Evaluation of NO\textsubscript{x} emissions and ozone production due to vehicular traffic via second-order models

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Abstract

The societal impact of traffic is a long-standing and complex problem. We focus on the estimation of ozone production due to vehicular traffic. For this, we couple a systems of conservation laws for vehicular traffic with a system of linear partial differential equations carefully modeling the production of ozone caused by emission from vehicles. The second-order model for traffic is obtained choosing a special velocity function for a Collapsed Generalized Aw-Rascle-Zhang second-order model and is tuned on NGSIM data. On the other side, the system of linear partial differential equations describes the main chemical reactions of NO\textsubscript{x} gases with a source term provided by a general emission model and the traffic ones. We analyze the ozone impact of various traffic scenarios and describe the effect of traffic light timing on such impact.

Keywords. Road traffic modeling; second-order traffic models; emissions; ozone production.

Mathematics Subject Classification. 35L65, 90B20, 62P12.

1 Introduction

The impact of road traffic and its inefficiencies on society is well known and was documented with quantitative estimates for more than a decade \cite{47, 45}. Moreover, the societal impact is high also in terms of pollution and environmental effects, with road traffic accounting for nearly one third of carbon dioxide (CO\textsubscript{2}) emissions \cite{46}. In general, the impact of air quality on public’s health is one of the world’s worst toxic pollution problems in this century, the current levels of air pollutants in urban areas are associated with large number of health conditions, including respiratory infections, heart disease \cite{13} and cancer. Air pollutants also contribute to the phenomena of greenhouse effect, ozone depletion, deforestation and the acidification of water and soils \cite{36} and they can induce certain diseases as well as damages on materials (plastic, metals, stones), including Cultural Heritage’s ones \cite{44, 12}.

While CO\textsubscript{2} is probably one of the most studied molecules, the effect on health is also related to other pollutants, such as particulate matters and nitrogen dioxide (NO\textsubscript{2}), see \cite{53}. Here we focus on the production of ozone which stems out of chemical reactions in the atmosphere of the NO\textsubscript{x} gases \cite{2, 49, 9}.

Much attention has been devoted in traffic literature to quantities such as flow, capacity and travel time. However, advanced modeling of fuel consumption and emission still faces limitations, especially for tools which can be integrated with the increasing flow of data from probe sensors. One of the main reasons is the high variability of fuel consumption and emissions, which are influenced by many factors as the vehicle type, make, model, year and others. Even if the estimation of fuel consumption and emission at the level of single vehicle presents such drawbacks, as shown in \cite{33}, it is possible to achieve reliable estimates using second-order macroscopic models paired with probe sensor data.
thus build-up on this idea by coupling a second-order macroscopic model with a system of ordinary differential equations (briefly ODEs) representing the complex chemical reactions of NO$_x$ gases, still subject to intensive research, which lead to ozone production.

Let us first discuss in detail the second-order model. First notice that most emission models use both the speed $v$ and acceleration $a$ of vehicles \[6\]. Thus a macroscopic model to be paired with an emission estimator must be of second-order, i.e. consists of an equation for conservation of mass and one for balance of momentum. In particular, the density-flow relation, also known as fundamental diagram, is typically multi-valued and allow a better fit of traffic data. General approaches have been proposed for second-order models \[17, 24\], extending the well-know Aw-Rascle-Zhang model \[4, 52\] and the paper \[33\] used a phase transition one \[7, 10\]. The recent paper \[15\] proposed to use a generalized second-order model with collapsed fundamental diagram in the free phase, thus allowing phase transitions with a simpler description and fitting well with probe and fixed sensor data. This modeling framework is called Collapsed Generalized Aw-Rascle-Zhang Models (briefly CGARZ) and we specify a model in this class by interpolating the Newell-Daganzo or triangular fundamental diagram with the Greenshield quadratic one.

The obtained second-order model is tuned and tested on NGSIM data. First we fix the model parameters using the NGSIM data to generate fundamental diagram data points. Then, as in \[33\], we compare emission predictions using the CGARZ model and a macroscopic emission formula with ground-truth emissions using the whole NGSIM dataset and a microscopic emission formula. The used emission formula is a general combination of velocity, acceleration and their powers, and we used parameters from \[31\] specifically tunes for NO$_x$ emissions of a petrol car. The resulting predictions need a correction factor, which is determined alternating the NGSIM data blocks (each of 15 minutes) as training and verification data. The overall relative error ranges between 5% and 23% with an average value of 14%. Notice that the relative error would be on the high end if the ultimate goal of the investigation would be the exact estimates of the emissions. However, here the tool is used to compare different traffic regimes and the model inaccuracies do not prevent to determine differences in emissions.

We also test the model accuracy in the two ways. First we compare the emissions obtained from the raw NGSIM dataset and that obtained numerically using aggregated macroscopic data obtained replacing cars with Gaussian kernels. The difference appears to be negligible, see Figure 3 (left). Then, we consider two different ways of measuring acceleration. The numerical one used in previous comparison and the theoretical one defined directly from the CGARZ model. Also in this case the discrepancies appear to be negligible, see Figure 3 (right).

Then we pass to model the chemical reactions at the base of ozone production in the atmosphere caused from NO$_x$ emissions due to vehicular traffic. Traffic is estimated to cause around one half of nitrogen oxide production, which in turn is one of the main precursor of ozone. The photodissociation of NO$_2$ is then responsible for the production of the highly reactive O atom and, finally, of ozone. The model capturing these reactions is comprised of a system of five ordinary differential equations (briefly ODEs). The production of NO$_2$ is tuned to 15% of the overall NO$_x$ production as suggested by the recent work \[8\].

Since we are mostly interested in the emissions and main reactions at street level, we pair the CGARZ model with simple linear partial differential equations (briefly linear PDEs) derived from the system of ODEs distributed along a one-dimensional parametrization of a road. The CGARZ system is responsible for the source term of the linear PDEs, representing NO$_x$ emissions and using the model tested on NGSIM data. The coupled system is then simulated using a Godunov-type scheme for the CGARZ paired with single step Runge-Kutta for the linear PDE.

We first run a simple test: the simulation of a simple interaction of a shock wave with a rarefaction. The shock represent a backward moving queue while the rarefaction an acceleration wave. The shock has minimal effect on the NO$_x$ emissions while the acceleration wave is the most responsible for the highest values.

We then consider a road with a traffic light and green-red cycles. The emissions are compared for
different length of the cycle and different proportions of the red-green times. The length of the cycle strongly affects NO\textsubscript{x} emissions: moving from 2.5 minutes to 7.5 minutes produces an increase of around 10\% of emissions, see Figure 9. On the other side, the variation of the red time versus green one does not affect significantly NO\textsubscript{x} emissions, except for an initial ramp up phase when starting from empty road, see Figure 10. These findings are in line with what observed in the first test, but quite different than common intuition.

We then focus specifically on ozone production. The overall coupled system of PDEs is simulated for 30 minutes corresponding to the two tests without and with the traffic light. The ozone rapidly increases and then reach a linear growth behavior in case of traffic light, while apparently saturate in case of no traffic light. Moreover, the ozone appear to be quite uniformly distributed along the road.

The paper is organized as follows. In Section 2 we introduce the CGARZ model. In Section 3 we define the emission model and we validate it with real data. In Section 4 we introduce a simplified set of chemical reactions which lead to ozone production. In Section 5 we merge the traffic model with the system of ODEs associated to the chemical reactions and finally, in Section 6 we propose some numerical tests to estimate the production of ozone.

2 CGARZ model and traffic data from mobile sensors

Traffic models are usually classified in categories, depending on the used scale: microscopic, with individual vehicles dynamics modeled by ordinary differential equations (ODE) \[5, 29, 35\]; cellular, with roads decomposed into cells containing more vehicles \[11, 16, 28\]; and continuum, where the aggregated car density evolves according to a partial differential equation (PDE), which can be of kinetic type \[23, 20\] or fluid-dynamic ones \[25, 4\]. For a review of models see \[19, 1, 17, 34\]. Here we focus on macroscopic fluid-dynamic ones.

Macroscopic fluid-dynamic traffic models are based on the conservation of vehicles, \(\rho_t + (\rho v)_x = 0\), where \(\rho(x, t)\) is the vehicle density and \(v(x, t)\) the average velocity. The first order Lighthill-Whitham-Richards (LWR) model \[25, 37\] assumes a functional relationship between velocity and density, \(v = v(\rho)\), and yields

\[
\rho_t + f(\rho)_x = 0, \tag{2.1}
\]

where \(f = \rho v(\rho)\) is the flow rate of vehicles. Second order models consider \(\rho\) and \(v\) as independent quantities and consists of balance laws:

\[
\rho_t + (\rho v)_x = 0, \quad v_t + g(\rho, v)_x = A(\rho, v), \tag{2.2}
\]

where \(A\) is an acceleration term. Among the most used models we recall the Aw-Rascle-Zhang (ARZ) model \[4, 18, 52\]. The LWR model \[2.1\] is able to capture the formation of traffic waves (shocks) but only due to network intersections or other triggers, while second-order models may give rise to waves from steady traffic situations. The latter, also referred to as phantom traffic jams, are observed experimentally \[43\]. Such waves are responsible for many drawbacks, including increase in fuel consumption and breaking events \[42\].

In this section we introduce the Collapsed Generalized Aw-Rascle-Zhang (CGARZ) model \[15, 14\], to describe the evolution of traffic flow. We propose new flux and velocity functions and we calibrate them by the NGSIM dataset.

2.1 CGARZ Model

The CGARZ model is one of the Generic Second Order Models (GSOM) \[24\], a family of macroscopic models which satisfy

\[
\begin{align*}
\rho_t + (\rho v)_x &= 0, \\
w_t + vw_x &= 0
\end{align*}
\]

with \(v = V(\rho, w),\)
for a specific velocity function $V$. The variables $\rho(x, t)$, $v(x, t)$ and $w(x, t)$ are respectively the traffic density, the velocity and a property of vehicles which is advected by traffic flow. The problem can be written in conservative form as:

$$
\begin{align*}
\rho_t + (\rho v)_x &= 0 \\
y_t + (yv)_x &= 0
\end{align*}
$$

with $v = V\left(\frac{y}{\rho}\right), \quad (2.4)$

where $y = \rho w$ is the conserved total property. The variable $w$ correlates different behaviors of drivers to the flow-density curves. Thus, the GSOM posses a family of fundamental diagrams $Q(\rho, w) = \rho V(\rho, w)$, parametrized by $w$. The peculiarity of the CGARZ model is that $w$ does not influence the traffic behavior in the low density regime. This means that vehicles may posses different properties, but the velocity and flow in free-flow is not affected by $w$. Thus, CGARZ possesses a single-valued fundamental diagram in free-flow, and a multi-valued function in congestion. The flux function has then the following form

$$Q(\rho, w) = \begin{cases} Q_f(\rho) & \text{if } 0 \leq \rho \leq \rho_f \\ Q_c(\rho, w) & \text{if } \rho_f \leq \rho \leq \rho_{\text{max}} \end{cases}, \quad (2.5)$$

where $\rho_f$ is the free-flow threshold density independent on $w$, and $\rho_{\text{max}}$ is the maximum density. Following [15], the flux function (2.5) has to satisfy the following properties:

**Q1.** $Q(\rho, w) \in C^1$ for each $w$, where $C^1$ is the set of continuously differentiable functions.

**Q2.** Flow-density curves have a common $\rho_{\text{max}}$ independent of $w$, $Q(\rho_{\text{max}}, w) = 0$ for all $w$.

**Q3.** The flux is strictly concave with respect $\rho$, $\frac{\partial^2 Q(\rho, w)}{\partial \rho^2} < 0$ for $\rho \in [0, \rho_{\text{max}}]$.

**Q4.** $\frac{\partial Q(\rho, w)}{\partial w} > 0$ if $\rho_f < \rho < \rho_{\text{max}}$.

The flux function (2.5) defines a velocity function $V(\rho, w) = \frac{Q(\rho, w)}{\rho}$. Thus, as a consequence of the properties of $Q$, the velocity function $V$ is in $C^1$ and is strictly decreasing with respect to $\rho$. Moreover, $V$ satisfies:

**V1.** Vehicles never go backwards, $V(\rho, w) \geq 0$.

**V2.** $\rho_{\text{max}}$ is the only density such that $V(\rho_{\text{max}}, w) = 0$.

**V3.** In the free-flow regime, the traffic velocity is independent of $w$, $\frac{\partial V(\rho, w)}{\partial w} = 0$ if $0 \leq \rho \leq \rho_f$.

**V4.** In the congestion regime, the traffic velocity is increasing with respect to $w$, $\frac{\partial V(\rho, w)}{\partial w} > 0$ if $\rho_f \leq \rho \leq \rho_{\text{max}}$.

In the next section we propose a new family of fundamental diagrams that satisfy the properties listed above.

### 2.1.1 Flux and velocity functions

Here we make a choice for the flux function of the CGARZ family, thus determining a unique model to be used. Differently from [15], we choose the flux function to be an interpolation between a triangular fundamental diagram, also known as Newell-Daganzo, and a Greenshield fundamental diagram. The reason for this choice is that those two diagrams are the most known and used in traffic modeling and they present two somehow opposite behavior, with the triangular one presenting a unique characteristic speed in congested regime, thus allowing contact discontinuities, while the Greenshield one being genuinely nonlinear in congested regime thus exhibiting rarefaction waves.
The model parameters to be calibrated from data are the following: the maximum speed $V_{\text{max}}$, the threshold density $\rho_f$ from the free-flow to the congested phase, the density $\rho_c$ in which the flux function reaches its maximum value, and a lower and upper bound for $w$, denoted by $w_L$ and $w_R$ respectively. Moreover, we set the maximal density $\rho_{\text{max}}$ as a property of the road. As in [15], we assume the Greenshields model in the free-flow regime, i.e. 

$$Q_f(\rho) = \rho V_{\text{max}} \left(1 - \frac{\rho}{\rho_{\text{max}}} \right),$$  

(2.6)

and as a novelty we define the flux function $Q_c(\rho, w)$ in the congested phase, as a convex combination of a lower-bound function $f(\rho)$ and an upper-bound function $g(\rho)$. In particular, we set

$$f(\rho) = \rho_f V_{\text{max}} \left(1 - \frac{\rho}{\rho_{\text{max}}} \right)$$  

(2.7)

as the straight-line which connects $(\rho_f, Q_f(\rho_f))$ with $(\rho_{\text{max}}, 0)$, and

$$g(\rho) = \rho V_{\text{max}} \left(1 - \frac{\rho}{\rho_{\text{max}}} \right)$$  

(2.8)

which corresponds to the free-flow phase flux function. Defining

$$\lambda(w) = \frac{w - w_L}{w_R - w_L},$$  

(2.9)

then our flux function $Q_c(\rho, w)$ is

$$Q_c(\rho, w) = (1 - \lambda(w))f(\rho) + \lambda(w)g(\rho),$$  

(2.10)

with $f$ and $g$ given in (2.7) and (2.8) respectively. The resulting flux function is

$$Q(\rho, w) = \begin{cases} 
\rho V_{\text{max}} \left(1 - \frac{\rho}{\rho_{\text{max}}} \right) & \text{if } 0 \leq \rho \leq \rho_f \\
(1 - \lambda(w))f(\rho) + \lambda(w)g(\rho) & \text{if } \rho_f < \rho \leq \rho_{\text{max}}.
\end{cases}$$  

(2.11)

Proposition 1. The flux function (2.11) verifies the properties $Q_2$-$Q_4$ and the property $Q_1$ for all $\rho \neq \rho_f$.

Proof. The function $Q$ is $C^1$ in $[0, \rho_{\text{max}}]\setminus\{\rho_f\}$ by construction: the free-flow part $Q_f$ is $C^1$ for all $\rho$, and the congested one is a convex combination of $C^1$ functions. Condition $Q_2$ follows directly from the definition of $f$ and $g$ which satisfy $f(\rho_{\text{max}}) = g(\rho_{\text{max}}) = 0$. To verify condition $Q_3$ we have that the second derivative is given by

$$\frac{\partial^2 Q(\rho, w)}{\partial \rho^2} = \begin{cases} 
\frac{V_{\text{max}}}{\rho_{\text{max}}} \rho_{\text{max}} & \text{if } 0 \leq \rho < \rho_f \\
-2\lambda(w)\frac{V_{\text{max}}}{\rho_{\text{max}}} & \text{if } \rho_f < \rho \leq \rho_{\text{max}},
\end{cases}$$

which is strictly negative for all $w$. Finally, condition $Q_4$ follows from the relation

$$\frac{\partial Q(\rho, w)}{\partial w} = \lambda'(w)(g(\rho) - f(\rho))$$

which is strictly positive since $g(\rho) > f(\rho)$ by construction.

Remark 2.1. To verify condition $Q_1$ for all $\rho \in [0, \rho_{\text{max}}]$, it is sufficient to choose a different function $f$ that joins with regularity to free-flow regime.
Once the flux function is defined, the velocity function is obtained as
\[ V(\rho, w) = \frac{Q(\rho, w)}{\rho}. \] (2.12)

To summarize, our model is
\[ \rho_t + (\rho v)_x = 0, \]
\[ w_t + vw_x = 0, \]
with \( v = V(\rho, w) = \begin{cases} 
V_{\text{max}} \frac{1 - \rho}{\rho_{\text{max}}} & \text{if } 0 \leq \rho \leq \rho_f \\
(1 - \lambda(w)) f(\rho) + \frac{\lambda(w)}{\rho} g(\rho) & \text{if } \rho_f \leq \rho \leq \rho_{\text{max}}
\end{cases} \] (2.13)
and \( \lambda(w) \) in (2.9).

### 2.1.2 Acceleration function

In time-continuous second-order models, the acceleration equation is a second partial differential equation of the general form
\[ \frac{Dv(x, t)}{Dt} = (v_t(x, t) + v(x, t) v_x(x, t)) = a(\rho(x, t), v(x, t)), \] (2.14)
where \( \frac{Dv}{Dt} \) is the total derivative (also called material derivative, convective derivative, Lagrangian derivative, or substantial derivative) and \( v \) is the speed function. This equation implies that the rate of change of the local speed \( \frac{Dv}{Dt} = (v_t + v v_x) \) in Lagrangian coordinates is equal to an acceleration function \( a(x, t) = a(\rho(x, t), v(x, t)) \).

In CGARZ model we derive the function acceleration by computing the total derivative of \( V(\rho, w) \), i.e.
\[ a(x, t) = \frac{Dv(x, t)}{Dt} = v_t(x, t) + v(x, t) v_x(x, t), \]
where
\[ v(x, t) = V(\rho(x, t), w(x, t)), \quad v_t = V_\rho \rho_t + V_w w_t, \quad v_x = V_\rho \rho_x + V_w w_x. \]

Then,
\[ a(x, t) = (\rho_t + \rho v_x) V_\rho + (w_t + v w_x) V_w, \]
and by applying the homogeneous equation in (2.3) for \( w \) we get
\[ a(x, t) = V_\rho (\rho_t + \rho v_x) = -V_\rho \rho v_x. \] (2.15)

In our case, by (2.11) and (2.12) we have
\[ V_\rho(\rho, w) = \begin{cases} 
-\frac{V_{\text{max}}}{\rho_{\text{max}}} & \text{if } 0 \leq \rho \leq \rho_f \\
-\frac{1 - \lambda(w)}{\rho^2} Q_f(\rho_f) \left( 1 - \frac{\rho_f^2}{\rho_{\text{max}}^2} \right) - \frac{\lambda(w)}{\rho_{\text{max}}} V_{\text{max}} & \text{if } \rho_f \leq \rho \leq \rho_{\text{max}}
\end{cases} \]

### 2.1.3 Calibrating a family of fundamental diagrams

As data for calibration we use the NGSIM dataset [48]. The database contains detailed vehicle trajectory data on the interstate I-80 in California, on April 13, 2005. The area under analysis is approximately 500 meters in length and consists of six freeway lanes. Several video cameras recorded vehicles moving through the monitored area, while a specific software has transcribed the vehicle trajectory data from video. The data include the precise location, velocity and acceleration of each

6
vehicle within the study area every 0.1 seconds. The period analyzed in this work refers to three time slots: 4:00 pm - 4:15 pm, 5:00 pm - 5:15 pm and 5:15 pm - 5:30 pm.

First of all we estimate the flow-density and velocity-density relationships from the dataset. We divide the study area into space-time cells $C^n_i = [x_i, x_{i+1}] \times [t^n, t^{n+1}]$ of length $120 \text{ m} \times 4 \text{ s}$. The density in $C^n_i$ is equal to the number of vehicles (denoted by veh) which cross the cell during the time interval $[t^n, t^{n+1}]$. The velocity in $C^n_i$ is the mean of all the velocities measured in the cell, and the flux is the product between density and velocity. The relationships between flow and density and between velocity and density are shown in Figure 1. In the two graphs we clearly see two “clouds” in which data are concentrated (except a small number of outliers accounting for less than 3% of points). From the analysis of these data we have estimated a possible set of model parameters, which is given in Table 1. Specifically, the parameters $V_{\text{max}}$ and $\rho_f$ are chosen such that the area enclosed between the curves $f$ and $g$ covers more than the 97% of data points of the real data clouds; $\rho_{\text{max}}$ is a property of the road, defined by

$$\rho_{\text{max}} = \frac{\text{Number of lanes}}{\text{Length of vehicles}} = \frac{6}{7.5 \times 10^{-3} \text{ km}},$$

and we set the two extreme $w_L$ and $w_R$ as

$$w_L = g(\rho_f) \quad \text{and} \quad w_R = g(\rho_c).$$

The family of curves generated by the data set given in Table 1 are shown in Figure 2.

![Figure 1](image1.png)

**Figure 1.** (Left) Flow-density relationship and (Right) velocity-density relationship from the NGSIM dataset.

### Table 1. Parameters for CGARZ model (2.13) calibrated on NGSIM dataset.

| $V_{\text{max}}$ | $\rho_f$ | $\rho_{\text{max}}$ | $\rho_c$ | $w_L$ | $w_R$ |
|-------------------|---------|---------------------|---------|-------|-------|
| 65 km/h           | 110 veh/km | 800 veh/km | $\rho_{\text{max}}/2$ | 5687   | 13000  |

3 Estimating emissions by traffic quantities

In this section we describe a microscopic and a macroscopic emission model appropriate for several air pollutants. Emitted by different sources, primary and secondary air pollutants mainly include: sulphur oxides (SO$_x$), nitrogen oxides (NO$_x$), volatile organic compounds (VOC), particulates (PM),...
free radicals, toxic metals, etc. [50, 40]. In areas with heavy street traffic and high amounts of UV radiation, ozone (O$_3$), NO$_x$ and hydrocarbons (HC) are of particular interest.

The existence of high concentration of ozone in the urban atmosphere suggests to have an effective control of some other pollutants such as carbon monoxide (CO) and sulphur dioxide (SO$_2$), ozone is a secondary pollutant formed in the ambient air through a complex set of sunlight initiated reactions of its precursor, primary emission of VOC, catalyzed by hydrogen oxide radicals, and of NO$_x$ [21, 41].

For the complexity of the phenomena involved, in this paper we focus on microscopic and macroscopic emission models for only NO$_x$. Numerical methods are designed for both models based on vehicle trajectories for the former and solution to the CGARZ model for the latter. Then we test the discrepancies between the two model estimates on NGSIM dataset and propose correction factors.

### 3.1 Emission Model

We use the microscopic emission model proposed in [31]. This model gives the instantaneous emission rate of four pollutant types: carbon dioxide, nitrogen oxides, volatile organic compounds and particulate matter. The emission rate $E_i$ of vehicle $i$ at time $t$ is computed using vehicle’s instantaneous speed $v_i(t)$ and acceleration $a_i(t)$

$$E_i(t) = \max\{E_0, f_1 + f_2 v_i(t) + f_3 v_i(t)^2 + f_4 a_i(t) + f_5 a_i(t)^2 + f_6 v_i(t)a_i(t)\}, \quad (3.1)$$

where $E_0$ is a lower-bound of emission and $f_1$ to $f_6$ are emission constants. Both the emission lower-bound and coefficients differ according to the type of pollutant and of vehicle (i.e. petrol car, diesel car, truck, etc.). We are particularly interested in the NO$_x$ emission rate, whose coefficients depend on whether the vehicle is in acceleration (defined as $a_i(t) \geq -0.5 \text{ m/s}^2$) or deceleration (with $a_i(t) < -0.5 \text{ m/s}^2$) mode. In Table 2 we report the NO$_x$ emission coefficients for a petrol car, for which $E_0 = 0$. See [31, Table 2] for the coefficients related to the other pollutants and vehicles type.

| Vehicle mode   | $f_1$ [kg/s] | $f_2$ [g/s] | $f_3$ [g/s/m] | $f_4$ [g/s/m$^2$] | $f_5$ [g/s/m$^2$] | $f_6$ [g/s/m$^2$] |
|----------------|-------------|-------------|---------------|------------------|------------------|------------------|
| $a_i(t) \geq -0.5 \text{ m/s}^2$ | 6.19e-04 | 8e-05 | -4.03e-06 | -4.13e-04 | 3.80e-04 | 1.77e-04 |
| $a_i(t) < -0.5 \text{ m/s}^2$ | 2.17e-04 | 0 | 0 | 0 | 0 | 0 |

Table 2. NO$_x$ parameters in emission rate formula (3.1) for a petrol car.
Assuming to have $N$ vehicles in a stretch of road going all at the same speed $\bar{v}$, with the same acceleration $\bar{a}$, the emission rate is given by the $N$ contributes of the vehicles, such that

$$E(t) = \sum_{i=1}^{N} E_i(t) = N \max\{E_0, f_1 + f_2 \bar{v}(t) + f_3 \bar{v}(t)^2 + f_4 \bar{a}(t) + f_5 \bar{a}(t)^2 + f_6 \bar{v}(t) \bar{a}(t)\}. \quad (3.2)$$

In particular this equation can be used in conjunction with quantities provided by a numerical solutions to a macroscopic model such as the CGARZ one.

Remark 3.1. We make use of a particular emission mode. However, the large majority of microscopic emissions models are based on a combination of polynomial expression in the velocity and acceleration. Thus our analysis can be easily adapted to other models.

3.2 Evaluating the acceleration

From the previous section it is clear that we need to compute the acceleration of vehicles to estimate the NO$_x$ emission rates. Here we describe a discrete formulation for the acceleration recovered by average quantities, as an alternative of (2.15) which is directly derived from the theoretical model.

Consider a road divided into cells both in space and time, with steps $\Delta x$ and $\Delta t$ respectively. Denote by $\rho^k_i$ the computed average density of the $i$-th cell at time $t^k = k\Delta t$ and by $V^k_i$ the computed average speed on the same cell. We follow the approach proposed in [26, 51] for the particular case of a single road with $n_l$ lanes. To define the average acceleration of a cell, we distinguish between the temporal acceleration and the spatial-temporal acceleration. The temporal acceleration refers to the change of the average speed for the vehicles which remain in the same cell $i$ between time $t^k$ and $t^{k+1}$,

$$a^{tmp}_i(k) = \frac{V^{k+1}_i - V^k_i}{\Delta t}. \quad (3.3)$$

Let $q^k_i$ be the flux of vehicles which cross the cell $i$ between time $t^k$ and $t^{k+1}$. The total number of vehicles which remain in the cell and therefore which are subjected to the temporal acceleration is $c^{tmp}_i(k) = n_l \Delta x \rho^k_i - \Delta t q^k_i$.

The spatial-temporal acceleration refers to the change of the average speed for the vehicles which move from a cell to the following one. It is defined as

$$a^{spt}_i(k) = \frac{V^{k+1}_{i+1} - V^k_i}{\Delta t}, \quad (3.4)$$

and the total number of vehicles subjected to this acceleration is $c^{spt}_i(k) = \Delta t q^k_i$.

Combining the definitions of temporal (3.3) and spatial-temporal (3.4) acceleration, we can introduce the average acceleration of vehicles in cell $i$ at time $t^k$ as

$$A^k_i = \frac{a^{tmp}_i(k)c^{tmp}_i(k) + a^{spt}_i(k)c^{spt}_i(k)}{c^{tmp}_i(k) + c^{spt}_i(k)},$$

which, after some computations, can be rewritten as

$$A^k_i = \frac{V^{k+1}_i - V^k_i}{\Delta t} + V^k_i \frac{V^{k+1}_{i+1} - V^{k+1}_i}{\Delta x}. \quad (3.5)$$

3.3 Estimating NO$_x$ emissions: a numerical test

In this section we compare the NO$_x$ emission rates given by (3.1) computed using the NGSIM dataset with that given by (3.2) computed along numerical solutions of the CGARZ model. In other words, the macroscopic CGARZ model is fed by real data only at initial time, then the emission rate is computed
along the numerical solution to CGARZ and compared with that resulting from the NGSIM complete dataset, considered as a ground truth.

The NGSIM dataset, introduced in Section 2.1.3, contains vehicle trajectory data, including microscopic speed and acceleration. These quantities can be fed directly in (3.1) providing microscopic NO\textsubscript{x} emissions produced by each vehicle. Then, we sum the emissions of vehicles along the entire road

\[ E_{true}^{(t_k)} = \sum_{i=1}^{N_{car}(t_k)} E_i(t_k), \tag{3.6} \]

where \( N_{car}(t_k) \) is the number of vehicles crossing the road at time \( t_k \) and \( E_i(t_k) \) is the emission rate of vehicle \( i \) at time \( t_k \).

The CGARZ model (2.13), calibrated with the NGSIM dataset in Section 2.1.3, is used here to estimate the average density and speed of vehicles along the road. We discretize the highway of the NGSIM dataset with a \( N_x \times N_t \) space-time grid whose cells are indexed by \((x_j, t^n) = (j \Delta x, n \Delta t)\). To numerically solve the model (2.13) we use the Second Order Cell Transmission Model (2CTM), described in [15].

**Remark 3.2.** As shown in [15] the 2CTM is equivalent to a Godunov type scheme.

The numerical solution is constructed in the following way. The initial density \( \rho_0 \) and velocity \( v_0 \) are obtained with a kernel density estimation of the ground-truth data, i.e. the Parzan-Rosenblatt window method [32] [33]. Given a vehicle location \( x_i(t) \) and velocity \( v_i(t) \), density and flow rate functions are obtained as superpositions of Gaussian profiles,

\[ \rho(x, t) = \frac{1}{h} \sum_{i=1}^{n} K(x, x_i), \]
\[ v(x, t) = \frac{\sum_{i=1}^{n} v_i K(x, x_i)}{\sum_{i=1}^{n} K(x, x_i)}, \tag{3.7} \]

where \( K(x, x_i) = \phi \left( \frac{x - x_i}{h} \right) + \phi \left( \frac{x - (2b - x_i)}{h} \right) + \phi \left( \frac{x - (2a - x_i)}{h} \right) \), \( \phi(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} \), \( h \) is a distance parameter, \( a \) and \( b \) are the extremes of the road. In this work \( h = 25 \text{ m} \). The initial \( w_0 \) is defined such that

\[ V(\rho_0(x_j), w_0(x_j)) = v_0(x_j), \quad \text{for } j = 1, \ldots, N_x, \]

and then \( y_0(x_j) = \rho_0(x_j) w_0(x_j) \). Once computed by the 2CTM the average density \( \rho^n_j \) and speed \( V^n_j \), we apply equation (2.15) to estimate the average acceleration \( A^n_j \) and finally equation (3.2) to compute the average emission rate \( E^n_j \) of the cell \( x_j \) at time \( t^n \), for all \( j \) and \( n \). Similar to microscopic case (3.6), we sum the emission rates all over the cells

\[ E_{mod}^{(t_k)} = \sum_{j=1}^{N_x} E^n_j, \tag{3.8} \]

where \( t_k = k \delta t \), with \( \delta t = 0.1 \text{ s} \) is the time frame of the NGSIM dataset.

Two formulas to compute the acceleration were proposed in (2.15) and (3.5). The first is analytical and adapted for macroscopic models, while the second is discrete and can be used to any type of data. In Figure 3 we compare the numerical results using the two formulations. The red-solid line of the left plot represents the NO\textsubscript{x} emission rate computed using the discrete acceleration on average density and speed values obtained via kernel density estimation (3.7) from NGSIM trajectory data. The blue-circles line, instead, represents the ground-truth emission rate (3.6). The results are quite similar, suggesting the accuracy of the discrete acceleration (3.5). Finally, on the right plot of Figure 3 we compare the emission rate of NO\textsubscript{x} computed with equation (3.2), using the two different definitions of the
acceleration function (2.15) and (3.5). The results are almost identical and have same computational cost, and this further certifies the efficiency of the CGARZ model (2.13) and suggests the use of the analytical formula (2.15) to estimate emissions.

We compare now the emission rate along the entire road obtained with (3.6) and (3.8) respectively, for each period of the NSGIM dataset. The results are computed with 13-minute simulations, in which we exclude the first and the last minute of recorded trajectories for corruption of data. We observe in Figure 3 that the emission rate obtained by the CGARZ model (3.8) (black-dotted) is lower than the ground-truth emission (3.6) (blue-solid). Improved results are obtained by multiplying the modeled emissions by a proper correction factor (red-circles). Specifically, for each data period \( j \), we have computed a correction factor \( r_j \) via linear regression between the ground-truth emission and the modeled one. Moreover, we define the following error

\[
\text{Error}(r_j) = \frac{\|E_{\text{true}} - r_j E_{\text{mod}}\|_{L^1}}{\|E_{\text{true}}\|_{L^1}}, \quad j = 1, 2, 3, \tag{3.9}
\]

where \( E_{\text{true}} \) and \( E_{\text{mod}} \) are vectors whose \( k \)-th components are given by (3.6) and (3.8) respectively. Table 3 shows the errors (3.9) obtained using the three different correction factors for all the time periods of the NSGIM dataset, where \( r_1 = 1.42, r_2 = 1.35 \) and \( r_3 = 1.15 \). We observe that the correction factors \( r_1, r_2 \) and \( r_3 \) give similar results.

| Period                | Error \( r_1 \) | Error \( r_2 \) | Error \( r_3 \) |
|-----------------------|-----------------|-----------------|-----------------|
| 4:01 pm - 4:14 pm     | 0.1604          | 0.1666          | 0.2204          |
| 5:01 pm - 5:14 pm     | 0.0819          | 0.0842          | 0.1625          |
| 5:16 pm - 5:29 pm     | 0.2304          | 0.1773          | 0.0586          |

Table 3. Errors given by (3.9) for the three slots of the NSGIM dataset and different correction factor \( r_1 = 1.42, r_2 = 1.35 \) and \( r_3 = 1.15 \).
Figure 4. Comparison of modeled (black-dotted), modeled with correction factors $r_j$ (red-circles) and ground-truth (blue-solid) emission rates along 500 meters of road during 13 minutes of simulation for the three time periods of the NSGIM dataset. The top row is computed for $r_1 = 1.42$, the central row for $r_2 = 1.35$ and the bottom row for $r_3 = 1.15$.
4 Estimating the production of O₃

Here we report the main chemical reactions of NOₓ gases which lead to the O₃ formation. NOₓ gases are usually produced from the reaction among nitrogen and oxygen (O₂) during combustion of fuels, such as hydrocarbons, in air, especially at high temperatures, such as occurs in car engines [30]. They include nitrogen oxide (NO) and nitrogen dioxide (NO₂), the latter is classified as a secondary pollutant. NO is produced according to the following reaction with O₂ and nitrogen (N₂), [27],

\[ \text{N}_2 + \text{O}_2 \rightarrow 2\text{NO}, \]

where the rate of the chemical reaction can be increased by raising the temperature. In the combustion mechanism, NO can react with O₂ thus forming NO₂,

\[ 2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2. \]

NO₂ is a very reactive compound that can be photo-dissociated into atomic oxygen (O), this mechanism is considered one of key steps in the formation of tropospheric ozone [3]. Nitrogen oxides and volatile organic compounds are considered ozone precursors, where traffic is considered the main source (more than 50% of anthropogenic source). The photolysis of NO₂ is speeded up in warmer conditions and with more UV-light. In the troposphere with strong solar irradiation, NO₂ is a relevant precursor substance for the ozone in photochemical smog and it is due to the following reactions:

\[ \text{NO}_2 + h\nu \xrightarrow{k_{1}} \text{O} + \text{NO} \quad (4.1) \]

\[ \text{O} + \text{O}_2 + \text{M} \xrightarrow{k_{2}} \text{O}_3 + \text{M}, \quad (4.2) \]

where \( h \) is Planck’s constant, \( \nu \) its frequency and \( k_1, k_2 \) are the reaction rate constants. M is a chemical species, such as O₂ or N₂, that adsorbs the excess of energy generated in reaction (4.2) [27]. Moreover, in presence of NO, O₃ reacts with it and this reaction destroys the ozone and reproduces the NO₂, with kinetic constant \( k_3 \):

\[ \text{O}_3 + \text{NO} \xrightarrow{k_3} \text{O}_2 + \text{NO}_2. \quad (4.3) \]

This means that the previous reactions do not result net ozone production, because the reactions only recycle O₃ and NOₓ. Net ozone production occurs, when other precursors, such as carbon monoxide, methane, non-methane hydrocarbons or certain other organic compounds (volatile organic compounds) are present in the atmosphere and fuel the general pathways to tropospheric O₃ formation. Although it would be interesting to consider the whole ground-level ozone production, here we focus only on the photochemical smog reactions (4.1), (4.2) and (4.3).

For vehicle’s emissions, the maximum NO₂ concentration is recorded at medium engine load and low engine speed. At high speed, the NO₂ emissions are reduced to a minimum (in most cases less than 4%) [39]. In older car diesel engines, approximately 95% of NOₓ are composed of NO and only 5% of NO₂. The proportion of NO₂ in total NOₓ in turbocharged diesel engines (without aftertreatment) is typically higher, reaching up to about 15%. According to a recent study using British data [8], the fraction of NO₃ in vehicle NOₓ emissions (all fuels) increased from around 5-7% in 1996 to 15-16% in 2009. For this reason we will consider in our simulation a NO₂ concentration equal to 15% of NOₓ.

Now, we set up the system of ordinary differential equations associated to the chemical reactions (4.1), (4.2) and (4.3). We assume that the reactions take place in a volume of dimension \( \Delta x^3 \), during the daily hours and that M in (4.2) is O₂. Moreover, we add the traffic emissions contribution as a source term for the concentration of NO and NO₂. Hence, we denote the chemical species concentration by \([·]\) = [weight unit \( \text{volume}^{-1} \)] and we define the variation of the concentration of NOₓ in \( \Delta x^3 \), at each time \( t \) as

\[ S_{\text{NO}_x} = \frac{E_{\text{NO}_x}(t)}{\Delta x^3}, \quad (4.4) \]
where the emission rate $E_{NO_x}(t)$ is given by (3.2).

The final system of equations, given by coupling the three reactions (4.1)-(4.3) and the source term (4.4), becomes

$$
\begin{align*}
\frac{d[O]}{dt} &= -k_2[O] [O_2]^2 + k_1[NO_2], \\
\frac{d[O_2]}{dt} &= -k_2[O] [O_2]^2 + k_3[O_3] [NO], \\
\frac{d[O_3]}{dt} &= k_2[O] [O_2]^2 - k_3[O_3] [NO], \\
\frac{d[NO]}{dt} &= k_1[NO_2] - k_3[O_3] [NO] + (1-p) S_{NO_x}, \\
\frac{d[NO_2]}{dt} &= -k_2[O] [O_2]^2 + k_3[O_3] [NO] + p S_{NO_x},
\end{align*}
$$

(4.5)

where $p = 0.15$ corresponding to 15% of NO$_2$ derived from the emission rate of NO$_x$, and the parameters $k_1$, $k_2$ and $k_3$, shown in Table 4, are estimated according to [22].

| $k_1$   | $k_2$   | $k_3$   |
|---------|---------|---------|
| 0.02 s$^{-1}$ | $6.09 \times 10^{-34}$ cm$^6$ molecule$^{-1}$ | $1.81 \times 10^{-14}$ cm$^3$ molecule$^{-1}$ |

Table 4. Parameters $k_1$, $k_2$, and $k_3$ of system (4.5).

5 From traffic quantities to the production of the ozone

In this section we merge the traffic model with air pollutants dynamics. As previously proposed, they are linked by the NO$_x$ emission rate.

The procedure is the following:

1. Estimate the traffic quantities, density $\rho = \rho(x,t)$ and speed $v = v(x,t) = V(\rho(x,t), w(x,t))$, with the CGARZ model (2.13).

2. Compute the analytical acceleration $a = a(x,t) = -\rho \partial \rho V \partial_x v$.

3. Estimate the source term $s = s(x,t)$, given by the emission rate (4.4) as a function of speed and acceleration, per unit of volume.

4. Solve the system (4.5) to estimate the chemical species concentration per unit of volume.

This procedure corresponds to solve the following system of equations. For $(x,t) \in [0,L] \times (0,T]$ and with suitable boundary and initial conditions,

$$
\begin{align*}
\partial_t \rho + \partial_x (\rho v) &= 0, \\
\partial_t w + v \partial_x w &= 0, \\
\partial_t \mu_1 + k_2 \mu_1 \mu_2^2 - k_1 \mu_5 &= 0, \\
\partial_t \mu_2 + k_2 \mu_1 \mu_2^2 - k_3 \mu_3 \mu_4 &= 0, \\
\partial_t \mu_3 - k_3 \mu_3 \mu_4 &= 0, \\
\partial_t \mu_4 - k_3 \mu_5 + k_3 \mu_3 \mu_4 &= (1-p) s, \\
\partial_t \mu_5 + k_1 \mu_5 - k_3 \mu_3 \mu_4 &= p s,
\end{align*}
$$

(5.1)

where we use the notations $\mu_1(x,t) = [O]$, $\mu_2(x,t) = [O_2]$, $\mu_3(x,t) = [O_3]$, $\mu_4(x,t) = [NO]$, $\mu_5(x,t) = [NO_2]$.!
In the following numerical tests, the space and time domain $[0, L] \times [0, T]$ is discretized via a grid of $N_x \times N_t$ cells of length $\Delta x \times \Delta t$. For each cell centered at $x_j$ and time $t^n$ of the numerical grid, we then compute density $\rho^n_j$, speed $v^n_j$, and concentrations $\{\mu^n_{i,j}\}_{i=1}^5$ solving system (5.1) by coupling the Godunov-type 2CTM scheme (see Section 3.3) with an ODEs solver. The latter is a single step Runge-Kutta method for stiff problem.

6 Numerical tests

In this section we show some examples illustrating the several steps which lead to the estimate of the production of ozone.

Let us consider the CGARZ traffic model (2.13) on a time horizon $[0, T]$ and on a road with one lane parametrized by $[0, L]$. We fix the maximum speed $V_{\text{max}}$, maximum density $\rho_{\text{max}}$, initial density $\rho_0(x)$ and left boundary condition $\rho(0, t) = u_0$, while we use Neumann boundary condition on the right, which corresponds to allowing all vehicles to leave the road. The parameters used in all simulations are shown in Table 5, and the initial density $\rho_0$ is

$$\rho_0(x) = \begin{cases} 42 & 0 \leq x \leq \ell \\ 110 & \ell < x \leq L, \end{cases}$$

with $\ell = 4.5$ km.

| $T$    | $L$    | $V_{\text{max}}$ | $\rho_{\text{max}}$ | $u_0$   | $\Delta x$ | $\Delta t$ |
|--------|--------|-------------------|----------------------|---------|------------|------------|
| 30 min | 10 km  | 120 km/h          | 133 veh/km           | 42 veh/km | 0.1 km     | 0.5$\Delta x/V_{\text{max}}$ |

Table 5. Parameters used in Tests 1, 2.

6.1 Test 1: Shock and rarefaction dynamic

The dynamic is described by an initial shock wave around the middle of the road and a rarefaction wave stemming from the right end of the road. The shock wave propagates backward for the first 10 minutes, when the interaction with the rarefaction wave, and the consequent cancellation, changes the shock speed to positive. In Figure 5 we compare the 3D plots of density, speed, acceleration and NO\textsubscript{x} emission rates. The four graphs have the same shape, since they depend on the density of vehicles. The acceleration reaches the minimum value along the blue curve shown in the graph, while the maximum value is reached at the beginning of the simulation at the end of the road, when the vehicles leave the road with maximum flux. Finally, the NO\textsubscript{x} emission rate has a peak in correspondence of the highest values of acceleration and it is equal to 0 along the curve with the darkest blue.

On the left plot of Figure 6 we show data points of speed, acceleration and emission obtained along the numerical test. More precisely, the horizontal and vertical axes denote speed and acceleration, respectively, while the color gives the NO\textsubscript{x} emission value. We observe that the NO\textsubscript{x} emission is higher for positive value of the acceleration and low speed, and it decreases with negative acceleration. On the right plot of Figure 6 we show the variation in time of the total emission, defined as the sum on the cells of the emission rates, at any time. For this test, the total emission increases until the dynamics is described by the shock wave, and then it starts to decrease.

6.2 Test 2: Dynamic with traffic lights

Here we test the effect of different traffic light cycles varying the time frame of the red phase. The latter corresponds to a Neumann boundary condition imposing vanishing outflow, while the green phase correspond to Neumann boundary condition allowing all cars to leave the road. We start by showing the solution obtained with a traffic light cycle of 5 minutes with a 2 minutes red phase. In
Figure 5. Test 1. Variation of density (top-left), speed (top-right), analytical acceleration (bottom-left) and NO\textsubscript{x} emissions (bottom-right) in space and time.

Figure 6. Test 1. (left) NO\textsubscript{x} emission rate as a function of speed and acceleration; (right) variation in time of the total emission rate along the entire road.
Figure 7 we show density, speed, acceleration and NO\textsubscript{x} emission rate in space and time. The wave with high density created by the red traffic lights takes about 18 minutes to reach the left boundary of the road. Indeed, at the beginning of the simulation the density of vehicles is too low to backward propagate the wave. Once it reaches the left boundary of the road we see a periodic behavior in all the graphs, determined by the traffic lights. The graphs related to density and speed have opposite behavior: when the density increases the speed decreases and vice versa. Similar to Test 1, the acceleration reaches the maximum values when the traffic light turns green and the vehicles leave the road. Again, the peaks of NO\textsubscript{x} emission rates correspond to the highest acceleration values.

In Figure 8 we show on the left the emission rate as a function of speed and acceleration, and on the right the total emission along the road in time on the right. Similar to Figure 6, the left graph shows higher emission levels at positive acceleration, but also at low speed and values of acceleration near to $-0.5 \text{ m/s}^2$. In the graph we can see two phases, horizontally divided at height $-0.5$. We observe that $-0.5 \text{ m/s}^2$ is the acceleration value which distinguishes the two possible choices of the parameters in (3.1), see Table 2. The right graph of Figure 8 shows the total emission in time, where the red and green lines represent the relative traffic light. We observe that, during the first 20 minutes, the emission rate increases faster when the traffic light is green and slower when it is red. Then, it reaches a maximum value after which it assumes a periodic behavior which depends on the traffic light.

![Graphs showing density, speed, acceleration, and NO\textsubscript{x} emissions](image)

**Figure 7.** Test 2. Variation of density (top-left), speed (top-right), analytical acceleration (bottom-left) and NO\textsubscript{x} emissions (bottom-right) in space and time.

Let now $r = t_g/t_r$ be the ratio between the time $t_g$ of the green phase and the time $t_r$ of the red phase respectively, and let $t_c$ be the time of the whole traffic light phase, i.e. $t_c = t_g + t_r$. We consider two different test cases: first we fix the ratio $r$ and we vary the time $t_c$; then, conversely we fix $t_c$ and...
we vary \( r \).

**Test 2.1: Emissions when the ratio \( r \) is constant.** In Figure 9 we show the NO\(_x\) emissions obtained with \( r = 3/2 \) and three different values of traffic light duration: on the left we set \( t_c = 7.5 \) min and \( t_r = 3 \) min, in the center \( t_c = 5 \) min and \( t_r = 2 \) min and on the right \( t_c = 2.5 \) min and \( t_r = 1 \) min. We observe that the maximum value of the NO\(_x\) emission rate increases when the frequency of vehicles restarts augments, namely when the time \( t_r \) of the red phase is lower.

**Test 2.2: Emissions when the traffic light duration \( t_c \) is constant.** In Figure 10 we show how the NO\(_x\) emissions vary with different ratio \( r \). Specifically, we plot NO\(_x\) total emissions (defined as the sum on the cells of the emission rates, at any time) for one hour of simulation with \( r = \{4, 3/2, 2/3\} \) which is equivalent to assume \((tg, tr) = (4 \text{ min}, 1 \text{ min}), (tg, tr) = (3 \text{ min}, 2 \text{ min}), (tg, tr) = (2 \text{ min}, 3 \text{ min}) \) respectively. We observe that until \( t_r \leq t_g \) (solid line and line with circle) the maximum of the emission rate increases when \( t_r \) grows, since the are more vehicle restarts; while it decreases with \( t_r > t_g \) (line with stars) when there are less vehicles restarts and more phases of stopped traffic.

To sum up, the two last examples developed in Test 2.1 and Test 2.2, suggest that the emissions grow with the increase of vehicles restarts. In particular, we observe from Figure 9 that the length of the traffic light cycle \( t_c \) has an highly influence on emissions, while Figure 10 shows that the ratio \( r \) between red-light and green-light has a less effect on the asymptotic emission values.
6.3 Test 3: Production of ozone

In this section we are interested in estimating the concentration of ozone along the entire road by means of the system (5.1). The reaction rate parameters \( k_1, k_2 \) and \( k_3 \) are listed in Table 4. For each cell \( x_j, j = 1, \ldots, N_x \), we set the initial concentrations \( \{ \mu_i(x_j, 0) \}_{i=1}^{5} \) as:
\[
\mu_1(x_j, 0) = \mu_3(x_j, 0) = 0, \quad \mu_2(x_j, 0) = 5.02 \times 10^{18} \text{ molecule/cm}^3,
\]
and, according to Section 4 and relation (4.4), for NO and NO\(_2\) we have
\[
\mu_4(x_j, 0) = (1 - p) \frac{E_{\text{NO}_x}(0)}{\Delta x^3}, \quad \mu_5(x_j, 0) = p \frac{E_{\text{NO}_x}(0)}{\Delta x^3} \text{ with } p = 0.15.
\]

For each time step \( n \) and for each \( x_j \), we compute the source term due to traffic by using the emission rate given in Test 1 and Test 2.

In Figure 11, we show the \( \text{O}_3 \) evolution along the entire road, during half an hour of simulation. We observe a behaviour amenable to the traffic variables dynamics given in Figure 5-7. To obtain now the total concentration of all the chemical species along the entire road, for every time \( t^n \) we sum the results on all the cells. In Figure 12 we show the variation in time of the concentration of \( \text{O}_3 \) and \( \text{O}_2 \). We observe that the ozone concentration has a huge growth, which is further amplified by the presence of the traffic light. Indeed the values of the red-circles line, which represent the solution with traffic light (Test 2), are considerably higher than those of the blue-solid line, which represent the solution without traffic light (Test 1). On the other hand, the oxygen concentration is almost constant in both the cases, with moderated dependence on traffic light.

To further investigate the impact of the traffic light on all the chemical species concentration, we solve our system starting from the \( \text{NO}_x \) emission rates computed in Test 2.1. Thus, we compute the total amount of \( \text{O}_3, \text{NO}, \text{NO}_2 \) and \( \text{O} \), obtained during the whole simulation along the entire road. Then, we measure the variation of each concentration with respect to the one obtained in the test case without traffic light, see Test 1. The results in Table 6 show that all the concentrations increase coherently with the behavior of the \( \text{NO}_x \) source term, see Figure 9.

7 Conclusions

The impact of vehicular traffic on society is evident and pervasive, but quantitative estimation of traffic effect on pollution is a difficult task. In this paper we proposed to couple a second-order model for traffic, comprised of conservation laws tested and tuned on NGSIM data, with a system of linear partial differential equations representing a simplified system of reactions in the atmosphere for ozone
Figure 11. Test 3. O$_3$ evolution along the entire road, for half an hour of simulation, in the case of dynamics without (left) and with (right) traffic light.

Figure 12. Test 3. Variation in time of the total concentration of O$_3$ (left) and O$_2$ (right), in the case of dynamics with (red-circles) and without (blue-solid) traffic light.

Table 6. Test 3. Variation of the total amount of O$_3$, NO, NO$_2$ and O concentration (g/km$^3$) computed with three different traffic light duration (Test 2.1) with respect the total amount of concentrations without traffic light (Test 1).

|       | $t_c = t_r + t_g$ (3 + 4.5) min | (2 + 3) min | (1 + 1.5) min |
|-------|-------------------------------|-------------|---------------|
| O$_3$ | 4.26e+05                      | 4.92e+05    | 5.75e+05      |
| NO    | 5.64e+06                      | 6.53e+06    | 7.67e+06      |
| NO$_2$| 1.73e+05                      | 2.02e+05    | 2.42e+05      |
| O     | 0.49                          | 0.54        | 0.59          |

production. The coupling is obtained via a general emission model, with parameters specifically tuned on NO$_x$ pollutants.

Via numerical simulations we tested various traffic scenarios obtaining three main results: 1) acceleration waves are most responsible for NO$_x$ emissions; 2) the length of traffic cycles impact emissions more than the ratio between green and red light; 3) ozone production is strongly impacted by traffic with linear growth regimes in presence of traffic light.

Future investigations will include extending the model to networks, to more complex chemical phe-
nomena and incorporating diffusion and transportation effects on emissions.

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