{m+1/2}) - f_0(\tfrac{3}{2} T_b^m - \tfrac{1}{2} T_b^{m-1}), \\ &\operatorname{div} e^{m+1} = 0, \\ &d_t \mathcal{T}^{m+1} - \Delta \overline{\mathcal{T}}^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big] \overline{\mathcal{T}}^{m+1/2} + \big[\overline{e}^{m+1/2} \cdot \nabla\big] \overline{T}_a^{m+1/2} \\ &\qquad = - \sum_{i=1}^{N} h_i \Big[W_i\big(\overline{Y}_a^{m+1/2}, \overline{T}_a^{m+1/2}\big) - W_i\big(\overline{Y}_b^{m+1/2}, \overline{T}_b^{m+1/2}\big)\Big], \\ &d_t \mathcal{Y}_i^{m+1} - \Delta \overline{\mathcal{Y}}_i^{m+1/2} + \big[\overline{u}_b^{m+1/2} \cdot \nabla\big] \overline{\mathcal{Y}}_i^{m+1/2} + \big[\overline{e}^{m+1/2} \cdot \nabla\big] \overline{Y}_{a,i}^{m+1/2} \\ &\qquad = W_i\big(\overline{Y}_a^{m+1/2}, \overline{T}_a^{m+1/2}\big) - W_i\big(\overline{Y}_b^{m+1/2}, \overline{T}_b^{m+1/2}\big). \end{aligned} \tag{53}$$

Now, we can use the regularity of f_0 to obtain the bound

$$\begin{aligned}\|f_0(\overline{T}_a^{m+1/2}) - f_0(\frac{3}{2}T_b^m - \frac{1}{2}T_b^{m-1})\| &= \|f_0(\overline{T}_a^{m+1/2}) - f_0(\overline{T}_b^{m+1/2} - \frac{1}{2}k^2 d_t^2 T_b^{m+1})\| \\ &\leq C\Big\{\|\mathcal{T}^m\| + \|\mathcal{T}^{m+1}\| + k^2\|d_t^2 T_a^{m+1}\|\Big\},\end{aligned} \tag{54}$$

and we can now benefit from Lemma 5.1 to bound the last term in (54) by $Ck^2(1+\log\frac{1}{k})$. (In fact, the logarithmic term can again be omitted).

The remainder of the proof is now straightforward, if we test (53) with $\{\overline{e}^{m+1/2}, \overline{\mathcal{T}}^{m+1/2}, \overline{\mathcal{Y}}^{m+1/2}\}$, and take into account the regularity properties of $\{W_i\}_{i=1}^N$. We omit the elaboration of this argument that verifies property $(P2)_0$. — The verification of (P1) can again be done analogously to the proof of Lemma (5.1) and will be omitted. □

5.3 The auxiliary problem (12). In here, we investigate the influence of an "explicit treatment" of the flow information in the chemical part. The results of the corresponding error analysis are formulated in the following lemma.

Lemma 5.3 *Suppose the assumptions (A1), (A2), (A3) and Postulate B to be valid for the solution of (1),(2). Then, the solution* $\{u_c^{m+1}, p_c^{m+1}, T_c^{m+1}, Y_c^{m+1}\} \in \mathcal{X}$ *of scheme (12) satisfies the properties (P1) and* $(P2)_0$, *for sufficiently small time-steps* $k \leq k_0(t_{M+1})$.

Proof. Since the verification of the stability property (P1) is not that evident, we start the proof with a short stability analysis.

Verification of property (P1):
If we test (12) with the triple $\{\overline{u}_c^{m+1/2}, \overline{T}_c^{m+1/2}, \overline{Y}_c^{m+1/2}\}$, we can easily find the following inequality,

$$\begin{aligned}&\|u_c^{M+1}\|^2 + \|T_c^{M+1}\|^2 + \sum_{i=1}^N \|Y_{c,i}^{M+1}\|^2 \\ &+ k\sum_{m=1}^M \Big\{\|\nabla \overline{u}_c^{m+1/2}\|^2 + \|\nabla \overline{T}_c^{m+1/2}\|^2 + \sum_{i=1}^N \|\nabla \overline{Y}_{c,i}^{m+1/2}\|^2\Big\} \leq C.\end{aligned} \tag{55}$$

Similarly, using the test functions $\{-\Delta\overline{u}_c^{m+1/2}, -\Delta\overline{T}_c^{m+1/2}, -\Delta\overline{Y}_c^{m+1/2}\}$, the following estimate can be obtained,

$$\begin{aligned}&\|\nabla u_c^{M+1}\|^2 + \|\nabla T_c^{M+1}\|^2 + \sum_{i=1}^N \|\nabla Y_{c,i}^{M+1}\|^2 \\ &+ k\sum_{m=1}^M \Big\{\|\Delta \overline{u}_c^{m+1/2}\|^2 + \|\Delta \overline{T}_c^{m+1/2}\|^2 + \sum_{i=1}^N \|\Delta \overline{Y}_{c,i}^{m+1/2}\|^2\Big\} \\ &\leq C + k\sum_{m=0}^M \Big\{\|\nabla u_c^m\|^6 + \|\nabla u_c^m\|^4 \|\nabla \overline{T}_c^{m+1/2}\|^2 + \|\nabla u_c^m\|^4 \sum_{i=1}^N \|\nabla \overline{Y_{i,c}}^{m+1/2}\|^2\Big\}.\end{aligned} \tag{56}$$

This implies local (in time) boundedness of the left-hand side of the latter inequalities for times $(0, t_{M+1}]$. — The verification of the following a-priori result then follows from (56) and system (12),

$$k \sum_{m=1}^{M} \Big\{ \|d_t u_c^{m+1}\|^2 + \|d_t T_c^{m+1}\|^2 + \sum_{i=1}^{N} \|d_t Y_{c,i}^{m+1}\|^2 \Big\} \le C. \tag{57}$$

The derivation of a-priori statements for difference-quotients of solution iterates is now straightforward, and we omit this part of the proof. In particular, the following bounds can be verified,

$$\begin{aligned} &\max_{0\le m\le M} \Big\{ \|d_t u_c^{m+1}\|_2^2 + \|d_t T_c^{m+1}\|_2^2 + \sum_{i+1}^{N} \|d_t Y_{c,i}^{m+1}\|_2^2 \Big\} \\ &\quad + k \sum_{m=0}^{M} \Big\{ \|\nabla d_t^2 \overline{u}_c^{m+1/2}\|^2 + \|\nabla d_t^2 \overline{T}_c^{m+1/2}\|^2 + \sum_{i=1}^{N} \|\nabla d_t^2 \overline{Y}_{c,i}^{m+1/2}\|^2 \Big\} \le C. \end{aligned} \tag{58}$$

Note that initial terms arising from final summation can be controlled owing to the supposed regularity of the actual solution given in Postulate B. This follows from an easy calculation in terms of errors (see below) and a corresponding of errors at initial steps.

Verification of property $(P2)_0$*:*
In order to show the validity of property $(P2)_0$, we can confine on the comparison of the solutions of the systems (11) and (12). By using the error functions for velocity field and pressure function,

$$e^{m+1} := u_b^{m+1} - u_c^{m+1}, \qquad \eta^{m+1} := p_b^{m+1} - p_c^{m+1},$$

the corresponding error identity for the momentum equation is as follows,

$$\begin{aligned} &d_t e^{m+1} - \Delta \overline{e}^{m+1/2} + \big[\{\tfrac{3}{2} u_c^m - \tfrac{1}{2} u_c^{m-1}\} \cdot \nabla\big] \overline{e}^{m+1/2} \\ &\quad + k^2 \big[d_t^2 u_b^{m+1} \cdot \nabla\big] \overline{u}_b^{m+1/2} - \big[\{\tfrac{3}{2} e^m - \tfrac{1}{2} e^{m-1}\} \cdot \nabla\big] \overline{u}_b^{m+1/2} \\ &\quad + \big[\{\tfrac{3}{2} e^m - \tfrac{1}{2} e^{m-1}\} \cdot \nabla\big] \overline{u}_b^{m+1/2} + \nabla \overline{\eta}^{m+1} \\ &\quad = \Big[f_0(\tfrac{3}{2} T_b^m - \tfrac{1}{2} T_b^{m-1}) - f_0(\tfrac{3}{2} T_c^m - \tfrac{1}{2} T_c^{m-1}) \Big]. \end{aligned} \tag{59}$$

We omit the elaboration of the remaining error identities. The verification property $(P2)_0$ is now straightforward if we test with $\overline{e}^{m+1/2}$ and test the remaining error identities with corresponding error functions for temperature and concentrations, since we can benefit from the stability results of the solution $\{u_b^m, p_b^m, T_b^m, Y_b^m\}$ given in Lemma 5.2 and the regularity of the functions f_0 and $\{W_i\}_{i=1}^N$. □

5.4 The auxiliary problem (13). This part is devoted to analyze the error effect coming from the semi-explicit treatment of the reaction part in the temperature and concentration equations. The preservation of the properties (P1) and $(P2)_0$ is assured through the next lemma.

Lemma 5.4 *Suppose the assumptions (A1),(A2) and (A3) to be valid and Postulat B to be satisfied for the solution of (1),(2). Then, the solution* $\{u_d^{m+1}, p_d^{m+1}, T_d^{m+1}, Y_d^{m+1}\} \in \mathcal{X}$ *of scheme (13) satisfies the properties (P1) and* $(P2)_0$*, provided time-steps* $k \leq k_0(t_{M+1})$ *are chosen sufficiently small.*

Proof. The verification of $(P2)_0$ uses an argument that is analogous to the one given in the proof of Lemma 5.2 for the function f_0, see formula (54). The proof of the stability statements (P1) will again be omitted. □

5.5 The auxiliary problem (14). This is the essential step in our investigation, because we pass from an incompressible velocity field to a slightly compressible one. The study of the error mechanisms of the projection scheme of Van Kan have been extended from the Stokes problem (see [12]) to the Navier-Stokes equations (16).

Lemma 5.5 *Suppose (A1), (A2), (A3) and Postulate B to be valid for the solution of (1),(2), and the initial pressure function* p_e^0 *to satisfy* $\|p_e^0 - p(0)\|_1 \leq Ck$*. Then, the solution* $\{u_e^{m+1}, p_e^{m+1}, T_e^{m+1}, Y_e^{m+1}\} \in \mathcal{X}$ *of scheme (14) satisfies the property* $(P2)_1$*, for sufficiently small time-steps* $k \leq k_0(t_{M+1})$.

Remark 5.1 *Note that the driving forces in the impulse equations in (13) and (14) are identical and that the 'chemical parts' are the same. Further, only provides us with an approximation result, whereas property (P1) is not subject of the consideration. In fact, this result cannot be established here but only averaged-type results apply. We refer to section 3.*

Proof. The right hand side of the first equation in (14) can be bounded in striking norms, owing to Lemma 5.4. Therefore, Theorem 3.1 can be applied to furnish the proof. □

5.6 The auxiliary problem (15). This section is devoted to gain further understanding in the effect the projection scheme has on the temperature and the concentration in scheme (4) through (7), or the reformulation (15). We emphasize that the subsequent lemma only provides us with approximation result $(P2)_1$ and thus concludes the proof of Theorem 1.1.

Lemma 5.6 *Suppose (A1), (A2), (A3) and Postulate B to be valid for the solution of (1),(2), and the initial pressure function* p_f^0 *to satisfy* $\|p_f^0 - p(0)\|_1 \leq Ck$*. Then, the solution* $\{u_f^{m+1}, p_f^{m+1}, T_f^{m+1}, Y_f^{m+1}\} \in \mathcal{X}$ *of scheme (15) satisfies property* $(P2)_1$*, for sufficiently small time-steps* $k \leq k_0(t_{M+1})$.

Proof. By using the error notation

$$e^{m+1} := u_e^{m+1} - u_f^{m+1}, \qquad \eta^{m+1} := p_e^{m+1} - p_f^{m+1},$$
$$\mathcal{T}^{m+1} := T_d^{m+1} - T_f^{m+1}, \qquad \mathcal{Y}_i^{m+1} := Y_{d,i}^{m+1} - Y_{f,i}^{m+1},$$

we obtain the following system of error equations,

$$\begin{aligned}
&d_t e^{m+1} - \Delta \overline{e}^{m+1/2} + \nabla \overline{\eta}^{m+1/2} = \frac{1}{2} k^2 \nabla d_t^2 \eta^{m+1} \\
&\quad + \big[P_{\mathbf{J}_0}\{\frac{3}{2}e^m - \frac{1}{2}e^{m-1}\} \cdot \nabla\big]\overline{u}_e^{m+1/2} + \big[P_{\mathbf{J}_0}\{\frac{3}{2}u_f^m - \frac{1}{2}u_f^{m-1}\} \cdot \nabla\big]\overline{e}^{m+1/2} \\
&\quad = f_0(\frac{3}{2}T_d^m - \frac{1}{2}T_d^{m-1}) - f_0(\frac{3}{2}T_f^m - \frac{1}{2}T_f^{m-1}), \\
&\mathrm{div} e^{m+1} - \beta k^2 \Delta d_t \eta^{m+1} = 0, \qquad \partial_n d_t \eta^{m+1}\big|_{\partial\Omega} = 0, \\
&d_t \mathcal{T}^{m+1} - \Delta \overline{\mathcal{T}}^{m+1/2} + \mathcal{H}(\overline{T}_d^{m+1/2}) + \big[P_{\mathbf{J}_0}\{\frac{3}{2}u_f^m - \frac{1}{2}u_f^{m-1}\} \cdot \nabla\big]\overline{\mathcal{T}}^{m+1/2} \\
&\quad = -\sum_{i=1}^{N} h_i \Big[W_i(\frac{3}{2}Y_d^m - \frac{1}{2}Y_d^{m-1}, \overline{T}_d^{m+1/2}) - W_i(\frac{3}{2}Y_f^m - \frac{1}{2}Y_f^{m-1}, \overline{T}_f^{m+1/2})\Big], \\
&d_t \mathcal{Y}_i^{m+1} - \Delta \overline{\mathcal{Y}}_i^{m+1/2} + \mathcal{H}(\overline{Y}_{d,i}^{m+1/2}) + \big[P_{\mathbf{J}_0}\{\frac{3}{2}u_f^m - \frac{1}{2}u_f^{m-1}\} \cdot \nabla\big]\overline{\mathcal{Y}}_i^{m+1/2} \\
&\quad = W_i(\overline{Y}_d^{m+1/2}, \frac{3}{2}T_d^m - \frac{3}{2}T_d^{m-1}) - W_i(\overline{Y}_f^{m+1/2}, \frac{3}{2}T_f^m - \frac{3}{2}T_f^{m-1}).
\end{aligned} \tag{60}$$

In this system of error equations, we made use of the abbreviative notation

$$\mathcal{H}(\overline{\phi}^{m+1/2}) = \Big[P_{\mathbf{J}_0}\Big\{\frac{3}{2}\{u_d^m - u_e^m + e^m\} - \frac{1}{2}\{u_d^{m-1} - u_e^{m-1} + e^{m-1}\}\Big\} \cdot \nabla\Big]\overline{\phi}^{m+1/2}. \tag{61}$$

The direct application of the error functions $\{\overline{e}^{m+1/2}, \overline{\mathcal{T}}^{m+1/2}, \{\overline{\mathcal{Y}}_i^{m+1/2}\}_{i=1}^N\}$ is now again not possible, owing to the fact that we are only provided with second order convergence results for the quantity $\max_{0\le m\le M} \|\overline{u}_d^{m+1/2} - \overline{u}_e^{m+1/2}\|$, see Lemma 3.1. The situation is quite the same as in the *3rd step* of the proof for Lemma 3.1. Therefore, we confine here on a sketchy argumentation. If we follow the lines presented there, we start with the derivation of a first suboptimal error result, compare (36), in particular

$$\begin{aligned}
&\|e^{M+1}\|^2 + \|\mathcal{T}^{M+1}\|^2 + \sum_{i=1}^{N} \|\mathcal{Y}_i^{M+1}\|^2 + k^2 \|\nabla \overline{\eta}^{M+1/2}\|^2 \\
&\quad + k \sum_{m=0}^{M} \Big\{\|\nabla \overline{e}^{m+1/2}\|^2 + \|\nabla \overline{\mathcal{T}}^{m+1/2}\|^2 + \sum_{i=1}^{N} \|\nabla \overline{\mathcal{Y}}_i^{m+1/2}\|^2\Big\} \le Ck^3(1 + \log\frac{1}{k}).
\end{aligned} \tag{62}$$

According to the considerations that follow formula (36), we find

$$
\begin{aligned}
(63) \qquad & \max_{0\le m\le M}\Big\{\|d_t u_f^m\| + \|d_t T_f^m\| + \sum_{i=1}^N \|d_t Y_{f,i}^m\| + \|\nabla u_f^m\| + \|\nabla T_f^m\| + \sum_{i=1}^N \|\nabla Y_{f,i}^m\| \\
& \quad + \|\Delta \overline{u}_f^{m+1/2}\| + \|\Delta \overline{T}_f^{m+1/2}\| + \sum_{i=1}^N \|\Delta \overline{Y}_{f,i}^{m+1/2}\|\Big\} \le C\big(1+\log\frac{1}{k}\big).
\end{aligned}
$$

Now, these are striking a-priori statements that can be made use of in an averaged approach, using the averaged version of error identities (60). For this purpose, we follow the chain of arguments given in the *3rd step, b)* of the proof of Theorem 3.1. The derivation of property $(P2)_1$ now follows from testing the system with the error functions $\{\overline{\overline{e}}^m, \overline{\overline{\mathcal{T}}}^m, \{\overline{\overline{\mathcal{Y}}}_i^m\}_{i=1}^N\}$, and inequality (63). Observe, that the pressure term on the right hand side of the first equation (60) can be bounded in terms of the velocity error through the second identity in (60). □

Now, the combination of the results of the Lemmata 5.1 through 5.6 furnishes the proof of Theorem (1.1).

6 Proof of Corollary 1.1.

The goal of the present section is to verify the improved error statements for the temperature gradient distribution and the mass fraction gradient that are stated in Corollary 1.1. For this purpose, we can benefit from the results that have been gained in the previous sections, see in particular the Lemmata 4.1, 5.1, 5.2, 5.3, 5.4, 5.5, and 5.6 for the results. Note that the latter two Lemmata just give statements concerning the convergence properties of the solution of the scheme (15). The subsequent analysis is split into several steps, dealing with each of the different auxiliary problems that have been introduced in section 2.

a) We start the proof of Corollary 1.1 by turning back to the system (47) of error equations. In order to make use of result (50) in the following, we have to add the corresponding equations for subsequent iterates for the last two identity. In order to outline the following steps, we can confine to the equation for the temperature error, since corresponding arguments can be given for the treatment of the equations that describe the evolution of the errors for the mass fractions. — Thus, if we test the equation with $\{-\Delta\overline{\overline{\mathcal{T}}}^m\}$, we end up with

$$
\begin{aligned}
& d_t\|\nabla \overline{\mathcal{T}}^{m+1/2}\|^2 + \|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \\
(64) \qquad & \le C\Big\{\|r_1^{m+1}(T)\|_1^2 + \|r_1^m(T)\|_1^2 + \|r_2^{m+1}(\Delta T)\|^2 + \|r_2^m(\Delta T)\|^2 + \|r_2^{m+1}(u)\|_1^2 \\
& + \|r_2^m(u)\|_1^2 + \sum_{i=1}^N \big\{\|r_2^{m+1}(Y_i)\|^2 + \|r_2^m(Y_i)\|^2\big\} + Ck^4\Big\}.
\end{aligned}
$$

In order to verify optimal error bounds for the quantities on the left hand side of the last inequality, we have to multiply it with a time-weight, i.e., $\tau_{m+1/2}$. Then, the quantities on the right hand side can easily be bounded by Ck^4, and the upper bound $\big(k\sum_{m=0}^{M}\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2\big)^{1/2}\le Ck^2$ is now a consequence of (50). As already mentioned, corresponding arguments apply for a consideration of the mass fraction error in (47).

b) In this step, we are dealing with the auxiliary problem (11), or, correspondingly, with the system of error equations (53). We can again confine ourselves to a consideration of the equation for the temperature error. Thus, testing the third identity in (53) with $-\Delta\overline{\mathcal{T}}^{m+1/2}$ amounts to the inequality

(65)
$$\|\nabla\mathcal{T}^{M+1}\|^2 + k\sum_{m=0}^{M}\|\Delta\overline{\mathcal{T}}^{m+1/2}\|^2 \le Ck^4 + k\sum_{m=0}^{M}\Big\{\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|\overline{e}^{m+1/2}\|_{0,q}^2\|\nabla\overline{T}_a^{m+1/2}\|_{0,r}^2\Big\},$$

for positive numbers q, r satisfying $\frac{1}{q}+\frac{1}{r}=\frac{1}{2}$. Furthermore, we made use of Lemma 5.2 in the last step of the last inequality. — In the following, we make use of Sobolev inequalities, which make the argumentation different for the two and the three dimensional case. Let us begin with the case $d=2$. Thanks to the Gagliardo-Nirenberg interpolation inequality (see [15], e.g.), we obtain for positive q,

$$\le Ck^4 + Ck\sum_{m=0}^{M}\Big\{\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|\overline{e}^{m+1/2}\|^{4/q}\|\nabla\overline{e}^{m+1/2}\|^{2-4/q}\|\nabla\overline{T}_a^{m+1/2}\|_{0,\frac{2q}{2-q}}^2\Big\}, \tag{66}$$

thanks to the Sobolev inequality $\|\phi\|_{0,p}\le C\|\phi\|_1,\ \forall\ 1\le p<\infty$. We can finally employ Gronwall's inequality, combined with the selection of an appropriate value q close to 2 in (66) to verify the upper bound $Ck^{4-\gamma}$, with $C=C(p)$ (and $C(p)\to\infty\ (p\to 2)$) and $\gamma=\gamma(p)>0$ arbitrarily. We note in particular that no summation of subsequent equations is necessary here, thanks to the structure of the convective term.
If we consider the case $d=3$, we get, instead of (66),

$$\le Ck^4 + Ck\sum_{m=1}^{M}\Big\{\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|\overline{e}^{m+1/2}\|\|\nabla\overline{e}^{m+1/2}\|\Big\} \le Ck^{7/2}. \tag{67}$$

The last inequality results from the bound $\big(\sum_{m=0}^{M}\|\nabla\overline{e}^{m+1/2}\|^2\big)^{1/2}\le k^{3/2}$ that was an outcome of the studies in subsection (5.2).

c) This step is devoted to auxiliary problem (12). In the error analysis, we can essentially follow the argumentation that has been given in step *b)*. In particular, for the new error functions we can verify

(68)
$$\|\nabla\mathcal{T}^{M+1}\|^2 + k\sum_{m=1}^{M}\|\Delta\overline{\mathcal{T}}^{m+1/2}\|^2 \le Ck^4 + k\sum_{m+1}^{M}\Big\{\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|\overline{e}^{m+1}\|_{0,q}^2\|\overline{T}_a^{m+1/2}\|_{0,r}^2\Big\},$$

Note that there is no averaging of the error function in the leading factor of the second term in the sum any more. This does not cause any problem for the two dimensional case, since we are provided with pointwise error statements in the $\ell^\infty\big(0, t_{M+1}; \mathbf{L}^2\big)$ norm for the velocity field. Contrary to this, in the three dimensional case we obtain the following slighlty modified version of the corresponding result (67),

$$\leq Ck^4 + Ck\sum_{m=1}^{M}\Big\{\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|e^{m+1}\|\|\nabla e^{m+1}\|\Big\} \leq Ck^3. \tag{69}$$

The latter bound is a consequence of the application of the Gronwall Lemma for the inequality (68), (69) and the further bound for the term $\max_{0\leq m\leq 1}\|\nabla e^{m+1}\| \leq Ck$. We skip the verification of this result.

d) In this step, we study the impact of perturbing the incompressibility constraint on the gradients of temperature and mass fraction iterates.
As we already know from (62), we can bound gradients of algebraic combinations of successive velocity error iterates. For pointwise control of the gradient, we get a decreased order of convergence, as we see, when we test the first equation in (60) with $-\Delta\overline{e}^{m+1/2}$,

$$\begin{aligned} d_t\|\nabla e^{m+1}\|^2 + \|\Delta\overline{e}^{m+1/2}\|^2 \leq C\Big\{&\|d_t e^{m+1}\|^2 + \|\nabla\overline{\eta}^{m+1/2}\|^2 \\ &+ \|\mathcal{T}^m\|^2 + \|\mathcal{T}^{m+1}\|^2\Big\} + \|\nabla e^m\|^2 + \|\nabla e^{m-1}\|^2, \end{aligned} \tag{70}$$

where we benefit from the second identity in (60) and elementary Sobolev inequalities to treat the convective part. The discrete version of Gronwall's lemma then gives, using (62),

$$\|\nabla e^{M+1}\|^2 + k\sum_{m=0}^{M}\|\Delta\overline{e}^{m+1/2}\|^2 \leq Ck\big(1+\log\frac{1}{k}\big). \tag{71}$$

We can now use this auxiliary result to tackle the derivation of the desired result, which is the verification of a result for gradients of algebraic combinations of temperature errors and mass fractions. We again restrict on the demonstration for the temperature errors. For this purpose, we sum error identities for subsequent errors, as they are given by the third equation in (60). If we then test the corresponding equality with $-\Delta\overline{\overline{\mathcal{T}}}^m$, we obtain

$$\begin{aligned} &d_t\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \\ &\quad\leq \big|\hat{b}\big(\overline{u}_f^{m-1/2} - \frac{1}{2}k^2 d_t^2 u_f^m, \overline{\overline{\mathcal{T}}}^m, \Delta\overline{\overline{\mathcal{T}}}^m\big)\big| \\ &\quad+ k\big|\hat{b}\big(\overline{u}_f^{m+1/2} - \frac{1}{2}k^2 d_t^2 u_f^{m+1}, d_t\overline{\mathcal{T}}^{m+1/2}, \Delta\overline{\overline{\mathcal{T}}}^m\big)\big| \\ &\quad+ \big|\hat{b}\big(\overline{\overline{\mathcal{E}}}^m - \frac{1}{2}k^2 d_t^2\overline{\mathcal{E}}^{m+1/2}, \overline{T}_d^{m+1/2}, \Delta\overline{\overline{\mathcal{T}}}^m\big)\big| \\ &\quad+ k\big|\hat{b}\big(\overline{\mathcal{E}}^{m-1/2} + \frac{1}{2}k^2 d_t^2\mathcal{E}^m, d_t\overline{T}_d^{m+1/2}, \Delta\overline{\overline{\mathcal{T}}}^m\big)\big| := I + II + III + IV. \end{aligned} \tag{72}$$

[2] Indeed, the bounds in (67) and (69) can be improved to $\mathcal{O}(k^4)$, but we omit the verification, since the restriction of the overall convergence order is limited in the subsequent step *d)*.

In the latter inequality, we introduced the shorthand notation $\mathcal{E}^{m+1} := u_d^{m+1} - u_f^{m+1}$. The analysis of the terms I through IV will now be done separately:

$$I \leq C\Big(\max_{-2\leq\ell\leq 0}\|\nabla u_f^{m+\ell}\|^4\Big)\|\nabla\overline{\overline{\mathcal{T}}}^m\|^2 + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2. \tag{73}$$

The second term is the sum of two terms, $II \leq II_a + II_b$:

$$II_a \leq C\|\Delta\overline{u}_f^{m+1/2}\|^2\|\nabla\overline{\mathcal{T}}^{m+1/2}\|^2 + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \tag{74}$$

In order to deal with II_b in an optimal way, we can benefit from (62) and Lemma 5.5. Further, we state without proof, that a corresponding result as stated in (71) for the velocity field is also valid for the temperature distribution. This can be verified by using corresponding arguments. — Since the subsequent considerations heavily rely on Sobolev inequalities, we will again distinguish the analysis for the two and three dimensional case. For the case $d = 2$, we are finally lead to

$$II_b \leq Ck^4\|d_t^2 u_f^{m+1}\|_q^2 \max_{\ell\in\{0,1\}}\|\nabla\overline{\mathcal{T}}^{m+1/2-\ell}\|^2_{\frac{2q}{2-q}} + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2, \tag{75}$$

and we can choose q arbitrarily close to 2 to find a constant $C = C(q)$.
In three dimensions, we obtain

$$\begin{aligned} II_b &\leq Ck^6\|d_t^2 u_f^{m+1}\|^2\|\nabla d_t^2 u_f^{m+1}\|\|\Delta d_t\overline{\mathcal{T}}^{m+1/2}\|^2 + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \\ &\leq Ck^3\big(1+\log\frac{1}{k}\big) + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2. \end{aligned} \tag{76}$$

The last bound is a consequence of (62) and (71).
We now deal with term III, and we restrict here on the analysis for the case of three dimensions ($d = 3$). Owing to the Lemmata 5.5, 5.6, and the formulae (62), (71), there holds

$$\begin{aligned} III &\leq C\|\overline{\overline{\mathcal{E}}}^m\|\|\nabla\overline{\overline{\mathcal{E}}}^m\| + Ck^4\|d_t^2\overline{\mathcal{E}}^{m+1/2}\|\|\nabla d_t^2\overline{\mathcal{E}}^{m+1/2}\| + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \\ &\leq Ck^3\big(1+\log\frac{1}{k}\big) + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2. \end{aligned} \tag{77}$$

Correspondingly, the last expression IV can be controlled in the way

$$\begin{aligned} IV &\leq Ck^2\Big\{\|\overline{\mathcal{E}}^{m+1/2}\|\|\nabla\overline{\mathcal{E}}^{m+1/2}\| + k^4\|d_t^2\mathcal{E}^m\|\|\nabla d_t^2\mathcal{E}^m\|\Big\}\|\Delta d_t\overline{T}_d^{m+1/2}\|^2 + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2 \\ &\leq Ck^3\big(1+\log\frac{1}{k}\big) + \frac{1}{8}\|\Delta\overline{\overline{\mathcal{T}}}^m\|^2. \end{aligned} \tag{78}$$

In particular, we employed (71) for this argument.

We can now come back to inequality (72). Thanks to (73) through (78), we can now employ the discrete Gronwall inequality and end up with the error bound

$$\|\nabla\overline{\mathcal{T}}^{M+1/2}\|^2 + \sum_{m=0}^{M} \|\Delta\overline{\overline{\mathcal{T}}}^{m}\|^2 \leq Ck^3\big(1+\log\frac{1}{k}\big). \tag{79}$$

e) We can now combine the sections *a)* through *d)* that furnish Corollary 1.1.

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