1 Comprehensive Automobile Research System (CARS) – a

2 Python-based Automobile Emissions Inventory Model

- Bok H. Baek¹, Rizzieri Pedruzzi², Minwoo Park³, Chi-Tsan Wang¹, Younha Kim⁴, Chul-Han
 Song⁵, and Jung-Hun Woo^{3,6}
- ⁵ ¹Center for Spatial Information Science and Systems George Mason University, Fairfax, VA, USA.
- ⁶ ²Department of Sanitary and Environmental Engineering, Federal University of Minas Gerais, Belo Horizonte,
- 7 Brazil.
- ⁸ ³Department of Technology Fusion Engineering, College of Engineering, Konkuk University, Seoul, Republic of
 ⁹ Korea
- ⁴Energy, Climate, and Environment program, International Institute for Applied Systems Analysis, Laxenburg,
 Austria
- ⁵School of Earth and Environmental Engineering, Gwangju Institute Science and Technology, Gwangju, Republic of
 Korea

14 ⁶Civil and Environmental Engineering, College of Engineering, Konkuk University, Seoul, Republic of Korea

15 corresponding to: Jung-Hun Woo (jwoo@konkuk.ac.kr)

17 Abstract

16

18 The Comprehensive Automobile Research System (CARS) is an open-source python-based 19 automobile emissions inventory model designed to efficiently estimate high quality emissions 20 from motor-vehicle emission sources. It can estimate the criteria air pollutants, greenhouse gases, 21 and air toxics in various temporal resolutions at the national, state, county, and any spatial 22 resolution based on the spatiotemporal resolutions of input datasets. The CARS is designed to 23 utilize the local vehicle activity data, such as vehicle travel distance, road link-level network 24 Geographic Information System (GIS) information, and vehicle-specific average speed by road 25 type, to generate a temporally and spatially resolved automobile emissions inventory for 26 policymakers, stakeholders, and the air quality modeling community. The CARS model adopted 27 the European Environment Agency's (EEA) onroad automobile emissions calculation 28 methodologies to estimate the hot exhaust, cold start, and evaporative emissions from onroad 29 automobile sources. It can optionally utilize average speed distribution (ASD) of all road types to 30 reflect more realistic vehicle speed variations. Also, utilizing high-resolution road GIS data allows 31 the CARS to estimate the road link-level emissions to improve the inventory's spatial resolution. 32 When we compared the official 2015 national mobile emissions from Korea's Clean Air Policy

33 Support System (CAPSS) against the ones estimated by the CARS, there is a moderate increase of 34 volatile organic compounds (VOCs) (33%), carbon monoxide (CO) (52%), and fine particulate 35 matter (PM_{2.5}) (15%) emissions while nitrogen oxides (NOx) and sulfur oxides (Sox) are reduced 36 by 24% and 17% in the CARS estimates. The main differences are driven by the usage of different 37 vehicle activities and the incorporation of road-specific ASD, which plays a critical role in hot 38 exhaust emission estimates but wasn't implemented in Korea's CAPSS mobile emissions 39 inventory. While 52% of vehicles use gasoline fuel and 35% use diesel, gasoline vehicles only 40 contribute 7.7% of total NOx emissions while diesel vehicles contribute 85.3%. But for VOC 41 emissions, gasoline vehicles contribute 52.1% while diesel vehicles are limited to 23%. While 42 diesel buses are only 0.3% of vehicles, each vehicle has the largest contribution to NO_x emissions 43 (8.51% of NO_x total) due to it having longest daily vehicle kilometer travel (VKT). In VOC 44 emission part, CNG buses are the largest contributor with 19.5% of total VOC emissions. For 45 primary PM_{2.5}, more than 98.5% is from diesel vehicles. The CARS model's in-depth analysis feature can assist government policymakers and stakeholders develop the best emission abatement 46 47 strategies.

48 Keywords: inventory: automobile, vehicle emissions, hot exhaust, cold start, evaporative, python

49 **1 Introduction**

50 Globally, ambient pollution causes more than 4.2 million premature deaths every year 51 (Cohen et al., 2017), and Burnett et al. estimate the health burden is closer to 9 million deaths from 52 ambient PM concentrations (Burneet et al, 2018). To effectively mitigate air pollutants, both 53 developed and developing countries' governments have been implementing stringent air pollution 54 abatement control policies to reduce harmful regional air pollutants (Hogrefe et al., 2001a; Hogrefe 55 et al., 2001b; Dennis et al., 2010; Rao et al., 2011; Appel et al., 2013; Luo et al., 2019). The CTM 56 simulation results strongly rely on precise input data, such as emission inventory, meteorology, 57 land surface parameters, and chemical mechanisms in the atmosphere.

58 The transportation emission sector is one of the major anthropogenic emissions in urban 59 areas. The tailpipe emissions from the vehicle's combustion process contain many air pollutants, 60 including nitrogen oxides (NOx), volatile organic compounds (VOCs), carbon monoxide (CO), 61 ammonia (NH_3), sulfur dioxide (SO_2), and primary particulate matter (PM) which will participate 62 in the formation of detrimental secondary pollutants like ozone and PM_{2.5} in the atmosphere. In 63 the Seoul Metropolitan Area (SMA) in South Korea, transportation automobile sources contribute 64 the most to the total NO_X and primary PM_{2.5} emissions across all emission sources. (Choi et al., 65 2014; Kim et al., 2017a; Kim et al., 2017b; Kim et al., 2017c). Thus, it is critical to understand and 66 represent better on the emission patterns from the transportation automobile sources in the CTM 67 model. The use of process-based automobile emission models is highly recommended to meet the

needs in CTM model because it can estimate the highly resolved spatiotemporal automobile
emissions. (Moussiopoulos et al., 2009; Russell and Dennis, 2000).

70 There are two methodologies known in emission inventory development: top-down and 71 bottom-up. The choice of methods is determined by the input data availability. The top-down 72 approach primarily relies on the aggregated and generalized country or regional information, 73 especially in developing countries where only limited datasets and information are available. It has 74 its limitations on representing the vehicle emission process realistically due to the lack of detailed 75 activity and ancillary supporting data. However, the bottom-up approach requires higher-quality 76 spatiotemporal activity datasets like road network information, vehicle composition (vehicle type, 77 engine size, vehicle age, and fuel-technology), pollutant-specific emissions factors, road segment 78 length, traffic activity data, and fuel consumption (EEA, 2019; Ibarra-Espinosa et al., 2018b; 79 IEMA, 2017). It can generate more accurate and detailed automobile emissions across various 80 operating processes, such as hot exhaust, evaporative, idling, and hot soak (Nagpure et al., 2016; 81 Ibarra-Espinosa et al., 2018a).

82 There are several bottom-up mobile emissions models available, like MOVES (MOtor 83 Vehicle Emissions Simulator) from the U.S. Environmental Protection Agency (USEPA), the 84 European Environment Agency's (EEA) model COPERT (COmputer Programmed to calculate 85 Emissions from Road Transport), the HERMES (High-Elective Resolution Modelling Emission 86 System) from Barcelona Supercomputing Center (Guevara et al., 2019), the VEIN (Vehicular 87 Emissions INventory) model developed by Ibarra-Espinosa et al. (2017), and the VAPI (Vehicular 88 Air Pollution Inventory) model developed by Nagpure and Gurjar (2012) for India (Nagpure et al., 89 2016). While these models are all bottom-up emission inventory models, a single model cannot 90 meet all modelers, policymakers, and stakeholders' needs because each model holds its own pros 91 and cons. They are developed differently to meet specific user needs based on the types of traffic 92 activity and emission factors, emission calculation methodologies, and other optional/available 93 traffic-related inputs such as average speed distribution and geographical resolution. Each model 94 is developed with different levels of specificity, underlying data set and modeling assumptions.

95 The MOVES model has the strength to generate high-quality emissions for up to 16 96 different emission processes (i.e., Running Exhaust, Start Exhaust, Evaporative, Refueling, 97 Extended Idling, Brake, Tire, etc.). It can simulate not only county-level but also road segment 98 level depending on data availability. It can also reflect local meteorological conditions, such as 99 ambient temperature and relative humidity, which can significantly impact both pollutants and 100 emissions processes (Choi et al., 2017; Perugu et al., 2018). Disadvantage of this model is it 101 difficult to update and apply to countries outside of the U.S. because MOVES model has a high 102 degree of specificity. The COPERT model that is widely used in European countries has its 103 advantages, such as the capability to model emissions in high resolution. Additionally, it is fully 104 integrated with the EEA's onroad vehicle emissions factors guidelines and can generate a complete 105 quality assurance (QA) and visualization summary (Ntziachristos et al., 2009). The cons are that it is a proprietary commercial licensed software, limited to EEA guidance, and challenging to
modify and update with any key input datasets like the latest emission factors from non-European
countries (Lejri et al., 2018; Rey DR, 2021; Li et al., 2019; Lv et al., 2019; Smit et al., 2019).

109 The HERMES and VEIN are both recently released bottom-up inventory models. They 110 have their pros in that they are both open-source models based on open-source computing 111 languages (Python and R), which provide transparency of emission calculations with a 112 considerable amount of data behind it (Ibarra-Espinosa et al., 2018b; Guevara et al., 2019). Both 113 models are driven by comma-separated value (CSV) formatted input files, making it very easy for 114 users to modify the input datasets. They are also based on the EEA's emission calculation method 115 and equipped with a complete OA and visualization tool based on Python and R libraries. However, 116 it is not an easy task to update the emission factors, and generate other required input datasets for 117 other countries, and lacks support for any control strategy plan feature to generate a responsive 118 reduced emissions inventory for policymakers, stakeholders, and modelers.

119 The VAPI (Vehicular Air Pollution Inventory) model was developed in India because the 120 country does not have an extensive and robust traffic-related dataset to run these kinds of vehicular 121 emissions inventory models (Nagpure et al., 2016; Perugu, 2019).

122 There are also a few shortcomings of incorporating these bottom-up models into CTM 123 studies. These models require strong programming skills to operate, such as collecting and 124 preparing the input data to fit the model requirement, configuring the model variables, and 125 changing specific variables that may be embedded in the code. Another downside is that while the 126 administration-level emissions inventory can be estimated by those models, it requires a 3rd party 127 emissions processor like the SMOKE (Sparse Matrix Operator Kerner Emissions) modeling 128 system (Baek and Seppanen, 2021) to process and generate spatially and temporally resolved 129 emissions inputs for CTM. Some detailed information, like link-level hourly driving patterns, can 130 be lost in the emissions processing steps.

131 There is no single model capable of meeting all the requirements across various spatial and 132 temporal scales (Pinto et al., 2020). However, transparency, simplicity, and a user-friendly 133 interface are requirements for those who mainly work in transportation policy and air quality 134 modeling development (Fallahshorshani et al., 2012; Kaewunruen et al., 2016; Sallis et al., 2016; 135 Sun et al., 2016; Tominaga and Stathopoulos, 2016). Thus, the ideal mobile emissions modeling 136 system would be computationally optimized, easy-to-use, and have a user-friendly interface. 137 Additionally, the model should easily adapt detailed local activity information and the state-of-art 138 emission factors as an input to represent them in the highest resolution possible in time and space.

We have developed the Comprehensive Automobile Research System (CARS) to meet these requirements, especially for the air quality research community, policymakers, and air quality modelers. The CARS is a stand-alone, fully modularized, computationally optimized, pythonbased automobile emission model. The modularization improves the efficiency of processing times. 143 Once district and road link-level annual/monthly/daily total emissions are computed, the rest of

144 the processes are optional. It can generate chemically speciated, spatially gridded hourly emissions

145 for CTMs without any 3rd party emissions modeling system to develop the highest quality CTM-

146 ready emissions inputs. All functions are operated by independent modules and can be enabled by

147 users. Details on modularization will be discussed later. The CARS model can be easily adopted

and is simple for users to add new functions or modules in the future. The application of the CARS

to South Korea will be described in detail later.

150 2 CARS Emissions Calculation

151 The CARS is an open-source Python-based customizable motor vehicle emissions 152 processor that estimates onroad and offroad emissions for specific criteria and toxic air pollutants. 153 Figure 1 is a schematic of the CARS overview. It applies vehicle, engine, and fuel specific 154 emission factors to traffic data to estimate the local level annual, monthly, and daily total emissions 155 inventory. The emissions inventory calculations require the list of pollutant-specific emissions 156 factors by vehicle age, local activity data, average speed profile/distribution by road type, and 157 geographic information system (GIS) road segment shapefiles inputs. The spatial resolution of 158 vehicle kilometer travel (VKT) defines the CARS geographic scale (i.e. district, county, state, and 159 country) for emission calculations. Unlike the district-level Korea Clean Air Policy Support 160 System (CAPSS) automobile emission inventory (Lee et al., 2011a; Lee et al., 2011b), the CARS applies high-resolution annual average daily traffic (AADT) data from the road GIS shapefiles to 161 162 distribute the total district emissions into road link-level emissions. Optionally, these road link-163 level emissions can be used to generate spatially gridded CTM-ready emissions input data once 164 the output modeling domain is defined. The summary of input files by categories are presented in 165 Appendix H. How the CARS estimates spatially and temporally enhanced automobile emissions 166 inventories will be discussed in detail next chapter.

167 South Korean traffic databases from the Korea CAPSS team (Lee et al., 2011b) from the 168 National Institute of Environmental Research (NIER) were used in this study to compute the 169 updated onroad automobile emissions inventory. The databases include individual vehicle activity 170 data (daily total VKT), road activity data (average speed distribution by road), vehicle age specific 171 emission factors, road type information, surface weather data, and GIS road shapefiles.

172 2.1 Individual Daily Average VKT Activity Data

The individual vehicle VKT data is used to reflect the human activity. This study imported the national registered vehicle-specific daily total VKT from South Korea's Vehicle Inspection Management System (VIMS), which belongs to the Korea Transportation Safety Authority (KTSA). It contains over 50 million records from 2013 to 2017. For the CARS model, we first sorted these records by the vehicle identification number (VIN) to remove any duplicates and then 178 built vehicle-specific daily total VKT traffic activity data in the CSV format. The summary of

those vehicle numbers and VKTs is presented in Fig. 2. Sedan vehicles using gasoline fuel

comprise the greatest percentage of total vehicles at 47% (~10.4 million) and have the highest
 VKT. Most vehicles demonstrate similar patterns between the number of vehicles and daily VKT.

181 VKT. Most vehicles demonstrate similar patterns between the number of vehicles and daily VKT.
182 However, as expected, LPG (liquefied petroleum gas)-fueled taxi are high in VKT compared to

183 the number of vehicles due to their daily long distance travel pattern.

184 The VIN (vin) information is used to calculate vehicle-specific daily average VKT (VKT_{vin}, 185 km d⁻¹). In Eq. (1), the individual daily average vehicle VKT (VKT_{vin}) is calculated based on the 186 cumulative mileage ($M_{f;vin}$) between the last inspection date ($D_{f;vin}$) and registration date ($D_{0;vin}$). 187 Each vehicle is categorized with Korea's NIER which defines the vehicle types (Ryu et al., 2003; 188 Ryu et al., 2004; Ryu et al., 2005; Lee et al., 2011a) based on a combination of vehicle types (e.g., 189 sedan, truck, bus, etc), engine sizes (e.g., compact, full size, midsize, etc) and fuel types (e.g., 190 gasoline, diesel, LPG, etc). Full details of vehicle types and daily total VKT are shown in Appendix 191 A and B.

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192
$$VKT_{vin} = \frac{M_{f;vin}}{D_{f;vin} - D_{0;vin}} \tag{1}$$

193 2.2 Emission Calculations

194 Automobile emission sources include motorized engine sources on the paved road network 195 and off the road network (e.g., drive way and parking lots). The CARS model doesn't simulate 196 emissions from nonroad emission sources, such as aviation, railways, construction, agricultures, 197 lawn mower, and boats yet. The CARS model simulates the onroad automobile emissions from 198 network roads using their local traffic-related datasets. The following section explains the 199 approach of the onroad automobile emission processes. The onroad emission (Eonroad) in the CARS 200 is defined in Eq. (2), which includes three major emission processes (Ntziachristos and Samaras, 201 2000):

$$E_{onroad} = E_{hot} + E_{cold} + E_{vap} \tag{2}$$

The hot exhaust emissions (E_{hot}) are the vehicle's tailpipe emissions when the internal combustion engine (ICE) combusts the fuel to generate energy under the average operating temperature. The cold start emissions (E_{cold}) are the tailpipe emissions from the ICE when the cold vehicle engine is ignited and the operational temperature is below average condition. The evaporative VOC emissions (E_{vap}) are the emissions evaporated/permeated from the fuel systems (fuel tanks, injection systems, and fuel lines) of vehicles.

The CARS first applies the hot exhaust emission factors by vehicle type, age, fuel, engine, and pollutants to individual daily total VKT to compute the hot exhaust emissions. The rest of the 211 processes for cold start and evaporative emissions are calculated afterwards. The emission

- 212 calculation methodologies used in the CARS model are based on tier 2 and tier 3 methodologies
- from the EEA's mobile emission inventory guidebook (EEA, 2019) to be consistent with Korea's
- 214 National Emission Inventory System (NEIS) (Lee et al., 2011a).

215 2.2.1 Hot Exhaust Emissions

Hot exhaust emissions, which is from the vehicle's tailpipe, is the exhaust gas from the combustion process in an ICE. The ICE combustion cycle generally causes incomplete combustion processes which emit hydrocarbons, carbon monoxide (CO), and particulate matter (PM) which not completely controlled from the aftertreatment equipment, such as three-way catalytic converter and released into the atmosphere. The sulfur compounds in the fuel are oxidized and become sulfur oxides (SO_x). Nitrogen oxides (NO_x) are produced due to the abundance of nitrogen (N₂) and oxygen (O₂) during the combustion process.

Equation 3 represents the calculation of daily individual vehicle hot exhaust emission rate, $E_{hot; p,vin,myr}$ (g d⁻¹) of pollutant (*p*). An individual vehicle-specific daily *VKT_{vin}* (km d⁻¹) is estimated by Eq. (1). The *EF_{hot;p,v,myr,s}* (g/km) is the hot exhaust emission factor of pollutants (*p*) for the vehicle type (*v*), vehicle manufacture year (*myr*), and average vehicle speed (*s*). The district's total emission rate is the total hot exhaust emissions from all individual vehicles within the same district.

228
$$E_{hot; p,vin,myr} = DF_{p,v,myr} \times VKT_{vin} \times EF_{hot; p,v,myr,s}$$
(3)

229 The deterioration factor (DF) in Eq. (3) is an optional function in the CARS. The 230 deterioration process is caused by vehicle aging and can lead to the increase of vehicle emissions. 231 The vehicle DF is varied by vehicle type (v), pollutant (p), and vehicle manufacture year (myr). 232 The CARS model computes vehicle ages based on the vehicle manufacture year and model 233 simulation year. According to the guidance of deterioration factors calculation from NIER, there 234 is no deterioration in a new vehicle during their first five years. After five years, the deterioration 235 factors can increase the 5~10% range depending on the type of vehicle and pollutants. 236 Deterioration processes can cause up to 100% increase of emissions in fifteen-year-old vehicles. 237 Currently, the DF is an empirical coefficient that varies by vehicle age (Lee et al., 2011a).

The hot exhaust emission factor, $EF_{hot;p,v,s}$ (g/km) is a function of vehicle speed (*s*) with other empirical coefficients: *a*, *b*, *c*, *d*, *f*, *k*. The emission factor formula and those coefficients were developed by NIER CAPSS (Lee et al., 2011a). These coefficients are varied by pollutants (*p*), vehicle type (*v*), vehicle manufacture year (*myr*), and vehicle speed (*s*). The vehicle speed affects the combustion efficiency of an ICE and impacts the emission rates and its composition from the tailpipe.

244
$$EF_{hot; p,v,myr,s} = k(a \times s^b + c \times s^d + f)$$
(4)

245 While vehicle speed plays a critical role in hot exhaust emissions from most vehicles, NOx 246 emissions from some diesel vehicles show sensitivity to local ambient temperature along with 247 vehicle speed (Ntziachristos and Samaras, 2000). Figure 3 shows the dependency of NO_x emission 248 factors from compact diesel vehicles to vehicle speed (Fig. 3a) and ambient temperature (Fig. 3b). 249 Figure 3a shows a significant decrease of NO_x emissions while speed increases between 0 and 70 250 km. Figure 3b demonstrates the significance of local meteorology on NO_x emissions from a 251 compact diesel sedan. Based on these NIER's CAPSS emission factors, the sensitivity to local 252 ambient temperature is limited to NO_x pollutant emissions from diesel vehicles.

253 Due to its high sensitivity to the vehicle operating speed, it is important for the CARS to 254 simulate realistic speed patterns for accurate emissions estimates. When a single speed is assigned 255 to compute hot exhaust emissions, it won't reflect the emissions under low-speed circumstances. 256 To overcome this limitation, the CARS has adopted the 16 average speed bins concepts for a better 257 representation of vehicle speed distribution that varies by road type (i.e., local, highway, 258 expressway). We have implemented a feature for the CARS optionally to apply road-specific 259 average speed distributions (ASD) $(A_{bin,r})$, which represents the fractions of 16-speed bins (bin) 260 (from 0 to 121 km h^{-1} defined in Appendix E) for eight different road types (r) (No.101-108, shown 261 in Appendix C) as classified by CAPSS (Fig. 4a). Although ASD patterns vary by region and time, 262 current CARS model version does not support ASD application by region and time of day due to 263 the lack of region and time-dependent ASD availability in South Korea.

264 We first developed the ASD (Fig. 4a) for eight different road types (No. 101-108) in South 265 Korea based on the latest road link-specific average speed and the length of link from the SK GIS 266 road network shapefiles (NIER, 2018). However, the ASD based on the SK GIS road shapefiles 267 did not capture low-speed range (<16 km h⁻¹) driving (Fig. 4a). This causes a significantly lower estimation of NOx and VOC emissions compared to the CAPSS (Appendix G). We believe the 268 269 SK average speed distribution is missing low-speed driving that can occur on links on different 270 days due to traffic congestion. To address this absence of low-speed driving in the SK ASD, we 271 incorporated data from the ASD (Figure 4b) from the state of Georgia developed by U.S. EPA to 272 the low-speed ranges (speed bin #1 and #2 for road type 1 to 7). We increased the total fractions 273 of low-speed bins (the 2:1 ratio of fractions of bin #1 and #2) by 2% for interstate expressways, 274 3% for urban expressways, 7% for all highways, and 15% for all local roads. The increases in low-275 speed bins lowered the distributions of other higher speed bins homogeneously due to the 276 renormalization of fractions by road type. Figure 4c shows the renormalized hybrid-ASDs of all 277 road types based on SK ASD and Georgia ASD. We understand, the hybrid-ASD approach is not 278 ideal for SK onroad emission inventory development. However, it clearly demonstrates the 279 CARS's capability and sensitivity to the vehicle speed representation and the impacts of ASD to 280 the local onroad mobile inventories.

While 16-speed bins ASD application is critical to computing more realistic hot exhaust emissions, there should be some restrictions on certain road types. Users can adjust the restricted roads control table input file to limit the vehicle types that can only be operated on a particular road type. For example, motorcycles are limited to local roads (No. 104, 106, and 107), but not on expressways (No. 101, 102, 103, 105, and 108) due to its traffic regulation rules. Heavy trucks are only allowed on the highway (No. 101, 102, 103, 105, and 108.) by law. The details of the road restriction control table format can be found on the CARS's user's guide from the CARS Github website (https://github.com/bokhaeng/CARS/tree/master/docs/User_Manual).

The 16-speed bins averaged speed distribution calculated by road type ($A_{bin,r}$) and road type weight factors ($\omega_{r,d}$) in a district (d) from Eq. (13) are added to the CARS hot exhaust emissions equation (Eq. 3). The hot exhaust emissions from individual vehicles ($E_{hot;p,vin,myr}$) can be calculated by considering road-specific speed bins distribution (Eq. 5). Although the vehicles may be operated in different districts from their registered district, this is our best method to estimate the vehicle speed for hot exhaust emissions.

295
$$E_{hot; p,vin,myr} = DF_{p,v,myr} \times \sum_{bin} (VKT_{vin} \times EF_{hot; p,v,myr,s} \times A_{bin,r})$$
(5)

296 2.2.2 Cold Start Emissions

The cold start emissions occur when a cold-engine vehicle is ignited. The lower temperature of the ICE is not an optimal condition for complete fuel combustion. This process lowers the combustion efficiency (CE) and increases the emissions of hydrocarbon and CO pollutants from the tailpipe exhaust (Jang et al., 2007). The CARS can estimate the cold start emissions for vehicles using gasoline, diesel, or liquefied petroleum gas (LPG) fuel. Besides the vehicle and engine type, road type also plays a critical role in the quantity of cold start emissions because it occurs mostly in parking lots and rarely on highways.

The cold start emission, E_{cold} (g d⁻¹), is derived from the hot exhaust emissions, the ratio of hot to cold exhaust emissions (EF_{cold}/EF_{hot} -1.0), and the percentage of the traveled distance with a cold engine (Eq. 6).

307
$$E_{cold; p,v} = \beta_T \times E_{hot; p,v} \times \left(\frac{EF_{cold; p,v}}{EF_{hot; p,v}} - 1.0\right)$$
(6)

The emission factor of cold start emissions (EF_{cold}) is not directly calculated from measurement data like hot exhaust emissions $(E_{hot;p,v})$, but measured under different ambient temperatures (*T*). The CARS model applies linear regression models developed by CAPSS to estimate the increasing ratio of cold start to hot exhaust emissions (EF_{cold}/EF_{hot}) under different temperatures (*T*) (Eq. 7). In this equation, *A* and *B* are the empirical coefficients that vary by the pollutants (*p*) and vehicle type (*v*).

314
$$\left(\frac{EF_{cold; p, \nu}}{EF_{hot; p, \nu}}\right) = A_{p, \nu} + B_{p, \nu} \times T \tag{7}$$

315 β is the percentage of the distance traveled under a cold engine. It also depends on the 316 ambient temperature. Cold ambient temperatures cause a longer distance traveled under a cold 317 engine due to the slower heating time. According to the CAPSS database for Seoul city (Lee et al., 318 2011a), the empirical linear equation for β is shown in Eq. (8). This formula represents how 319 ambient temperature affects β . For example, when the average temperature is -2°C, β is 34.8%. 320 In summer, the monthly average temperature is 25.7°C, which causes β to drop to 21%.

321
$$\beta = 0.647 - 0.025 \times 12.35 - (0.00974 - 0.000385 \times 12.35) \times T$$
 (8)

322 **2.2.3** Evaporative VOC Emissions

332

323 Evaporative emissions are emissions from vehicle fuel that are evaporated into the 324 atmosphere. This occurs in the fueling system inside the vehicle, such as fuel-tanks, injection 325 systems, and fuel lines. Diesel vehicles, however, can be exempted due to diesel fuel's low vapor 326 pressure. The primary sources of evaporative emissions are breathing losses through tank vents 327 and fuel permeation/leakage. The CARS model adopted the EEA's emission inventory guidebook 328 (EEA, 2019) to account for three mechanisms to estimate the evaporative VOC emissions (E_{vap}): 329 diurnal emissions from the tank (e_d) , hot and warm soak emissions by fuel injection type (S_{fi}) , and 330 running loss emissions (R) (Eq. 9). Unlike CAPSS, there is a conversion factor (0.075) applied to 331 E_{vap} for motorcycles to prevent an over-estimation of VOC.

$$E_{vap; p,v} = \left(e_{d; p,v} + S_{fi; p,v} + R_{l; p,v}\right)$$
(9)

333 Diurnal emissions, e_d (g d⁻¹), during the daytime are caused by the ambient temperature 334 increase and the expansion of fuel vapors inside the fuel tank. Most of the current fuel tank systems 335 have emission control systems to limit this kind of evaporative VOC emissions. The e_d can be 336 calculated with the empirical Eq. (10), which was developed by CAPSS. T_l is the monthly average 337 of the daily lowest temperatures and T_h is the monthly average of the daily highest temperatures. 338 The empirical coefficient α is 0.2, which represents how 80% of emissions are eliminated by the 339 vehicle emission control system.

340
$$e_d = \alpha \times 9.1 exp[0.3286 + 0.0574 \times (T_l) + 0.0614 \times (T_h - T_l - 11.7)] (10)$$

Soak emissions (S_{fi}) occur when a hot ICE is turned off; the remaining heat from the ICE can increase the fuel temperature in the system. The carburetor float bowls are the major source of the soak emissions. Newer vehicles with fuel injection and return-less fuel systems do not emit soak emissions. Because most of the current vehicles in South Korea have a new fuel system, soak emissions (S_{fi}) in the CARS model are set to 0.

The running loss emissions (R_l) are from vapors generated in the fuel tank when a vehicle is in operation (Eq. 11). In some older vehicles, the carburetor and engine operation can increase the temperature in the fuel tank and carburetor, which can cause a significant increase in evaporative VOC emissions. VOC emissions from running loss can be greatly increased during warmer weather. However, newer vehicles with fuel injection and return-less fuel systems are not affected by the ambient temperature. Because most vehicles in South Korea do not use carburetor technology, we expect running loss emissions to have the least impact (Lee et al., 2011b).

353
$$R_l = \alpha \times L_{r,v} \times [(1 - \beta) \times R_h + \beta \times R_w]$$
(11)

The empirical coefficient α is 0.1 here, which represents that 90% of the running loss is avoided by the newer fuel system. *L* is the distance traveled (km) by road and is the same one used in hot exhaust emission calculations. β is the same parameter from Eq. (8). The R_h and R_w are the average emission factors from running loss under hot and warm/cold conditions, respectively.

358 2.3 Road Link-Level Emissions Calculations

359 In general, district-level automobile emissions calculations are driven by district-level 360 averaged vehicle activity and operating data, which do not reflect realistic spatial patterns of 361 onroad automobile emissions. The CARS model introduces road link-specific traffic data by 362 default to develop spatially enhanced road link-specific emissions that reflect more representative 363 emissions by road link. This high-resolution traffic data is a GIS shapefile that is composed of 364 many connected segments, which are called "road links." All road links hold information such as 365 start/end location coordinates, AADT, road link length, averaged vehicle speed, and road type (No. 366 101-108).

The CARS model applies link-level AADT ($AADT_{d,r,l}$, d⁻¹) and road length ($L_{d,r,l}$) to compute the road link-specific VKT ($VKT_{d,r,l}$, km d⁻¹) in Eq. (12). The road links are identified by district (*d*), road type (*r*), and link (*l*) labels. The road VKT is a parameter that reflects the traffic activity of each road link and it is different from individual daily vehicle activity data ($VKT_{v,age}$) in Eq. (1).

$$372 VKT_{d,r,l} = AADT_{d,r,l} \times L_{d,r,l} (12)$$

373 Road link-specific VKT ($VKT_{d,r,l}$) is used to redistribute the district total emissions (E_{onroad}) 374 from Eq. 2 into road link-level emissions. The following three weight factors are computed: the 375 district weight factors, ω_d (Eq. 13), the road type weight factors, $\omega_{d,r}$ (Eq. 14), and the road-link 376 weight factors, $\omega_{d,l}$ (Eq. 15). The weight district factors (ω_d) are the renormalization of each 377 district's total VKT over state-level total VKT (N is the number of districts). The main reason we 378 performed the renormalization over state-level total VKT is to reflect daily traffic patterns from 379 multiple districts under the assumption that most vehicles travel within the same state. The road 380 type weight factors by district ($\omega_{r,d}$) are used to compute road-specific emissions, while road381 specific averaged speed distributions (ASD; $A_{s,r}$) from Eq. (5) are applied to capture vehicle 382 operating speeds by road type. The road link weight factors ($\omega_{d,l}$) are then applied to redistribute 383 the district emissions into road link-level emissions.

384

385
$$\omega_d = \frac{\sum_r \sum_l VKT_{d,r,l}}{\frac{1}{N} \sum_d \sum_r \sum_l VKT_{d,r,l}}$$
(13)

386
$$\omega_{d,r} = \frac{\sum_{l} VKT_{d,r,l}}{\sum_{r} \sum_{l} VKT_{d,r,l}}$$
(14)

387
$$\omega_{d,l} = \frac{VKT_{d,r,l}}{\sum_r \sum_l VKT_{d,r,l}}$$
(15)

388 **3 CARS Configuration**

389 The CARS model is an open-source program based on Python (Guido van Rossum, 2009) 390 that allows the users to efficiently apply open-source modules to develop programs. Users can 391 easily install Python development tools and load customized packages and modules to set up the 392 CARS development environment. All CARS modules are developed using Python v3.6. Other than 393 the GIS road shapefiles, all input files are based in the ASCII CSV format, which can be easily 394 handled by both spreadsheet programs and programming languages, making it more accessible for 395 users of all skillsets. The CARS can not only estimate district-level and spatially enhanced road 396 link-level emissions, but can also generate hourly chemically speciated gridded emissions for 397 CTMs. In addition, the CARS also generates various summary reports, graphics, and 398 georeferenced plots for quality assurance.

The required Python modules for the CARS are: "*geopandas*," "*shapely.geometry*", and "*csv*" modules to read the shapefiles and table data files. The "*NumPy*" and "*pandas*" modules are used to operate the memory arrays and scientific calculations while the "*pyproj*" module deals with converting the projection coordinate systems. "*matplotlib*" is for generating any type of figures/plots. Furthermore, the CARS model can also read and write Climate and Forecast (CF)compliant NetCDF-formatted files using "*NetCDF4*".

405 The first process in the CARS is "Loading function path"; it allows users to define and 406 check the input file paths. Once all input files are checked, there are six process modules in CARS 407 to process inputs, compute emissions, and generate various output files, including QA reports. 408 Figure 5 is the schematic of the CARS that consists of six process modules with various functions. 409 The six process modules are (1) "Process activity data", (2) "Process emission factors", (3) 410 "Process shapefile, (4) "Calculate district emissions", (5) "Grid4AQM", and (6) "Plot figures". 411 The main purpose of modularizing the CARS is to meet the needs of various communities, such 412 as policymakers, stakeholders, and air quality modelers. While modules (1) through (4) are

required to develop the district-level and road link-level emissions inventories, module (5) 413 414 "Grid4AQM" is optional depending on if users want to develop chemically-speciated gridded 415 hourly emissions for CTMs. Also, the modularity system in the CARS allows users to bypass 416 certain modules if it has been previously processed without any changes. For example, if there is 417 no change in traffic activity, emission factors table, or GIS shapefiles, users do not need to run 418 these modules and can simply read the data frame outputs and then run "Grid4AQM" for the 419 modeling dates and domain. The "Grid4AQM" module will not only improve the computational time for CTMs but also eliminate the need for a 3rd party emissions modeling system like SMOKE 420 421 (Baek and Seppanen, 2021).

The rectangle boxes in Fig. 5 represent the data array and the boxes with rounded edges are the functions in the CARS. Details on the CARS code, input table format, and functions setup information can be found on the CARS GitHub website (Pedruzzi *et al.*, 2020).

425 The "Process activity data" module first reads the vehicle activity data, such as an 426 individual vehicle's daily total VKT based on its registered district. The "Process emission factors" 427 module reads and stores the emission factors table that holds all pollutant emission factors to 428 estimate the emissions for all vehicles. Meteorology-sensitive emission factors are only limited to 429 NO_x pollutants. District boundary GIS shapefiles and road network shapefiles are processed 430 through "**Process shape file**" to generate the VKT-based redistribution weighting factors from Eq. 431 (13), (14) and (15) for the "Calculate district emissions" module to compute district-level and 432 road link-level emission rates (metric tons per year, t yr⁻¹).

The redistributed emission rates (t yr⁻¹) from the "Calculate district emissions" module 433 434 present annual total emission rates until district-level VKTs from the "Process activity data" 435 module are added. Then, the "Grid4AQM" module can generate CTM-ready chemically speciated 436 emissions. The "Read_chemical" function from the "Grid4AQM" module is designed to process 437 the chemical speciation profile that can convert the inventory pollutants such as CO, NO_X , SO_2 , 438 PM₁₀, PM_{2.5}, VOC, and NH₃, into the chemically lumped model species that CTM requires for 439 chemical mechanisms, such as SAPRC (L. and Heo, 2012) and Carbon Bond version 6 (CB6) 440 (Yarwood and Jung, 2010). The "Read temporal" function processes the complete set of monthly, 441 weekly, and hourly temporal allocation profiles that can convert annual total emissions to hourly 442 emissions. "Read griddesc" defines the CTM-ready modeling domain and computes the gridding 443 fractions for all road link-level emissions by overlaying the modeling domain over the GIS 444 shapefiles. Once annual total emissions are chemically speciated, spatially gridded, and temporally 445 allocated into hourly emissions, the "Gridded_emis" function will combine emission source-level 446 conversion fractions from each function (*Read_chemical, Read_temporal*, and *Read_griddesc*) to 447 generate the CTM-ready chemically speciated, gridded hourly emissions in the NetCDF binary 448 format. The "Plot Figures" module is designed for generating various summary reports and 449 graphics to assist users in understanding the estimated automobile emissions inventory computed

by the CARS. The following section will describe the detailed processes of the "Grid4AQM"module, which includes chemical, spatial, and temporal allocations.

452 The influence of temperature on emission processes are considered in the CARS model. 453 There are three temperature parameters in current CARS model such as "temp max" for maximum 454 temperature, "temp mean" for mean temperature, and "temp min" for minimum temperature. 455 These temperature parameters will be applied to over the entire modeling domain during the simulation period. Current CARS model version does not support to process gridded meteorology 456 data from the 3rd party meteorology models like Meteorology-Chemistry Interface Processor 457 (MCIP) from U.S. EPA., and Weather Research Forecasting (WRF) model from National Center 458 459 for Atmospheric Research (NCAR) yet. However, CARS can easily adopt various temporally 460 resolved temperature values by adjusting the CARS simulation period (i.e., day, week, month, 461 season, or annual).

462 **3.1 Chemical Speciation**

463 To support CTMs applications, the CARS needs to be able to convert inventory pollutants 464 into chemical lumped model species based on the choice of CTM chemical mechanisms. NO_x 465 includes nitric oxide (NO), nitrogen dioxide (NO₂), and nitrous acid (HONO). VOCs can represent 466 hundreds of different organic carbon species, such as benzene, acetaldehyde, and formaldehyde. 467 These grouped inventory pollutants cannot be directly imported into the chemical mechanism 468 modules in the CTM system and require chemical speciation allocation for CTMs to process them 469 during their chemical reactions. Therefore, the "Grid4AQM" module performs the chemical 470 species allocation step prior to the temporal and spatial allocations to generate the gridded hourly 471 emissions. The "Read_chemical" function in "Grid4AQM" module allows users to assign these 472 emission inventory pollutants to CTM-ready surrogate chemical species (a.k.a lumped chemical 473 species) by vehicle, engine, and fuel type. For example, VOC emissions from diesel busses can be 474 converted into the following composition based on its chemical allocation profile: alkanes (68%), 475 toluene (9%), xylenes (8%), alkenes (4%), ethylene (2%), benzene (1.3%), and unreactive 476 compounds (7%) when CB6 chemical mechanism is selected. Further details on the chemical 477 speciation profile input formats are available in the CARS user's guide.

478 **3.2 Spatial Allocation**

The "**Calculate district emissions**" module calculates not only the total district emissions but also road link-specific emissions based on road link-specific AADT data from road network GIS shapefiles. The "**Calculate district emissions**" module first gets the district total vehicle emissions (Eq. 2) based on the district-level VKTs, and then the normalized district total emissions by district weight factor, ω_d (Eq. 13). Afterwards, the normalized district total emissions are redistributed into every road link using road link-level weight factors ($\omega_{d,l}$) (Eq. 15). The district total emissions from Eq. (2) and from Eq. (15) remain the same. Then the computed road linklevel emissions then will be converted into grid cell emissions using the modeling domain grid cell
fractions computed in the "*Read_griddesc*" function in the "Grid4AQM" module.

488 **3.3 Temporal Allocation**

489 Once chemical and spatial allocations are completed, the final step to support CTM 490 application is a temporal allocation that converts the annual total emissions from the "Calculate district emissions" module into hourly emissions. The "Read temporal" temporal allocation 491 492 function in the "Grid4AOM" module converts the annual emission rate (t yr⁻¹) to the hourly 493 emission rate (mol hr⁻¹) using monthly, weekly, and weekday/weekend diurnal temporal profiles. 494 This module processes these temporal profile inputs, which are the monthly (January - December), 495 weekly (Monday - Sunday), and weekday/weekend 24 hour profile tables (0:00-23:00 LST). The 496 users can assign these temporal profiles with a combination of vehicle, engine, fuel, and road types 497 to enhance their temporal representations in detail.

498 **3.4** Chemical Transport Model Emissions

499 The main goal of the "Grid4AQM" module is to generate temporally, chemically, and 500 spatially enhanced CTM-ready gridded hourly emissions. First, it reads the CTM modeling domain 501 configuration and then overlays it over the road network GIS shapefile and district-boundary 502 shapefile to define the modeling domain. This overlaying process between the road network, 503 district boundary GIS shapefiles, and modeling domain allows the "Grid4AQM" module to 504 compute the fraction of road links that intersects with each grid cell. Figure 6 demonstrates how 505 the district boundary and road network GIS shapefiles are used to perform the spatial allocation 506 processes in CARS. Figure 6a is a native road link shapefile of Seoul with AADT, VKT, district 507 ID, and road type. Figure 6b presents an overlay of two districts's road links (purple and blue) over 508 the selected region. State total emissions will be renormalized into weighed district total emission 509 data and then redistributed into the road link. Figure 6c illustrates how the weighted road linklevel emissions get allocated into modeling grid cells for CTMs. The link-level VKT ($VKT_{d,r,l}$) 510 511 from Eq. (12) will be used to compute a total of traffic activity fractions by grid cell and then use 512 that to assign the link-level emissions from Eq. (2) into each grid cell. When a road link intersects with multiple grid cells, the "Grid4AQM" module will weigh the emissions by the length of the 513 514 link that intersects with each grid cell. It should be noted that current CARS model can only 515 generate the Community Multiscale Air Quality (CAMQ)-ready gridded hourly emissions in 516 format of IOAPI (Input/Output Applications Programming Interface) based on NetCDF format.

517 Through the overlay process, the CARS model can generate various types of output data, 518 such as total district emissions, link-level emissions, and CTM-ready gridded emissions. For 519 example, the CO vehicle emissions from the Seoul metropolitan in South Korea are presented in 520 three different output formats in Fig. 7. Figure 7a shows the annual mobile $PM_{2.5}$ emissions by

district. The road link level annual emissions are presented in Fig. 7b. Furthermore, the CARS
 applies the link-level emissions from Fig. 7b to generate the hourly grid cell emission data with a

523 $1 \text{ km} \times 1 \text{ km}$ resolution for the CTM in Fig. 7c.

524 **3.5** National Control Strategy Application

525 One of the unique features in the CARS compared to other mobile emissions models is that 526 it can promptly develop controlled mobile emissions responding to the national emergency high 527 PM_{2.5} episodes. It is very common to experience high PM_{2.5} episodes, especially during the 528 wintertime in South Korea due to domestic and international primary and secondary air pollutants 529 emissions. When the 72 hour forecasted PM_{2.5} concentration exceeds the average 50 μ g/m³ (0:00-530 16:00 LST), the national PM_{2.5} emergency control strategy is activated for ten days. It applies a 531 nationwide vehicle restriction policy within 24 hours. It enforces a limit on what kind of vehicles 532 can be operated on a certain date. The restrictions can be applied in the following ways: the 533 closures of public parks and government facilities, and restrictions of certain vehicles based on 534 their fuel type and age, which is a major factor of engine deterioration. This policy will limit the 535 number of vehicles on the network roads significantly, which could reduce primary PM_{2.5} and 536 precursor pollutant (NOx, NH₃, and VOC) emissions, especially from heavily populated 537 metropolitan regions (Choi et al., 2014; Kim et al., 2017a; Kim et al., 2017b; Kim et al., 2017c).

538 To understand the impacts of an even/odd vehicle restriction policy in real-time, we need to 539 quickly develop a rapid control response emissions for the air quality forecast modeling system. 540 The process of generating the controlled mobile emissions can take a long time if we start fresh. 541 Thus, we have implemented this control strategy as an optional "Control Factors" function in the 542 "Calculate district emissions" in the module for users to quickly and easily generate the 543 controlled mobile emissions with consideration of the limited number of vehicles based on the 544 vehicle, engine, fuel, and vehicle manufactured year. A one hundred percent (100%) control factor 545 means that there are no emissions from those selected vehicles.

Because of the modularization system in the CARS, we can bypass some computationally expensive data processing modules (i.e., "**Process activity data**", "**Process emission factors**", and "**Process shape file**") and let the "**Calculate district emissions**" module quickly apply control factors while it computes the district-level mobile emission inventory from Eq. (2). This will allow users to reduce the computational time to generate the controlled mobile emissions under a specific control scenario and develop the controlled CTM-ready gridded hourly emissions using the "**Grid4AQM**" module.

553 **3.6 Computational Time**

While the CARS can generate a high-quality spatiotemporal emission inventory for policymakers, stakeholders, and air quality modelers, it is quite critical for the CARS to generate these complex mobile emissions effectively and accurately without being at the expense of computational time. This is especially important to meet the needs for an air quality forecast modeling system responding to a national emergency control strategy implementation.

559 In this section, we will discuss the details of the CARS computational modeling performance. 560 While the CARS model has been highly optimized, the modularization of CARS has also improved 561 its modeling performance with optional module runs. The breakdown of module-specific 562 computational time estimates based on the benchmark CARS runs are listed in Table 1. The 563 benchmark CARS case includes a total of 24,383,578 daily VKT datasets from KSTA over two 564 different years, 84,608 emission factors for all pollutants across a combination of vehicle-age-565 engine-fuel types, 385,795 road links from the GIS road network shapefiles, 5,150 districts/16-566 states boundary GIS shapefile, and 5,494 grid cells (=82 rows and 67 columns) for CTMs. Without 567 any computational parallelization, the total processing time of all six modules usually takes around 568 a half hour to generate a single day CTM-ready gridded hourly emission file. However, it can be 569 further shortened to 25-30 minutes on a higher performance computer. Because of the modular 570 system implemented in the CARS, generating one month (31 days) long gridded hourly emissions 571 from CTMs do not require over 15 computational hours, but only around 100 minutes on high-572 performance computers. The maximum usage of RAM can reach up to 11 GB. Table 1 shows the 573 breakdown of computational time by each module from two different hardwares (desktop and 574 laptop computers). The numbers in parentheses beside the "Grid4AQM" module is the 575 computational time for a single day versus 31 days. While the "Grid4AQM" module takes an 576 average of 4.9 minutes for a single day emissions generation, processing a consecutive 31 days 577 saves 46% more time, decreasing from 151.9 minutes (=4.9 minutes * 31 days) to 81.6 minutes.

578 **4 Results**

579 CARS and CAPSS Comparison

580 The CARS model calculates the 2015 onroad automobile emissions based on the latest 581 2015 emission factors and the 2015-2017 vehicle activity database in South Korea. The annual 582 total emissions from CARS are compared against the ones from NIER CAPSS in Table 2. The 583 CARS model estimated the following annual total emissions in units of metric tons per year (t yr 584 ¹): NO_x (301,794); VOC (61,186); CO (373,864), NH₃ (12,453); PM_{2.5} (10,108), and SO_x (172.0). 585 Compared to NIER CAPSS, the CARS overestimated all pollutants except for NO_x (-18% decrease) 586 and SO_x (-17% decrease). It overestimated the emissions of VOC by 33%, PM_{2.5} by 15%, CO by 587 52%, and NH_3 by 24%. Both NIER CAPSS and CARS shared the same emission factor tables,

which hold over 84,608 emission factors for all pollutants across a combination of vehicle, age,engine, and fuel types.

590 The difference between CAPSS and CARS approaches are caused by three reasons: First, 591 the number of vehicles used in CARS is slightly higher (6%) than CAPSS data (1.3 out of 23 592 million), as well as other key traffic-related activity inputs (i.e., vehicle age distribution, averaged 593 speed distribution, etc). Secondly, the vehicle speed information assigned by vehicle and road type 594 play a critical role in the differences between CAPSS and CARS. The CAPSS calculation was 595 based on the road-specific mean speed value or 80% of the speed limit as an input of vehicle 596 operating speed by three road types (rural, urban, and expressway). In other words, CAPSS only 597 assigns a "single-speed value" for each road type, and does not encounter the variation of vehicle speed during its operation on roads into the emissions calculation. Most running exhaust emissions 598 599 occur during a vehicle's low-speed operation due to its incomplete combustion of fuel, and it is 600 critical to accurately represent the emissions across various speed bins in order to compute the 601 correct emissions. The CARS model has an option to apply the average speed distribution (ASD) 602 over 16 speed bins for eight road types (Fig. 4). The CARS speed distribution process can better 603 represent the speed variations of vehicle speeds for each road type. A detailed analysis of the 604 impact of vehicle speed will be discussed later in this chapter. Lastly, other advanced processes in 605 the CARS, such as link-level AADT and district-level vehicle data (5,150 districts in South Korea), 606 can reflect more spatial detail and variation than the CAPSS. The CAPSS only considers state-607 level data (17 states in South Korea) and five road types (interstate expressway, urban highway, 608 rural highway, urban local, and rural local).

Figure 8 illustrates more details about the difference between the annual emissions from CARS to the CAPSS by pollutants and vehicle types. Sedan vehicles show the largest increase of VOC (33%), CO (41%), and NH₃ (23%) in the CARS relative to CAPSS because almost 56% of total vehicle count (13.5 million) is composed of sedan vehicles. Also, sedan vehicles contribute 51% of total VOC and 61% of total CO annual emissions. The VOC and CO emissions from sedans are largely affected by the average speed distribution process when compared to other vehicle types. Similarly, the largest decreases of NO_x (-16%) and SO_x (-18%) are from trucks because they

- are significant NO_x (~50%) and SO_x contributors (~27%) and their emission factors are sensitive
- 617 to vehicle speed.

618 Onroad Emissions Analysis

The CARS is a bottom-up emissions model, which utilizes local individual vehicle activity data, detailed local emission factors for every vehicle and fuel type, and localized inputs such as average speed distribution by road type and deterioration factor. It allows users to assess the detailed breakdown of localized emission contributions. Table 3 represents the individual air pollutants (NO_x, VOC, PM_{2.5}, CO, NH₃, and SO_x) emission contributions (t yr⁻¹), fractions (%), and impact factors (IF) by the vehicle type and fuel system. The IF is defined by the normalized annual emissions with vehicle counts of each category (kg yr⁻¹ per vehicle). The CARS also can provide the average daily VKT per vehicle, which is the total daily VKT divided by vehicle numbers, to explain the emission contributions in Appendix D.

628 Diesel-fueled vehicles contribute the most of NO_x emissions, which is over 85.3% (257,305) t yr⁻¹), although the number of diesel vehicles only amounts to approximately 35% of the total 629 vehicles (Table 3a). While the diesel trucks emitted 49.1% (148,246 t yr⁻¹) of total NO_x with an IF 630 value of 47.9 (kg yr⁻¹), the highest impact (IF = 340 kg yr⁻¹) occurred from diesel buses with only 631 a 8.51% contribution to the total NOx emissions. This is caused by the highest average daily VKT 632 633 from diesel buses compared to other vehicles, which is expected in a highly populated metropolitan area like Seoul, South Korea. A diesel bus generally has a 3-5 times higher daily VKT (180 km d⁻ 634 ¹) than other common vehicles (gasoline sedan: 34 km d⁻¹, diesel truck: 57 km d⁻¹). The second-635 largest vehicle type is the CNG (compressed natural gas) bus (248 kg yr⁻¹), which also has a higher 636 VKT. Their average daily VKT is 212 km d^{-1} , with only a 3.1% NO_x contribution. 637

638 For VOC emissions, over 12 million gasoline vehicles cause 52.1% (31,885 t yr⁻¹) of the 639 total VOC emissions, and the gasoline sedan is the highest contributor across all vehicle types, which is over 28,434 t yr⁻¹ (46.5%) (Table 3b). Unlike NOx emissions, diesel vehicles only 640 contribute 23.0% (14.070 t yr⁻¹) of the total VOC emissions. Across the vehicle fuel types, the IF 641 642 outcome indicates that CNG vehicles have the highest IF values for VOC, which is 247 kg yr⁻¹ due 643 to the relatively high VOC contribution (19% over total VOC) and a low number of heavy CNG vehicles. The IF of CNG trucks are 77.2 kg yr⁻¹, but only contribute 0.2% to total VOC emissions. 644 645 The IF of the CNG bus is 320 kg yr⁻¹ and emits 19.5% of the total VOC. Comparing the IFs of 646 buses across fuel types, the CNG bus emits less NO_x but higher VOC than a diesel vehicle. Each 647 CNG bus has about 33 times higher IF of VOC (320 kg yr⁻¹) than a diesel bus (9.51 kg yr⁻¹), and CNG buses released slightly lower NO_x (248 kg yr⁻¹) than diesel buses (340 kg yr⁻¹) (Table 3a and 648 649 3b).

650 The current South Korea NIER currently does not have the PM emission factors from tire 651 and brake wear, which are the highest contributors of PM_{2.5} emissions from onroad vehicles (Hugo A.C. et al., 2013; Fulvio Amato et al., 2014). Once the emission factors of tire and brake wear are 652 653 prepared, those emissions can be computed by CARS. For that reason, diesel vehicles become the major source of PM_{2.5} emissions, which contributes over 98.5% (9,959 t yr⁻¹) of the PM_{2.5} 654 655 emissions based on the CARS 2015 emissions (Table 3c). The diesel truck, SUV, and van are the 656 three major sources, and their contributions of total PM_{2.5} are 53.6%, 21.4%, and 11.2%, 657 respectively. Although over 52% of the vehicles are gasoline vehicles, their primary PM_{2.5} contribution is limited to 1.44%. The diesel bus has the highest IF (2.83 kg yr⁻¹), which is caused 658 659 by the largest average daily VKTs.

660 Similar to VOC emissions, CO is mostly emitted through the tailpipe due to incomplete internal combustion of fuel and share similar emissions distributions across vehicle and fuel types 661 662 (Table 3d). Gasoline vehicles contribute most of the CO (220,390 t yr⁻¹, 59.0%), and sedan vehicles are the primary source (178,121 t yr⁻¹, 47.6%) of this out of all gasoline vehicles. Across vehicle 663 types, bus shows the highest IF of CO (81.2 kg yr⁻¹) due to its largest daily VKT. CO is the most 664 abundant pollutant released from vehicles (373,864 t yr⁻¹) across all pollutants from onroad 665 666 automobile sources. Although CO is much less reactive than other vehicle VOCs (Rinke and 667 Zetzsch, 1984; Liu and Sander, 2015), the majority of CO emissions from onroad automobile sources plays a critical role in generating 30% of hydroperoxyl radicals (HO₂) and causing ozone 668 669 formation in urban areas (Pfister et al., 2019). Thus, CO is also another crucial precursor to ozone 670 formation in urban areas.

671 SO_x emissions are related to the sulfur content within the fuel component; diesel has a 672 higher sulfur content than any other fuels. Most SO_x is contributed by diesel vehicles (93.8 t yr⁻¹, 673 54.5%) (Table 3e). Within diesel vehicles, trucks provide 26.5% of SO_x (45. t yr⁻¹). Although the 674 SO_x from sedan vehicles are slightly higher (~3.3%) than diesel trucks, the number of diesel trucks 675 is only 29.6% of the number of gasoline sedans. Thus, diesel trucks have a higher IF than gasoline 676 sedans. Across vehicle types, buses have the highest IF (0.095 kg yr⁻¹) of SO_x, and diesel buses in 677 particular have the largest IF at 0.143 kg yr⁻¹.

678 The NH₃ emissions table (table 3f) indicates that 98.7% of NH₃ is from gasoline vehicles 679 while diesel trucks only contribute 1.13%. The IF result also shows that the gasoline sedan has the 680 most significant impact per vehicle (1.17 kg yr⁻¹).

681 According to the vehicle activity and the CARS model results, nearly half of the total 682 vehicles (24.3 million) are gasoline sedans (10.4 million, 42.8%), and gasoline sedan vehicles 683 contributed most of the VOC and CO emissions (46.5% and 47.6%), but only 7.7% of the total 684 NO_x emissions. The number of diesel vehicles is 8.6 million (35.4%); however, they emitted about 85.3% of the total NO_x and 98.5% of the primary PM_{2.5}. These results indicated that the annual 685 traffic-related mobile emissions are not only affected by the number of vehicles, but also by 686 687 different vehicle and fuel types. Therefore, this study normalized the annual emissions by the 688 number of vehicles to confirm the emission composition by individual vehicle types.

689 Average Speed Impact Study

The CARS can also optionally apply the average speed distribution (ASD) by road type to compute more realistic mobile emissions on the road network when compared to using a current single average speed value for each road type (Appendix E). Applying the ASD will generate a better representation of actual traffic patterns from each road type. To understand the impacts of ASD application, we performed sensitivity runs between using a single-speed to the ASD application (Appendix F). The ASD data was described in Fig. 4, and the road-specific average single-speed values were developed based on the weighted average method using the same ASDdata. Appendix E and S6 describe the details of ASD as well as road-specific speed values.

Figure 9a shows the differences in total emissions between two scenarios and is organized by pollutant. The single-speed scenario largely underestimates the emissions across all pollutants compared to the ones from the ASD scenario. NO_x (16%), VOC (40%), and CO (30%) were especially underestimated. The difference is caused by the lack of low-speed bins (<16 km h⁻¹) representation when a single average speed approach was used. Higher emissions are emitted while vehicles are operated with low-speed bins, which decreases the combustion efficiency of ICE and releases more pollutants.

705 Figure 9b shows the road-specific breakdown between the ASD and single speed scenarios 706 to understand the impacts of vehicle operating speeds on onroad automobile emissions. In this 707 figure, each color indicates the emissions percentage differences by road types. Other than NH₃, 708 significant discrepancies happened between local urban roads (5.8%), highways (3.9%), and urban 709 highways (3.0%). Other pollutants, VOC, PM_{2.5}, CO, and SO_x, have similar fractions of road types. 710 This phenomenon is caused by low-speed conditions (<16 km h⁻¹) and the fractions of road VKT 711 contributions (Appendix C). The lower speeds cause the incomplete combustion of ICE and 712 increase the emission rate. Also, local urban roads, highways, and urban highways have higher 713 road VKT contributions at 17%, 18%, and 12%, respectively (Appendix C) than rural roads. 714 Higher emissions from low speed conditions from these high contribution roads (urban local, urban 715 highway, and highway) caused these significant differences between the ASD and single-speed 716 approaches. Although the interstate expressway has the largest VKT contribution (41%), it also 717 has the lowest fraction of low-speed bins (2%). That is why the difference between the ASD and 718 single speed scenarios on interstate expressways is less than 1%. In general, NH₃ emission factors 719 do not change by vehicle operating speed, so the ASD impact is quite minimal.

720 **5 Conclusions**

The CARS is a bottom-up automobile emissions model that utilizes the localized traffic-721 722 related activity and emission factors input datasets to generate high quality localized bottom-up 723 emissions inventories for policymakers, stakeholders, and research community as well as 724 temporally and spatially enhanced hourly gridded emissions for CTMs. First, the CARS model 725 employs the daily VKTs for all registered vehicles and the emission factors function to compute 726 district-level total daily emissions for each vehicle. To reflect realistic traffic patterns, the CARS 727 model computes and utilizes link-level VKTs (=link-length×AADT) from the road network GIS 728 shapefiles to redistribute the original district-level total emissions into spatially enhanced road 729 link-level emissions. It can also optionally implement a control strategy as well as road restriction 730 rules to improve the quality of local emission inventories and meet the needs of users.

731 The CARS model is a fully modularized and computationally optimized python-based 732 bottom-up mobile emissions model that can effectively process a huge dataset to calculate high 733 quality spatiotemporal county-level, road link-level and grid cell-level mobile emissions. We 734 believe that the implementation of the ASD into the CARS improves the representation of onroad 735 automobile emissions from the road network when compared to a single-speed for each road type 736 approach. It allows the CARS to have a better representation of low speed (<16 km h-1) vehicle 737 emissions. We believe that CARS model's versatile spatiotemporal bottom-up automobile 738 emissions and the in-depth analysis feature can assist government policymakers and stakeholders 739 to develop the rapid responsive emission abatement strategies as a response to the South Korea's 740 national PM_{2.5} emergency control strategy that enforces the nationwide vehicle restriction policy 741 within 24 hours.

742 Code Availability:

The source code of the CARS model public release version 1.0 can be downloaded from theGithub release website:

- 745 <u>https://github.com/bokhaeng/CARS/releases/tag/CARSv1.0</u>
 746
- 747

748 Digital Object Identifier (DOI) for the CARS version 1.0:

- 749 https://zenodo.org/record/5033314#.YNzDrC1h001
- 750 751

752 Installation Package for CARS version 1.0:

The CARS version 1.0 installation package comes with the complete inputs and outputs datasets for users to confirm their proper installation on their computers and can be downloaded from the

- 755 Github release website:
- https://github.com/bokhaeng/CARS/releases/download/CARSv1.0/CARS_v1.0_public_release_
 package_25June2021.zip
- 758
- 759760 User's Guide Documentation:
- 761 The CARS version user's guide documentation can be accessed through the Github repository:
- 762 <u>https://github.com/bokhaeng/CARS/tree/master/docs/User_Manual</u>
- 763 764

765 Data availability:

All the datasets, excel and python scripts used in this manuscript for the data analysis are uploaded through GMD website along with a supplemental appendix document.

768

769 Author contribution

Dr. B.H. Baek and Dr. Jung-Hun Woo are lead researchers in this study. Dr. Rizzieri Pedruzzi
develop the source code of CARS model, Dr. Minwoo Park tested the model and provided the
model input data. Dr. Chi-Tsan Wang analyzed the model result and prepared the manuscript.
Younha Kim, Chul-Han Song, analyzed the model result and provided comments.

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- 775

776 Competing interests

The Authors declare that they have no conflict of interest.

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989 Tables

990	Table 1. Computational processing time by CARS module based on the modeling setup: Tota
991	number of activity data = 24,383,578; Emission Factors = 84,608; GIS road links=385,795

000	$1^{1} + 1^{1} + 1^{2} + 1^{2} + 1^{2} = 5$ 150/16 01-00-01-00 - 01-01 - 11- 5 404 (02 - 1-00-01-00-01-00-01-00-00-00-00-00-00-00
997	$\alpha_1 s_1 c_1 s_2 s_1 a_1 e_1 = 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - $
<i>))</i>	$(02 \text{ columns} \times 07 \text{ columns} \times 07 \text{ columns})$

No	Module	Desktop i7	Laptop i9	Averaged Time
110	11100010	(minutes)	(minutes)	(minutes)
1	Process activity data	1.8	1.5	1.7
2	process emission factors	1.1	0.8	1.0
3	Process shape file	9.9	7.3	8.6
4	Calculate district emissions	6.4	5.7	6.1
5	Grid4AQM [31days]	4.8 [75.9]	5.0 [87.2]	4.9 [81.6]
6	Plot figures	6.2	5.4	5.8
	Total [31days]	30.2 [101.3]	25.7 [107.9]	28.1[104.8]

Pollutants (t yr⁻¹) **Emission Inventory** VOC NO_{x} SO_x NH₃ PM2.5 CO 301,794 61,186 10,108 373,864 172 12,453 CARS 2015 CAPSS 2015 369,585 46,145 8,817 245,516 209 10,079

Table 2. The total emissions comparison between CARS and CAPSS for the 2015 emission.

Table 3. The summary tables of emissions (t yr⁻¹), contributions (%), and impact factor (IF, kg yr⁻¹) per vehicle for criteria air pollutants (CAPs) by vehicle and fuel types: (a) for NO_x; (b) VOC;

(c) for $PM_{2.5}$; (d) for CO; (e) for SO_x; and (f) for NH₃.

(a) NOx

Vehicle	Gasoline		Diesel		LPG		CNG		Hybric	1	Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	20,219 (6.70%)	1.94	14,783 (4.90%)	12.8	8,159 (2.77%)	4.49	12 (0.00%)	1.26	65 (0.02%)	0.39	43,239 (14.3%)	3.19
Truck	23 (0.01%)	5.54	148,246 (49.1%)	47.9	920 (0.31%)	4.55	88 (0.03%)	66.4	-	-	149,277 (49.5%)	45.2
Bus	0 (0.00%)	0.97	25,677 (8.51%)	340	-	-	9,260 (3.07%)	248	0 (0.00%)	1.77	34,938 (11.6%)	333
SUV	159 (0.05%)	1.19	39,565 (13.1%)	11.4	175 (0.06%)	8.54	0 (0.00%)	1.60	1 (0.00%)	0.42	39,900 (13.2%)	11.0
Van	14 (0.00%)	4.78	16,659 (5.52%)	22.6	1,337 (0.44%)	6.80	0 (0.00%)	1.25	0 (0.00)	0.37	18,012 (6.00%)	19.2
Taxi	-	-	-	-	1,217 (0.40%)	2.11	-	-	-	-	1,217 (0.40%)	2.11
Special	1 (0.00%)	20.1	12,347 (4.10%)	152	0 (0.00%)	0.52	-	-	-	-	12,375 (4.10%)	151
Motorcycle	2,836 (0.94%)	1.31	-		-	-	-	-	-	-	2,836 (0.94%)	1.32
Total	23,253 (7.70%)	1.83	257,305 (85.3%)	29.9	11,809 (3.91%)	4.20	9,361 (3.10%)	36.7	66 (0.02%)	0.39	301,794 (100%)	13.3

(b) VOC

/												
Vehicle	Gasoline		Diesel		LPG	LPG			Hybrid		Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	28,434 (46.5%)	2.73	629 (1.03%)	0.55	2,107 (3.44%)	1.16	3 (0.01%)	0.33	77 (0.13%)	0.47	31,250 (51.1%)	2.30
Truck	23 (0.04%)	5.44	8,194 (13.4%)	2.65	286 (0.47%)	1.41	102 (0.17%)	77.2	-	-	8,605 (14.1%)	2.61
Bus	0 (0.00%)	1.65	717 (1.17%)	9.51	-	-	11,942 (19.5%)	320	0 (0.00%)	0	12,659 (20.7%)	112
SUV	246 (0.40%)	1.84	2,441 (3.99%)	0.71	46 (0.08%)	2.25	0 (0.00%)	0.75	1 (0.00%)	0.55	2,733 (4.47%)	0.76
Van	21 (0.03%)	7.04	1,185 (1.94%)	1.61	393 (0.64%)	2.00	0 (0.00%)	0.45	0 (0.00%)	0	1,599 (2.61%)	1.71
Taxi	-	-	-	-	273 (0.45%)	0.47	-	-	-	-	273 (0.45%)	0.47
Special	1 (0.00%)	25.8	904 (1.48%)	11.1	0 (0.00%)	0.23	-	-	-	-	905 (1.48%)	11.0
Motorcycle	3,160 (5.16%)	1.46	-		-	-	-	-	-	-	3,160 (5.16%)	1.46
Total	31,885 (52.1%)	2.50	14,070 (23.0%)	1.64	3,106 (5.08%)	1.10	12,047 (19.7%)	247	78 (0.13%)	0.47	61,186 (100%)	2.51

(c) PM2.5												
Vehicle	Gasoline		Diesel		LPG		CNG		Hybrid	t	Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	144 (1.42%)	0.01	809 (8.00%)	0.70	0	0	0	0	3 (0.03%)	0.02	956 (9.46%)	0.07
Truck	0 (0.01%)	0	5,415 (53.6%)	1.75	0	0	0	0	-	-	5,415 (53.6%)	1.64
Bus	0	0	214 (2.11%)	2.83	-	-	0	0	0 (0.01%)	0.09	214 (2.11%)	1.89
SUV	2 (0.02%)	0.02	2,165 (21.4%)	0.63	0	0	0	0	0	0.02	2,167 (21.4%)	0.60
Van	0	0	1,127 (11.2%)	1.53	0	0	0	0	0	0.02	1,127 (11.2%)	1.20
Taxi	-	-	-	-	0	0	-	-	-	-	0	0
Special	0	0	230 (2.28%)	2.82	0	0	-	-	-	-	230 (2.28%)	2.81
Motorcycle	0	0	-		-	-	-	-	-	-	0	0
Total	146 (1.44%)	0.01	9,959 (98.5%)	1.16	0	0	0	0	3 (0.03%)	0.02	10,108 (100%)	0.41

(d) CO

Vehicle	Gasoline		Diesel		LPG		CNG		Hybrid		Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	178,121 (47.6%)	17.1	3,436 (0.92%)	2.98	42,886 (11.5%)	23.6	29 (0.01%)	2.91	177 (0.05%)	1.07	224,649 (60.1%)	16.6
Truck	254 (0.07%)	61.1	47,065 (12.6%)	15.2	9,088 (2.43%)	44.9	68 (0.02%)	51.4	-	-	56,475 (15.1%)	17.1
Bus	0 (0.00%)	19.3	7,633 (2.05%)	101	-	-	1542 (0.41%)	41.3	1 (0.00%)	4.64	9,176 (2.45%)	81.2
SUV	2,616 (0.70%)	19.6	13,401 (3.58%)	3.87	791 (0.21%)	38.6	0 (0.00%)	4.09	2 (0.00%)	1.15	16,808 (4.50%)	4.65
Van	131 (0.04%)	43.4	6,611 (1.77%)	8.97	8,032 (2.15%)	40.9	2 (0.00%)	6.53	0 (0.00%)	1.00	14,777 (3.95%)	15.8
Taxi	-	-	-	-	8,481 (2.27%)	14.7	-	-	-	-	8,481 (2.27%)	14.7
Special	13 (0.00%)	269	4,224 (1.13%)	51.7	1 (0.00%)	3.69	-	-	-	-	4,239 (1.13%)	51.7
Motorcycle	39,256 (10.5%)	18.2	-		-	-	-	-	-	-	39,256 (10.5%)	18.2
Total	220,390 (59.0%)	17.3	82,372 (22.0%)	9.57	69,281 (18.5%)	24.6	1641 (0.44%)	33.6	180 (0.05%)	1.07	373,864 (100%)	15.4

1013

(e) SO_x												
Vehicle	Gasoline		Diesel		LPG		CNG		Hybrid		Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	51.3 (29.8%)	0.005	6.5 (3.79%)	0.006	8.28 (4.81%)	0.005	0	0	1.14 (0.67%)	0.007	67.2 (39.1%)	0.005
Truck	0.03 (0.02%)	0.008	45.5 (26.5%)	0.015	0.97 (0.57%)	0.005	0	0	-	-	46.5 (27.1%)	0.014
Bus	0 (0.00%)	0.003	10.8 (6.26%)	0.143	-	-	0	0	0.01 (0.01%)	0.047	10.8 (6.26%)	0.095
SUV	0 (0.00%)	0.000	18.2 (10.6%)	0.005	0.00 (0.00%)	0.000	0	0	0.01 (0.01%)	0.007	18.2 (10.6%)	0.005
Van	0.02 (0.01%)	0.006	5.5 (3.20%)	0.007	0.77 (0.45%)	0.004	0	0	0 (0.00%)	0.010	6.30 (3.66%)	0.007
Taxi	-	-	-	-	7.71 (4.49%)	0.013	-	-	-	-	7.71 (4.48%)	0.013
Special	0 (0.00%)	0.003	7.3 (4.27%)	0.090	0.00 (0.00%)	0.005	-	-	-	-	7.34 (4.27%)	0.090
Motorcycle	7.94 (4.62%)	0.004	-		-	-	-	-	-	-	7.94 (4.62%)	0.004
Total	59.3 (34.5%)	0.006	93.8 (54.5%)	0.011	17.7 (10.3%)	0.006	0	0	1.17 (0.68%)	0.007	172 (100%)	0.007

1015 1016

(e) NH₃

Vehicle	Gasoline		Diesel		LPG		CNG		Hybrid		Total	
	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF	Emission	IF
Sedan	12,225 (98.3%)	1.17	20 (0.16%)	0.02	0	0.00	0	0	19 (0.15%)	0.11	12,284 (98.6%)	0.91
Truck	0 (0.00%)	0.03	82 (0.66%)	0.03	0	0.00	0	0	-	-	82 (0.66%)	0.02
Bus	0 (0.00%)	0.09	15 (0.12%)	0.19	-	-	0	0	0 (0.00%)	0.51	15 (0.12%)	0.13
SUV	0 (0.00%)	0.00	0 (0.00%)	0.00	0	0.00	0	0	0 (0.00%)	0.16	0 (0.00%)	0.00
Van	0 (0.00%)	0.02	14 (0.11%)	0.02	0	0.00	0	0	0 (0.00%)	0.09	14 (0.11%)	0.01
Taxi	-	-	-	-	0	0.00	-	-	-	-	0 (0.00%)	0.00
Special	0 (0.00%)	0.01	10 (0.08%)	0.12	0	0.00	-	-	-	-	10 (0.08%)	0.12
Motorcycle	49 (0.39%)	0.02	-		-	-	-	-	-	-	49 (0.39%)	0.02
Total	12,293 (98.7%)	0.97	141 (1.13%)	0.02	0	0.00	0	0	19 (0.16%)	0.12	12,453 (100%)	0.51

1019 Figures



Figure 1. CARS schematic methodology to estimate mobile emissions.



Figure 2. (a) The number of vehicles by vehicle and fuel types and **(b)** the total daily VKT by

1025 vehicle and fuel types in South Korea.



Figure 3. Variation of NOx emission factors from diesel compact engines by vehicle speed and 1030 ambient temperatures: (a) NO_x emission factors function to vehicle speed; (b) NO_x emission 1031 factors of diesel compact truck function to vehicle speed and ambient temperature.



Figure 4. (a) The South Korea speed distribution by road types. (b) The Georgia state speed distribution by road types. (c) The average speed distribution (ASD) by road types used in this study for South Korea.



$\begin{array}{c} 1040 \\ 1041 \end{array}$

Figure 5. The schematic of modules and their functions in the CARS.



1044 Figure 6 (a) the road network GIS shapefile of Seoul, South Korea; (b) two districts with different

1045 colors (purple and blue); (c) the modeling grid cells over road segments.



1048Figure 7. Three different formats of CO emissions from CARS, (A) District-level total emissions1049 $(t yr^{-1})$ (B) Link-level total emissions $(t yr^{-1})$, (C) CTM-ready gridded hourly total emissions (moles1050 s^{-1}).



1053 1054 **Figure 8**. Comparison between CARS 2015 and CAPSS 2015 onroad mobile emissions inventories by vehicle types. The standard line is CAPSS 2015 data.



1059 emission differences by pollutant; (b) The road-specific difference (%) by pollutant.

1061 Appendices

1062

1063

1064 Appendix A: The vehicle types classified by fuel type, vehicle body type, and engine size. The 1065 emission factors of the diesel vehicle with the star (*) are depended on the ambient temperature (*T*).

Vehicle	Fuel Types										
Types	Gasoline	Diesel	LPG	CNG	HYBRID_G	HYBRID_D	HYBRID_L	HYBRID_C			
	Supercompact	Supercompact*	Supercompact	-	-	-	-	-			
G 1	Compact	compact*	compact	compact	compact	compact	compact	-			
Sedan	Fullsize	Fullsize*	Fullsize	Fullsize	Fullsize	Fullsize	Fullsize	-			
	Midsize	Midsize*	Midsize	Midsize	Midsize	Midsize	Midsize	-			
	Supercompact	Supercompact	Supercompact	-	-	-	-	-			
	Compact	Compact*	Compact	Compact	-	-	-	-			
	Fullsize	Concrete	-	Fullsize	-	-	-	-			
Truck	Midsize	Fullsize	Midsize	Midsize	-	-	-	-			
	-	Midsize	-	-	-	-	-	-			
	-	Dump	-	-	-	-	-	-			
	-	Special	Special	Special	-	-	-	-			
Buc	Urban	Urban	Urban	Urban	-	Urban	-	-			
Bus	-	Rural	-	Rural	-	Rural	-	Rural			
SUV	Compact	Compact*	Compact	-	-	-	-	-			
50 1	Midsize	Midsize*	Midsize	Midsize	Midsize	-	-	-			
	supercompact	supercompact	supercompact	-	-	-	-	-			
Van	Compact	Compact	Compact	Compact	-	-	-	-			
v all	-	-	Fullsize	Fullsize	Fullsize	Fullsize	Fullsize	Fullsize			
	Midsize	Midsize	Midsize	Midsize	Midsize	Midsize	Midsize	Midsize			
	-	-	Compact	-	-	-	-	-			
Taxi	-	-	Fullsize	-	-	-	-	-			
	-	-	Midsize	-	-	-	-	-			
	-	Tow	-	-	-	-	-	-			
Special	Wrecking	Wrecking	Wrecking	Wrecking	-	-	-	-			
	Others	Others	Others	-	-	-	-	-			
	Compact	-	-	-	-	-	-	-			
Motorcycle	Midsize	-	-	-	-	-	-	-			
monoreyere	Fullsize	-	-	-	-	-	-	-			

- no existence
- * ambient temperature-dependent diesel vehicle
- 1067 1068 1069 1070 1071 1072 1073 1074 LPG: Liquefied Petroleum Gas
- CNG: Connecticut Natural Gas
- Hybrid_G: hybrid vehicle with gasoline
- Hybrid_D: hybrid vehicle with diesel
- Hybrid_L: hybrid vehicle with LPG
- Hybrid_C: hybrid vehicle with CNG
- 1075
- 1076

1077 Appendix B, The summary of activity data (number of vehicles and daily total VKTs) in South 1078 Korea by vehicle type with engine size.

Wabiala						Fuel Ty	pes				
Venicle	Engine sizes	Gaso	oline	Di	iesel	LF	PG	CI	NG	H	/brid
Types		Numbers	Daily VKT	Numbers	Daily VKT	Numbers	Daily VKT	Numbers	Daily VKT	Numbers	Daily VKT
	Supercompact	1,792,471	50,197,345	46	1,761	83,226	4,000,067	6	237	-	-
C . d	Compact	1,372,317	39,543,668	51,324	2,570,086	8,040	257,060	276	12,115	3,802	137,360
Sedan	Fullsize	2,403,327	100,632,702	428,831	20,928,552	292,850	15,910,588	5,296	323,852	21,533	1,086,509
	Midsize	4,858,533	167,454,032	672,960	33,126,318	1,431,970	66,640,378	4,310	625,717	140,527	6,717,856
	Supercompact	850	9,595	816	354	111,051	6,550,476	-	-	-	-
	Compact	3,185	143,510	2,655,089	133,480,216	87,650	3,567,109	42	2,694	-	-
Trueste	Fullsize	3	422	180,991	25,774,819	-	-	72	4,676	-	-
Truck	Midsize	98	7,430	258,509	17,477,685	1,434	47,870	14	483	-	-
	Dump	-	-	-	-	-	-	-	-	-	-
	Special	20	970	-	-	2,292	99,124	1,194	60,886	-	-
Buc	Urban	1	126	40,448	7,282,593	1	652	6,543	1,466,854	2	282
Dus	Rural	-	-	34,997	6,334,278	-	-	30,792	6,460,001	216	50,873
SUV	Compact	42,348	1,395,153	2,341,397	105,962,626	6,946	275,728	13	551	-	
30 1	Midsize	91,002	3,520,552	1,120,128	5,277,861	13,567	595,426	15	706	1,719	88,683
	supercompact	88	1,645	-	-	44,947	2,058,014	-	-	-	-
	Compact	2,937	87,507	685,317	34,781,937	151,654	6,135,138	7	255	-	-
Van	Fullsize	-	-	19,452	1,318,221	1	14	97	7,598	3	136
	Midsize	2	1,303,795	31,790	1,433,407	15	416	160	15,216	2	85
	Special	-		-	-	-		-	-	-	-
	Compact	-	-	-	-	8,380	576,378	-	-	-	-
Taxi	Fullsize	-	-	-	-	92,861	10,827,756	-	-	-	-
	Midsize	-	-	-	-	474,455	69,087,721	-	-	-	-
	Tow	-	-	40,807	7,447,773	-	-	-	-	-	-
Special	Wrecking	2	138	12,568	813,746	128	6,607	3	94	-	-
	Others	47	553	28,275	989,988	180	9,966	-	-	-	-
	Compact	184,822	3,507,948	-	-	-	-	-	-	-	-
Motorcycle	Fullsize	65,964	3,493,728	-	-	-	-	-	-	-	-
	Midsize	1,910,988	61,676,824	-	-	-	-	-	-	-	-

- no existence

1079 1080 1081 1082 LPG: Liquefied Petroleum Gas

CNG: Connecticut Natural Gas

Hybrid: all hybrid vehicles, electric power mixed with fossil fuel (gasoline, diesel, LPG, or CNG)

1083

1084

1087 Appendix C, Eight road types with assigned average vehicle operating speed and VKT fractions.

Road	Description	Average Speed	Road VKT
types	Description	$({\rm km} {\rm h}^{-1})$	fraction
101	Interstate Expressway	90	41%
102	Urban Expressway	60	5%
103	Highway	58	18%
104	Urban Highway	36	12%
105	Rural Highway	55	3%
106	Rural Local Road	45	4%
107	Urban Local Road	32	17%
108	Ramp	50	0.4%

Appendix D, The daily average VKT (km d⁻¹) per vehicle by vehicle and fuel types.

Vehicle types	Fuel Types								
	Gasoline	Diesel	LPG	CNG	Hybrid	Average			
Sedan	34	49	48	97	48	38			
Truck	39	57	51	52	-	57			
Bus	126	180	-	212	237	191			
SUV	37	46	42	45	52	46			
VAN	29	51	42	87	44	49			
Taxi	-	-	140	-	-	140			
Special	14	113	54	31	-	113			
Motorcycle	32	-	-	-	-	32			

1093Appendix E, Average speed distribution (ASD) for each road type: The table columns are1094different road types, and the table rows are average speed of each speed bin.

Speed	Speed Speed		Road Types							
bins	(km/h)	101	102	103	104	105	106	107	108	
1	speed < 4	1.50%	2.00%	5.00%	5.00%	5.00%	10.00%	10.00%	0.00%	
2	$4 \leq speed < 8$	0.50%	1.00%	2.00%	2.00%	2.00%	5.00%	5.00%	0.00%	
3	$8 \leq \text{speed} \leq 16$	0.00%	0.33%	0.40%	3.59%	0.41%	0.30%	2.76%	0.11%	
4	$16 \leq \text{speed} \leq 24$	0.00%	1.09%	3.64%	14.35%	1.45%	2.91%	11.75%	5.85%	
5	$24 \leq speed \leq 32$	0.01%	3.04%	6.82%	35.25%	6.85%	6.15%	40.80%	12.80%	
6	$32 \leq speed \leq 40$	0.17%	6.43%	9.28%	17.14%	14.70%	12.00%	12.69%	24.53%	
7	$40 \leq speed \leq 48$	0.52%	14.76%	10.70%	10.86%	16.20%	23.30%	7.49%	23.74%	
8	$48 \leq speed \leq 56$	0.53%	16.66%	12.52%	5.72%	15.42%	20.72%	4.24%	6.60%	
9	$56 \leq speed \leq 64$	1.94%	23.49%	12.83%	2.68%	6.08%	10.06%	2.56%	10.90%	
10	$64 \leq speed < 72$	5.05%	16.30%	10.51%	1.90%	13.21%	3.84%	1.45%	5.30%	
11	$72 \leq speed \leq 80$	11.70%	10.19%	12.69%	0.74%	9.98%	2.85%	0.53%	5.30%	
12	$80 \leq \text{speed} \leq 89$	28.73%	4.30%	12.21%	1.04%	6.75%	2.21%	0.65%	4.59%	
13	$89 \leq \text{speed} \leq 97$	34.24%	0.51%	1.82%	0.15%	1.90%	0.62%	0.08%	0.00%	
14	$97 \leq \text{speed} < 105$	14.99%	0.00%	0.02%	0.00%	0.04%	0.03%	0.00%	0.30%	
15	$105 \leq \text{speed} \leq 113$	0.18%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
16	$113 \leq \text{speed} < 121$	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	

1095 Appendix F: Single average speed for each road type

Speed	peed Speed		Road Types						
bins	(km/h)	101	102	103	104	105	106	107	108
1	speed < 4	0%	0%	0%	0%	0%	0%	0%	0%
2	$4 \leq speed < 8$	0%	0%	0%	0%	0%	0%	0%	0%
3	$8 \leq speed < 16$	0%	0%	0%	0%	0%	0%	0%	0%
4	$16 \leq \text{speed} \leq 24$	0%	0%	0%	0%	0%	0%	0%	0%
5	$24 \leq speed \leq 32$	0%	0%	0%	0%	0%	0%	100%	0%
6	$32 \leq speed \leq 40$	0%	0%	0%	100%	0%	0%	0%	0%
7	$40 \leq speed \leq 48$	0%	0%	0%	0%	0%	100%	0%	100%
8	$48 \leq speed \leq 56$	0%	0%	100%	0%	100%	0%	0%	0%
9	$56 \leq \text{speed} \leq 64$	0%	100%	0%	0%	0%	0%	0%	0%
10	$64 \leq speed < 72$	0%	0%	0%	0%	0%	0%	0%	0%
11	$72 \leq speed \leq 80$	0%	0%	0%	0%	0%	0%	0%	0%
12	$80 \le \text{speed} \le 89$	100%	0%	0%	0%	0%	0%	0%	0%
13	$89 \leq \text{speed} \leq 97$	0%	0%	0%	0%	0%	0%	0%	0%
14	$97 \leq speed < 105$	0%	0%	0%	0%	0%	0%	0%	0%
15	$105 \leq speed \leq 113$	0%	0%	0%	0%	0%	0%	0%	0%
16	$113 \leq \text{speed} < 121$	0%	0%	0%	0%	0%	0%	0%	0%

Appendix G:

The annual emission rate between original road type ASD, adjusted road type ASD, and CAPSS result for 2015

Gg/year	СО	NOx	SOx	PM10	PM2.5	VOC	NH3
CARS data 2015 org ASD	269.3	258.4	0.2	9.5	8.8	38.9	12.4
CARS data 2015 adj ASD	373.9	301.8	0.2	11.0	10.1	61.2	12.5
CAPSS 2015	245.5	369.6	0.2	9.6	8.8	46.1	10.1

Appendix H:

CARS model input data summary table

Input data type	Parameters	Variable Name in CARS	File format
Human activity data of each vehicle	Fuel, vehicle, type, daily VKT, region code, manufacture data activity_file		CSV
Emission factor table	Vehicle, engine, fuel, SCC ,Pollutant, year, temperature, v,a,b,c,d,f,k Emis_factor_list		CSV
Link level Shape file	Link ID, region code, region name, road rank, speed, VKT, Link length, geometry	region code, region name, road eed, VKT, Link length, geometry	
County Shape File	Region code, region name	county_shape	shape file
Average speed distribution table	Speed bins, the distribution of each road type avg_SPD_Dist_file		CSV
road restriction table	Vehicle, engine, fuel, road types	road_restriction	csv
Vehicle deterioration table	Vehicle, engine, SCC, fuel, Pollutant, Manufacture date	Deterioration_list	CSV
Control strategy factors table	Vehicle, engine, fuel, year, data, region code, control factor	control_list	csv
Model domain description	Projection method name, parameters for prjection method, domain name, bottum left coner X and Y, grid cell size, numbers of grid cell in X, Y, and Z-axis	gridfile_name	text file in griddesc format
Temporal	Profile reference number, Year to Monthly profile (12 columns)	temporal _monthly_file	CSV
profile tables	Profile reference number, week to daily profile (7 columns)	temporal _week_file	CSV

	Profile reference number, week day to hourly profile (24 columns)	temporal_weekday_file	CSV
	Profile reference number, weekend day to hourly profile (24 columns)	temporal_weekend_file	CSV
	Vehicle, types, fuel, road type, month reference number, week reference number, weekday reference number, weekend reference number	temporal_CrossRef	CSV
Chemical profile	Species code, species name, target species name, fraction, molecular weight,	Chemical_profile	txt or csv
table	Vehicle, engine, fuel, species reference codes	speciation_CrossRef	CSV