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Publication Date

2022-07-01

DOI

10.7922/G2F18X2S

Data Availability

The data associated with this publication are available at:

<https://zenodo.org/doi/10.5281/zenodo.11575091>

Network-wide Emissions Estimation Using the Macroscopic Fundamental Diagram

July 2022

A Research Report from the National Center
for Sustainable Transportation

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TECHNICAL REPORT DOCUMENTATION PAGE

1. Report No. NCST-GT-RR-22-45	2. Government Accession No. N/A	3. Recipient's Catalog No. N/A	
4. Title and Subtitle Network-wide Emissions Estimation Using the Macroscopic Fundamental Diagram		5. Report Date July 2022	
		6. Performing Organization Code N/A	
7. Author(s) Jorge A. Laval, Ph.D., https://orcid.org/0000-0002-0986-4046 Rafegh Aghamohammadi, Ph.D., https://orcid.org/0000-0003-3100-0145		8. Performing Organization Report No. N/A	
		9. Performing Organization Name and Address Georgia Institute of Technology School of Civil and Environmental Engineering 790 Atlantic Dr, Atlanta, GA 30332	
12. Sponsoring Agency Name and Address U.S. Department of Transportation Office of the Assistant Secretary for Research and Technology 1200 New Jersey Avenue, SE, Washington, DC 20590		10. Work Unit No. N/A	
		11. Contract or Grant No. USDOT Grant 69A3551747114	
		13. Type of Report and Period Covered Final Research Report (January 2020 – April 2022)	
		14. Sponsoring Agency Code USDOT OST-R	
15. Supplementary Notes DOI: https://doi.org/10.7922/G2F18X2S Dataset DOI: https://zenodo.org/doi/10.5281/zenodo.11575091			
16. Abstract This report presents a review of the studies incorporating the Macroscopic Fundamental Diagram (MFD) dynamics for emissions estimation using various microscopic estimation frameworks. These studies show the potential of applicability of the MFD-based tools for emissions estimation. However, the accuracy of existing models in estimating the emissions of large-scale urban networks is questionable due to their inability in capturing the variations in traffic conditions across such networks. As a solution to this problem, we have proposed to develop a multi-reservoir emissions estimation framework by partitioning large-scale networks into smaller regions with homogeneous traffic conditions and low-scatter MFDs like the multi-reservoir Dynamic Traffic Assignment (DTA) models, which can result in more accurate network-wide emissions estimation. The key component of this framework is finding a method to accurately estimate the emissions using aggregated network representation and its corresponding variables. A numerical experiment on an arbitrary network shows that the estimation efficiency can increase significantly by implementing aggregated network representation, albeit the results will be less accurate the more aggregated the representation becomes. The possible reasons and considerations for future applications have been discussed, which would lead to developing calibrated aggregated-level methods, which can estimate the emissions efficiently and accurately. After calibrating the MFD-based emissions estimation method to acceptable levels of accuracy and efficiency, traffic control strategies can be proposed to optimize the energy consumption and emissions of CO, CO ₂ , NO _x , PM _{2.5} , CH ₄ , VOC, etc. The proposed control strategies can include perimeter control strategies in the boundaries of the regions, ramp-metering strategies at the connections to the freeways and signal timing strategies, which is known to influence the shape of the MFD.			
17. Key Words Emissions estimation, macroscopic fundamental diagram, aggregated models		18. Distribution Statement No restrictions.	
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 32	22. Price N/A

Form DOT F 1700.7 (8-72)

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Acknowledgments

This study was funded, partially or entirely, by a grant from the National Center for Sustainable Transportation (NCST), supported by the U.S. Department of Transportation (USDOT) through the University Transportation Centers program. The authors would like to thank the NCST and the USDOT for their support of university-based research in transportation, and especially for the funding provided in support of this project.

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A National Center for Sustainable Transportation Research Report

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Network-wide Emissions Estimation Using the Macroscopic Fundamental Diagram

EXECUTIVE SUMMARY

This report presents a comprehensive review of studies incorporating Macroscopic Fundamental Diagram (MFD) dynamics for emissions estimation using various microscopic estimation frameworks. These studies show the potential of applicability of MFD-based tools for emissions estimation. However, the accuracy of existing models in estimating the emissions of large-scale urban networks is questionable due to their inability in capturing the variations in traffic conditions across such networks.

As a solution to this problem, we have proposed to develop multi-reservoir emissions estimation framework by partitioning large-scale networks into smaller regions with homogeneous traffic conditions and low-scatter MFDs similar to the multi-reservoir Dynamic Traffic Assignment (DTA), which can result in more accurate network-wide emissions estimation. The key component of this framework is finding a method to accurately estimate the emissions using aggregated network representation and its corresponding variables. A numerical experiment on an arbitrary network shows that the estimation efficiency can increase significantly by implementing aggregated network representation, albeit the results will be less accurate the more aggregated the representation becomes. The possible reasons and considerations for future application have been discussed, which would lead to developing calibrated aggregated-level methods, which can estimate the emissions efficiently and accurately.

After calibrating the MFD-based emissions estimation method to acceptable levels of accuracy and efficiency, traffic control strategies can be proposed to optimize the energy consumption and emissions of CO, CO₂, NO_x, PM_{2.5}, CH₄, VOC, etc. The proposed control strategies can include perimeter control strategies in the boundaries of the regions, ramp-metering strategies at the connections to the freeways and signal timing strategies, which is known to influence the shape of the MFD.

Introduction

The continuously increasing mobility demand in developing communities is resulting in several consequences where (i) delays caused by congestion directly result in economic loss, (ii) uncurbed fuel consumption exacerbates the depletion of non-renewable energy resources, and (iii) emissions from the vehicles provoke local (air pollution, acid rain, health issues) and global (climate change, global warming effect) damages. Therefore, from a sustainable development perspective, such effects must be studied and controlled to prevent any hindrance to the development process.

The motor vehicles emissions can be categorized into two general categories: (i) the air pollutants such as Particular Matter (PM), Non-Methane Hydrocarbons (NMHC), Nitrogen Oxides (NO_x), Carbon Monoxide (CO) and Sulfur Dioxide (SO₂), which impact the air quality and can result in human health issues, and (ii) Greenhouse Gases (GHG) including Carbon Dioxide (CO₂), Methane (CH₄) and Nitrous Oxide (N₂O), which have broader impacts such as climate change and global warming. Although the predominant GHG emitted from motor vehicles is CO₂, the latter two GHGs have higher Global Warming Potential (GWP) despite their lower emission rates (Azar & Johansson, 2012).

According to a recent fact sheet published by the United States Environmental Protection Agency (EPA), transportation sector accounted for the largest portion (28%) of total U.S. GHG emissions in 2016 (EPA, 2018). Between 1990 and 2016, GHG emissions in the transportation sector has increased more in absolute terms than any other sector (i.e., electricity generation, industry, agriculture, residential, or commercial) due in large part to increased demand for travel.

Several national and international policies including 1990 Clean Air Act Amendment, Kyoto Protocol and Paris Agreement have been proposed to control the GHG and pollutants emissions. The kernel technical basis of all these policies is the requirement of reliable emissions data, which is estimated using emission models. Emission models can be categorized as microscopic and macroscopic models (Rakha, et al., 2003). Macroscopic models such as EPA's MOBILE and California Air Resources Board's EMFAC models use average aggregate network parameters to estimate network-wide energy consumption and emission factors. The major drawback of these macroscopic models is in the use of a single traffic-related variable to estimate emissions, thereby ignoring other important explanatory variables that can significantly affect emission estimates.

The project level of EPA's state-of-the-science emissions model, MOVES (MOTOR Vehicle Emission Simulator) (EPA, 2020), is a microscopic model that incorporates the effects of different instantaneous speed and acceleration profiles on vehicle emissions, thereby trying to reflect the real driving conditions as much as possible. The latest approved version of MOVES is required by the regulations to be used in all transportation and air quality planning and assessment work. However, the complicated interface of MOVES, the need to comprehensive data and analysis for each link of the network and exhaustive run-time make it impractical for

real-time analysis and control purposes on large-scale city streets networks with hundreds of thousands of links.

Up until recently, the main objective of most traffic control strategies has been to alleviate congestion and to reduce the delay incurred by travelers and emission and fuel consumption control have only gained interest in the past few years. However, the optimal emission and fuel consumption strategy may not lead to minimal delay and congestion (Csikos & Varga, 2011). Therefore, the optimal control strategy considering all aspects must be a tradeoff between optimum emissions and optimum delay conditions.

The emissions and energy consumption calculations using MOVES or other microscopic models are resource intensive for large-scale networks and intractable for real-time analysis and control purposes. Several efforts have lately been made to improve the efficiency of MOVES model, e.g., MOVES Lite (Liu & Frey, 2013) and MOVES-Matrix (Liu, et al., 2016), but still the need to link-level computations is a hurdle to the real-time emission estimation for traffic control purposes.

The idea of an aggregated relationship between the network-wide traffic variables dates back to 1960s (Smeed, 1967; Godfrey, 1969) and a few other studies in 1980s (Herman & Prigogine, 1979; Mahmassani, et al., 1984; Ardekani & Herman, 1987). However, the recent empirical verification of existence of a network-level Macroscopic Fundamental Diagram (MFD) on urban areas has opened up a new paradigm (Geroliminis & Daganzo, 2008).

The MFD gives average traffic variables as a function of the number of vehicles inside the region, n . For instance, the average flow MFD:

$$Q = Q(n), \quad \text{(average flow MFD)} \quad (1)$$

gives the average flow, Q , on network arguably independently of trip origins and destinations, and route choice. This makes the MFD an invaluable tool to overcome the difficulties of the traditional link-level planning and control models including the microscopic emissions estimation models. If the MFD is accurately derived using empirical data or estimated using the analytical models on a region with homogeneous traffic distribution, it can be used to replace the links inside the region with a single entity, whose traffic dynamics is given by the MFD variables, in the emissions estimation method without significant loss of accuracy. The MFD has been widely used in other aspects of traffic planning and management such as dynamic traffic assignment (Yildirimoglu, et al., 2015; Batista, et al., 2019; Aghamohammadi & Laval, 2020; Aghamohammadi & Laval, 2020), optimal control (Ramezani, et al., 2015; Haddad, 2017; Kouvelas, et al., 2017), parking (Cao & Menendez, 2015; Leclercq, et al., 2017) and pricing (Zheng, et al., 2016; Yang, et al., 2019).

Nevertheless, the implementation of MFD in emissions estimation is yet an underdeveloped field of research and practice, with only a handful of studies conducted on this topic up until now. Furthermore, since emissions analysis is required to be done according to certain regulations or using specific models by the national or local agencies, many authorities are limited to use the specific models and software packages for the emissions estimation

purposes. Therefore, researchers tend to explore innovative ways to incorporate the state-of-the-art developments in the traffic modeling realm into the existing emissions estimation methods to improve their efficiency. Furthermore, the MFD has the potential to provide a tool to control the congestion and emissions of urban networks simultaneously.

In this project, we will first conduct a review of the existing literature on implementation of the MFD for emissions estimation purposes in the recent years. Of foremost importance is the studies which try to incorporate the MFD dynamics into the existing well-established emissions estimation models mandated by the authorities to be used for emissions analysis. Later, we will use the MFD-based aggregated traffic conditions at different aggregation levels to estimate the emissions from a grid network using the MOVES model and the efficiency and accuracy of the results will be discussed.

Background

Considering the monotonous increase of the share of transportation industry in the pollutants and GHG emissions (EPA, 2021), there will be a need to develop traffic control and routing strategies in the near future not only based on the travel time minimization criterion, but also seeking to optimize the pollutants and GHG emissions and energy consumption, which would require accurate real-time emissions estimations. In general, the emissions estimation models can be categorized into three different approaches based on their need to different levels of data (Yin, et al., 2013):

- 1) The *emission factor models*, which assign an emission factor derived from repetitive experiments to the whole analysis period. The emission factor can be multiplied by correction factors to incorporate different vehicle speeds, fuel type, vehicle age, etc. The total amount of emission for any specific pollutant or GHG is found by multiplying the corresponding emission factor by the total vehicle miles travelled (VMT) for the analysis period.
- 2) The *physical power-demand models*, which consider the vehicle's operational conditions and driving environment to provide second-by-second emissions. These models usually consider different operational characteristics of vehicles such as engine power, engine speed, air/fuel ratio, fuel use, etc. for different vehicle operation states. This type of models estimates the emissions more accurately, however, their extensive need to obtain a large variety of detailed data is an obstacle in their application.
- 3) The *acceleration and speed-based models*, which compute emission rates as nonlinear functions of instantaneous speed and acceleration values. This approach has gained more popularity recently, since they provide more accurate estimates compared to the emission factor models and require less information compared to physical power-demand models.

The current microscopic methods of emission estimation such as the MOVES model are unsuitable for real-time applications in large-scale networks with thousands of links despite their higher accuracy compared to the previous models. In this section, we will perform a review of the state of the art in incorporating MFD in vehicular emissions estimation. It is worth

mentioning that we have changed the mathematical notation of some of the reviewed studies in order to keep the consistency of the notations throughout this report.

Reservoir-based Models

Most of the MFD-based emissions estimation models in the literature model the entire network as a reservoir, whose traffic dynamics are given by the MFD of the reservoir. The network wide aggregated MFD variables are then used to estimate the vehicular emissions inside the network.

Shabihkhani and Gonzales (2014) developed a methodology for GHG emissions estimation using the MFD of a single homogeneous network for estimating driving cycle components, i.e., (i) time spent cruising at free-flow speed, T_c , (ii) time spent idling while stopped, T_i , and (iii) the number of vehicle stops per distance traveled, s , without the need for extensive trajectory analysis using conventional microscopic methods. Then, the total emissions per vehicle distance traveled, E , is computed as:

$$E = e_c T_c + e_i T_i + e_s s, \quad (\text{total emissions per distance travelled}) \quad (2)$$

where e_c is the emission factor per unit cruising time, e_i is the emission factor per unit idling time and e_s is the emission factor associated with complete cycle of deceleration from the free-flow speed, v_f , to 0 and then acceleration from 0 to v_f . To estimate the emission factors, a traffic simulation has been conducted on a simple ring network with a single intersection representing a long arterial or a network with homogeneous traffic conditions. The ring network has been loaded with the full range of possible densities from an empty network to complete jam. The vehicle trajectories are extracted to be used for microscopic emissions estimation via the project level of the MOVES model as a comparison benchmark to compute the emission factors and the duration of a full deceleration and acceleration cycle, τ .

The next step is to approximate the aforementioned driving cycle components using the MFD. It has been assumed that the vehicles stop only once during each traffic signal cycle, C . The driving cycle components for each traffic state, with average MFD speed v are estimated as:

$$s = \frac{1}{vC}, \quad (\text{number of stops per unit distance travelled}) \quad (3a)$$

$$T_c = \frac{1}{v_f} - \frac{\tau}{2} s, \quad (\text{cruising time}) \quad (3b)$$

$$T_i = \frac{1}{v} - \frac{1}{v_f} - \frac{\tau}{2} s. \quad (\text{idling time}) \quad (3c)$$

Later, sensitivity analysis has been done to see the impact of the three main factors, the green time to cycle length ratio, the signal cycle length, and the block length on GHG emissions estimates and their relative error compared to the benchmark emissions rate computed using the MOVES model. It has been found that the green time to cycle length ratio plays a key role in both the shape of the MFD and the rate of emissions and the estimation errors are significant and consistently positive at near-to-jam density values. A significant shortcoming of the proposed model is not being capable of taking different vehicle types into account.

Csikos, et al. (2015) developed an optimal perimeter control model aiming to minimize the emissions from the vehicles inside the perimeter built on the emissions estimation model proposed in Csikos (2012) using the average speed (v), total travel distance (TTD) and total time spent (TTS) variables obtained using the MFD. The emission factors for different traffic states for the network are calculated similar to the linkwise emission factors formulation provided by (Ntziachristos, et al., 2009) using the MFD average speed, which has later been multiplied by the TTD of the network to find the total emissions of the network. The CO emission estimates for two different case studies indicate that the proposed method has a 20% error compared to the link-level microscopic Versit+Micro model (Smit, et al., 2007) but yields in very similar results compared to the link-level Copert IV model (Ntziachristos, et al., 2009).

Amirgholy, et al. (2017) proposes a model for optimal design of public transportation systems in congested urban networks. As a component of the total cost of the transportation system, the external cost of emissions is approximated by using the average speed of the network MFD in a VMT-based emissions estimation model proposed by Affum, et al. (2003). In this model, the external cost of emissions (E_N) is computed as a function of the fuel consumption of automobiles (F_A) and transit vehicles (F_T), where the MFD speed for any given average density state in the network is only used for computation of the fuel consumption of the average automobile per unit distance traveled in the network.

Ingole, et al. (2020) proposed an optimal perimeter control model for a network comprised of an inner city modeled as a reservoir with entrances and exits at three locations on the perimeter and bypass freeways connecting and exit points. The model aims to minimize the NO_x emissions inside the reservoir using a gating strategy based on Nonlinear Model Predictive Control (NMPC). The reservoir emissions are computed by integrating the fourth-degree polynomial formulation proposed by Lejri, et al. (2018) into the COPERT IV model (Ntziachristos, et al., 2009). The total emissions of pollutant $m \in \{CO_2, NO_x\}$ between t and $t + dt$, $E_{dt}^m(t)$, in [g] is found as:

$$E_{dt}^m(t) = EF^m(v(t)) \times n(t) \times v(t) \times dt, \quad (4)$$

where $EF^m(v(t))$ is the emission factor of pollutant m in [g/km], $n(t)$ is the accumulation of vehicles inside the reservoir at time t , $v(t)$ is the MFD mean speed at time t in [km/h] and dt is the time step in [h]. The emission factors are calibrated through curve fitting to the actual microscopic emissions for different MFD mean speeds. The emissions of each internal route i inside the reservoir is found by replacing n in Eq. (4) with the partial accumulation of the route n_i . Furthermore, the emissions of each bypass link can be calculated by replacing the accumulation and average speed of the link in Eq. (4).

Saedi, et al. (2020) developed a model to estimate the network-wide emissions by incorporating the MFD into the microscopic emission model considering different light and heavy-duty vehicle compositions. The benchmark microscopic emission rates are obtained using the polynomial model proposed in Panis, et al. (2006) as:

$$E_m(t) = \max[0, (f_1)_i^m + (f_2)_i^m v_i + (f_3)_i^m v_i^2 + (f_4)_i^m a_i + (f_5)_i^m a_i^2 + (f_6)_i^m v_i a_i], \quad (5)$$

where $i \in \{\text{gasoline car, diesel car, LPG car, heavy-duty vehicles}\}$ is the vehicle type, $m \in \{\text{CO}_2, \text{NO}_x\}$ represents different emission types, v_i is the vehicle's speed in [m/s], a_i is the vehicle's acceleration in [m/s²] and $(f_1)_i^m$ to $(f_6)_i^m$ are model constants determined by non-linear multiple regression methods. For the macroscopic emissions estimation the authors propose:

$$E_m(t) = (\sum_{i=1}^N \alpha_i^m p_i) k(t) (\beta_m + v(t)) = (\sum_{i=1}^N \alpha_i^m p_i) (\beta_m k(t) + q(t)), \quad (6)$$

where $E_m(t)$ is the rate of emission in [g/s] of pollutant $m \in \{\text{CO}_2, \text{NO}_x\}$ at time step t in the observation period, p_i is the penetration rate of vehicle type i in the traffic stream, $k(t)$, $v(t)$, and $q(t)$ are the network-wide average density, speed, and flow, respectively, and α_i^m and β_m are the model parameters for vehicle type i and pollutant m . β_m can be perceived as a penalty factor for high density scenarios, when the traffic is congested and repeated stop and go movements have a significant toll on the emissions.

A micro-simulation is used to produce traffic data for different demand and vehicle composition scenarios in order to calibrate the proposed macroscopic emission model parameters using the microscopic emission estimates found by Eq. (5). The significant difference between the calibrated parameters for a congested central business district (CBD) inside the network and the entire network, which is less congested on average, demonstrate that the model parameters are very sensitive to the network topology and demand intensity and that the parameters must be calibrated for each network. The results indicate that different vehicle compositions only have a scaling factor on the resulting total emissions. Using the results, 3-dimensional Network Emission Diagrams (NED) are developed showing the emission rate for any average flow and density pair for the studied network.

The next subsection will review another class of MFD-based emissions estimation models, which do not explicitly state the incorporation of MFD in their model but in fact are using MFD for their local traffic flow relationships like the continuum-space DTA models presented in Aghamohammadi & Laval (2020).

Continuum-space Models

Another major approach observed in the literature is to model the network as a continuum space where the vehicles can circulate at any point $x = (x, y)$ of a Euclidean two-dimensional domain $\Omega \subset R^2$, see Figure 1(a). The basic notion behind the continuum-space traffic models is that when the network is dense enough such that the distances between road segments are small compared to the size of network, the network can be approximated by a continuum space. There is a vast body of literature on continuum-space Dynamic Traffic Assignment (DTA), emanating from the seminal pedestrian flow model by Hughes (2002). Later, researchers have adapted this framework to the vehicular traffic and have proposed various DTA models in continuum space, see e.g., (Jiang, et al., 2011; Du, et al., 2013; Lin, et al., 2017), which consist of a conservation law partial differential equation (PDE) in two dimensions, supplemented with an Eikonal or Hamilton-Jacobi PDE for the route choice component.

The connection between the continuum-space models and the MFD theory lies in the numerical solution of these models, where the continuum space is partitioned into a grid of small regions,

see Figure 1(b), and the traffic dynamics inside each region is described by a local speed-density relationship. Several recent studies in the continuum-space DTA literature have mentioned the local speed-density relationship as MFD (Du, et al., 2013; Du, et al., 2015; Long, et al., 2017). Aghamohammadi & Laval (2020) shows that the speed-density relationship can in fact be interpreted as the MFD, since it is defined on a portion of the network and must also take the network effects such as signal timing into account. Note that the local MFDs in the continuum-space models are defined only on a small portion of the network, while in the reservoir-based models there is a single MFD defined over the entire network.

As the first study investigating the emissions in the continuum space, Yin, et al. (2013) proposes a bi-level optimization problem to optimize housing allocation to minimize vehicular emissions in an integrated land use and transportation modeling framework. The lower-level subprogram formulates the traffic assignment problem to achieve the user optimum (UE) solution, where the total cost for each user is consisted of the travel and housing costs and solves the resulting system of PDEs using the finite element method (FEM). For a complete review of formulation and different solution methods of continuum-space traffic assignment models refer to Aghamohammadi & Laval (2020).

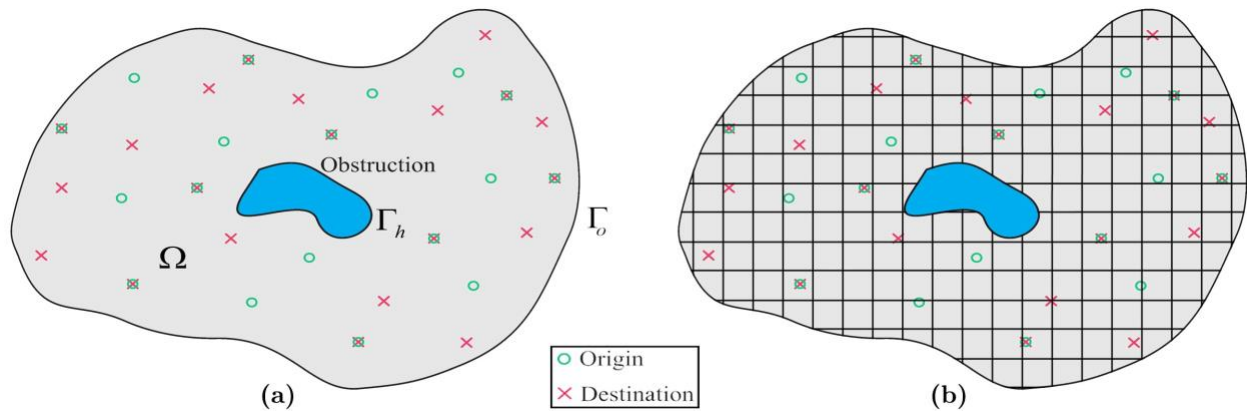


Figure 1. Illustration of (a) continuum space and (b) typical solution grid

In the upper-level subprogram, the housing allocation is optimized to minimize the CO₂ emissions. The emissions and fuel consumption estimation model proposed by Ahn, et al. (2002) is adopted to estimate the emission rate of each type of emission as:

$$E^m(v, a) = \exp(\sum_{i=0}^3 \sum_{j=0}^3 \omega_{i,j}^m v^i a^j), \quad (7)$$

where E^m is the instantaneous emission rate and fuel consumption with superscript m denoting different kind of emissions, HC and CO in [mg/s] and fuel consumption in [gal/h], v is the speed in [km/h], a is the acceleration in [km/h²] and $\omega_{i,j}^m$ denotes the model regression coefficient for emission type m , speed power i , and acceleration power j . However, this model cannot be directly used to estimate the CO₂ emissions and the CO₂ emission rate can be found using the carbon balance between fuel consumption and emissions of other gases including carbon as:

$$E^{CO_2}(v, a) = 2458.29F(v, a) - 3.17E^{HC}(v, a) - 1.57E^{CO}(v, a), \quad (8)$$

where F , E^{HC} and E^{CO} are Fuel consumption in [gal/h], HC emission rate in [mg/s] and CO emission rate in [mg/s], respectively, which all can be computed using Eq. (7) using the available model coefficients. The total CO₂ emissions in the network are found by integrating the CO₂ emission rate multiplied by the norm of the optimum flow vector at any point $f^*(x, y)$ over the entire network considering that the speed and acceleration values at the vicinity of any point is given by the local MFDs described earlier.

Jiang, et al. (2018) proposes a second-order continuum-space DTA model, where the travelers seek to minimize their travel cost based on the dynamic user equilibrium (DUE) principle considering that the travelers only perceive their instantaneous travel times as the travel cost. After solving the DTA problem using the standard PDE solution methods, the instantaneous emission rate $E_i^m(x, t)$ in [g/s/veh] for each vehicle type i and emission type $m \in \{CO_2, NO_x, PM, VOC\}$ at any location $x \in \Omega$ and time t is found using the Panis, et al. (2006) model given by Eq. (5). The rate of the emission for the i -th vehicle type and the m -th emission type at location $x \in \Omega$ and time t is expressed as $DE_i^m(x, t)$ in [kg/km²/h] and is calculated as:

$$DE_i^m(x, t) = 3.6 \times \rho_i(x, t)E_i^m(x, t), \quad (\text{emission rate at location } x) \quad (9)$$

where $\rho_i(x, t)$ is the density of i -th vehicle type at location x and time t . The total emission rate for the i -th vehicle type and the m -th emission type in the entire continuum space at time t is denoted by $TE_i^m(t)$ in [kg/h] and is obtained as:

$$TE_i^m(t) = \iint_{\Omega} DE_i^m(x, y, t) dx dy, \quad (\text{total emission rate}) \quad (10)$$

The corresponding cumulative emission for the i -th vehicle type and the m -th emission type in the entire network since the beginning of analysis until time t , $CE_i^m(t)$ in [kg], can be found as:

$$CE_i^m(t) = \int_0^t TE_i^m(s) ds, \quad (\text{cumulative emission}) \quad (11)$$

Discussion and Outlook

In this section, we discuss the main findings in terms of the observed trends in the literature and identify the issues and challenges that deserve further research. Table 1 presents an overview of the studied papers, their specifications, and main contributions.

Table 1. Overview of the studied papers

Source	Estimated Emissions	MFD Variables	Base Model	Main contribution
Reservoir-based Models				
Shabihkhani & Gonzales (2014)	GHG	v	MOVES (EPA, 2020)	Computed driving cycle components to be used in the MOVES model
Csikos, et al. (2015)	CO	v , TTD , TTS	COPERT IV (Ntziachristos, et al., 2009)	Replaced the MFD-based variables for network into the link-level COPERT IV model
Amirgholy, et al. (2017)	External cost of emission	v	Affum, et al. (2003)	Proposed optimal transit system design by incorporating external emissions cost in the total cost
Ingole, et al. (2020)	CO ₂ , NO _x	v, n	COPERT IV (Ntziachristos, et al., 2009)	Proposed optimal perimeter control minimizing the emissions inside the reservoir
Saedi, et al. (2020)	CO ₂ , NO _x	v, q, k	Panis, et al. (2006)	Developed the most detailed MFD-based emissions model in the literature using mean MFD v, q and k
Continuum-space Models				
Yin, et al. (2013)	CO ₂	v, a	Ahn, et al. (2002)	Developed a housing allocation optimization model by minimizing the CO ₂ emissions in the network
Jiang, et al. (2018)	CO ₂ , NO _x , PM, VOC	v, a	Panis, et al. (2006)	Developed a comprehensive method to estimate emissions in continuum space

From Single-reservoir to Multi-reservoir Models

The studies reviewed here demonstrate that the MFD can be a powerful tool in making the microscopic emissions estimation models less resource intensive and more efficient for real-time network control and management purposes. However, due to the heterogeneity of realistic large-scale networks, the single-reservoir models presented here cannot accurately estimate the emissions in large-scale networks. The current trend of dealing with heterogeneity in large-scale networks is to partition the network into smaller regions with homogeneous traffic conditions, which will exhibit accurate low-scatter MFDs. This approach has been

recently very popular among the researchers for network control and traffic assignment purposes (Yildirimoglu, et al., 2015; Haddad, 2017; Aghamohammadi & Laval, 2020).

In a similar way, for emissions estimation purposes the large-scale networks can be divided into smaller regions in order to estimate the emissions inside the network more accurately. The size of regions can be determined based on the physical reality of the networks or in a way to make a balance between the accuracy and efficiency of the model. The smaller the regions inside the network, the more accurate the emissions estimations will be but on the other hand the higher number of regions would increase the computation times and reduce the model efficiency.

After appropriately partitioning the network into smaller regions, the same single-reservoir emissions estimation methods presented here can be applied to estimate the emissions from each region, which would sum up to the emissions from the entire network. Furthermore, the knowledge about emissions at each part of the network will pave the path to develop traffic control and routing strategies aiming to minimize the emissions inside the network.

Challenges in Estimation of the MFD

Although the proposed multi-reservoir approach sounds promising, a main concern which can be a hurdle in implementation of this approach is deriving the MFDs for each region inside the network. The MFD can be empirically derived using empirical data such as loop detector data (LDD). However, the required empirical data is not available for many networks and even when available it is subject to significant errors and bias.

Another approach is to determine the MFD analytically, which does not require empirical data and estimates the shape of the MFD using network topology and control characteristics such as block length, existence of turn-only lanes, and traffic signal settings. Up until recently, the analytical estimation of the MFD was not an easy task because the Method of Cuts (MoC) in Daganzo & Geroliminis (2008) becomes intractable for real-life networks and one needs to resort to simulation methods, which defeats the purpose of macroscopic modeling. Laval & Castrillon (2015) develops the Stochastic Method of Cuts (SMoC) by extending the MoC to stochastic corridors with different block lengths and signal timing settings and shows that (the probability distribution of) the MFD can be well approximated by a function of mainly two parameters: the density of traffic signals (λ) and the mean red to green ratio of traffic signals (μ).

Adopting the analytical methods discussed above or other analytical MFD estimation methods in the literature can help to overcome the obstacle of determining the MFDs of regions in the multi-reservoir approach by only needing some information about the network topology and control characteristics. Moreover, if the data for analytical methods are not easy to obtain, one can resort to micro-simulation methods to derive the MFD, which would need precise calibration and validation to represent the ground truth accurately.

Incorporating the MFD in the MOVES model

Out of the studied papers, only one study builds an MFD-based emissions estimation model based on the MOVES model (EPA, 2020) required by the US EPA for emissions analysis. The European researchers tend to utilize the COPERT IV model (Ntziachristos, et al., 2009), which is developed and required by the European Environment Agency. Therefore, it would be better if the researchers in the US put more emphasis on incorporating recent advances in traffic modeling domain such as the MFD in order to improve the efficiency of the MOVES model. It is worth noting that there are efforts in the literature to improve the efficiency of the MOVES model, such as MOVES Lite (Liu & Frey, 2013) and MOVES-Matrix (Liu, et al., 2016), but in this project, our focus is on increasing the efficiency of the MOVES model by implementing aggregated representation of the traffic dynamics inside urban networks. In addition to increasing the efficiency of the emissions estimations, the MFD can help to reduce monitor the traffic conditions in a macroscopic level and has the potential to be implemented for control purposes aiming to reduce the congestion and emissions simultaneously.

The project level of the MOVES model allows the traffic data to be included in the model via three different methods: (i) the average link speed for the analysis period, (ii) the second-by-second link drive schedule demonstrating instantaneous link speeds, or (iii) the operating mode distribution for all links in the network. The derivation of the second set of data might be unattainable from the MFD only, unless we have information about the evolution of the MFD over time. The sequential MFD data can help us to derive the driving cycle components more accurately compared to the method presented in Shabihkhani & Gonzales (2014), which uses only the mean MFD speed in order to find the driving cycle components. Furthermore, the variance of MFD at any given density value might be helpful in determining the driving cycle components, which needs further investigation.

On the other hand, the average link speed input method provides a straight-forward method to incorporate MFD variables in the MOVES model. Following the aforementioned recommendations, after dividing the network into several regions with homogeneous traffic conditions, all the links inside each region can be replaced by a single entity with its average speed given by the mean MFD speed. However, case-specific correction factors may be needed to estimate the emissions accurately by this approach, which can be found by calibrating the results using the results of link-level emissions estimates.

The next section will present the results from a numerical experiment incorporating the aggregated traffic variables in the MOVES model and will compare the efficiency and accuracy attained by 4 different aggregation levels of network representation.

Numerical Experiment

In this section, we will try to estimate the *running exhaust* emissions of several pollutants in the MOVES model for a grid network by implementing the aggregated representation of traffic (i.e., the MFD) in different aggregation levels. Due to the limitations of this project, we did not delve deeper into estimation of the MFDs and have used the aggregated traffic conditions as a proxy

to the MFD in this numerical experiment. The project scale is the most in-detail module of the MOVES model requiring detailed inputs describing the vehicle population and activity at the site. This module is capable of estimating the emissions of different pollutants emitted from a transportation network for a one-hour period in a specific month of the year at a specific county given information on network geometry, vehicle type, fuel type and age distribution of the fleet, meteorology data, and any ongoing maintenance programs at the project location.

The numerical experiment here aims to demonstrate the potential of implementing aggregated-level representation of a network in the MOVES model by comparing the accuracy and efficiency of emissions estimations conducted in 4 different aggregation levels: (i) lane, (ii) link, (iii) corridor, and (iv) network. The corridor aggregation level implemented here might not be applicable to networks with arbitrary shapes, where no clear corridors can be observed. This aggregation level has been included in the analysis here to showcase an intermediate step between the link-level and network-level aggregations to balance off the accuracy and efficiency levels. Toward this purpose, a 5-by-5 homogeneous grid network with identical block lengths of 200 meters, 2 lanes in each direction and traffic signals with a cycle length of 90 seconds at all intersections, as shown in Figure 2, has been loaded with a constant demand rate of 5 vehicles per second for 2100 seconds with randomly distributed origins and destinations across the network using the SUMO traffic simulation package (Lopez, et al., 2018). The evolution of departures, arrivals, accumulation, and network average speed during the analysis period is demonstrated in Figure 3. The accumulation curve, indicating the number of running vehicles on the network, can be derived as the difference between the cumulative departures and arrivals curves at any time.

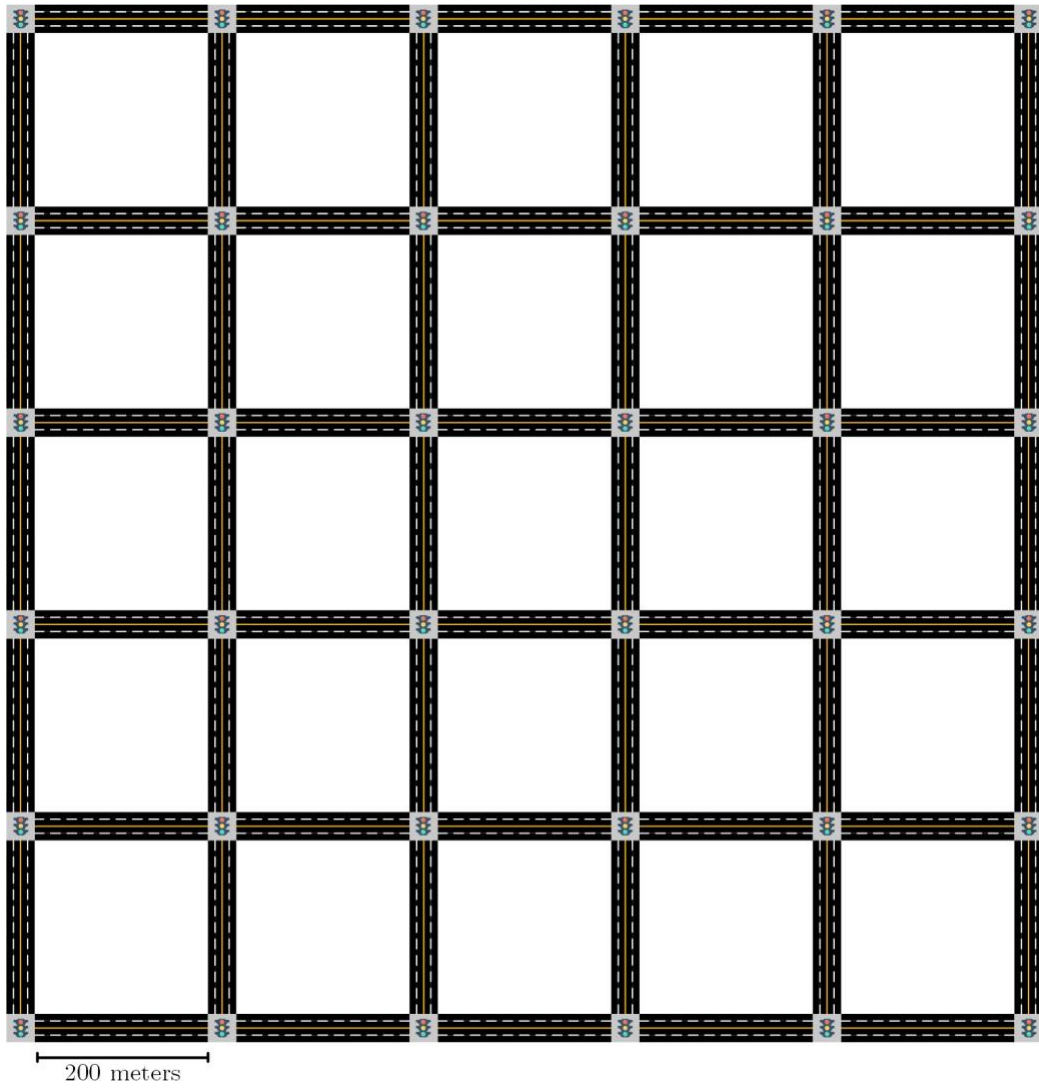


Figure 2. Illustration of the 5-by-5 grid network

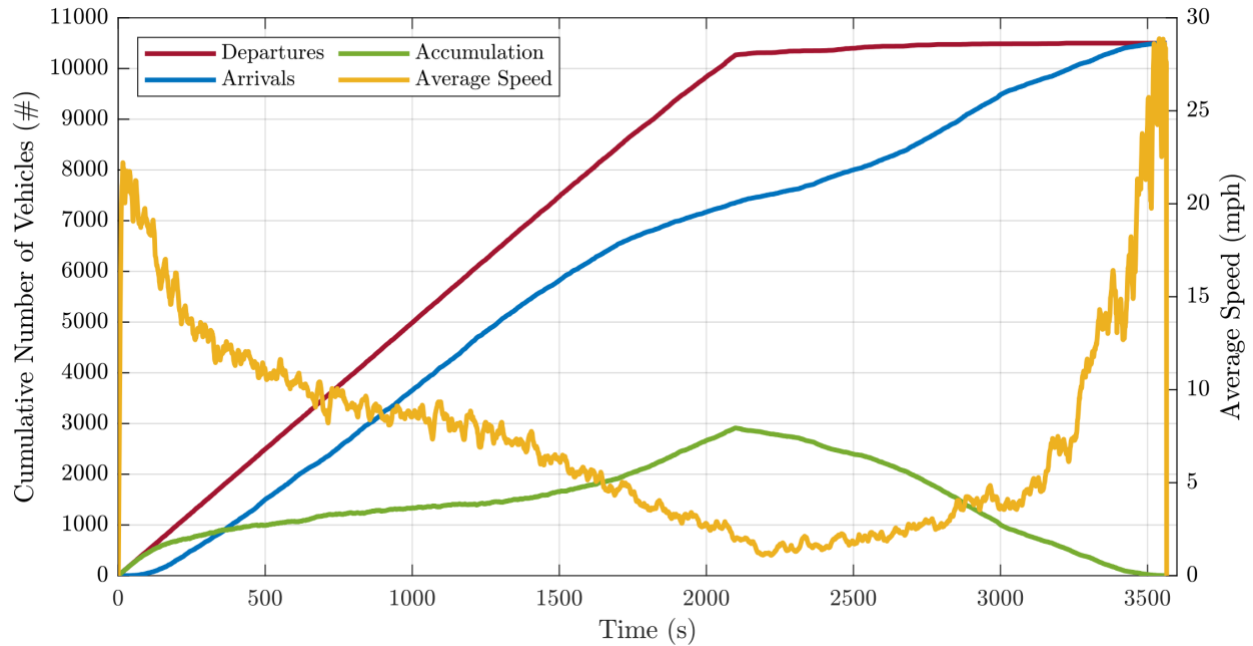


Figure 3. Evolution of the cumulative curves and average speed over time

Figure 4 exhibits the average speed versus accumulation and average flow versus average density MFD plots for the network. The two different branches in each of these diagrams, known as the “hysteresis loops” in the literature, are associated with the loading and unloading phases of the network and different behavior of the urban networks in loading and unloading periods due to abrupt and immense changes in the demand as in this experiment. However, in real life, the changes in demand pattern are usually gradual and the networks do not exhibit distinct loading and unloading behavior. This will reduce the likelihood of observing hysteresis loops and will result in well-defined MFD functions. The analysis in this experiment will not be impacted by this phenomenon since we can directly obtain the speed values at any point of time, needless of referring to the MFD.

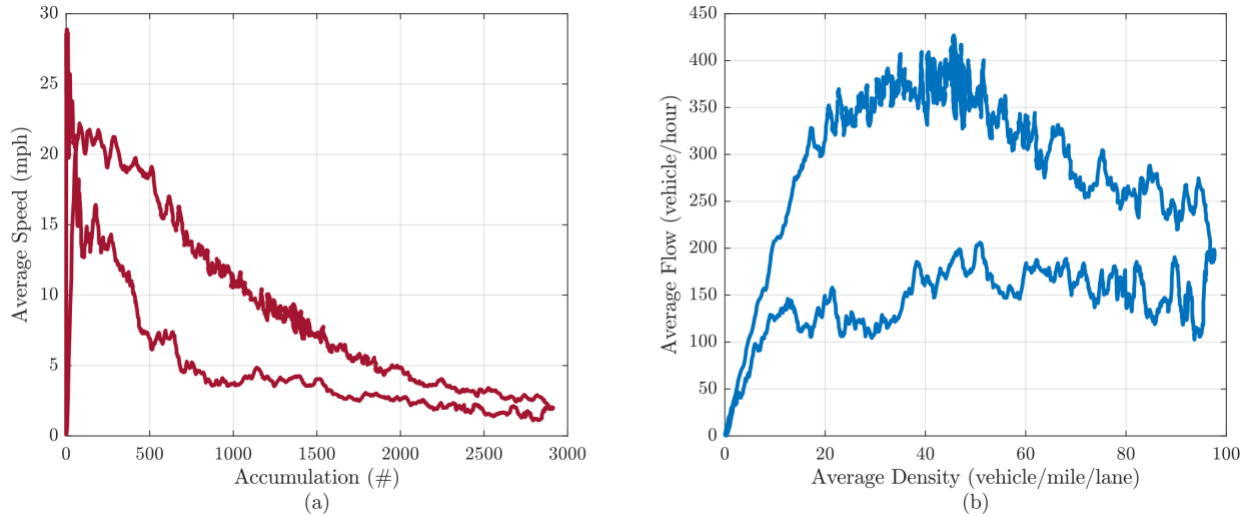


Figure 4. (a) Average speed vs. Accumulation, and (b) Average Flow vs. Average Density MFDs

The simulation provides second-by-second speed, density, and flow measurements for each lane in the network, which can be inputted to the MOVES model to compute the lane-level emissions, which results in the most accurate estimates and will be used as a benchmark for comparison purposes. Furthermore, 3 other emissions estimations have been performed the link, corridor, and network levels by replacing all the lanes inside each of the aggregated representations by a single entity, whose traffic conditions are computed by averaging the traffic variables of all lanes inside them. The other required inputs of the MOVES model, which will be the same through all runs, are given in Table 2.

Table 2. MOVES input parameters for the numerical experiment

Parameter	
Year, Month, Day	Weekday in June 2021
Time of day	17:00 to 18:00
Location	Fulton county, Georgia
Vehicle type	Passenger cars
Fuel type	Gasoline
Road type	Urban unrestricted access

The estimated emissions, total energy consumption and MOVES run-times for different aggregation levels are presented in Table 3. The provided run-times only include the computation times by the MOVES model, and it has been assumed that the computational time for aggregating the traffic conditions is similar for different aggregation levels once the traffic conditions is known and is negligible compared to the MOVES computation times. The lane-level network representation estimates are the most accurate results and have been selected as a benchmark to compare the accuracy and efficiency of the estimates using other aggregation levels.

The numbers in parentheses in this table show the relative percent change in the estimates with respect to the lane-level estimates, which have been further plotted against the run-time of each estimation process in Figure 5. The results indicate that using an aggregated network representation in link, corridor, and network levels, will result in 1.8, 5.3, and 13.1 times faster estimation, respectively, compared to the lane-level estimation. However, this higher efficiency comes at the expense of losing some accuracy. While the link-level estimates have a maximum relative error rate of 8%, the relative error of network-level estimates is as high as 25%. On the other hand, the relative error of the corridor-level results for all components except PM_{2.5} is below 10%. Considering the 81% reduction in the execution time, the corridor-level aggregation looks as an efficient and plausible approximation method for the microscopic emissions estimation at the lane level.

Table 3. Emissions estimates and run-times for different aggregation levels

Component	Aggregation Level			
	Lane	Link	Corridor	Network
Carbon Monoxide (CO) [kg]	64.51	59.36 (-7.97%)	66.14 (2.53%)	76.4 (18.43%)
Carbon Dioxide Equivalent (CO ₂) [kg]	3646.90	3753.68 (2.92%)	3875.27 (6.26%)	4162.17 (14.12%)
Oxides of Nitrogen (NO _x) [g]	996.26	923.57 (-7.29%)	896.41 (-10.02%)	744.6 (-25.25%)
Primary Exhaust PM _{2.5} [g]	32.95	31.13 (-5.51%)	27.95 (-15.14%)	24.71 (-24.99%)
Methane (CH ₄) [g]	127.43	126.03 (-1.09%)	130.19 (2.17%)	116.9 (-8.25%)
Total Energy Consumption [10 ⁹ J]	50.59	52.07 (2.92%)	53.75 (6.26%)	57.75 (14.15%)
MOVES Run-time [s]	1098.7	612.5 (-44.25%)	206.2 (-81.24%)	84.0 (-92.35%)

* Relative percent change with respect to the lane-level results in parentheses

Although the results presented here are for an arbitrary and simplified network, the two main impacting factors for the aggregated-level emissions estimation in the MOVES model can be listed as:

- 1) The lengths provided in the network configuration to the MOVES model serve as the trip length on the given entity. This is valid for the lane- and link-level network representations; however, in the corridor and network levels, the travelers do not necessarily travel the entire length and their trip length is usually lower than the length of the corridor or network. Therefore, using the actual corridor and network lengths will most probably result in overestimation of the emissions. Using average trip length instead of entity length in corridor- and network-level representations can help to mitigate this issue and increase the accuracy of the results.

- 2) Implementing an aggregated representation will result in a less-detailed rendition of the traffic flow evolution in the emissions estimation process, which will prevent the estimation process from capturing the entire driving cycles in the network and presumably result in underestimation of the emissions. Although this was expected by implementing aggregated representations of the network, it can be diminished by calibrating the aggregated estimates to the microscopic estimates.

As it can be seen in Figure 5, the error rate varies with different pollutants stemming from individual formulations with different weights of the impacting factors used to compute the emissions of each component, except for the CO₂ emissions and the total energy consumption which have totally similar behaviors due to similar computations in the MOVES model (EPA, 2020). Therefore, any calibration process for the emissions estimates in different aggregation levels should be network and component specific.

Once the results from a training set have been calibrated for a network, a general recipe can be provided to estimate the emissions with high accuracy using the aggregated traffic variables. Furthermore, the driving cycles capturing the drivers' behaviors in the MOVES model may need to be updated if the aggregated representation of traffic conditions is implemented to estimate the emissions considering that the aggregated traffic conditions provide less details on the variations of traffic flow inside the urban networks or zones (Shabihkhani & Gonzales, 2014). The main advantage of such method in addition to its significantly higher efficiency would be that the emissions inside any region of the network can be easily estimated by tracking a single traffic variable: *the number of vehicles inside the region or accumulation*. This will enable the practitioners to develop perimeter control strategies aiming to minimize the emission of any component for a multi-region network with well-known MFDs and calibrated MFD-based emissions estimation methods.

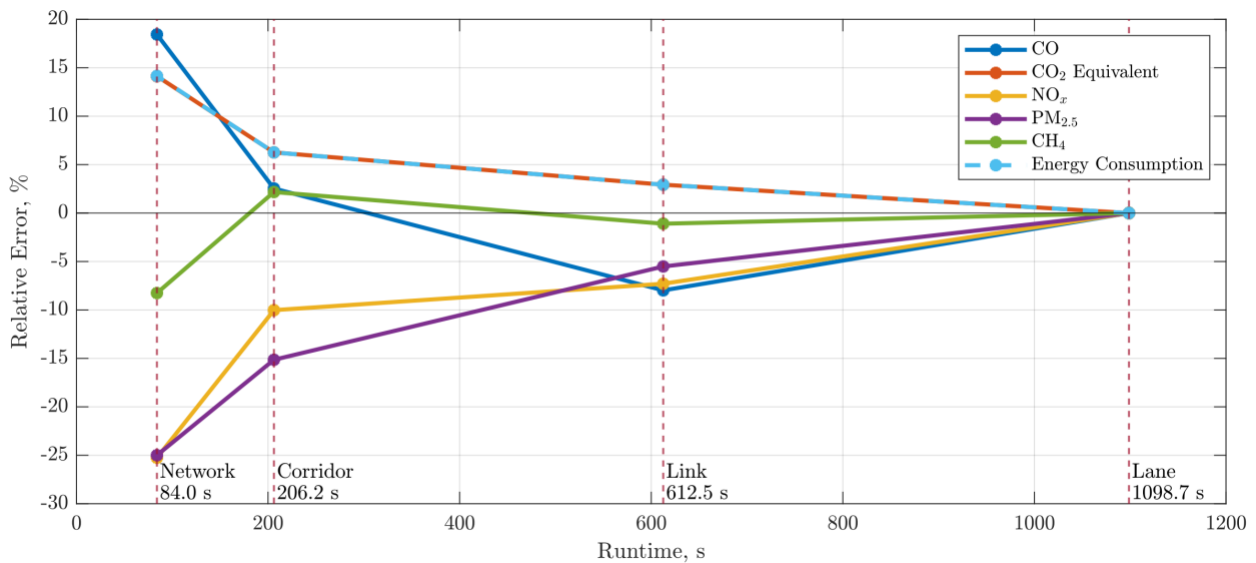


Figure 5. Emission estimates vs. Run-times for different aggregation levels

Although the network-level emissions estimation using the MFD outputs can increase the efficiency of the emissions estimation, the results will only reveal the total emissions inventory of the entire network and will not be helpful in identifying the emissions hotspots inside the network. To overcome this shortcoming, one can partition the network into smaller zones and feed the zone-level traffic conditions produced by their respective MFDs to the MOVES model to estimate the emissions in the zone level. Not only this will increase the accuracy of the estimated emissions, but also it will help to identify the zones with higher emissions. If the hotspot zones are still large, link-level emission estimations can be conducted in these zones to detect the exact links with the highest emissions.

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Data Summary

Products of Research

This study has produced simulation traffic data for the numerical experiment and the emissions estimations outputs by the MOVES model in 4 different aggregation levels for the numerical experiment.

Data Format and Content

The data includes:

- 1) The second-by-second traffic conditions of the network in the numerical experiment in 4 different aggregation levels: (i) lane, (ii) link, (iii) corridor, and (iv) network, in csv format.
- 2) The outputs of the MOVES model for different aggregation levels in MySQL database format.

Data Access and Sharing

The data can be publicly accessed at <https://zenodo.org/doi/10.5281/zenodo.11575091>.

Reuse and Redistribution

The data can be reused and redistributed by the general public using the following citation:

Laval, J., & Aghamohammadi, R. (2024). Network-wide Emissions Estimation Using the Macroscopic Fundamental Diagram [Data set]. Zenodo.
<https://zenodo.org/doi/10.5281/zenodo.11575091>