A posteriori error estimates with application of adaptive mesh refinement for thermal multiphase compositional flows in porous media*

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Abstract

We consider in this work thermal multiphase multicomponent flows in porous media. We derive fully computable a posteriori error estimates for the dual norm of the residual supplemented by a nonconformity evaluation term. The estimators are general and valid for a variety of discretization methods. We also show how to estimate separately the space, time, linearization, and algebraic errors giving the possibility to formulate adaptive stopping and balancing criteria. Moreover, a space–time adaptive mesh refinement algorithm based on the estimators is proposed. We consider the application of the theory to an implicit finite volume scheme with phase-upwind and two-point discretization of diffusive fluxes. Numerical results on an example of real-life thermal oil-recovery in a reservoir simulation illustrate the performance of the refinement strategy and in particular show that a significant gain in term of mesh cells can be achieved.

Key words: a posteriori error analysis, adaptive mesh refinement, compositional Darcy flow, thermal flow, finite volume method

1 Introduction

The thermal multiphase compositional model in porous medium describes the flow of several fluids through a subsurface under a non-isothermal condition. The governing equations are the conservation of the amount of each component and the conservation of energy, which are partial differential equations, supplemented by algebraic equations expressing the conservation of volume, the conservation of the quantity of matter, and the thermodynamic equilibrium, see [18, 19, 14].

Thermal models are especially important for simulation of the enhanced oil recovery, where the increase of temperature reduces the oil viscosity which in turn improves mobility and makes the production easier and leading to better recovery indexes. Several methods of thermal simulation have been considered. We can cite, e.g., the recent works [35, 17, 41, 39, 33, 38, 20, 36]. Thermal processes play also an important role in the modeling of geothermal reservoirs, see, e.g., [40] and the references therein.

A mathematical structure of multiphase thermal models of flow in porous media is proposed in [47]. The authors give a formulation and numerical solution of equations for modeling multicomponent, two-phase, thermal fluid flow in porous media. For this purpose they develop an algorithm that achieves a

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better balance between stability and accuracy. This approach was used previously for reservoir simulation of black-oil model [9] and also for compositional models [8]. Recently, it has been proposed in [10, 36] to formulate the phase transitions as a set of local inequality constraints and use the complementarity approach.

Many numerical methods have been proposed for the discretization of the multiphase compositional model: finite differences and finite element methods in, e.g., [3, 7, 18, 50], mixed finite element methods in, e.g., [24, 13, 15, 16], finite volume methods in, e.g., [34, 37, 30, 5, 1, 4], and recently vertex-centered methods on general 3D meshes in [29]. Many adaptive mesh refinement algorithms have been considered, cf. [31, 26, 17] for dynamic griding to thermal and isothermal models, and other recent works, cf. [46, 44, 39, 41, 33, 38, 42, 43].

The discretization of the thermal multiphase multicomponent model leads to a nonlinear, strongly coupled systems of differential and algebraic equations. The resolution of these systems requires an important computational effort. Therefore, proposing an adaptive algorithm to optimize this resolution holds a special interest in reservoir modeling. To the best of our knowledge, this work is the first to develop a posteriori error estimates to control the error and stopping criteria for the iterative algebraic and nonlinear solvers for the general version of the thermal multiphase compositional model. We follow [49, 12] where a rigorous a posteriori error analysis for the immiscible incompressible two-phase flow was given under the assumption that the flow process is isothermal, and [22], where a generalization to arbitrary number of phases and components, still in the isothermal case, was done.

The paper is organized as follows. Section 2 details the unknowns and the physical properties related to the general thermal multiphase compositional model and describes the governing equations that constitute the mathematical system of the model. In Section 3 we consider a discretization of the thermal model based on the two-points finite volume scheme in space and the backward Euler scheme in time. Linearization by the Newton method and algebraic resolution by an arbitrary iterative solver is also discussed. In Section 4 we postprocess the original phase pressures and temperature and we devise their $H_0^1(\Omega)$-conforming reconstructions, as well as $H(\mathrm{div};\Omega)$-conforming fluxes needed in the a posteriori analysis. In Section 5 we introduce the weak formulation of the problem, define the corresponding error measure, and derive the a posteriori error estimate. Section 6 finally illustrates the numerical results on an enhanced oil recovery thermal process for heavy oil. We show results corresponding to adaptive mesh refinement strategy saving an important number of mesh cells during the simulation, without affecting the precision of the resolution.

2 The thermal multiphase compositional model

We consider the flow through a porous medium of several fluid phases, each composed of a finite number of components from a given set. Mass exchange between phases as well as thermal effects are accounted for. The precise formulation we use extends that of Eymard, Guichard, Herbin, and Masson [29] based on the original paper of Coats [19]; see also [32] and [22].

Let $\Omega \subset \mathbb{R}^d$, $d \geq 1$, denote a bounded connected polygonal domain with boundary $\partial\Omega$, and let $t_F > 0$. In petroleum-related applications, Ω typically represents a reservoir, while t_F is the simulation time. We denote by $\mathcal{P} = \{p\}$ and $\mathcal{C} = \{c\}$ respectively the set of phases and components. A synthetic description of the fluid system is given in terms of the component-phase matrix $\mathbf{M} = [m_{cp}]_{c\in\mathcal{C},\, p\in\mathcal{P}} \in \{0,1\}^{\mathcal{C},\mathcal{P}}$ such that, for all $c \in \mathcal{C}$ and all $p \in \mathcal{P}$,

$$m_{cp} = \begin{cases} 1 & \text{if the component } c \text{ is contained in the phase } p, \\ 0 & \text{otherwise.} \end{cases}$$

Given the component-phase matrix, we can define, for all $p \in \mathcal{P}$, the set of components present in the phase p as $\mathcal{C}_p = \{c \in \mathcal{C};\ m_{cp} = 1\}$. Conversely, for each component $c \in \mathcal{C}$, the set of phases containing c is given by $\mathcal{P}_c = \{p \in \mathcal{P};\ m_{cp} = 1\}$.

2.1 Unknowns

The unknowns of the model are (i) the *reference pressure* P; (ii) the *temperature* T; (iii) the *saturations* $\boldsymbol{S} = (S_p)_{p\in\mathcal{P}}$, representing the fraction of the pore volume occupied by each phase; (iv) for all $p \in \mathcal{P}$,

the *molar fractions* of the components present in p, $\boldsymbol{C}_p := (C_{p,c})_{c\in\mathcal{C}_p}$. The unknowns of the model are collected in the vector

$$\mathcal{X} := \begin{pmatrix} P \\ T \\ (S_p)_{p\in\mathcal{P}} \\ (C_{p,c})_{p\in\mathcal{P},c\in\mathcal{C}_p} \end{pmatrix}.$$

Finally, for each phase $p \in \mathcal{P}$ the (average) *phase pressure* is given by

$$P_p = P_p(P, \boldsymbol{S}) := P + P_{\mathrm{c}_p}(\boldsymbol{S}), \tag{2.1}$$

where $P_{\mathrm{c}_p}(\boldsymbol{S})$ is a *generalized capillary pressure*.

2.2 Fluid and medium properties

The porous medium is characterized by the following properties (the usual dependency on the unknowns is provided in brackets): (i) the *porosity* ϕ; (ii) the symmetric tensor $\mathbb{K}$ of *absolute permeability*; (iii) the *thermal conductivity* λ; (iv) the *rock energy* $e_{\mathrm{r}}(P_p, T, \mathbf{C}_p)$; (v) the *rock molar density* ζ_r. These properties can additionally depend on the space variable when heterogeneous media are considered, but it is assumed for the sake of simplicity that the dependence on time is only via the variables of the model. Next, each fluid phase $p \in \mathcal{P}$ is characterized by the following properties: (i) the *molar density* $\zeta_p(P_p, T, \boldsymbol{C}_p)$; (ii) the *mass density* $\rho_p(P_p, T, \boldsymbol{C}_p)$; (iii) the *viscosity* $\mu_p(P_p, T, \boldsymbol{C}_p)$; (iv) the *relative permeability* $k_{\mathrm{r},p}(\boldsymbol{S})$; (v) for all $c \in \mathcal{C}_p$, the *fugacity* $f_{c,p}(P_p, T, \boldsymbol{C}_p)$; (vi) the *phase enthalpy* $H_p(P_p, T, \boldsymbol{C}_p)$; (vii) the *phase internal energy* $e_p(P_p, T, \boldsymbol{C}_p)$. It is also convenient to define for each phase $p \in \mathcal{P}$ the *mobility* given by $\nu_p(P_p, T, \boldsymbol{S}, \boldsymbol{C}_p) := \zeta_p(P_p, T, \boldsymbol{C}_p)\frac{k_{\mathrm{r},p}(\boldsymbol{S})}{\mu_p(P_p,T,\boldsymbol{C}_p)}$.

2.3 The thermal multiphase compositional model

We summarize in this section the equations that govern the non-isothermal multiphase compositional flow. For each component $c \in \mathcal{C}$, we let l_c denote the *amount* (in moles) *of component* c per unit volume given by

$$l_c = l_c(\mathcal{X}) = \phi \sum_{p\in\mathcal{P}_c} \zeta_p(P_p, T, \boldsymbol{C}_p) S_p C_{p,c}. \tag{2.2}$$

The *conservation of the amount of each component* is expressed by the following system of PDEs:

$$\partial_t l_c + \nabla\cdot\boldsymbol{\Phi}_c = q_c, \qquad \forall c \in \mathcal{C}, \tag{2.3}$$

where, for each $c \in \mathcal{C}$, $q_c \in L^2((0, t_{\mathrm{F}}); L^2(\Omega))$ denotes a *source* or *sink* and the *component flux* $\boldsymbol{\Phi}_c$ has the following expression:

$$\boldsymbol{\Phi}_c := \sum_{p\in\mathcal{P}_c} \boldsymbol{\Phi}_{p,c}, \qquad \boldsymbol{\Phi}_{p,c} = \boldsymbol{\Phi}_{p,c}(P_p, T, \boldsymbol{S}, \boldsymbol{C}_p) := \nu_p(P_p, T, \boldsymbol{S}, \boldsymbol{C}_p) C_{p,c} \boldsymbol{v}_p(P_p, T, \boldsymbol{C}_p), \tag{2.4}$$

with $\boldsymbol{v}_p$ denoting the *average phase velocity* given by Darcy's law (in the following, $\boldsymbol{g}$ denotes the gravity vector acting along $-z$ and g its Euclidian norm),

$$\boldsymbol{v}_p = \boldsymbol{v}_p(P_p, T, \boldsymbol{C}_p) := -\mathbb{K}\left(\nabla P_p - \rho_p(P_p, T, \boldsymbol{C}_p)\boldsymbol{g}\right) = -\mathbb{K}\left(\nabla P_p + \rho_p(P_p, T, \boldsymbol{C}_p) g \nabla z\right). \tag{2.5}$$

The *molar energy* per unit volume is given by

$$e_H = e_H(\mathcal{X}) = \phi \sum_{p\in\mathcal{P}} \zeta_p(P_p, T, \mathbf{C}_p) e_p(P_p, T, \mathbf{C}_p) S_p + (1-\phi)\zeta_{\mathrm{r}} e_{\mathrm{r}}(P_p, T, \mathbf{C}_p). \tag{2.6}$$

The *conservation of energy* is then expressed by the following scalar PDE:

$$\partial_t e_H + \nabla\cdot\boldsymbol{\Phi}_H = Q_H, \tag{2.7}$$

where $Q_H \in L^2((0, t_{\mathrm{F}}); L^2(\Omega))$ denotes a *thermal source* or *sink* and

$$\boldsymbol{\Phi}_H := \mathbf{J} + \sum_{p\in\mathcal{P}} \boldsymbol{\Phi}_{p,H}, \tag{2.8}$$

with *Fourier flux* $\mathbf{J} = \mathbf{J}(T) := -\lambda\nabla T$ and *phase enthalpy fluxes* given by

$$\mathbf{\Phi}_{p,H} := \nu_p(P_p, T, \boldsymbol{S}, \mathbf{C}_p)H_p(P_p, T, \mathbf{C}_p)\boldsymbol{v}_p(P_p, T, \mathbf{C}_p).$$

For the sake of simplicity, we assume *no-flow boundary conditions*,

$$\mathbf{\Phi}_c\cdot\boldsymbol{n}_\Omega = 0 \text{ for all } c \in \mathcal{C} \quad \text{and} \quad \mathbf{\Phi}_H\cdot\boldsymbol{n}_\Omega = 0 \text{ on } \partial\Omega \times (0, t_{\mathrm{F}}), \tag{2.9}$$

where $\partial\Omega$ denotes the boundary of Ω and $\boldsymbol{n}_\Omega$ its outward normal. At $t = 0$ we prescribe the *initial molar energy* and the *initial amount of each component* by setting

$$e_H(\cdot, 0) = e_H^0, \qquad l_c(\cdot, 0) = l_c^0 \quad \forall c \in \mathcal{C}. \tag{2.10}$$

The system is closed by the algebraic equations

$$\sum_{p\in\mathcal{P}} S_p = 1, \qquad \sum_{c\in\mathcal{C}_p} C_{p,c} = 1 \quad \forall p \in \mathcal{P}, \tag{2.11}$$

and enforcing the thermodynamic equilibrium expressed by $\sum_{c\in\mathcal{C}}(N_{\mathcal{P}_c}-1) = \sum_{p\in\mathcal{P}} N_{\mathcal{C}_p} - N_{\mathcal{C}}$ inequalities of fugacities (we have used the notation $N_{\mathcal{X}}$ for the cardinality of the set $\mathcal{X}$).

To fix the ideas, we now present an example of a thermal multiphase multicomponent model which is the case considered in the numerical experiment of Section 6 below. It is the thermal Dead Oil model a steam-assisted gravity drainage process (SAGD), a technique of steam injection designed to increase the oil mobility.

Example 1 (Dead Oil model)**.** *In the Dead Oil model we have three phases: the oil phase, the water phase, and the steam phase, represented respectively by lowercase indices (*$\mathrm{w}, \mathrm{o}, \mathrm{s}$*). We use also the uppercase indices (*W, O*) to represent the two components of the model: water and oil, respectively. The system of governing equations consists of the mass conservation equation of the water component*

$$\partial_t\big(\phi(\zeta_{\mathrm{w}}S_{\mathrm{w}} + \zeta_{\mathrm{s}}S_{\mathrm{s}})\big) + \nabla\cdot(\nu_{\mathrm{w}}\boldsymbol{v}_{\mathrm{w}} + \nu_{\mathrm{s}}\boldsymbol{v}_{\mathrm{s}}) = q_{\mathrm{W}},$$

of the mass conservation equation of the oil component

$$\partial_t(\phi\zeta_{\mathrm{o}}S_{\mathrm{o}}) + \nabla\cdot(\nu_{\mathrm{o}}\boldsymbol{v}_{\mathrm{o}}) = q_{\mathrm{O}},$$

and of the energy conservation equation

$$\partial_t e_H + \nabla\cdot(\boldsymbol{u} - \lambda\nabla T) = Q_H.$$

Here,

$$e_H := \phi e + (1-\phi)\zeta_r e_r, \quad e := \sum_{p\in\{\mathrm{w},\mathrm{o},\mathrm{s}\}} \zeta_p e_p S_p, \quad \boldsymbol{u} := \sum_{p\in\{\mathrm{w},\mathrm{o},\mathrm{s}\}} \nu_p H_p \boldsymbol{v}_p.$$

The algebraic closure equations are stated as follows: the volume conservation gives

$$S_{\mathrm{w}} + S_{\mathrm{o}} + S_s = 1,$$

the structure of the model together with the conservation of the quantity of matter imply

$$C_{\mathrm{w,W}} = C_{\mathrm{s,W}} = C_{\mathrm{o,O}} = 1,$$

and the thermodynamic liquid–steam equilibrium relation reads

$$S_{\mathrm{s}}S_{\mathrm{w}}(T - T_{\mathrm{sat}}(P)) = 0.$$

We consider no-flow boundary conditions prescribed for the component fluxes,

$$\begin{aligned}(\nu_{\mathrm{w}}\boldsymbol{v}_{\mathrm{w}} + \nu_{\mathrm{s}}\boldsymbol{v}_{\mathrm{s}})\cdot\boldsymbol{n}_\Omega = 0, &\qquad \text{on } \partial\Omega\times(0,t_F),\\ (\nu_{\mathrm{o}}\boldsymbol{v}_{\mathrm{o}})\cdot\boldsymbol{n}_\Omega = 0, &\qquad \text{on } \partial\Omega\times(0,t_F),\end{aligned}$$

and also a condition of no-flow for the total energy flux,

$$(-\lambda\nabla T + \boldsymbol{u})\cdot\boldsymbol{n}_\Omega = 0, \qquad \text{on } \partial\Omega\times(0,t_F).$$

Finally the initial conditions are fixed as

$$\begin{aligned}e_H(\cdot,0) &= e_H^0,\\ \phi(\zeta_{\mathrm{w}}S_{\mathrm{w}} + \zeta_{\mathrm{s}}S_{\mathrm{s}}) &= l_{\mathrm{W}}^0,\\ \phi\zeta_{\mathrm{o}}S_{\mathrm{o}} &= l_{\mathrm{O}}^0.\end{aligned}$$

3 Discretization and resolution

We consider here a discretization of the thermal multiphase compositional model of Section 2.3 which naturally extends the scheme of [22, Section 2.2] to the non-isothermal case, see also [32].

3.1 Space-time meshes

Let $(\tau_n)_{1\le n\le N}$ denote a sequence of positive real numbers corresponding to the discrete time steps such that $t_{\rm F} = \sum_{n=1}^N \tau_n$. We consider the discrete times $(t^n)_{0\le n\le N}$ such that $t^0 := 0$ and, for $1 \le n \le N$, $t^n := \sum_{i=1}^n \tau_i$; then we define the time intervals $I_n := (t^{n-1}, t^n)$. For a function of time v with sufficient regularity we let $v^n := v(t^n)$, $0 \le n \le N$, and, for $1 \le n \le N$, we define the backward differencing operator

$$\partial_t^n v := \frac{1}{\tau^n}(v^n - v^{n-1})$$

that we shall use for both scalar- and vector-valued functions.

Let $(\mathcal{M}^n)_{0\le n\le N}$ denote a family of meshes of the space domain Ω. For every element $M \in \mathcal{M}^n$, we denote by $|M|$ its d-dimensional Lebesgue measure and by h_M its diameter. For $0 \le n \le N$, we denote by $\mathcal{E}^n$ the set of mesh faces. Boundary faces are collected in the set $\mathcal{E}^{{\rm b},n} := \{\sigma \in \mathcal{E}^n;\ \sigma \subset \partial\Omega\}$ and we let $\mathcal{E}^{{\rm i},n} := \mathcal{E}^n \setminus \mathcal{E}^{{\rm b},n}$. We let also $\mathcal{E}_M^{{\rm i},n}$ denote the faces of an element $M \in \mathcal{M}^n$ not lying on $\partial\Omega$. For an internal face $\sigma \in \mathcal{E}^{{\rm i},n}$ we fix an arbitrary orientation and denote the corresponding unit normal vector by $\boldsymbol{n}_\sigma$. For a boundary face $\sigma \in \mathcal{E}^{{\rm b},n}$, $\boldsymbol{n}_\sigma$ coincides with the exterior unit normal $\boldsymbol{n}_\Omega$ of Ω. We assume that the family $(\mathcal{M}^n)_{0\le n\le N}$ is super admissible in the sense of [27, Definition 3.1]. Super admissibility requires that for all cells $M \in \mathcal{M}^n$ there exists a point $\boldsymbol{x}_M \in M$ (the *cell center*) and for all faces $\sigma \in \mathcal{E}^n$ there exists a point $\boldsymbol{x}_\sigma \in \sigma$ (the *face center*) such that, for all faces σ lying on the boundary of M, the line segment joining $\boldsymbol{x}_M$ with $\boldsymbol{x}_\sigma$ is $\mathbb{K}^{-1}$-orthogonal to σ. Common examples of super admissible meshes are Cartesian orthogonal grids (for diagonal permeability tensor $\mathbb{K}$) or matching triangular meshes that satisfy the (strict) Delaunay condition. In what follows we let, for all $M \in \mathcal{M}^n$ and all $\sigma \in \mathcal{E}_M^{{\rm i},n}$, $d_{M,\sigma} := {\rm dist}(\boldsymbol{x}_M, \boldsymbol{x}_\sigma)$ and $\mathtt{K}_M^\sigma := \mathbb{K}\cdot\boldsymbol{n}_\sigma$.

3.2 Two-point finite volume discretization

In the context of two-point finite volume methods, the unknowns of the model are discretized using one value per cell: For all $0 \le n \le N$ we let

$$\mathcal{X}_\mathcal{M}^n := (\mathcal{X}_M^n)_{M\in\mathcal{M}^n}, \qquad \mathcal{X}_M^n := \begin{pmatrix} P_M^n \\ T_M^n \\ (S_{p,M}^n)_{p\in\mathcal{P}} \\ (C_{p,c,M}^n)_{p\in\mathcal{P},c\in\mathcal{C}_p} \end{pmatrix} \quad \forall M \in \mathcal{M}^n.$$

For all time steps $0 \le n \le N$ and all $M \in \mathcal{M}^n$, the discrete phase saturations are collected in the vector $\boldsymbol{S}_M^n := (S_{p,M}^n)_{p\in\mathcal{P}}$ while, for all $p \in \mathcal{P}$, the discrete molar fractions are collected in the vector $\boldsymbol{C}_{p,M}^n := (C_{p,c,M}^n)_{c\in\mathcal{C}_p}$. The initial condition (2.10) is augmented to

$$\mathcal{X}_\mathcal{M}(\cdot,0) = \mathcal{X}_\mathcal{M}^0, \tag{3.1}$$

with $\mathcal{X}_\mathcal{M}^0$ resulting from a steady-state equilibrium computation. For each phase $p \in \mathcal{P}$, the corresponding phase pressure inside each cell $M \in \mathcal{M}^n$ at time step $0 \le n \le N$ is given by

$$P_{p,M}^n = P_{p,M}^n(P_M^n, \boldsymbol{S}_M^n) := P_M^n + P_{{\rm c}_p}(\boldsymbol{S}_M^n). \tag{3.2}$$

The PDEs (2.3) and (2.7) expressing, respectively, the conservation of the amount of each component and of energy, are discretized by requiring, for all $1 \le n \le N$ and all $M \in \mathcal{M}^n$,

$$R_{c,M}^n(\mathcal{X}_\mathcal{M}^n) := |M|\partial_t^n l_{c,M} + \sum_{\sigma\in\mathcal{E}_M^{{\rm i},n}} F_{c,M,\sigma}(\mathcal{X}_\mathcal{M}^n) - |M| q_{c,M}^n = 0, \qquad \forall c \in \mathcal{C}, \tag{3.3}$$

$$R_{H,M}^n(\mathcal{X}_\mathcal{M}^n) := |M|\partial_t^n e_{H,M} + \sum_{\sigma\in\mathcal{E}_M^{{\rm i},n}} \Big(F_{H,M,\sigma}(\mathcal{X}_\mathcal{M}^n) + G_{M,\sigma}(\mathcal{X}_\mathcal{M}^n)\Big) - |M| Q_{H,M}^n = 0, \tag{3.4}$$

where $q^n_{c,M} := \int_{I_n}\int_M q_c/(|M|\tau_n)$, $Q^n_{H,M} := \int_{I_n}\int_M Q_H/(|M|\tau_n)$, and the accumulation terms are given, for all $0 \le n \le N$, by the following discrete versions of (2.2) and (2.6), respectively: For all $M \in \mathcal{M}^n$,

$$l^n_{c,M} = l_{c,M}(\mathcal{X}^n_M) := \phi \sum_{p\in\mathcal{P}_c} \zeta_p(P^n_{p,M}, T^n_M, \boldsymbol{C}^n_{p,M}) S^n_{p,M} C^n_{p,c,M} \qquad \forall c \in \mathcal{C}, \tag{3.5}$$

$$e^n_{H,M} = e_{H,M}(\mathcal{X}^n_M) := \phi \sum_{p\in\mathcal{P}} \zeta_p(P^n_{p,M}, T^n_M, \mathbf{C}^n_{p,M}) S^n_{p,M} e_p(P^n_{p,M}, T^n_M, \mathbf{C}^n_{p,M}) + (1-\phi)\zeta_{\mathrm{r}} e_{\mathrm{r}}(P^n_{p,M}, T^n_M, \mathbf{C}^n_{p,M}). \tag{3.6}$$

The total flux of a generic component $c \in \mathcal{C}$ across an interface σ results from the sum of the corresponding fluxes for each phase $p \in \mathcal{P}_c$, i.e.,

$$F_{c,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) := \sum_{p\in\mathcal{P}_c} F_{p,c,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}), \tag{3.7}$$

and, similarly, the flux $F_{H,M,\sigma}$ is given by the sum of the fluxes for each phase $p \in \mathcal{P}$, i.e.,

$$F_{H,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) := \sum_{p\in\mathcal{P}} F_{p,H,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}), \tag{3.8}$$

where, for a given phase p, any $M \in \mathcal{M}^n$, and any $\sigma \in \mathcal{E}^{\mathrm{i},n}_M$ with $\sigma = \partial M \cap \partial L$,

$$F_{p,c,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) = \nu^{\uparrow}_p(\mathcal{X}^n_{\mathcal{M}}) C^n_{p,c,M^{\uparrow}_p} F_{p,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}), \qquad F_{p,H,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) = \nu^{\uparrow}_p(\mathcal{X}^n_{\mathcal{M}}) H^{\uparrow}_{p,M^{\uparrow}_p} F_{p,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}), \tag{3.9}$$

with phase upstream cell

$$M^{\uparrow}_p = \begin{cases} M & \text{if } P^n_{p,M} - P^n_{p,L} \ge 0, \\ L & \text{otherwise,} \end{cases}$$

and $C^n_{p,c,M^{\uparrow}_p}$, $H^{\uparrow}_{p,M^{\uparrow}_p}$, and $\nu^{\uparrow}_p(\mathcal{X}^n_{\mathcal{M}}) := \nu_p(P^n_{p,M^{\uparrow}_p}, T^n_{M^{\uparrow}_p}, \boldsymbol{S}^n_{M^{\uparrow}_p}, \boldsymbol{C}^n_{p,M^{\uparrow}_p})$ denoting, respectively, the upstream molar fraction, upstream enthalpy, and upstream mobility. In (3.9), we have introduced the two-point finite volume approximation of the normal component of the average phase velocity on σ given by

$$F_{p,M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) := |\sigma| \frac{\alpha_M \alpha_L}{\alpha_M + \alpha_L} \left[P^n_{p,M} - P^n_{p,L} + \rho^n_{p,\sigma} g\,(z_M - z_L)\right], \qquad \alpha_K := \frac{\mathtt{K}^{\sigma}_K}{d_{K\sigma}} \quad \forall K \in \{M, L\}, \tag{3.10}$$

where $\rho^n_{p,\sigma}$ is an interface mass density of the phase p obtained by averaging the cell values in M and L; cf. [22] for further details. Finally, for all $M \in \mathcal{M}^n$ and all $\sigma \in \mathcal{E}^{\mathrm{i},n}_M$ with $\sigma = \partial M \cap \partial L$, the discrete Fourier flux $G_{M,\sigma}$ is given by

$$G_{M,\sigma}(\mathcal{X}^n_{\mathcal{M}}) := |\sigma| \frac{\beta_M \beta_L}{\beta_M + \beta_L}(T^n_M - T^n_L), \qquad \beta_K := \frac{\lambda_K}{d_{K\sigma}} \quad \forall K \in \{M, L\}. \tag{3.11}$$

All boundary fluxes are set to zero to account for the homogeneous natural boundary condition (2.9).

To close the system, we enforce, for all $1 \le n \le N$ and all $M \in \mathcal{M}^n$,

$$\sum_{p\in\mathcal{P}} S^n_{p,M} = 1, \qquad \sum_{c\in\mathcal{C}_p} C^n_{p,c,M} = 1 \quad \forall p \in \mathcal{P}, \tag{3.12}$$

and require that the thermodynamic equilibrium expressed in terms of $\left(\sum_{p\in\mathcal{P}} N_{\mathcal{C}_p} - N_{\mathcal{C}}\right)$ equalities of fugacities is satisfied in each cell. For further details we refer to [22] and the references therein.

3.3 Linearization and algebraic resolution

The discretization method of Section 3.2 requires to solve a system of nonlinear algebraic equations at each time step, which we do using the Newton algorithm. For $1 \le n \le N$ and $\mathcal{X}^{n,0}_{\mathcal{M}}$ fixed (typically,

$\mathcal{X}_{\mathcal{M}}^{n,0} = \mathcal{X}_{\mathcal{M}}^{n-1}$), the Newton algorithm generates a sequence $(\mathcal{X}_{\mathcal{M}}^{n,k})_{k\geq 1}$ with $\mathcal{X}_{\mathcal{M}}^{n,k}$ solution to the following linear system: For all $M \in \mathcal{M}^n$,

$$\sum_{M'\in\mathcal{M}^n} \frac{\partial R_{c,M}^n}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k} - \mathcal{X}_{M'}^{n,k-1}) + R_{c,M}^n(\mathcal{X}_{\mathcal{M}}^{n,k-1}) = 0, \qquad \forall c \in \mathcal{C}, \tag{3.13}$$

$$\sum_{M'\in\mathcal{M}^n} \frac{\partial R_{H,M}^n}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})\left(\mathcal{X}_{M'}^{n,k} - \mathcal{X}_{M'}^{n,k-1}\right) + R_{H,M}^n(\mathcal{X}_{\mathcal{M}}^{n,k-1}) = 0. \tag{3.14}$$

The (approximate) solution to (3.13)–(3.14) is typically obtained using an iterative algebraic solver. For $1 \leq n \leq N$, a given Newton iteration $k \geq 1$, and $\mathcal{X}_{\mathcal{M}}^{n,k,0}$ fixed (typically, $\mathcal{X}_{\mathcal{M}}^{n,k,0} = \mathcal{X}_{\mathcal{M}}^{n,k-1}$), the iterative solver generates a sequence $(\mathcal{X}_{\mathcal{M}}^{n,k,i})_{i\geq 1}$ solving the linear system up to the residuals given, for all $M \in \mathcal{M}^n$, by

$$\begin{aligned} R_{c,M}^{n,k,i} &= \frac{|M|}{\tau^n}\frac{\partial l_{c,M}}{\partial \mathcal{X}_M^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_M^{n,k,i} - \mathcal{X}_M^{n,k-1}) \\ &\quad + \sum_{M'\in\mathcal{M}^n}\sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}} \frac{\partial F_{c,M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_M^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}) + R_{c,M}^n(\mathcal{X}_{\mathcal{M}}^{n,k-1}), \qquad \forall c \in \mathcal{C}, \end{aligned} \tag{3.15}$$

$$\begin{aligned} R_{H,M}^{n,k,i} &= \frac{|M|}{\tau^n}\frac{\partial e_{H,M}}{\partial \mathcal{X}_M^n}(\mathcal{X}_M^{n,k-1})(\mathcal{X}_M^{n,k,i} - \mathcal{X}_M^{n,k-1}) \\ &\quad + \sum_{M'\in\mathcal{M}^n}\sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}} \frac{\partial F_{H,M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}) \\ &\quad + \sum_{M'\in\mathcal{M}^n}\sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}} \frac{\partial G_{M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}) + R_{H,M}^n(\mathcal{X}_{\mathcal{M}}^{n,k-1}). \end{aligned} \tag{3.16}$$

Thus, at time step n, Newton iteration $k \geq 1$, and linear solver iteration $i \geq 1$, the residual vectors $R_{c,M}^{n,k,i}$, $R_{H,M}^{n,k,i}$ are given for all $M \in \mathcal{M}^n$ by

$$R_{c,M}^{n,k,i} = \frac{|M|}{\tau^n}\left(l_{c,M}(\mathcal{X}_{\mathcal{M}}^{n,k-1}) + \mathfrak{L}_{c,M}^{n,k,i} - l_{c,M}^{n-1}\right) + \sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}} F_{c,M,\sigma}^{n,k,i} - |M|q_{c,M}^n \qquad \forall c \in \mathcal{C}, \tag{3.17}$$

$$R_{H,M}^{n,k,i} = \frac{|M|}{\tau^n}\left(e_{H,M}(\mathcal{X}_{\mathcal{M}}^{n,k-1}) + \mathfrak{E}_M^{n,k,i} - e_{H,M}^{n-1}\right) + \sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}}\left(F_{H,M,\sigma}^{n,k,i} + G_{M,\sigma}^{n,k,i}\right) - |M|Q_{H,M}^n, \tag{3.18}$$

where $\mathfrak{L}_{c,M}^{n,k,i}$ and $\mathfrak{E}_M^{n,k,i}$ are linear perturbations of the mass and energy accumulation terms defined as, respectively,

$$\mathfrak{L}_{c,M}^{n,k,i} := \frac{\partial l_{c,M}}{\partial \mathcal{X}_M^n}(\mathcal{X}_M^{n,k-1})(\mathcal{X}_M^{n,k,i} - \mathcal{X}_M^{n,k-1}), \qquad \mathfrak{E}_M^{n,k,i} := \frac{\partial e_{H,M}}{\partial \mathcal{X}_M^n}(\mathcal{X}_M^{n,k-1})(\mathcal{X}_M^{n,k,i} - \mathcal{X}_M^{n,k-1}),$$

whereas the linearized fluxes $F_{c,M,\sigma}^{n,k,i}$ and $F_{H,M,\sigma}^{n,k,i}$ read

$$F_{c,M,\sigma}^{n,k,i} := \sum_{p\in\mathcal{P}_c} F_{p,c,M,\sigma}^{n,k,i}, \qquad F_{H,M,\sigma}^{n,k,i} := \sum_{p\in\mathcal{P}} F_{p,H,M,\sigma}^{n,k,i}, \tag{3.19}$$

with linearized phase fluxes

$$F_{p,c,M,\sigma}^{n,k,i} := F_{p,c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k-1}) + \sum_{M'\in\mathcal{M}^n} \frac{\partial F_{p,c,M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}), \tag{3.20}$$

$$F_{p,H,M,\sigma}^{n,k,i} := F_{p,H,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k-1}) + \sum_{M'\in\mathcal{M}^n} \frac{\partial F_{p,H,M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}). \tag{3.21}$$

Finally, the linearized energy flux reads

$$G_{M,\sigma}^{n,k,i} := G_{M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k-1}) + \sum_{M'\in\mathcal{M}^n} \frac{\partial G_{M,\sigma}}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_{\mathcal{M}}^{n,k-1})(\mathcal{X}_{M'}^{n,k,i} - \mathcal{X}_{M'}^{n,k-1}). \tag{3.22}$$

4 Approximate solution and reconstructions

In this section, we first postprocess the original piecewise constant finite volume phase pressures and temperature approximations. We then detail how to obtain the flux reconstructions and smoothed phase pressure and temperature that enter the definitions of the a posteriori estimators proposed in Section 5. We will employ, for each time step n, $H(\mathrm{div};\Omega)$-conforming discrete fluxes belonging to the lowest-order Raviart–Thomas–Nédélec space $\mathbf{RTN}(\mathcal{M}^n)$ (see Brezzi and Fortin [11]). Recall that, for rectangular parallelepipeds meshes such as the ones used in the numerical examples of Section 6 below,

$$\begin{aligned}\mathbf{RTN}(\mathcal{M}^n) := \{&\boldsymbol{v}_h \in \mathbf{H}(\,\mathrm{div}\,;\Omega);\ \boldsymbol{v}_h|_M \in \mathbb{Q}_{0,1}(M)\times\mathbb{Q}_{1,0}(M) \text{ if } d=2,\\ &\mathbb{Q}_{0,1,1}(M)\times\mathbb{Q}_{1,0,1}(M)\times\mathbb{Q}_{1,1,0}(M) \text{ if } d=3,\quad \forall M\in\mathcal{M}^n\}.\end{aligned}$$

For more general meshes one can either introduce a matching simplicial submesh of $\mathcal{M}^n$ and use the simplicial version of $\mathbf{RTN}(\mathcal{M}^n)$, or use the construction proposed in [23, Appendix A].

4.1 Post-processing of the phase pressures and temperature

The original finite volume approximations of the phase pressures and of the temperature are piecewise constant. To evaluate their gradient inside each cell, we define piecewise quadratic, possibly discontinuous phase pressures and temperature as described in the following. Let a time step $1 \le n \le N$, a Newton linearization iteration $k \ge 1$, and an algebraic solver iteration $i \ge 1$ be fixed. Following [28], we define the fluxes $\mathbf{\Gamma}_{p,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$, $p \in \mathcal{P}$, and $\mathbf{\Gamma}_{T,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ such that, for all $M \in \mathcal{M}^n$ and all $\sigma \in \mathcal{E}_M^{\mathrm{i},n}$,

$$(\mathbf{\Gamma}_{p,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma = F_{p,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}) \quad \forall p\in\mathcal{P}, \qquad (\mathbf{\Gamma}_{T,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma = G_{M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}), \tag{4.1}$$

with $F_{p,M,\sigma}$ and $G_{M,\sigma}$ defined by (3.10) and (3.11), respectively, and $\mathbf{\Gamma}_{p,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = 0$ on $\partial\Omega$, $\mathbf{\Gamma}_{T,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = 0$ on $\partial\Omega$, thereby accounting for the no flux boundary conditions (2.9). The fluxes $\mathbf{\Gamma}_{p,h}^{n,k,i}$, $p\in\mathcal{P}$, defined by (4.1) are discrete Darcy phase velocities. Motivated by (2.5) and following [48], we introduce for each $p\in\mathcal{P}$ the piecewise quadratic phase pressure $P_{p,h}^{n,k,i}$ such that, for all $M\in\mathcal{M}^n$,

$$(-\mathbb{K}\nabla P_{p,h}^{n,k,i})|_M = (\mathbf{\Gamma}_{p,h}^{n,k,i})|_M - (\mathbb{K}\rho_p(P_{p,M}^{n,k,i},T_M^{n,k,i},\boldsymbol{C}_{p,M}^{n,k,i})\boldsymbol{g})|_M \quad\text{and}\quad \frac{(P_{p,h}^{n,k,i},1)_M}{|M|} = P_{p,M}^{n,k,i}.$$

Similarly, we define the piecewise quadratic temperature reconstruction $T_h^{n,k,i}$ such that, for all $M\in\mathcal{M}^n$,

$$-\lambda\nabla T_h^{n,k,i}|_M = \mathbf{\Gamma}_{T,h}^{n,k,i}|_M \quad\text{and}\quad \frac{1}{|M|}(T_h^{n,k,i},1)_M = T_M^{n,k,i}.$$

From the above reconstructions we define the space-time functions $P_{p,h\tau}^{n,k,i}$, $p\in\mathcal{P}$, and $T_{h\tau}^{n,k,i}$ assuming an affine-in-time behavior from the converged values at t^{n-1} and the (possibly non converged) values $P_h^{n,k,i}$, $p\in\mathcal{P}$, and $T_h^{n,k,i}$ at t^n. For further use we also define the vector of reconstructed phase pressures $\boldsymbol{P}_{h\tau}^{n,k,i} := (P_{p,h\tau}^{n,k,i})_{p\in\mathcal{P}}$. Henceforth, ∇ is to be understood as the broken gradient operator on $\mathcal{M}^n$ when used for $P_{p,h\tau}^{n,k,i}$ or $T_{h\tau}^{n,k,i}$.

4.2 Saturations, molar fractions, amounts of components, and molar energy

The approximations of saturations, molar fractions, amounts of components, and molar energy obtained using the finite volume discretization detailed in Sections 3 are piecewise constant in space. We define for all $0\le n\le N$, $k\ge 1$, and $i\ge 1$, the functions of space such that

$$\begin{aligned}
(S_{p,h}^{n,k,i})|_M &= S_{p,M}^{n,k,i} && \forall p\in\mathcal{P}\\
(C_{p,c,h}^{n,k,i})|_M &= C_{p,c,M}^{n,k,i} && \forall p\in\mathcal{P},\ \forall c\in\mathcal{C}_p,\\
(l_{c,h}^{n,k,i})|_M &= l_{c,M}^{n,k,i} := l_{c,M}(\mathcal{X}_{\mathcal{M}}^{n,k,i}) && \forall c\in\mathcal{C},\\
(e_{H,h}^{n,k,i})|_M &= e_{H,M}^{n,k,i} := e_{H,M}(\mathcal{X}_{\mathcal{M}}^{n,k,i}),
\end{aligned}$$

with $l_{c,M}$ and $e_{H,M}$ defined by (3.5) and (3.6), respectively. The space–time functions $S_{p,h\tau}^{n,k,i}$, $p \in \mathcal{P}$, $C_{p,c,h\tau}^{n,k,i}$, $p \in \mathcal{P}$, $c \in \mathcal{C}_p$, $l_{c,h\tau}^{n,k,i}$, $c \in \mathcal{C}$, and $e_{H,h\tau}^{n,k,i}$ are then defined therefrom while being continuous and piecewise affine in time.

Remark 4.1. *As detailed in [22, Section 4.2.2], the relations* (3.2), (3.5)*, and* (3.6) *may not hold precisely for the discrete approximations $P_{h\tau}^{n,k,i}$, $T_{h\tau}^{n,k,i}$, $S_{p,h\tau}^{n,k,i}$, $C_{p,c,h\tau}^{n,k,i}$, $P_{p,h\tau}^{n,k,i}$, $e_{H,h\tau}^{n,k,i}$, and $l_{c,h\tau}^{n,k,i}$ (the capillary pressure function applied to a piecewise polynomial is typically no more a piecewise polynomial and a product of two piecewise affine-in-time functions is a piecewise quadratic-in-time function). Similarly, whereas the algebraic closure equations* (3.12) *hold precisely, the equality of fugacities will be violated if the local fugacity equations are not resolved exactly. We suppose the error from all these non-satisfactions as negligible.*

4.3 H_0^1-conforming phase pressures and temperature reconstructions

The approximations defined in Section 4.1 have sufficient regularity for the application of the piecewise gradient operator, but are nonconforming. In order to define our a posteriori estimators below, following [21, 6] in the model cases, we introduce space-continuous phase pressures and temperature reconstructions defined by $\mathfrak{P}_{p,h}^{n,k,i} = \mathcal{I}_{\rm av}(P_{p,h}^{n,k,i})$, $\mathfrak{T}_{h\tau}^{n,k,i} = \mathcal{I}_{\rm av}(T_{h\tau}^{n,k,i})$, where $\mathcal{I}_{\rm av}$ denotes the vertex-averaging interpolator, cf., e.g., [2].

4.4 $H(\mathrm{div};\Omega)$-conforming flux reconstructions

Let a time step $1 \le n \le N$, a Newton linearization iteration $k \ge 1$, and an algebraic solver iteration $i \ge 1$ be fixed. We define the following flux reconstructions for use in the a posteriori estimates of Section 5:

- The *discretization fluxes* $\mathbf{\Theta}_{{\rm dis},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$, $c \in \mathcal{C}$, and $\mathbf{\Theta}_{{\rm dis},H,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ such that, for all $M \in \mathcal{M}^n$ and all $\sigma \in \mathcal{E}_M^{{\rm i},n}$,

$$(\mathbf{\Theta}_{{\rm dis},c,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma := F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}), \qquad (\mathbf{\Theta}_{{\rm dis},H,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma := F_{H,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}) + G_{M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}), \tag{4.2}$$

  with $F_{c,M,\sigma}$, $F_{H,M,\sigma}$, and $G_{M,\sigma}$ defined by (3.7), (3.8), and (3.11), respectively, while $\mathbf{\Theta}_{{\rm dis},c,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = \mathbf{\Theta}_{{\rm dis},H,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = 0$ on $\partial\Omega$ coherently with (2.9).

- The *linearization error fluxes* $\mathbf{\Theta}_{{\rm lin},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$, $c \in \mathcal{C}$, and $\mathbf{\Theta}_{{\rm lin},H,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ such that, for all $M \in \mathcal{M}^n$ and all $\sigma \in \mathcal{E}_M^{{\rm i},n}$,

$$\begin{aligned}(\mathbf{\Theta}_{{\rm lin},c,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma &= F_{c,M,\sigma}^{n,k,i} - F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}),\\ (\mathbf{\Theta}_{{\rm lin},H,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_\sigma &= F_{H,M,\sigma}^{n,k,i} - F_{H,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}) + G_{M,\sigma}^{n,k,i} - G_{M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i}),\end{aligned} \tag{4.3}$$

  with $F_{c,M,\sigma}^{n,k,i}$, $F_{H,M,\sigma}^{n,k,i}$, and $G_{M,\sigma}^{n,k,i}$ defined by (3.19)–(3.22), while $\mathbf{\Theta}_{{\rm lin},c,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = \mathbf{\Theta}_{{\rm lin},H,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = 0$ on $\partial\Omega$.

- The *algebraic error fluxes* $\mathbf{\Theta}_{{\rm alg},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$, $c \in \mathcal{C}$, and $\mathbf{\Theta}_{{\rm alg},H,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ such that, for all $M \in \mathcal{M}^n$ and for all $\sigma \in \mathcal{E}_M^{{\rm i},n}$,

$$(\mathbf{\Theta}_{{\rm alg},c,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_{\partial M} := -R_{c,M}^{n,k,i}, \qquad (\mathbf{\Theta}_{{\rm alg},H,h}^{n,k,i}\cdot\boldsymbol{n}_M,1)_{\partial M} := -R_{H,M}^{n,k,i}, \tag{4.4}$$

  with $R_{c,M}^{n,k,i}$ and $R_{H,M}^{n,k,i}$ defined by (3.17) and (3.18), respectively, with $\mathbf{\Theta}_{{\rm alg},c,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = \mathbf{\Theta}_{{\rm alg},H,h}^{n,k,i}\cdot\boldsymbol{n}_\Omega = 0$ on $\partial\Omega$.

- The *total fluxes* $\mathbf{\Theta}_{c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$, $c \in \mathcal{C}$, and $\mathbf{\Theta}_{H,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ are then obtained from the above quantities letting

$$\mathbf{\Theta}_{c,h}^{n,k,i} := \mathbf{\Theta}_{{\rm dis},c,h}^{n,k,i} + \mathbf{\Theta}_{{\rm lin},c,h}^{n,k,i} + \mathbf{\Theta}_{{\rm alg},c,h}^{n,k,i}, \qquad \mathbf{\Theta}_{H,h}^{n,k,i} := \mathbf{\Theta}_{{\rm dis},H,h}^{n,k,i} + \mathbf{\Theta}_{{\rm lin},H,h}^{n,k,i} + \mathbf{\Theta}_{{\rm alg},H,h}^{n,k,i}. \tag{4.5}$$

5 A posteriori error estimate

In this section we describe the weak solution for the thermal multiphase compositional model of Section 2.3, we define an error measure composed of the dual norm of the residual augmented by a nonconformity evaluation term, and derive an a posteriori estimate allowing to distinguish the different sources of the error.

5.1 Weak solution

We proceed in the same spirit as for the isothermal case considered in [22]. In the following, $(\cdot,\cdot)_D$ stands for the L^2-scalar product on $D \subset \Omega$ and $\|\cdot\|_D$ for the associated norm; the same notation is used for both scalar and vector arguments, and the subscript is dropped whenever $D = \Omega$. We define

$$X := L^2((0,t_{\mathrm{F}}); H^1(\Omega)), \qquad Y := H^1((0,t_{\mathrm{F}}); L^2(\Omega)). \tag{5.1}$$

Let $\varepsilon > 0$ be a (small) parameter which only needs to satisfy $\varepsilon \le 1$. We equip the space X with the following norm:

$$\|\varphi\|_X := \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{M\in\mathcal{M}^n} \|\varphi\|_{X,M}^2 \,\mathrm{d}t \right\}^{\frac{1}{2}}, \qquad \|\varphi\|_{X,M}^2 := \varepsilon h_M^{-2} \|\varphi\|_M^2 + \|\nabla\varphi\|_M^2 . \tag{5.2}$$

This choice is motivated by the homogeneous Neumann boundary conditions (2.9). Taking $\varepsilon = 0$ is possible and classical when Dirichlet (pressure and temperature) boundary conditions are prescribed at least on a part of the boundary, cf. [25, 49, 12]. We suppose sufficient regularity to satisfy:

Assumption 5.1 (Regularity of the exact solution)**.** *The weak solution of the multiphase compositional thermal problem of Section 2.3 can be characterized as follows:*

$$l_c \in Y \qquad \forall c \in \mathcal{C}, \tag{5.3a}$$
$$e_H \in Y, \tag{5.3b}$$
$$P_p(P,\boldsymbol{S}) \in X \qquad \forall p \in \mathcal{P}, \tag{5.3c}$$
$$T \in X, \tag{5.3d}$$
$$\boldsymbol{\Phi}_c \in [L^2((0,t_{\mathrm{F}}); L^2(\Omega))]^d \qquad \forall c \in \mathcal{C}, \tag{5.3e}$$
$$\boldsymbol{\Phi}_H \in [L^2((0,t_{\mathrm{F}}); L^2(\Omega))]^d, \tag{5.3f}$$
$$\int_0^{t_{\mathrm{F}}} \{(\partial_t l_c,\varphi)(t) - (\boldsymbol{\Phi}_c,\nabla\varphi)(t)\}\,\mathrm{d}t = \int_0^{t_{\mathrm{F}}} (q_c,\varphi)(t)\mathrm{d}t \qquad \forall \varphi \in X,\ \forall c \in \mathcal{C}, \tag{5.3g}$$
$$\int_0^{t_F} \{(\partial_t e_H,\varphi)(t) - (\boldsymbol{\Phi}_H,\nabla\varphi)(t)\}\,\mathrm{d}t = \int_0^{t_F} (Q_H,\varphi)(t)\mathrm{d}t \qquad \forall \varphi \in X, \tag{5.3h}$$
the initial condition (2.10) *holds,* (5.3i)
the algebraic closure equations (2.11) *and the inequalities of fugacities hold,* (5.3j)

where P_p, l_c, e_H, $\boldsymbol{\Phi}_c$, and $\boldsymbol{\Phi}_H$ are defined, respectively, by (2.1), (2.2), (2.6), (2.4), *and* (2.8).

We mention that existence and uniqueness of a weak solution has to our knowledge not been established for the general thermal multiphase compositional model.

Remark 5.2 (PDEs fluxes)**.** *It follows from* (5.3b)–(5.3a), *the assumptions $q_c \in L^2((0,t_{\mathrm{F}});\, L^2(\Omega))$, $Q_H \in L^2((0,t_{\mathrm{F}});\, L^2(\Omega))$,* (5.3e)–(5.3f), *and* (5.3g)–(5.3h) *that actually*

$$\boldsymbol{\Phi}_c, \boldsymbol{\Phi}_H \in L^2((0,t_{\mathrm{F}}); \mathbf{H}(\mathrm{div},\Omega)), \tag{5.4a}$$
$$\nabla\cdot\boldsymbol{\Phi}_c = q_c - \partial_t l_c \qquad \forall c \in \mathcal{C}, \tag{5.4b}$$
$$\nabla\cdot\boldsymbol{\Phi}_H = Q_H - \partial_t e_H, \tag{5.4c}$$
$$\boldsymbol{\Phi}_c\cdot\boldsymbol{n}_\Omega = 0 \quad \text{on } \partial\Omega\times(0,t_{\mathrm{F}}) \qquad \forall c \in \mathcal{C}, \tag{5.4d}$$
$$\boldsymbol{\Phi}_H\cdot\boldsymbol{n}_\Omega = 0 \quad \text{on } \partial\Omega\times(0,t_{\mathrm{F}}). \tag{5.4e}$$

Thus, the component fluxes $\boldsymbol{\Phi}_H, \boldsymbol{\Phi}_c$ have continuous normal trace in a proper weak sense, the governing equations (2.3) *and* (2.7) *are satisfied with a weak divergence, and the boundary conditions* (2.9) *hold in the normal trace sense. This in particular motivates the flux reconstructions* (4.5).

5.2 Error measure

Consider the approximate solution as specified in Sections 4.1–4.2, defined on the whole space–time slab $\Omega \times (0, t_{\rm F})$ (we omit here the indices n, k, i for simplicity). The error measure from [22, Section 3.3] for the isothermal multiphase compositional model consists here of the quantities $\mathcal{N}_c, c \in \mathcal{C}$, and $\mathcal{N}_p, p \in \mathcal{P}$, depending on $\boldsymbol{P}_{h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, (\boldsymbol{C}_{p,h\tau})_{p\in\mathcal{P}}$, defined as, respectively,

$$\mathcal{N}_c := \sup_{\varphi\in X, \|\varphi\|_X=1} \int_0^{t_{\rm F}} \left\{ (\partial_t l_c - \partial_t l_{c,h\tau}, \varphi)(t) - \left(\boldsymbol{\Phi}_c - \boldsymbol{\Phi}_{c,h\tau}, \nabla\varphi\right)(t) \right\} \mathrm{d}t, \tag{5.5}$$

with the exact component fluxes $\boldsymbol{\Phi}_c$ defined by (2.4) and $\boldsymbol{\Phi}_{c,h\tau}$ given by

$$\boldsymbol{\Phi}_{c,h\tau} := \sum_{p\in\mathcal{P}_c} \boldsymbol{\Phi}_{p,c,h\tau}, \qquad \boldsymbol{\Phi}_{p,c,h\tau} := \nu_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, \boldsymbol{C}_{p,h\tau}) C_{p,c,h\tau} \boldsymbol{v}_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{C}_{p,h\tau}), \tag{5.6}$$

and

$$\mathcal{N}_p := \inf_{\delta_p\in X} \left\{ \sum_{c\in\mathcal{C}_p} \int_0^{t_{\rm F}} \left\| \boldsymbol{\Psi}_{p,c}(P_{p,h\tau})(t) - \boldsymbol{\Psi}_{p,c}(\delta_p)(t) \right\|^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \tag{5.7}$$

where, for a space–time function $\varphi \in L^2((0, t_{\rm F}); H^1(\mathcal{M}))$ (piecewise regular in space with respect to the partitions $\mathcal{M}^n$), we have let

$$\boldsymbol{\Psi}_{p,c}(\varphi) := \nu_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, \boldsymbol{C}_{p,h\tau}) C_{p,c,h\tau} \mathbb{K} \nabla\varphi. \tag{5.8}$$

As we consider a non-isothermal flow, we need to add some other contributions to define an error measure taking into account the energy equation. We define

$$\begin{aligned} \mathcal{N}_H &= \mathcal{N}_H(\boldsymbol{P}_{h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, (\boldsymbol{C}_{p,h\tau})_{p\in\mathcal{P}}) \\ &:= \sup_{\varphi\in X, \|\varphi\|_X=1} \int_0^{t_F} \left\{ (\partial_t e_H - \partial_t e_{H,h\tau}, \varphi)(t) - \left(\boldsymbol{\Phi}_H - \boldsymbol{\Phi}_{H,h\tau}, \nabla\varphi\right)(t) \right\} \mathrm{d}t, \end{aligned} \tag{5.9}$$

with $\boldsymbol{\Phi}_H$ defined by (2.8) and $\boldsymbol{\Phi}_{H,h\tau}$ given by

$$\boldsymbol{\Phi}_{H,h\tau} := \mathbf{J}_{h\tau}(T_{h\tau}) + \sum_{p\in\mathcal{P}} \boldsymbol{\Phi}_{p,H,h\tau}, \tag{5.10}$$

where

$$\boldsymbol{\Phi}_{p,H,h\tau} := \nu_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, \boldsymbol{C}_{p,h\tau}) H_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{C}_{p,h\tau}) \boldsymbol{v}_p(P_{p,h\tau}, T_{h\tau}, \boldsymbol{C}_{p,h\tau}), \tag{5.11}$$

and for a space-time function $\varphi \in L^2((0, t_{\rm F}); H^1(\mathcal{M}))$, we have let

$$\mathbf{J}_{h\tau}(\varphi) := -\lambda \nabla\varphi. \tag{5.12}$$

Note here that the definition (5.9) corresponds to the dual norm of the residual inspired from the weak formulation (5.3h) related to the energy equation. We supplement this term by defining a nonconformity measure for the temperature,

$$\mathcal{N}_T = \mathcal{N}_T(\boldsymbol{P}_{h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, (\boldsymbol{C}_{p,h\tau})_{p\in\mathcal{P}}) := \inf_{\theta\in X} \left\{ \int_0^{t_F} \left\| \mathbf{J}_{h\tau}(T_{h\tau})(t) - \mathbf{J}_{h\tau}(\theta)(t) \right\|^2 \mathrm{d}t \right\}^{\frac{1}{2}}. \tag{5.13}$$

Collecting all the previous contributions, we define the error measure for the multiphase thermal compositional model as

$$\mathcal{N}_e = \mathcal{N}_e(\boldsymbol{P}_{h\tau}, T_{h\tau}, \boldsymbol{S}_{h\tau}, (\boldsymbol{C}_{p,h\tau})_{p\in\mathcal{P}}) := \left\{ \sum_{c\in\mathcal{C}} {\mathcal{N}_c}^2 + {\mathcal{N}_H}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p\in\mathcal{P}} {\mathcal{N}_p}^2 + {\mathcal{N}_T}^2 \right\}^{\frac{1}{2}}. \tag{5.14}$$

A localized version of this error measure can be obtained as follows: For each approximation as defined in Sections 4.1–4.2, we let

$$\mathcal{N}_e^{n,k,i} := \left\{ \sum_{c\in\mathcal{C}} \mathcal{N}_c^{n,k,i^2} + \mathcal{N}_H^{n,k,i^2} \right\}^{\frac{1}{2}} + \left\{ \sum_{p\in\mathcal{P}} \mathcal{N}_p^{n,k,i^2} + \mathcal{N}_T^{n,k,i^2} \right\}^{\frac{1}{2}}, \tag{5.15}$$

with $\mathcal{N}_c^{n,k,i}$, $c\in\mathcal{C}$, $\mathcal{N}_p^{n,k,i}$, $p\in\mathcal{P}$, $\mathcal{N}_H^{n,k,i}$, and $\mathcal{N}_T^{n,k,i}$ localized versions of respectively (5.5), (5.7), (5.9), and (5.13), where time integration is performed on I_n instead of $(0,t_F)$.

The error measure for the exact solution satisfying Assumption 5.1 is zero. Conversely, shall the approximate solution satisfy exactly the initial condition and have the error measure zero, then it satisfies Assumption 5.1.

5.3 An a posteriori error estimate distinguishing the space, time, linearization, and algebraic errors

In this section we propose an a posteriori estimate for the time-localized error measure (5.15) that we subsequently adapt to distinguish the different sources of error.

5.3.1 A basic time-localized a posteriori error estimate

For $1\le n\le N$, we define the piecewise constant space functions $q_{c,h}^n$, $c\in\mathcal{C}$, and $Q_{H,h}^n$, such that $q_{c,h}^n|_M = \int_{I_n}\int_M q_c/(|M|\tau_n)$, $c\in\mathcal{C}$, and $Q_{H,h}^n|_M = \int_{I_n}\int_M Q_H/(|M|\tau_n)$, respectively. For further use we also define the piecewise constant space-time functions $q_{c,h\tau}$, $Q_{H,h\tau}$, such that $q_{c,h\tau}|_{I_n} = q_{c,h}^n$, $Q_{H,h\tau}|_{I_n} = Q_{H,h}^n$, respectively, for all $1\le n\le N$.

Let $1\le n\le N$, a Newton linearization iteration $k\ge 1$, and an algebraic solver iteration $i\ge 1$ be fixed. It follows from (3.17), (3.18), the definition (4.5) of the flux reconstructions $\mathbf{\Theta}_{c,h}^{n,k,i}$, $c\in\mathcal{C}$, and $\mathbf{\Theta}_{H,h}^{n,k,i}$, and Green's theorem that there holds,

$$\left(q_{c,h}^n - \frac{l_{c,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) + \mathfrak{L}_{c,M}^{n,k,i} - l_{c,M}^{n-1}}{\tau^n} - \nabla\cdot\mathbf{\Theta}_{c,h}^{n,k,i}, 1\right)_M = 0 \qquad \forall M\in\mathcal{M}^n,$$

$$\left(Q_{H,h}^n - \frac{e_{H,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) + \mathfrak{E}_{c,M}^{n,k,i} - e_{H,M}^{n-1}}{\tau^n} - \nabla\cdot\mathbf{\Theta}_{H,h}^{n,k,i}, 1\right)_M = 0 \qquad \forall M\in\mathcal{M}^n.$$

Let $C_M := \min\{C_{\mathrm{P},M}, \varepsilon^{-\frac{1}{2}}\}h_M$. Then following [22] we define the following estimators:

$$\eta_{\mathrm{R},M,c}^{n,k,i} := C_M \left\| q_{c,h}^n - (\tau^n)^{-1}\big(l_{c,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) + \mathfrak{L}_{c,M}^{n,k,i} - l_{c,M}^{n-1}\big) - \nabla\cdot\mathbf{\Theta}_{c,h}^{n,k,i}\right\|_M, \qquad \forall c\in\mathcal{C}, \tag{5.16a}$$

$$\eta_{\mathrm{R},M,H}^{n,k,i} := C_M \left\| Q_{c,h}^n - (\tau^n)^{-1}\big(e_{H,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) + \mathfrak{E}_{c,M}^{n,k,i} - e_{H,M}^{n-1}\big) - \nabla\cdot\mathbf{\Theta}_{H,h}^{n,k,i}\right\|_M, \tag{5.16b}$$

$$\eta_{\mathrm{F},M,c}^{n,k,i}(t) := \left\| \mathbf{\Theta}_{c,h}^{n,k,i} - \mathbf{\Phi}_{c,h\tau}^{n,k,i}(t)\right\|_M \qquad \forall t\in I_n,\ \forall c\in\mathcal{C}, \tag{5.16c}$$

$$\eta_{\mathrm{F},M,H}^{n,k,i}(t) := \left\| \mathbf{\Theta}_{H,h}^{n,k,i} - \mathbf{\Phi}_{H,h\tau}^{n,k,i}(t)\right\|_M, \qquad \forall t\in I_n, \tag{5.16d}$$

$$\eta_{\mathrm{NC},M,p,c}^{n,k,i}(t) := \left\| \mathbf{\Psi}_{p,c}(P_{p,h\tau}^{n,k,i})(t) - \mathbf{\Psi}_{p,c}(\mathfrak{P}_{p,h\tau}^{n,k,i})(t)\right\|_M \qquad \forall t\in I_n,\ \forall c\in\mathcal{C},\ \forall p\in\mathcal{P}_c, \tag{5.16e}$$

$$\eta_{\mathrm{NC},M,T}^{n,k,i}(t) := \left\| \mathbf{J}_{h\tau}^{n,k,i}(T_{h\tau}^{n,k,i})(t) - \mathbf{J}_{h\tau}^{n,k,i}(\mathfrak{T}_{h\tau}^{n,k,i})(t)\right\|_M, \qquad \forall t\in I_n, \tag{5.16f}$$

$$\eta_{\mathrm{NA},M,c}^{n,k,i} := \varepsilon^{-\frac{1}{2}} h_M (\tau^n)^{-1} \left\| l_{c,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k,i}\big) - l_{c,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) - \mathfrak{L}_{c,M}^{n,k,i}\right\|_M, \qquad \forall c\in\mathcal{C}, \tag{5.16g}$$

$$\eta_{\mathrm{NA},M,H}^{n,k,i} := \varepsilon^{-\frac{1}{2}} h_M (\tau^n)^{-1} \left\| e_{H,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k,i}\big) - e_{H,M}\big(\mathcal{X}_{\mathcal{M}}^{n,k-1}\big) - \mathfrak{E}_{c,M}^{n,k,i}\right\|_M, \tag{5.16h}$$

where the functions $\mathbf{\Psi}_{p,c}$, $p\in\mathcal{P}$, $c\in\mathcal{C}_p$, are defined by (5.8), and $\mathbf{\Phi}_{c,h\tau}^{n,k,i}$ and $\mathbf{\Phi}_{H,h\tau}^{n,k,i}$ respectively as in (5.6) and (5.10).

The proof of the following result is a straightforward generalization of that of [22, Theorem 3.3] and is omitted for the sake of brevity.

Corollary 5.3 (Time-localized a posteriori error estimate)**.** *Consider a time step $1 \le n \le N$, a Newton linearization iteration $k \ge 1$, and an algebraic solver iteration $i \ge 1$. Under Assumption 5.1 there holds, with estimators given by* (5.16)*,*

$$\mathcal{N}_c^n \le \left\{ \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta_{\mathrm{R},M,c}^{n,k,i} + \eta_{\mathrm{F},M,c}^{n,k,i}(t) + \eta_{\mathrm{NA},M,c}^{n,k,i}\right)^2 \mathrm{d}t \right\}^{\frac12} \qquad c\in\mathcal{C}, \tag{5.17a}$$

$$\mathcal{N}_p^n \le \left\{ \sum_{c\in\mathcal{C}_p} \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta_{\mathrm{NC},M,p,c}^{n,k,i}(t)\right)^2 \mathrm{d}t \right\}^{\frac12} \qquad p\in\mathcal{P}, \tag{5.17b}$$

$$\mathcal{N}_H^{n,k,i} \le \left\{ \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta_{\mathrm{R},M,H}^{n,k,i} + \eta_{\mathrm{F},M,H}^{n,k,i}(t) + \eta_{\mathrm{NA},M,H}^{n,k,i}\right)^2 \mathrm{d}t \right\}^{\frac12}, \tag{5.17c}$$

$$\mathcal{N}_T^{n,k,i} \le \left\{ \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta_{\mathrm{NC},M,T}^{n,k,i}(t)\right)^2 \mathrm{d}t \right\}^{\frac12}. \tag{5.17d}$$

5.3.2 Distinguishing the different error components

For all $1 \le n \le N$, $k \ge 1$, $i \ge 1$, and $M \in \mathcal{M}^n$, we define the *spatial estimators* evaluating the error related to the spatial mesh choice,

$$\eta_{\mathrm{sp},M,c}^{n,k,i}(t) := \eta_{\mathrm{R},M,c}^{n,k,i} + \left\| \boldsymbol{\Theta}_{\mathrm{dis},c,h}^{n,k,i} - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t^n) \right\|_M + \left\{ \sum_{p\in\mathcal{P}_c} \left(\eta_{\mathrm{NC},M,p,c}^{n,k,i}(t)\right)^2 \right\}^{\frac12} \qquad t\in I_n, \tag{5.18a}$$

$$\eta_{\mathrm{sp},M,H}^{n,k,i}(t) := \eta_{\mathrm{R},M,H}^{n,k,i} + \left\| \boldsymbol{\Theta}_{\mathrm{dis},H,h}^{n,k,i} - \boldsymbol{\Phi}_{H,h\tau}^{n,k,i}(t^n) \right\|_M + \eta_{\mathrm{NC},M,T}^{n,k,i}(t) \qquad t\in I_n, \tag{5.18b}$$

the *temporal estimators* evaluating the error related to the size of the time step,

$$\eta_{\mathrm{tm},M,c}^{n,k,i}(t) := \left\| \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t^n) - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t) \right\|_M \qquad t\in I_n, \tag{5.18c}$$

$$\eta_{\mathrm{tm},M,H}^{n,k,i}(t) := \left\| \boldsymbol{\Phi}_{H,h\tau}^{n,k,i}(t^n) - \boldsymbol{\Phi}_{H,h\tau}^{n,k,i}(t) \right\|_M \qquad t\in I_n, \tag{5.18d}$$

the *linearization estimators* measuring the error in the linearization of the nonlinear system (3.3)–(3.4),

$$\eta_{\mathrm{lin},M,c}^{n,k,i} := \left\| \boldsymbol{\Theta}_{\mathrm{lin},c,h}^{n,k,i} \right\|_M + \eta_{\mathrm{NA},M,c}^{n,k,i}, \tag{5.18e}$$

$$\eta_{\mathrm{lin},M,H}^{n,k,i} := \left\| \boldsymbol{\Theta}_{\mathrm{lin},H,h}^{n,k,i} \right\|_M + \eta_{\mathrm{NA},M,H}^{n,k,i}, \tag{5.18f}$$

and the *algebraic estimators* that quantify the error in the algebraic iterative resolution of the linear system (3.13)–(3.14),

$$\eta_{\mathrm{alg},M,c}^{n,k,i} := \left\| \boldsymbol{\Theta}_{\mathrm{alg},c,h}^{n,k,i} \right\|_M, \tag{5.18g}$$

$$\eta_{\mathrm{alg},M,H}^{n,k,i} := \left\| \boldsymbol{\Theta}_{\mathrm{alg},H,h}^{n,k,i} \right\|_M. \tag{5.18h}$$

Global versions of these estimators are given by

$$\eta_{\mathrm{sp},c}^{n,k,i} := \left\{ 4 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{sp},M,c}^{n,k,i}(t) \right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \tag{5.19a}$$

$$\eta_{\mathrm{tm},c}^{n,k,i} := \left\{ 2 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{tm},M,c}^{n,k,i}(t) \right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \tag{5.19b}$$

$$\eta_{\mathrm{lin},c}^{n,k,i} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{lin},M,c}^{n,k,i} \right)^2 \right\}^{\frac{1}{2}}, \tag{5.19c}$$

$$\eta_{\mathrm{alg},c}^{n,k,i} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{alg},M,c}^{n,k,i} \right)^2 \right\}^{\frac{1}{2}} \tag{5.19d}$$

and

$$\eta_{\mathrm{sp},H}^{n,k,i} := \left\{ 4 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{sp},M,H}^{n,k,i}(t) \right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \tag{5.20a}$$

$$\eta_{\mathrm{tm},H}^{n,k,i} := \left\{ 2 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{tm},M,H}^{n,k,i}(t) \right)^2 \mathrm{d}t \right\}^{\frac{1}{2}}, \tag{5.20b}$$

$$\eta_{\mathrm{lin},H}^{n,k,i} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{lin},M,H}^{n,k,i} \right)^2 \right\}^{\frac{1}{2}}, \tag{5.20c}$$

$$\eta_{\mathrm{alg},H}^{n,k,i} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{alg},M,H}^{n,k,i} \right)^2 \right\}^{\frac{1}{2}}. \tag{5.20d}$$

Using the triangle and Cauchy–Schwarz inequalities and Corollary 5.3, we can estimate the time-localized norm $\mathcal{N}_e^n$ of (5.15) as follows:

Corollary 5.4 (Distinguishing the space, time, linearization, and algebraic errors)**.** *Under the assumptions of Corollary 5.3, there holds, with the estimators given by* (5.19)–(5.20)*,*

$$\begin{aligned} \mathcal{N}_e^{n,k,i} \le \Bigg\{ \sum_{c \in \mathcal{C}} & \left(\eta_{\mathrm{sp},c}^{n,k,i} + \eta_{\mathrm{tm},c}^{n,k,i} + \eta_{\mathrm{lin},c}^{n,k,i} + \eta_{\mathrm{alg},c}^{n,k,i} \right)^2 \\ & + \left(\eta_{\mathrm{sp},H}^{n,k,i} + \eta_{\mathrm{tm},H}^{n,k,i} + \eta_{\mathrm{lin},H}^{n,k,i} + \eta_{\mathrm{alg},H}^{n,k,i} \right)^2 \Bigg\}^{\frac{1}{2}}. \end{aligned} \tag{5.21}$$

Criteria can be proposed in the same spirit as for the isothermal case considered in [22] for stopping the iterative algebraic solver and the iterative linearization solver when the corresponding error components do not affect significantly the overall error.

6 Test case

In this Section we present one of the SAGD process simulation, more precisely the Dead Oil model presented in Example 1.

6.1 Model description

The reservoir considered in this test case is a 3-dimensional parallelepiped (100m × 1400m × 55m) discretized by a nonuniform Cartesian grid, see Figure 1 cbrown, right. We consider a homogeneous anisotropic reservoir with 35% porosity, $1.94 \cdot 10^{-12}$ m^2 horizontal permeability, and $0.97 \cdot 10^{-12}$ m^2

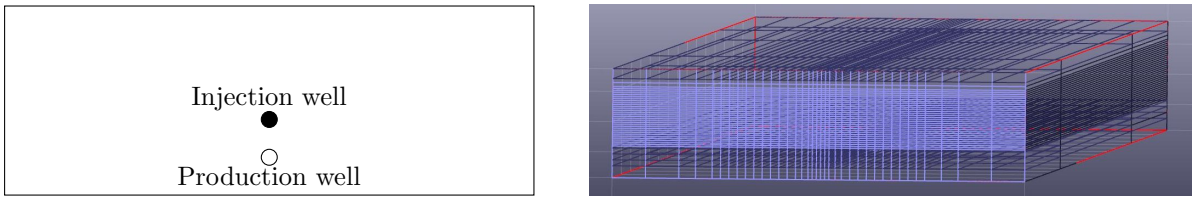


Figure 1: Reservoir mesh

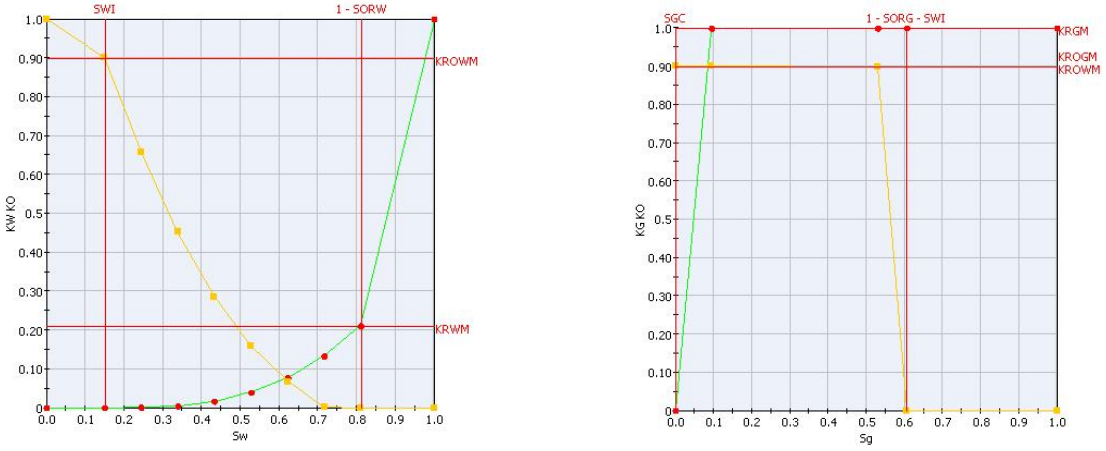


Figure 2: Relative permeability

vertical permeability. Two horizontal wells, injection and production well (in the Y direction) perforate the reservoir, see Figure 1 cbrown, left.

The fluid is a heavy, viscous oil. Viscosity range is tabulated as a function of temperature, from $1.68 \cdot 10^3$Pa·s (at 23.89°C) to $0.741 \cdot 10^{-3}$Pa·s (at 455.44°C). The initial water saturation is equal to 0.15 so that the initial oil saturation is equal to 0.85.

The mass density of the oil for this test case is given by the following formula

$$\rho_{\mathrm{o}}(P,T) = \rho_{\mathrm{o,O}}(P,T) = \rho_{\mathrm{o}}^{\mathrm{ref}}\left[1 + c_{\mathrm{O}}(P - P^{\mathrm{ref}}) + d_{\mathrm{O}}(T - T^{\mathrm{ref}})\right],$$

with a constant compressibility of the oil component $c_{\mathrm{O}} = 72.5 \cdot 10^{-11}\mathrm{Pa}^{-1}$, a constant thermal expansion of the oil component $d_{\mathrm{O}} = 8.5 \cdot 10^{-4}\mathrm{K}^{-1}$, and a constant reference mass density $\rho_o^{\mathrm{ref}} = 63.304$. The water mass density is given by

$$\rho_{\mathrm{w}}(T) = \alpha_1 + \alpha_2 T + \alpha_3 T^2,$$

with $\alpha_1 = 7.81 \cdot 10^2, \alpha_2 = 1.63 \cdot 10^0$, and $\alpha_3 = -3.06 \cdot 10^{-3}$. Water viscosity is given as for a standard water following [45], ($1.002 \cdot 10^{-3}$Pa·s at 20°C).

The capillary pressure is set to zero and the relative permeability is shown in Figure 2. The thermal conductivity $\lambda(t)$ of the rock is constant equal to 33. We mention that the thermal properties of the rock are those of the so-called saturated rock. The compressibility of the rock is constant equal to $43.5 \cdot 10^{-10}\mathrm{Pa}^{-1}$ and the lost in heat in the foot-wall is not simulated.

The SAGD (steam assisted gravity drainage) process is simulated for $t_{\mathrm{F}} = 10$ years. The reservoir is initially assumed at hydrostatic equilibrium with a constant temperature equaling to 11°C. The initial pressure is $7.27 \cdot 10^5$Pa at -400m. To get started the production of the reservoir we begin with a heating phase of the surrounding region of production and injection wells in a period of 90 days. Then, the production well is put into production for one day with high rate of liquid flow without injection to bring down the pressure in the injection zone. Finally a period of injection/production (until 10 years) is held during the simulation. In the model, the injection and production rates are controlled by the pressure ($24.81 \cdot 10^5$Pa for the producer and $25.36 \cdot 10^5$Pa for the injector).

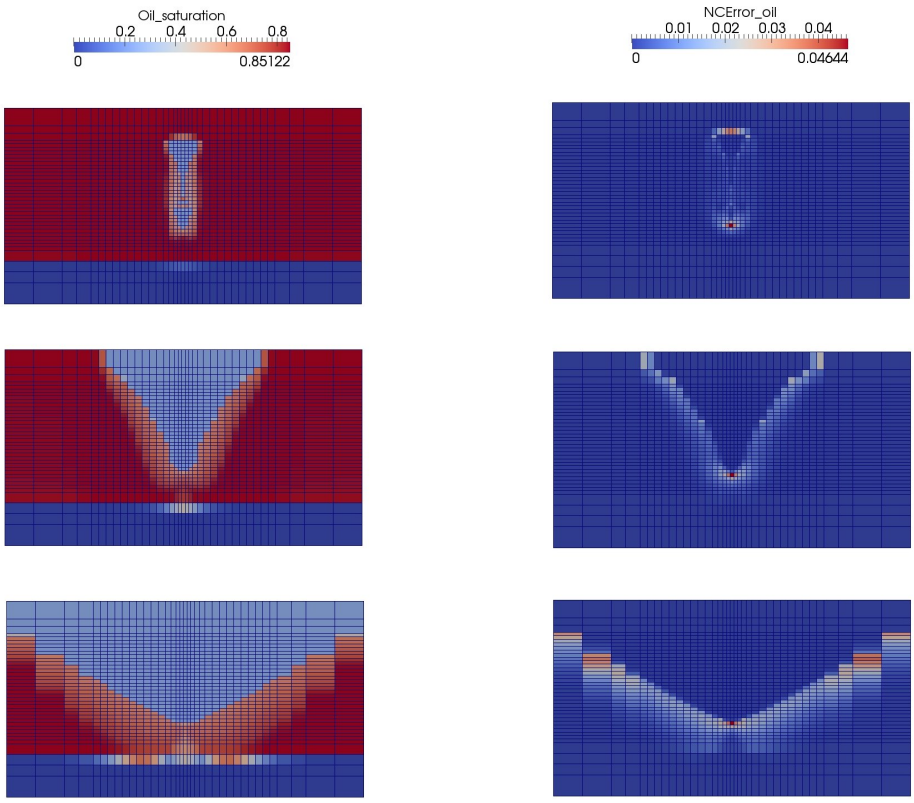


Figure 3: Approximate oil saturation (left) and spatial estimator of the oil phase (right) at 400, 1100, and 2800 days (fixed mesh)

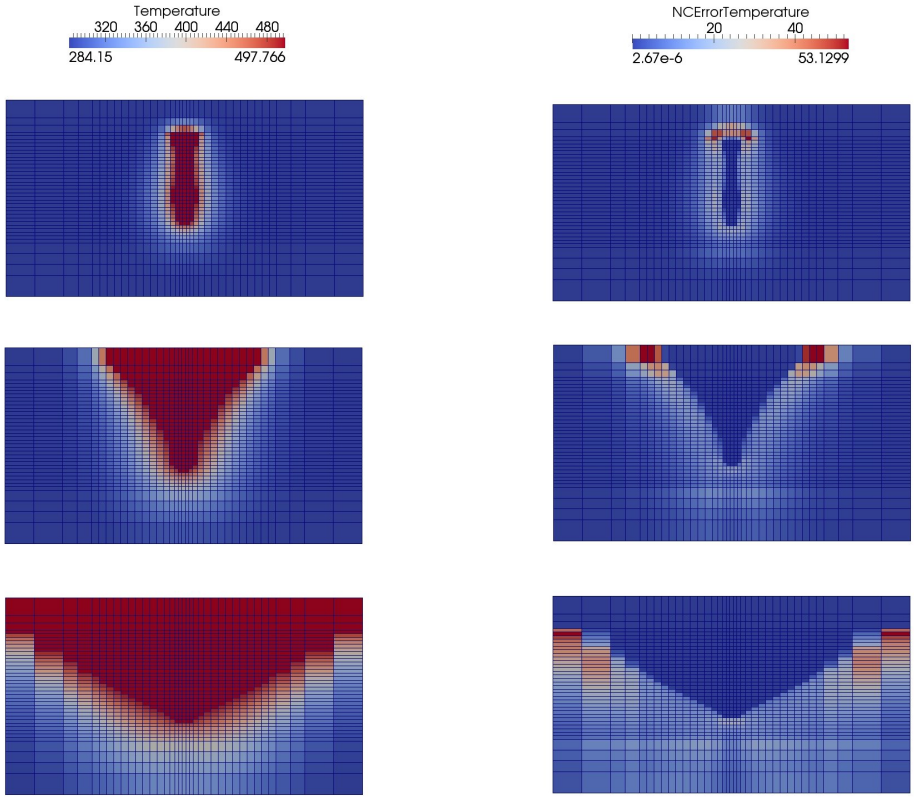


Figure 4: Approximate temperature (left) and temperature spatial estimator (right) at 400, 1100, and 2800 days (fixed mesh)

6.2 Approximate solution and a posteriori estimate

We show here the behavior of the approximate solution and the corresponding a posteriori estimate during the simulation on a fine fixed grid.

Figure 3 shows the evolution of the oil saturation and the corresponding spatial estimator of the oil phase $\eta^n_{\mathrm{sp},M,\mathrm{o}}$ (5.18a) at different time steps. We see an error detected by the estimator around the wells; importantly, this estimator detects the error that follows the movement of the oil front in the reservoir. This result demonstrates that we have a good indicator of the corresponding error and suggests its use in an algorithm of mesh adaptivity.

The results of the evolution of temperature and the temperature's spatial estimator ($\eta^n_{\mathrm{sp},M,T}$ (5.18b)) are summarized in Figure 4. Remark that the predicted error points out an important error in the zone that follows the diffusion of the temperature during the simulation, which shall help us to choose wisely the mesh to refine in order to equilibrate the distribution of the error over the domain and then reduce the size of the system for resolution.

6.3 Adaptive mesh refinement

In this section we numerically assess an adaptive mesh refinement (AMR) strategy based on the space error indicators derived in Section 5.3.2 by comparing the results with a reference solution obtained on a fine grid. As we have a symmetry in the domain, of the flow of the fluid Figure 3, and of the diffusion of temperature Figure 4, we present the results in what follows on the half of the domain only. To refine the mesh adaptively we use a space criterion based on the spatial estimator of the oil phase $\eta^n_{\mathrm{sp},M,\mathrm{o}}$ (5.18a). The algorithm that describes the adaptive strategy can be sketched as follows:

Algorithm 6.1 (Adaptive algorithm)**.**

Fix the fractions of cells to refine, ζ_{ref}, and to derefine, ζ_{deref}
while $t^n \leq t_{\mathrm{F}}$ **do** {Time loop}
  Solve the system (3.3)–(3.4).
  Compute $\eta^n_{\mathrm{tm},M,\mathrm{o}}, \eta^n_{\mathrm{sp},M,\mathrm{o}}$.
  Refine the cells $M \in \mathcal{M}^n$ such that $\eta^n_{\mathrm{sp},M,\mathrm{o}} \geq \zeta_{\mathrm{ref}} \max_{L\in\mathcal{M}^n} \left\{\eta^n_{\mathrm{sp},L,\mathrm{o}}\right\}$.
  Derefine the cells $M \in \mathcal{M}^n$ such that $\eta^n_{\mathrm{sp},M,\mathrm{o}} \leq \zeta_{\mathrm{deref}} \max_{L\in\mathcal{M}^n} \left\{\eta^n_{\mathrm{sp},L,\mathrm{o}}\right\}$.
  Adapt the time step if necessary.
end while

Figure 5 shows the evolution of the approximate oil saturation at different simulation times. We remark that the refinement follows the front of saturation as time evolves, and then the derefinement process is effected in the zones abandoned by the front of oil saturation.

Similar results can be appreciated in Figure 6 where we present the evolution of the temperature at several chosen time steps. A refinement that follows the diffusion of temperature can be observed, as well as a derefinement in the non-exposed zone.

The efficiency of the adaptive algorithm based on the spatial a posteriori estimator can be appreciated in Figure 7. Figure 7a illustrates the cumulated rate of oil production during the simulation; we compare here the result on the fine grid and the result with adaptive mesh refinement. We observe that applying the refinement strategy does not affect the accuracy of the predicted oil production, which is industrially the most important quantity.

The cumulative number of cells during the simulation is shown in Figure 7b. We remark an important reduction in term of the number of cells using the adaptive refinement strategy in comparison with the resolution on the fine grid. On average, the number of cells is reduced by 75%, which is a very important gain.

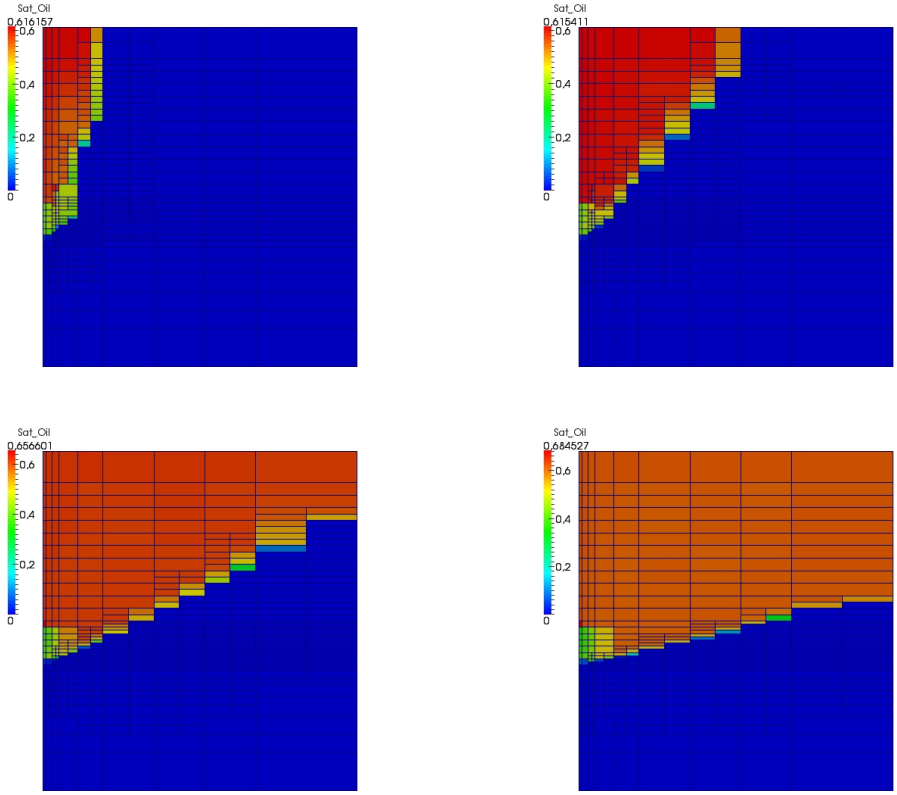


Figure 5: Approximate oil saturation at 2, 4, 8, and 10 years (adaptively refined mesh)

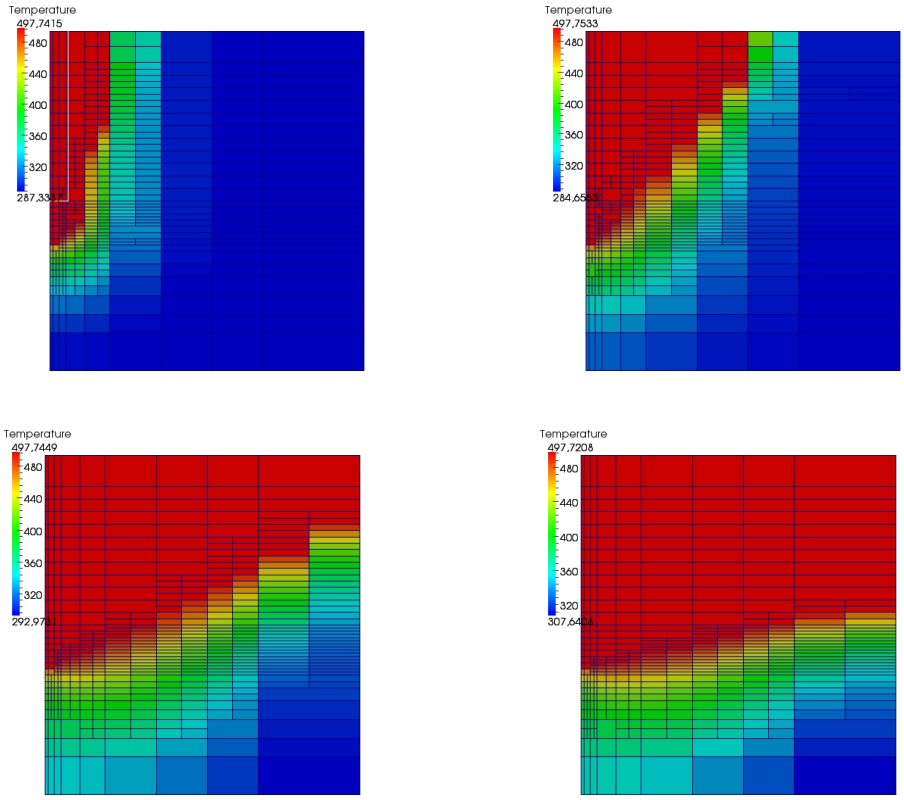
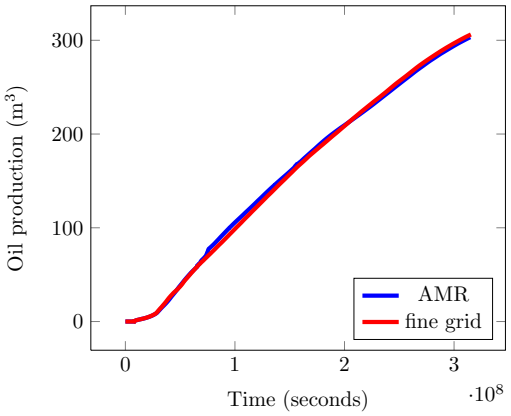
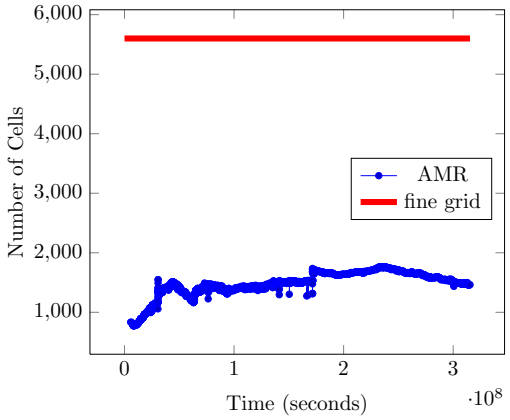


Figure 6: Approximate temperature at 2, 4, 8, and 10 years (adaptively refined mesh)



(a) Cumulated rate of oil production as a function of time



(b) Number of cells as a function of time

Figure 7: Fine grid vs. adaptive mesh refinement. Average reduction of the number of cells : 75%.

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