SELF-ADAPTIVE ALGORITHM BASED ON A POSTERIORI ANALYSIS OF THE ERROR APPLIED TO AIR QUALITY FORECASTING USING THE FINITE VOLUME METHOD

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Abstract. In this work, we present a self-adaptive algorithm based on the techniques of the a posteriori estimates for the transport equation modeling the dispersion of pollutants in the atmospheric boundary layer at the local scale (industrial accident, urban air quality). The goal is to provide a powerful model for forecasting pollutants concentrations with better manipulation of available computing resources.

This analysis is based on a vertex-centered Finite Volume Method in space and an implicit Euler scheme in time. We apply and validate our model, using a self-adaptive algorithm, with real atmospheric data of the Grand Casablanca area (Morocco).

1. Introduction. According to the World Health Organization’s annual report (May 2018 [14]), the contribution of human activities is the main factor negatively influencing the air quality that we breathe. This human contribution together with some natural sources cause pollution of the atmosphere.

In this work, we are interested in pollutant dispersion at the local scale where, at ground level, pollutant has contact with the population, animals, and agriculture. Some dangerous pollutants in the first part of the atmosphere are formed by photochemical reactions like ozone (O_3) or directly issued from road traffic and industry emissions like sulfur dioxide (SO_2) [14].

The goal of this paper is to present a powerful numerical tool to improve the numerical model of pollutants concentration forecasting, this model is based on Partial Differential Equation (PDE) modeling the transport of the pollutant considered at ground level. This model describes the diffusion mechanism, advection due to the wind, and the chemical reactions to which pollutants participate.

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The solution of our model represents the pollutant concentration, and is a function belonging to a functional space of infinite dimension. We will approximate this solution by a vertex-centered Finite Volume discretization of the domain, and will use an implicit Euler scheme for the time discretization. The numerical methods generally give rise to a large linear system whose resolution is expensive in terms of CPU time and computing resources. So, does the resolution of such system provide a good approximation of solution to the model? and are the available computing resources well used? That is why we propose a mesh self-adaptive algorithm based on the a posteriori analysis of the error established in the energy norm in order to obtain an approximate solution very close to the exact one with low calculation costs.

The importance of the a posteriori estimators in the self-adaptation of the mesh is proved in many theoretical works, these estimators are applied in several domains and concrete problems (see for instance [1, 3, 4]). The main results consist of calculating error indicators explicitly in terms of the approximate solution and the data, which make possible estimating the error in all meteorological conditions, at every part in a given simulation domain at every time. We note that in the absence of observations, an estimation of the uncertainty is essentially the only means to assess the quality of the results [10]. To simplify the spatial indicator, we approached the advection flux by a different kind than the one presented in the work of Amaziane et al. [2] and which is different from the approximations treated for this problem in Mallet’s works (see [8]). Another strong point of our approach based on the a posteriori analysis is the calculation of the jump indicator, allowing to detect the zones of the field where there is a strong emission or consumption of the considered pollutant.

Outline. The remainder of the paper is organized as follows:

In Section 1, we introduce the transport model and define all used notations. We use, in Section 2, the Finite Volume Method to build an approximation of our transport model. Then, Section 3 provides the a posteriori analysis; we develop a family of error indicators for the mesh adaptivity. In Section 4, we present numerical results obtained by applying our model to forecast the ozone concentration with a real atmospheric data concerning the Grand Casablanca area (in the north-west of Morocco), where the importance of this work has been valued by comparing the CPU time and the number of elements in the domain of dispersion before and after the use of the self-adaptive algorithm; we had the same tolerance in reducing the number of elements from 22887 to 1374 in 29.37% of the initial CPU time. Finally, we give a comparison of some forecasted concentration obtained in two parts of the domain before and after the use of our algorithm.

2. Numerical model of the transport equation. In this work, we restricted to the first part of the troposphere called the atmospheric boundary layer [13], which can be defined as the part of the troposphere influenced in one hour or less by changes in the neighborhood of the earth surface (heating, evaporation, emissions of pollutants ...), so its height can vary between several tens of meters (night) and a few kilometers.

Since the concentration of pollutants in the atmosphere is not only subject to diffusion mechanism and advection due to the wind transport, but also subject to chemical reactions. These reactions can increase or decrease the presence of such
pollutant and its lifespan in the mechanism, therefore we find in our model a term ("rc") related to the balance of production and chemical reaction losses.

The equation modeling the pollutant transport in the atmospheric boundary layer is given by [9]:

$$\frac{\partial c}{\partial t} - \text{div}(D \nabla c) + \text{div}(V c) + rc = S_i - L_i.$$  \hspace{1cm} (1)

The first term $\partial c/\partial t$ represents the accumulation of the pollutant concentration $c$ over time in the domain of dispersion. $\text{div}(D \nabla c)$ is the diffusion term, $D$ is the diffusion matrix, representing the diffusive mobility of the pollutant. Furthermore, $\text{div}(V c)$ is the advection term, $V$ is the wind velocity vector. The term $rc$ is the balance of production and loss by chemical reaction of the pollutant with $r$ is the reaction coefficient, it is expressed by the use of a suitable chemical mechanism [6], we cite two examples of mechanisms that include a fixed number of species; RADM2 [12] and RACM [11]. Finally, $S_i$ is the sources term (emissions) of the pollutant and the last term $L_i$ represents leaching losses (rain for example).

We note that the different parameters used in this PDE depend on time and space, but also on weather illumination (for the photolysis), temperature, pressure, and humidity. In Section 4, we use Louiss parametrizations [7] to calculate these parameters.

To complete the description of the model, we must add the boundary conditions; in the ground, the only flows taken into account are those related to the dry deposition denoted $D_i$ and emissions denoted $S_i$, we have the Neumann boundary condition given by:

$$D \frac{\partial c}{\partial n} = S_i - D_i,$$

where $n$ is the unit outer-normal vector in ground oriented in the direction of increasing altitudes [15]. For the initial condition, we take $c(\cdot, t_0) = c_0$ the given initial concentration of pollutant.

Since the main wind components are horizontal [8, 15], then our simplified model will be treated in two dimensions. In fact, in the atmospheric boundary layer, the horizontal wind is typically of order a few meters per second (2 to 10 $m.s^{-1}$), the vertical winds are very weak; they are of order millimeters or centimeters per second, so they are negligible.

In this paper, we deal with the following problem (P), without losing generality, by choosing a simple boundary conditions in order to simplify the a posteriori analysis of the error. However, the problem can be treated using other boundary conditions, it’s depending on the studied case,

\begin{equation}
(P) \begin{cases}
\text{Find } c \in L^2(0, T; H^1(\Omega)) \text{ such that } \frac{\partial c}{\partial t} \in L^2(0, T; H^{-1}(\Omega)) \text{ and } \\
\frac{\partial c}{\partial t} - \text{div}(D \nabla c) + \text{div}(V c) + rc = f \text{ in } \Omega \times ]0, T[, \\
D \frac{\partial c}{\partial n} = g \text{ on } \Gamma_1 \times ]0, T[, \\
D \frac{\partial c}{\partial n} = 0 \text{ on } \Gamma_i \times ]0, T[, \; i = 2, \cdots, 4, \\
c(\cdot, 0) = c_0 \text{ in } \Omega,
\end{cases}
\end{equation}
where $\Omega = [0, 1] \times [0, 1]$ is a bounded polygonal domain in $\mathbb{R}^2$, with Lipschitz boundary $\Gamma = \bigcup_{i=1}^{4} \Gamma_i$ such that: $\Gamma_1 = [0, 1] \times \{0\}$, $\Gamma_2 = \{0\} \times [0, 1]$, $\Gamma_3 = [0, 1] \times \{1\}$, and $\Gamma_4 = \{1\} \times [0, 1]$. The time interval is $[0,T]$ with $T > 0$.

$D$ is a space uniform continuous and a time differentiable function in $\Omega \times [0,T]$, satisfying:

$\forall x \in \Omega, \forall t \in [0,T]$, $0 < D_{\min} \leq D(x,t) \leq D_{\max} < +\infty$.

We suppose $f \in L^2(0,T; L^2(\Omega))$, $c_0 \in H^1(\Omega)$, $V \in C(0,T; W^{1,\infty}(\Omega))^2$, $r \in C(0,T; L^\infty(\Omega))$, and furthermore, there exist two constants $\beta \geq 0$ and $\alpha \geq 0$ such that:

$\frac{1}{2} \text{div} V + r \geq \beta$ and $\|r\|_{L^\infty(\Omega)} \leq \alpha \beta$ in $[0,T]$.

Afterwards, we will use the standard notations of Sobolev spaces.

We write the weak formulation (WF) of the problem $(P)$:

$$
(WF) \quad \begin{cases}
\text{Find } c \in L^2(0,T; H^1(\Omega)) \text{ such that } \frac{\partial c}{\partial t} \in L^2(0,T; H^{-1}(\Omega)) \text{ and } \\
\int_{\Omega} \frac{\partial c}{\partial t} v dx + \int_{\Omega} D \nabla c \cdot \nabla v dx + \int_{\Omega} \text{div}(Vc)v dx \\
+ \int_{\Omega} r c v dx = \int_{\Omega} f v dx + \int_{\Gamma_1} g v ds, \forall v \in H^1(\Omega) \\
c(.,0) = c_0.
\end{cases}
$$

This problem admits a unique solution [5].

3. Finite volume discretizations of the model. For the space discretization, we consider $T_h^n$ a regular triangulation of $\Omega$ by $N$ closed triangles $T$, and denote by $V_h^n$ the Vertex-centered dual mesh associated to $T_h^n$ formed by $M$ volumes $V_i$, each volume is obtained by connecting the middle points of edges and circumcenter of each neighboring pair of triangles having a common edge with a straight line segment (shown in Figure 1). Then we have $\Omega = \bigcup_{i=1}^{M} V_i$. We denote by $\gamma$ the boundary of the volume $V_i$ and by $E_h^n$ the set of edges $E$ of the primal triangulation $T_h^n$. Let $\Gamma_h^n$ be the set of edges $\gamma$ of the dual decomposition $V_h^n$.

We denote by $c^n$, $D^n$, $r^n$, $f^n$, and by $g^n$ approximations of $c(t_n)$, $D(t_n)$, $r(t_n)$, $f(t_n)$, and of $g(t_n)$, respectively.

For the time discretization, we consider a partition of the time interval $[0,T]$ into sub-intervals $[t_{n-1}, t_n]$, $n = 1, \ldots, M_n$ such that $0 = t_0 < t_1 < t_2 < \cdots < t_{M_n-1} < t_{M_n} = T$, $\Delta t_n$ is the length $t_n - t_{n-1}$.
We consider the following semi-implicit time discretization of the problem (P):

$$\frac{c^n - c^{n-1}}{\Delta t_n} - \text{div}(D^nc^n) + \text{div}(V^{n-1}c^{n-1}) + r^n c^n = f^n \text{ in } \Omega, \quad (4)$$

**Numerical finite volume scheme:** Over each control volume $V_i$ in $\Omega$, we integrate the previous equation (4) and obtain:

$$\int_{V_i} \frac{c^n - c^{n-1}}{\Delta t_n} dx - \sum_{\gamma \subset \partial V_i} \left\{ \int_{\gamma} D^nc^n \cdot n_{\gamma} ds - \int_{\gamma} V^{n-1}c^{n-1} \cdot n_{\gamma} ds \right\}$$

$$+ \sum_{\gamma \subset \Gamma_i \cap \partial V_i} \int_{\gamma} V^{n-1}c^{n-1} \cdot n_{\gamma} ds + \int_{V_i} r^n c^n dx = \int_{V_i} f^n dx + \sum_{\gamma \subset \Gamma_i \cap \partial V_i} \int_{\gamma} g^n ds,$$

where $n_{\gamma}$ is the unit outward normal vector on $\gamma$ and $V_i^{\text{int}}$ is the set of interior control volumes.

Let $c^n_i$ be a constant approximation of $c^n$ in volume $V_i$ and $c^n_j$ a constant approximation of $c^n$ in volume $V_j$ sharing a common edge $\gamma$ with $V_i$.

The finite volume discretization will be ended by considering the numerical flux functions $F(c^n_i, c^n_j, n_{\gamma})$ and $G(c^{n-1}_i, c^{n-1}_j, n_{\gamma})$ such that:

$$\int_{\partial V_i} D^n_h \nabla c^n \cdot n_{\gamma} dx \approx \sum_{\gamma \subset \partial V_i} |\gamma| F(c^n_i, c^n_j, n_{\gamma}),$$

and

$$\int_{\partial V_i} V^{n-1}c^{n-1} \cdot n_{\gamma} ds \approx \sum_{\gamma \subset \partial V_i} |\gamma| G(c^{n-1}_i, c^{n-1}_j, n_{\gamma}),$$

where $D^n_h$ is an approximation of $D$ as piecewise polynomial.

The discrete problem will be defined at each instant $t_n$ by:

$$(P^n_h) \left\{ \begin{array}{l}
\text{Find } c^n_i; i = 1 \ldots M \text{ such that :}
\left. \begin{array}{l}
|V_i| \frac{c^n_i - c^{n-1}_i}{\Delta t_n} - \sum_{\gamma \subset \partial V_i} |\gamma| \left\{ F(c^n_i, c^n_j, n_{\gamma}) - G(c^{n-1}_i, c^{n-1}_j, n_{\gamma}) \right\}
+ \sum_{\gamma \subset \Gamma_i \cap \partial V_i} \int_{\gamma} V^{n-1}c^{n-1} \cdot n_{\gamma} ds + |V_i|r^n c^n_i
= |V_i|f^n_i + \sum_{\gamma \subset \Gamma_i \cap \partial V_i} \int_{\gamma} g^n ds,
\end{array} \right\}
\end{array} \right\}$$

where $f^n_i$ and $r^n_i$ are respectively the average values of $f^n$ and $r^n$ in $V_i$:

$$f^n_i := \frac{1}{|V_i|} \int_{V_i} f^n(x) dx \text{ and } r^n_i := \frac{1}{|V_i|} \int_{V_i} r^n(x) dx.$$

For every $n$, we obtain the values $(c^n_i)_{i=1, \ldots, M}$ that will be considered as an approximation of the solution at instant $t_n$ in the triangulation $T^n_h$.

We define the spaces $\mathcal{P}_1(T^n_h)$ and $\mathcal{P}_0(V^n_h)$ by:

$$\mathcal{P}_1(T^n_h) := \left\{ u_h \in C^0(\Omega) : u_h|_T \in \mathcal{P}_1; \forall T \in T^n_h \right\},$$

and

$$\mathcal{P}_0(V^n_h) := \left\{ u_h \in C^0(\Omega) : u_h|_V \in \mathcal{P}_0; \forall V \in V^n_h \right\},$$

where $\mathcal{P}_l$ is the set of polynomial functions of degree $\leq l$. 
Let \( X_{(\Omega, h)} := \left\{ v_h \in H^1(\Omega) : \forall T \in T_h^n, v_h|_T \in P_1(T_h^n) \right\} \).

We denote by \( c^n_h \) an element of \( X_{(\Omega, h)} \) constructed by an interpolation using 
\( (c^n_i)_{i=1}^M \),

ie: \( c^n_h = \sum_{i=1}^M \psi_i c^n_i \) where \( \{\psi_i\}_{i=1}^{N_n} \) is the set of basis functions of \( P_1(T_h^n) \) such that:

\[
\psi_i(x_j) := \begin{cases} 
1 & \text{if } i = j, \\
0 & \text{else}.
\end{cases}
\]

Let \( c_{h, \Delta t} \) be an interpolation of \( (c^n_h), n = 0, \ldots, N_n \), with respect to time \( t \) in \([0, T]\),
which is defined by:

\[
c_{h, \Delta t} := c^n_{h-1} + \frac{t - t_{n-1}}{\Delta t_n} (c^n_h - c^n_{h-1}), \quad \forall t \in [t_{n-1}, t_n],
\]

or

\[
c_{h, \Delta t} := c^n_h - \frac{t_n - t}{\Delta t_n} (c^n_h - c^n_{h-1}), \quad \forall t \in [t_{n-1}, t_n].
\]

We give in the last section the numerical simulation using the finite volume scheme (5) proved in this work for the transport equation of the ozone. The discrete problem is given by this linear system:

\[
A c^n = b,
\]

where \( A = (1 + r \Delta t) I + A_1 \), \( I \) is the identity matrix, \( A_1 \) is the matrix representing the diffusion term, and \( b = (I - A_2) c^{n-1} + F \), \( A_2 \) is the matrix corresponding to the advection term and \( F = \Delta t [f(x_1), \ldots, f(x_M)]^T \).

4. A posteriori error analysis. A simulation carried out by a numerical method can take a lot of time especially if we treat a concrete problem on a field of diffusion of large dimensions. A delicate phase in this process is the construction of the mesh. Indeed, if the mesh is too coarse, the duration of the computations will be short, but we lose the quality of the approximate solution. On the other hand, if the mesh is very fine, there are two disadvantages; first, the fact that the calculation may be unnecessarily long because some areas do not require a fine mesh; secondly, the process itself may end in an external interruption (limit of time exceeded for example). We must therefore find a good compromise so that the mesh is fine only where it is necessary.

In order to be able to develop an adaptive method, one will resort to a posteriori error estimates. The interest of these estimates is to provide bounds on the error that can be evaluated as soon as the approximate solution has been calculated. Indeed, these limits are evaluated only according to the discreet solution and the data of the problem and of the mesh.

Before giving the upper bound for the error using the finite volume approximation, we need to consider \( Q^n_h \), another partition of \( \Omega \) formed by the quadrilaterals \( Q \) defined by \( Q = V \cap T \) where \( V \in \mathcal{V}_n^h \) and \( T \in T^n_h \), we also define the set \( K^n_h = \cup T \) formed by the triangles \( T \) having \( x_i \) (the center of the control volume \( V_i \)) as a vertex and \( \gamma \) as an edge.

In this work, the estimates are established in the energy norm defined as follows:

\[
|[c - c_{h, \Delta t}](t)| := \left\{ ||(c - c_{h, \Delta t})(t)||^2_{0, \Omega} + \int_0^t ||(c - c_{h, \Delta t})(s)||^2 ds \right\}^{1/2},
\]
where
\[ ||c|| := \left\{ \|D^{1/2} \nabla c\|_{0,\Omega}^2 + \beta ||c||_{0,\Omega}^2 \right\}^{1/2}. \]

In the following, we are interested in building a family of indicators simultaneously estimating errors related to time and space discretization.

Then, we define the space error indicator of the approximation \( c_h^n \) by:
\[
(\eta_h^n)^2 := \sum_{V \in \mathcal{V}_h} \sum_{Q \subset V} \alpha_Q^2 ||f^n_Q - c_h^n - c_h^{n-1} \Delta t||_Q + \text{div}(D_h^n \nabla c_h^n) - \text{div}(V^{n-1} c_h^{n-1}) - r_h^n c_h^n ||_0,\Omega
\]
\[ + D_{\text{min}}^{-1/2} \sum_{E \in \mathcal{E}_h} \alpha_E \left\| \left[ D_h^n \frac{\partial c_h^n}{\partial n_E} \right]_E \right\|_{0,E}^2 + \sum_{\gamma \in \Gamma_\partial P} \| g^n - D_h^n c_h^n ||_{0,\gamma}. \tag{9} \]

The first term of \( \eta_h^n \) is the norm of the residual of the transport equation \( (P) \), the second measures the jumps of \( \nabla c_h^n \) across edges, and the last term measures the error in the boundary.

The time error indicator is given at each instant explicitly, and measures the error committed between two successive iterations as a function of the approximate solution and discretization data. This indicator is defined by:
\[
(\theta_h^n)^2 := \frac{\Delta t_n}{3} \left( \| (D_h^n)^{1/2} \nabla (c_h^n - c_h^{n-1}) \|_{0,\Omega}^2 + \| \text{div}(V^{n-1}(c_h^{n-1} - c_h^n)) \|_{0,\Omega}^2 \right.
\]
\[ + \| (r_h^n)^{1/2} (c_h^n - c_h^{n-1}) \|_{0,\Omega}^2 \). \tag{10} \]

Finally, we denote also \( \mu_h^n(t) \) the interpolation error defined by:
\[
\mu_h^n(t) := \max \left( \beta^{-1/2}, D_{\text{min}}^{-1/2} \right) \left( \| f - f_h^n + \text{div}(V^{n-1} - V)c_h,\Delta t \|_{0,\Omega} + \| (D_h^n - D) \nabla c_h,\Delta t \|_{0,\Omega} + \| g^n - g \|_{0,\gamma} \right). \tag{11} \]

**An upper bound for the error.** The previous indicators will be used to give an upper bound of the error between the exact solution and the approximate one. We have this theorem:

**Theorem 4.1.** Let be \( c \) the exact solution of the problem \( (P) \). Then there exists a constant \( C \) independent of mesh, such that:
\[
\|[c - c_h,\Delta t]\|(t_n) \leq C \left\{ \|c_0 - \Pi_0 c_0\|_{0,\Omega}^2 + \sum_{m=1}^{n} \left( (\Delta t_m \eta_h^n)^2 + (\theta_h^m)^2 + \int_{t_{m-1}}^{t_m} \| \mu_h^n(t) \|^2 \right) \right\}^{1/2}, \tag{12} \]

where \( \eta_h^n, \theta_h^m, \) and \( \mu \) are defined by \( (9), (10), \) and \( (11), \) respectively.

The proof of this theorem is close to that treated for the problem of porous media (see [2]).
5. Numerical simulation. In this section, in order to give numerical simulation of the treated phenomena, we begin by describing the domain of the study (Grand Casablanca area) where we will apply our numerical model to forecast the concentration of the ozone. Then we present a self-adaptive algorithm based on the techniques of the a posteriori analysis of the error. Finally, we show the effectiveness of our algorithm to minimize computing costs.

5.1. Grand Casablanca area. The Grand Casablanca area is located on the Atlantic coast, in the center-west of Morocco in north-western Africa, it is bounded by the Atlantic Ocean to the west. The study area covers an area of 1615 $Km^2$, or about 0.16% of the total area of the country, (Figure 2).

The climate of this area is oceanic; it is mild and rainy in winter and humid and temperate in summer with absence of frost in winter and high humidity during the year. The signatures in terms of precipitation are quite similar and winter appears as the rainiest season while the months of July are dry.

![Figure 2. The measurement stations on the Grand Casablanca area.](image)

5.2. Numerical results of the ozone transport. The ozone has a harmful effect to humans, animals, and vegetation when it reaches too high concentrations in the air. This is why WHO [14] and also legislators in all countries, set limit values not to exceed or even target values to improve air quality. Prolonged exposure to this pollutant can have a lasting impact on the body, causing cardiopulmonary diseases, asthma, and allergies.

According to the measurements history of ozone concentration on the Grand Casablanca area, it is noticed that the peak of ozone is lived during the summer, that is why, in this simulation we use the real meteorological data of 1st July 2015 to calculate the parameters of our numerical model. We assume that the initial concentration over the entire zone is zero and that the only source of ozone is punctual, this source emits an initial concentration of $64 \mu g.m^{-3}$ at instant $t = 0$.

Since the Grand Casablanca area is of $60 \ km \times \ 60 \ km$ dimension, we will addimensionalize our system by introducing a characteristic concentration of ozone and also a characteristic length $L = 6 \times 10^{-4} \ m$. Then we consider the characteristic time and we get a new variable to see that the differential operators (div) and $\nabla$ are related to the new variable.
We will implement our model with a fast algorithm of the finite volume method. We have based on the Louis parameterizations [7] to calculate the diffusion coefficient $D$, the wind components and the other parameters that appeared during the calculation of the Richardson number ($R_i$). The later allows to determine the stability function ($F(R_i)$)[7]. The advantage of this method of calculation is the fact that it only uses the main characteristics of the flow (speed, pressure, temperature ...) and no longer secondary characteristics that are not always available (the height of the atmospheric boundary layer, the length of Monin-Obukhov, ...). We find in Table 1 the different parameters used in this test.

| Parameter | Signification | Value       |
|-----------|---------------|-------------|
| $D$       | Diffusion coefficient | $95.3 \text{ m}^2\text{s}^{-1}$ |
| $V$       | Velocity vector | $[3.9 \text{ m.s}^{-1}, 1.58 \text{ m.s}^{-1}]$ |
| $r$       | Reaction balance | 3.9         |
| $f$       | Second member  | $2.95 \mu g.m^{-3}$ |
| $c_0$     | Initial concentration | $64 \mu g.m^{-3}$ |

**Self-adaptive algorithm.** We propose a self-adaptive algorithm which ensures the control of the total error with respect to a user-defined precision by refining the spatial mesh automatically. This algorithm is described as follows:

**Table 2.** The self-adaptive algorithm at an iteration.

| Step 1: | Mesh generating and data input. |
| Step 2: | Solve the discrete problem. |
| Step 3: | Calculate the local error indicators. |
| Step 4: | Mark mesh cells and adapt mesh. |
| Step 5: | Solve the discrete problem in the new adapted mesh. |
| Step 6: | if the stopping test is satisfied, go to the step 7 else, go to the step 3. |
| Step 7: | Interpolate solution and visualization. |

To set up our algorithm, we start with the data processing, then we discretize the domain of diffusion, the Grand Casablanca area, by a regular spatial primal mesh with step $h = 0.1$, and by a dual mesh of the vertex-centered type (see Figure 1). We discretize the time interval with a fixed time step 1s, in the next step, we solve the discrete problem (5) on the first mesh. Afterward, we interpolate the approximate solution obtained which represents the concentration of ozone in each part of the domain $\Omega$ at each instant $t \in [12h, 13h]$. This approximate solution will be used to calculate the local error indicators (9) and (10), which will be used later to implement the self-adaptation algorithm of the first mesh. Figures 3 gives numerical simulations obtained using a uniform mesh with 443 elements at two instants $t = 50$ and $t = 1400$.

To improve the quality of the approximate solution, we totally refine the spatial mesh by taking $h = 0.01$, which minimizes the relative error, as shown in Figure 4, but the number of elements and also the CPU time are increased.
Figure 3. Numerical simulations obtained using a uniform mesh with 443 elements at two times $t = 50$, (A), and $t = 1400$, (B).

Figure 4. Numerical simulations obtained using a uniform mesh with 22887 elements at two times $t = 50$, (A), and $t = 1400$, (B).

In order to minimize computing costs without losing the quality of solution, we use the self-adaptive mesh algorithm; the numerical simulation obtained using this algorithm is given in Figure 5, whose quality is clearly improved compared to Figure 3 with less number of elements that automatically decrease the CPU time. The self-adaptation of the used mesh is done in 3 levels at each time, the meshes obtained using our self-adaptive algorithm in each level at instants $t = 50$ and $t = 1400$ are given in Figures 6 and 7.

In Table 3, we give the numerical results at instant $t = 50$.

As shown in Table 4, we notice that at instant $t = 1400$ we obtained the same order of the error after the implementation of the self-adaptive algorithm. However, the number of elements was reduced from 22887 to 1374, which, in turn, reduce the computation time by 70.63%.

In the following, we present in Figure 8 the comparison of numerical simulation results concerning the forecasting of the ozone concentration in two positions: the
Figure 5. (A) and (B) are the approximate solution using a adaptive mesh at $t = 50$ and $t = 1400$ respectively in level 2.

Figure 6. (A), (B) and (C) are the adaptively refined meshes at $t = 50$ in level 1, 2 and 3 respectively.

Table 3. The results obtained before and after the application of the self-adaptive algorithm of the mesh at $t = 50$.

| Level     | Number of elements | jump indicator | residual indicator | CPU time  |
|-----------|--------------------|----------------|--------------------|-----------|
| primal mesh | 443                | $5.0132e-03$   | $1.6088e-04$       | 1.4053 s  |
| $t = 50$  |                    |                |                    |           |
| 1         | 196                | $9.8885e-05$   | $9.4178e-04$       | 6.0905 s  |
| 2         | 278                | $3.1335e-05$   | $2.6348e-04$       | 7.2734 s  |
| 3         | 629                | $7.8928e-06$   | $3.1045e-06$       | 8.2617 s  |
| uniform mesh | 22887            | $1.3548e-07$   | $1.9964e-06$       | 53.4408 s |

Jahid station and the Khansae station before and after the implementation of our algorithm.

6. Conclusion and future works: To obtain a good pollutant dispersion forecasted by a numerical model, it is necessary to minimize the error between the exact
Figure 7. (A), (B) and (C) are the adaptively refined meshes at $t = 1400$ in level 1, 2 and 3 respectively.

Table 4. The results obtained before and after the application of the self-adaptive algorithm of the mesh at $t = 1400$.

| Level       | Number of elements | Jump indicator | Residual indicator | CPU time  |
|-------------|--------------------|----------------|--------------------|-----------|
| Primal mesh | 443                | 1.6483e−05     | 1.9601e−05         | 1.4053 s  |
| Adaptive    |                    |                |                    |           |
| 1           | 828                | 1.3212e−07     | 1.9516e−06         | 18.1240 s |
| 2           | 1374               | 7.2050e−08     | 1.5499e−07         | 25.0560 s |
| uniform mesh| 22887              | 1.1405e−08     | 1.2477e−07         | 95.6868 s |

Figure 8. Forecasted concentration of ozone before and after the implementation of our algorithm in two positions: Jahid station, (A) and Khansae station, (B).

This relative error is due either to the physical parameters or the choice of the numerical method. At this end, we used the Louis parametrizations and applied the techniques of mesh self-adaptation based on the a posteriori estimations.
The numerical study revealed the influence of using a mesh self-adaptive algorithm with respect to computational cost and the accuracy of the simulations. Indeed, as shown in Figure 8 and Table 4, we got a better approximation of the solution by considering the self-adaptive algorithm, based on a posteriori analysis; this algorithm reduced the number of nodes by 70.63% and the CPU time by 73.81% comparing to classical algorithm without losing the quality of the simulation. Summarizing, mesh self-adaptive algorithm is an effective tool to obtain accurate solutions with less computational cost.

The jump term in the spatial indicator gives additional information on the studied phenomena; it could detect areas where there is an unnatural flow of possible pollutants source. So, the detection of pollutant sources could be done using the jump without developing inverse problems which are often difficult to solve. Our approach will serve all stakeholders in air quality issues. Especially, we cite organizations requiring prompt information to react and make decision, such as government departments, civil protection, airports, toxicology and poison control centers.

In next works, we will introduce an algorithm using the both spatial and temporal indicators for self-adaptive mesh with respect to space and time. Furthermore, we will extend this study into 3D problem, bearing in mind building effects, topology, and pollutant sources due to the road traffic. This approach will allow us to give comparison results between the approximate forecasting and the corresponding measured concentrations for several pollutants.

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