AMERICAN UNIVERSITY OF BEIRUT

SIMULATING IN-VEHICLE EXPOSURE: FIELD AND MODELING BASED ASSESSMENT

by

GHINWA GEORGES HARIK

A thesis
submitted in partial fulfillment of the requirements
for the degree of Master of Engineering
to the Departement of Civil and Environmental Engineering
of the Faculty of Engineering and Architecture
at the American University of Beirut

Beirut, Lebanon
January 2015

AMERICAN UNIVERSITY OF BEIRUT

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by
GHINWA GEORGES HARIK

Approved by:

Dr. Mutasem El-Fadel, Professor Civil and Environmental Engineering	Advisor
Dr. Ibrahim Alameddine, Assistant Professor Civil and Environmental Engineering	Co-Advisor
Dr. Alan Shihadeh, Professor Mechanical Engineering	Member of Committee

Date of thesis defense: 23-January-2015

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# ACKNOWLEDGEMENTS

I am using this opportunity to express my gratitude to everyone who supported me throughout this program.

I first dedicate this work to the one above all, giving me the grace of being here, Saint Mary Mother of God and to my Husband, Anthony, for your perseverance, encouragement and reluctant support.

I would like to express my deepest appreciation to my advisor, Dr. Mutasem El Fadel, a brilliant scholar and a noble person, your knowledge and experience were the essence of this work. To Dr. Ibrahim Alameddine, for all the time and effort you spent helping me, this work could not have been achieved without your support. To Dr. Alan Shehadi, for your interference and advice, your knowledge substantially improved the work. To Dr. Layal Abi Esber, your work was an inspiration and your tremendous help made this work achievable.

Finally I would like to thank my family for their everlasting love and understanding.

AN ABSTRACT OF THE THESIS OF

Ghinwa Georges Harik for Master of Engineering

Major: Environmental and Water Resources Engineering

Title: Simulating in-vehicle exposure: Field and Modeling based assessement

This study examines ambient contaminant infiltration to in-vehicle microenvironments to assess in-vehicle exposure and potential self-pollution from vehicular exhaust. For this purpose, in and out-vehicle CO and $PM_{2.5}$ concentrations were monitored in several cars under idle and moving conditions using common ventilation modes. Field measurements were coupled with mathematical modeling to define air exchange rates (AER), $PM_{2.5}$ deposition rates (DR), and equivalent emission rates (ER) representing potential self-pollution. Using CO as an indicator, the AER ranged between 1.8 and 112.2 h^{-1} and generally increased with vehicle speed under all tested ventilation modes. The DR of $PM_{2.5}$ ranged between 0.6 and 12.6 h^{-1} and was also dependent of speed and ventilation conditions. Self-pollution varied widely with car make, speed and ventilation mode with corresponding average equivalent ERs of 2.86 to 238.3 mg/h for CO and 0.01 to 2.5 mg/h for $PM_{2.5}$.

Keywords: In-vehicle exposure, PM2.5, CO, Self-Pollution, CONTAM, Mass Balance

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ABBREVIATIONS

AC FA	:	Air Conditionning on Fresh Air
AC Rec	:	Air Conditionnig on Recirculation
AER	:	Air Exchange Rate
CFD	:	Computational Fluid Dynamics
Cin	:	In-vehicle Concentration
CO	:	Carbon Monoxide
Cout	:	Out-vehicle Concentration
DR	:	Deposition Rate
EPA	:	Environmental Protection Agency
ER	:	Emission Rate
HV	:	Hyundai Verna
IO	:	Indoor to Outdoor
MBE	:	Mass Balance Equation
NIST	:	National Institute of Standards and Technology
P206	:	Peugeot 206
P307	:	Peugeot 307
PM	:	Particulate Matter
Ppm	:	Part per million
RMSE	:	Root Mean Square Error
V	:	Volume
W1/2	:	Window half-opened
WHO	:	World Health Organization
%	:	Percent

CHAPTER 1 INTRODUCTION

The interest in in-vehicle air quality has increased in recent years due to prolonged commute and travel distances as well as traffic congestion (Müller *et al.*, 2011; Kimbrell *et al.*, 2000). In-vehicle air pollution is mainly due to infiltration of poor ambient air quality and vehicle exhaust. The in-cabin of small size vehicles is invariably the most vulnerable to contamination compared to other commuting means (Duci *et al.*, 2003; Dan, 2008) due often to inadequate air exchange rate, the small cabin volume, as well as the low intake point of ventilation that is near the exhaust emissions of other vehicles (Chan *et al.*, 1999). In parallel, indoor air quality is highly dependent on the 1) outdoor environment whereby roadway vehicles can be simulated as commuting in a tunnel with the in-vehicle air being an extension of the outdoor air through infiltration and 2) ventilation means through passive or forced air intrusion (Lazaridis, 2011; Chan, 2002; Chan *et al.*, 2003). At the ambient air level, vehicle exhaust, fuel burning, tire scuff and other motorized emissions constitute a major source of pollutants(NOx, CO, and PM) (Müller *et al.*, 2011).Poor ambient air quality coupled with prolonged commute and travel distances are often associated with increased in-vehicle exposure and adverse health effects. Concurrently, in-vehicle self-pollution, which is defined as the intrusion of the vehicle's own exhaust into the passenger's compartment by either exhaust return or infiltration through firewalls, was demonstrated to represent a significant source of in-vehicle exposure (Abi-Esber *et al.* 2013). In the same context, several studies reported poorer in-cabin air quality compared to the ambient environment and was attributed to the existence of an inside pollution source (Zagury *et al.*, 2000; Chan, 2002; Chan *et al.*, 2003).

An apparent shortcoming in the reported literature is related to the lack of certain critical physical parameters (observations such as the vehicle Air Exchange Rate and in-cabin $PM_{2.5}$

Deposition Rate) that allow for a better analysis and understanding of field. These parameters were targeted in the current study using a hybrid approach of a field experimental program coupled with mathematical modeling to assess potential self-pollution from vehicular exhaust.

CHAPTER 2 MATERIALS AND METHODS

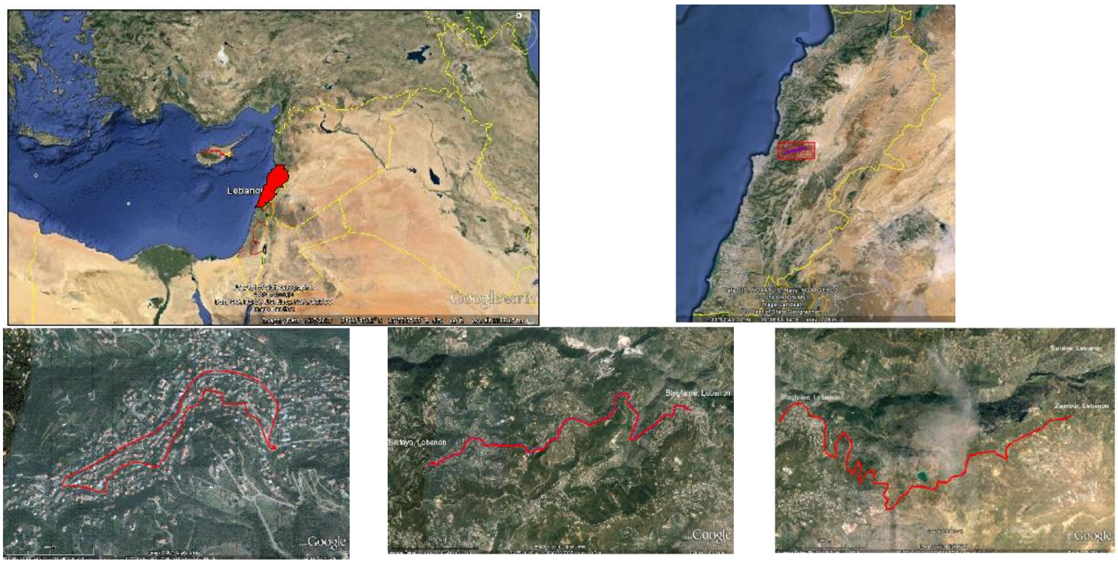
2.1. Field Experimental Program

Self-pollution tests were conducted using three different vehicles at speeds of 40, 60 and 80 km/h. All three vehicles were small in size: Peugeot 206 (2006, V=2 m^3), Peugeot 307 (2008, V= 2.24 m^3), and a Hyundai Verna (2011, V= 2.55 m^3). The Air Conditioning (AC) filters of all vehicles were removed to exclude the effect of filtering. The tests were run under three common ventilation modes, namely:

- Driver's window half opened, Air Conditioning off, vents closed
- Windows closed, Air Conditioning on fresh air, with the fan setting on medium (2)
- Windows closed, Air Conditioning on recirculation, with the fan setting on medium (2)

All experiments were conducted during the period ranging between May 22 and June 21, 2014 in Mount-Lebanon (Metn region) along a road located at an altitude ranging between 900 m (Bikfaya) to 1600 m (Zaarour) above sea level characterized with a relatively cleaner air particularly at higher elevations. Tests were conducted under idle conditions (to assess self-pollution potential in a relatively pristine area (Bteghrine) away from traffic to exclude potential pollution effect from surrounding vehicles) and moving conditions (to assess in-vehicle pollution from surrounding traffic). For the latter, three trajectories were chosen based on vehicle speeds (Figure 1).

- Trajectory A: a 3.5 km closed circuit in a relatively well inhabited residential area (Bikfaya) with frequent traffic stops and an average speed of 40 km/h.
- Trajectory B: a 9.9 km sketched highway with less residents and traffic stops (between Bikfaya and Bteghrine) and an average speed of 60 km/h.
- Trajectory C: a 13.9 km along a road with low traffic (between Bteghrine to Zaarour) and an average speed of 80 km/h.



(a)Trajectory A: 3.5km *(b)Trajectory B: 9.9km* *(c)Trajectory C: 13.5km*

Figure 1 Location of field testing and trajectories

Concentrations of $PM_{2.5}$ were monitored using two Portable DustTrak analyzers (TSI Inc.) of type 8531. The precision of the analyzers was previously determined experimentally and shown to be 4% at roadsides (Abi-Esber *et al.*, 2013). They have an accuracy of 0.1% or 0.001mg/m3; but different studies reflected conflicting results on their tested accuracy (compared to gravitational methods) reporting an underestimation of 0.97 (Kim *et al.*, 2004) and overestimation by 2 (Chang *et al.*, 2001) and 2.8 (Levy *et al.*, 2002) at different locations. Even though no accuracy test has been done for on-road vehicles, these analyzers have been long used and relied upon in particulate measurements for these cases. They are factory calibrated and zeroed before each test (TSI, 2011). Two portable Langan CO analyzers of type L76n (Langan Products Inc.) were used to monitor in and out vehicle CO concentrations. The CO analyzers have a 40 sec response time with a maximum range of 200 ppm, a resolution of 0.1 ppm and accuracy between 0 and 3 ppm tested compared to a non-dispersive infrared spectrometry process (Chang *et al.*, 2001). A two point calibration process was applied prior to testing with zero and a 50 ppm gas span. In and out- vehicle concentrations were monitored at 1 min intervals. The in-vehicle CO and $PM_{2.5}$ analyzers were placed inside the cabin. The out-vehicle analyzers were also placed inside the cabin and linked to the outside air by a Telfon tube placed in the front right area of the car which is expected to result in the highest exposure (Abi-Esber *et al.*, 2013). During testing the window was slightly opened to allow the passage of the tube to capture out-vehicle air sampling; the window was tightly sealed with an adhesive tape to control infiltration (Figure 2).

Figure 2 Experimental setup

A total of 144 experiments were carried out (3 cars, 2 indicators, 3 ventilation modes, 4 speeds) which are presented in Table 1 with corresponding purposes. During all tests smoking was prohibited and each car had two occupants, a driver and a passenger to record the trip schedule.

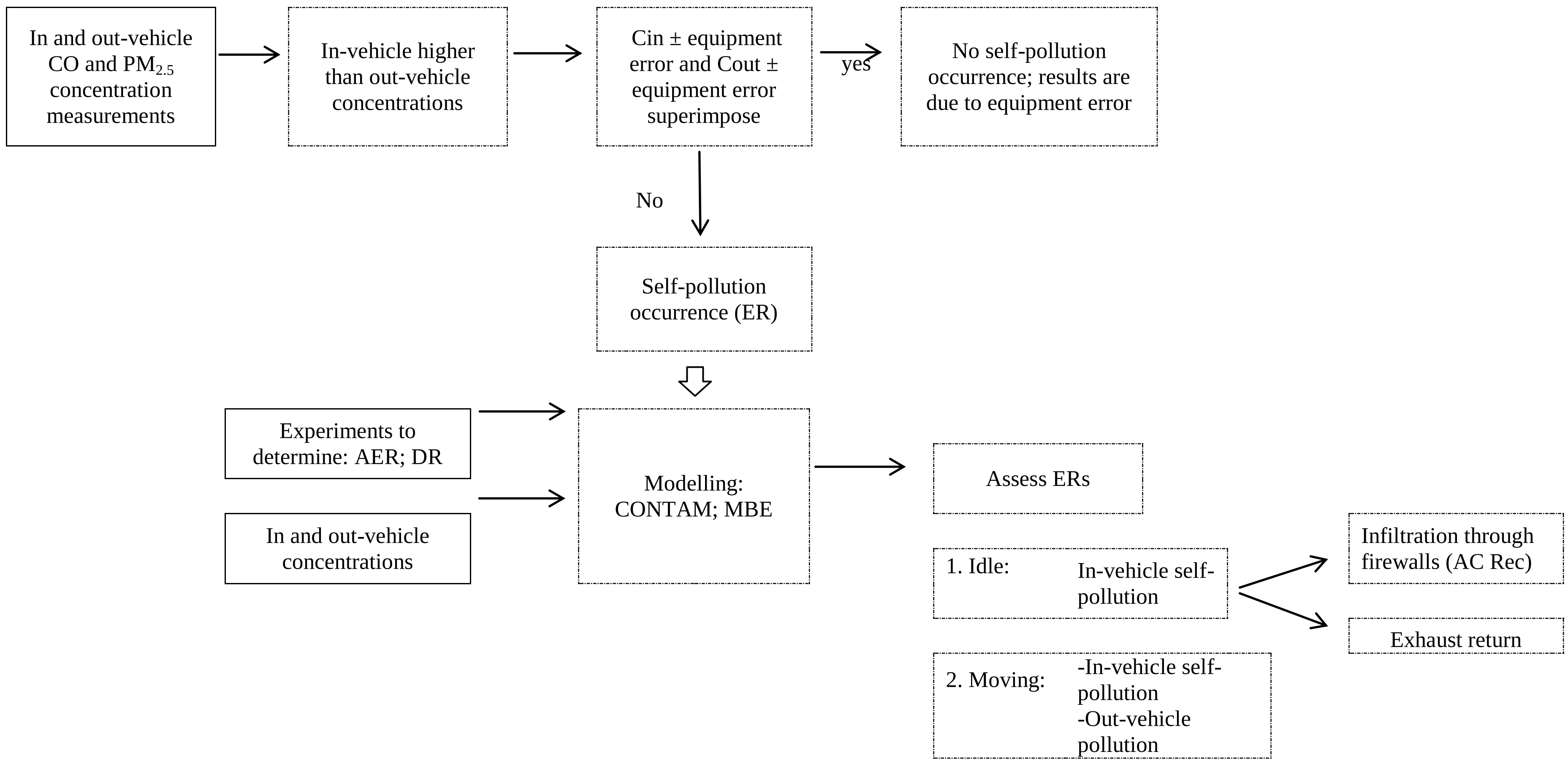


Figure 3 Summary of the overall experimental and modeling work

Table 1 Experimental and modeling program

Indicator	**Number of tests**	**[a]Car type**	**Model year**	**Engine**	**[b]Ventilation**	**Speed (km/h)**	**Location**	**Duration of test (min)**	**Purpose**	**Model**	**Number of simulations**
CO	36	P206	2006	65kW; 87hp	W1/2	0	Idle: Away from traffic	5 – 100	Determine the Air Exchange Rate (AER)		
		P307	2007	81kW; 108hp	AC FA	40	Moving: Rural roads				
		HV	2011	66kW; 89hp	AC Rec	60					
						80					
$PM_{2.5}$	36	P206	2006	65kW; 87hp	W1/2	0	Idle: Away from traffic	5 – 50	Determine the deposition rate of $PM_{2.5}$ (DR)		
		P307	2007	81kW; 108hp	AC FA	40	Moving: Rural roads				
		HV	2011	66kW; 89hp	AC Rec	60					
						80					
CO	72	P206	2006	65kW; 87hp	W1/2	0	Idle: Away from traffic	30	Assess equivalent Emission rates (ER)	MBE	72
$PM_{2.5}$		P307	2007	81kW; 108hp	AC FA	40	Moving: Rural roads			CONTAM	72
		HV	2011	66kW; 89hp	AC Rec	60					
						80					
Total tests	**144**									**Total simulations**	**144**

[a]P206: Peugeot 206; P307: Peugeot 307; HV: Hyundai Verna
[b]W1/2: Window half opened; AC FA: AC on fresh air mode; AC Rec: AC on recirculation mode

Trips of 20 - 30 min were conducted with continuous monitoring of in and out-vehicle CO and $PM_{2.5}$ concentrations under the same predefined conditions (vehicle, speed, ventilation mode and trajectories). Average pollutant in-vehicle concentrations were calculated and compared to the World Health Organization permissible exposure limit (8h guideline for CO, 9ppm and 24h guideline for $PM_{2.5}$, 25 µg/m3) (WHO, 2005). Field measurements coupled with mathematical modeling were used to assess potential self-pollution with corresponding equivalent in-vehicle source ERs. This process requires first the definition of physical parameters like the AERs and $PM_{2.5}$ DRs.

A. Estimation of the Air Exchange Rate (AER)

A tailored set of tests were conducted to estimate the Air Exchange Rate (AER) for each vehicle under each ventilation and speed condition. During this set of experiments, a high initial CO source was introduced by burning charcoal until reaching an in-vehicle CO concentration between 60 and 100 ppm. During this process, the cabin air was mixed using a fan while the charcoal was still burning to ensure well mixed conditions inside the entire cabin. The charcoal was extinguished and the measurements were initiated at 1 minute intervals, until equilibrium is reached between in and out-vehicle levels. The AER was then estimated using Equations 1 to 3 (He *et al.* 2005; Calver *et al.* 2005).

$$\frac{dC}{dt} = AER\ C_O + \frac{S}{V} - (AER + k)\ C \qquad (1)$$

$$AER = \frac{\ln(C_O - C_{O_0}) - \ln(C - C_o)}{t - t_0} \qquad \text{When } S = 0 \text{ (charcoal extinguished)} \qquad (2)$$

$$C = C_0\ e^{-AER\ t} \qquad \text{When } C >> C_O \qquad (3)$$

Where AER Air Exchange Rate, h^{-1}

C In-vehicle concentration at time t, mg/m^3

C_O Out-vehicle concentration at time t, mg/m^3

S Source generation rate, mg/h

V Volume of the cabin, m^3

k Deposition or decay rate, h^{-1} (in the case of CO, k=0 and decay rate=0 due to the short duration of the experiment in comparison to the half-life of CO in the air)

C_0 In-vehicle concentration at time 0, mg/m^3

C_{O0} Out-vehicle concentration at time 0, mg/m^3

B. Estimation of the $PM_{2.5}$ deposition rate (DR)

Similarly, another tailored set of tests was conducted to estimate the $PM_{2.5}$ deposition rate (DR). A $PM_{2.5}$ source was introduced using tobacco smoke until a high in-cabin concentration is reached, between 9 and 35 mg/m^3. A fan was also used to ensure well mixed conditions before turning off the cigarettes and starting the measurements at 1 minute interval until equilibrium is reached between in and out-vehicle levels. In-vehicle $PM_{2.5}$ concentrations can be estimated using Equations 4 and 5 (Chen *et al.*, 2000; He *et al.*, 2005) where P is the filter penetration factor (= 1 since all filters were removed from the vehicles and the relatively high in-vehicle $PM_{2.5}$ concentration compared to the ambient air). All other parameters are as defined above.

$$\frac{dC}{dt} = P\, AER\, C_O + \frac{S}{V} - (AER + k)\, C \qquad (4)$$

$$C = C_0\, e^{-(AER+k)\,t} \qquad \text{When } S = 0 \text{ (Cigarettes turned off) and } C >> C_O \qquad (5)$$

2.2. In-vehile Air Quality Simulations and ER Estimation

In-vehile Air Quality simulations fall into two categories namely zonal (microscopic view) and multi-zonal (macroscopic view). Zonal modeling relies on Computational Fluid Dynamics (CFD) whereas multi-zonal modeling, a less complex technique, does not consider spatial variation and assess average volume concentration (Emmerich, 2001). Multi-zone simulations are generally faster and hold wider assumptions than the CFDs but can be equally accurate for small volumes, which is the case for in-vehicle cabins thus justifying their usage in this study. A general mass balance (Equations 6 to 9) was first used to simulate various scenarios (Figure 4) followed by the application of the multi-zone model CONTAM (Equation 10) developed by the National Institute of Standards and Technology (NIST) for contaminant and airflow analysis (Walton *et al.*, 2013). The two approaches were adopted for cross validation in assessing potential self-pollution and in-vehicle exposure with simulations using a 1 minute time step which is consistent with field measurements. The simulations were compared to the actual data using the Root Mean Squared Error (RMSE). RMSE values between 0 and 1/2 a standard deviation of the measured data were deemed acceptable. For both models, the ultimate objective was to estimate the temporal variation of the contaminant source in the vehicles and equivalent Emission Rates (ERs) for self-pollution potential.

$$\frac{dC}{dT} = (AER_{inf} + AER_{w})\,C_O - (AER_{inf} + AER_{w})\,C + S - R \quad (6)$$

$$\frac{dC}{dT} = (AER_{inf} + (1-\eta)\,AER_{hvac})\,C_O - (AER_{inf} + AER_{hvac})\,C + S - R \quad (7)$$

$$\frac{dC}{dT} = (AER_{inf})\,C_O - (AER_{inf} + \eta\,AER_{hvac})\,C + S - R \quad (8)$$

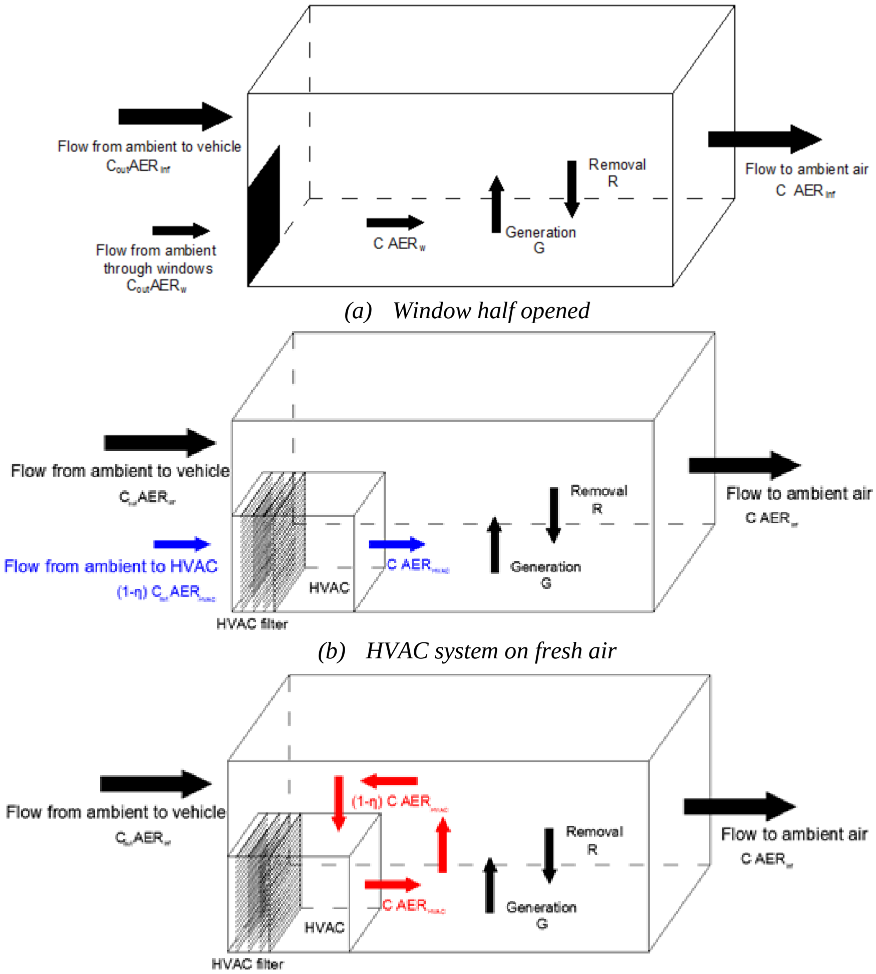
$$\frac{dC}{dT} = AER\,C_O - AER\,C + S \qquad \text{When } \eta = 0 \quad (9)$$

$$\rho_i V_i C_{i\,(t+\Delta t)} = \rho_i V_i C_{i(t)} + \Delta t\left[\textstyle\sum_j F_{j\to i}(1-\eta_j)C_j - \sum_i F_{i\to j}C_i + m_i k C_i + G_i - R_i C_i\right]_{(t+\Delta t)} \quad (10)$$

C	In-vehicle concentration, mg/m^3
AER_{inf}	Air exchange rate from infiltration, h^{-1}
AER_w	Air exchange rate through windows, h^{-1}
AER_{hvac}	Air exchange rate from HVAC, h^{-1}
η	Filter efficiency
i,j	Control volume i and j
ρ_i	Density of air in i, kg/m^3
V_i	Volume of air in i, m^3
C_i	Concentration of species in i, kg/kg
$F_{j\text{->}i}$	Rate of air mass flow from j to i, kg/h
η_j	Filter efficiency
m_i	Mass of air in i, kg
K	Kinetic reaction coefficient between, h^{-1}

G_i Generation rate of species, kg/h

R_i Removal rate of species, kg/h



(a) Window half opened

(b) HVAC system on fresh air

(c) HVAC system on recirculation

Figure 4 Representation of simulated Mass balance scenarios

CHAPTER 3 RESULTS AND DISCUSSIONS

3.1. Field Experimental Program

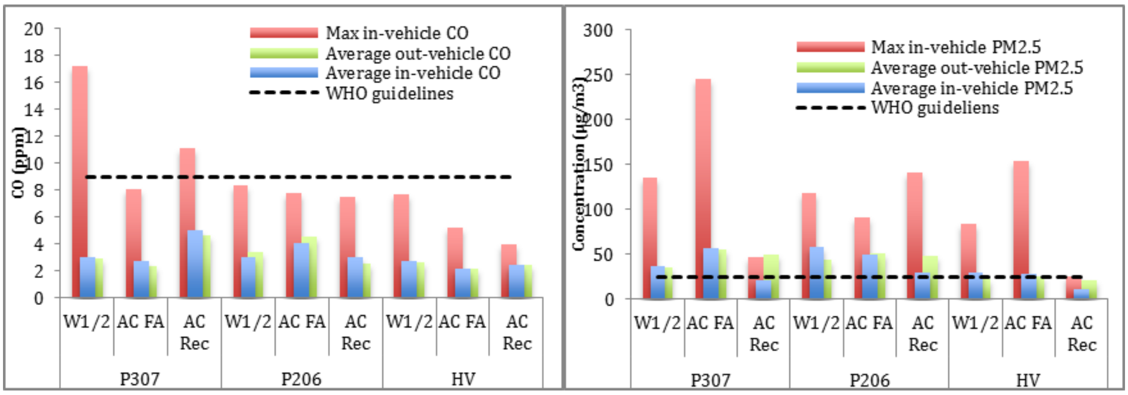
Observed sources of ambient CO and $PM_{2.5}$ concentrations included mainly traffic and quarry emissions in the general area with minor effect contribution expected from tire and breaks (Keuken *et al.*, 2013). Field testing results are summarized in Table 2 showing the minimum, maximum and mean CO and $PM_{2.5}$ out- and in-vehicle concentrations for all vehicle types under various ventilation modes and speeds. Detailed minute to minute results are presented in Figures B-3.1 – B-3.2 (Appendix B.3).

Table 2 Measured in and out-vehicle CO and $PM_{2.5}$ concentrations

	[a]Vehicle-[b]Ventilation	In-vehicle concentration			Out-vehicle concentration		
		Min	**Max**	**Mean**	**Min**	**Max**	**Mean**
CO (ppm)	**P307-W1/2**	1.19	17.24	2.99	1.2	10.4	2.95
	P307-AC FA	1.43	8.03	2.72	1.2	10.9	2.37
	P307-AC Rec	1.92	11.14	4.16	1.1	49.8	4.68
	P206-W1/2	1.19	8.33	2.9	1.7	12.9	3.39
	P206-AC FA	2.47	7.78	4.04	1.6	43	4.52
	P206-AC Rec	1.13	7.48	2.08	1.5	11	2.52
	HV-W1/2	1.01	7.66	2.39	1	9.1	2.63
	HV-AC FA	1	5.22	1.84	1	8.3	2.13
	HV-AC Rec	1.13	3.94	2.08	1	15.1	2.44
$PM_{2.5}$ (µg/m3)	**P307-W1/2**	1	136	33	12	105	36
	P307-AC FA	7	245	46	16	396	56
	P307-AC Rec	2	47	22	15	247	50
	P206-W1/2	43	118	58	30	131	44
	P206-AC FA	19	92	50	16	95	51
	P206-AC Rec	12	142	30	15	500	49
	HV-W1/2	20	84	30	14	81	23
	HV-AC FA	14	154	28	12	119	26
	HV-AC Rec	7	25	11	14	199	22

[a] P307: Peugeot 307; P206: Peugeot 206; HV: Hyundai Verna;
[b]W1/2: Window half opened; AC FA: AC on fresh air mode; AC Rec: AC on recirculation mode

During the entire testing program, CO measurements fluctuated between 1 and 49.8 ppm for out-vehicle concentrations and between 1 and 17.2 ppm for in-vehicle measurements. With the exception of a few peaks, average in-vehicle CO concentrations did not exceed the 8h air quality guideline of the WHO or 9 ppm (WHO, 2005) reflecting the low traffic conditions along the test routes. In contrast, the average in-vehicle $PM_{2.5}$ concentrations exceeded often the 24 h WHO exposure limits of 25 μg/m^3 (WHO, 2005) with a variation pattern ranging between 1 and 245 μg/m^3 for in-vehicle conditions (Figure 5) and between 12 and 500 μg/m^3 for out-vehicle conditions which can be attributed to the impact of quarries in the general area.



(a) CO concentrations *(b) $PM_{2.5}$ concentrations*

Figure 5 In and out-vehicle CO and $PM_{2.5}$ concentrations

The profiles of in and out-vehicle concentrations under the window half opened mode exhibited similar fluctuations (84.05%) for all tested vehicles at various speeds with decreasing correspondence when shifting to AC on fresh air (66%) and AC on recirculation mode (55%). This can be attributed to the air exchange rate that stabilizes in and out-vehicle concentrations and helps in reaching a quasi-steady state between the two environments. Average in-vehicle concentrations are mostly higher than ambient air levels which would normally indicate the existence of an in-vehicle source or a self-pollution potential after accounting for the accuracy of the monitoring equipment.

A. Estimation of the Air Exchange Rate (AER)

Temporal measurements of in and out-vehicle CO concentrations in the three testing vehicles under variable speeds and ventilation modes (see Appendix B.2) were used to estimate the AER (Equations 1 to 3). The AERs tended to increase with vehicle age and speed and ventilation type (Table 3). The corresponding AERs ranged between 15.6 – 112.2h^{-1}, 29.4 – 72.9h^{-1}, and 1.8 – 18h^{-1} under W1/2 (window half opened); AC FA (AC on fresh air); and AC Rec (AC on recirculation), respectively. While no values for AER were reported in the literature at speeds exceeding 40 km/hr, a range from 1.6 to 120 h^{-1} was reported for various ventilation modes at a speed of 32 km/hr (Table 2).

Table 3 Estimated AER under variable speed and ventilation modes

[a]Ventilation	Speed (km/h)	Hyundai Verna	Peugeot 307	Peugeot 206	Literature reported ranges	Source
W1/2	**0**	16.8	21	15.6	13.3-13.7	Park et al. (1998)
	32	-	-	-	120	Ott et al. (1992)
	32	-	-	-	12	Park et al. (1998)
	32	-	-	-	28.9-30.8	Ott et al. (2007)
	40	55.2	51.6	37.2	-	-
	60	88.8	85.8	52.8	-	-
	80	112.2	102	109.2	-	-
AC FA	**0**	29.4	31.8	48	36	Hayes, 1989
	0	-	-	-	36.2-47.5	Park et al. (1998)
	40	35.4	33	67.2	-	-
	60	41.4	39	72	-	-
	80	49.2	35.4	72.6	-	-
AC Rec	**0**	7.2	10.8	1.8	1.96-3.23	Engelmann et al. (1992)
	0	-	-	-	1.8-3.7	Park et al. (1998)
	0	-	-	-	0.92	Ott et al. (2007)
	32	-	-	-	1.6-2.4	Ott et al. (2007)
	40	9.6	10.8	15	-	-
	60	9.6	10.8	15	-	-
	80	10.8	17.4	18	-	-

[a]W1/2: Window half opened; AC FA: AC on fresh air mode; AC Rec: AC on recirculation mode

B. Estimation of the $PM_{2.5}$ deposition rate (DR)

Similarly measurements of in and out-vehicle $PM_{2.5}$ concentrations were collected for the different vehicles, speeds and ventilation conditions (see Appendix B.2) and used to estimate the $PM_{2.5}$ DR (Equations 4 and 5). The results changed noticeably with speed and ventilation conditions (Table 4) with corresponding values ranging between 0.6 – 9.6 h^{-1}, 0.6 – 12.6 h^{-1} and 0.6 – 12.6 h^{-1} under W1/2, AC FA and AC Rec, respectively.

Table 4 $PM_{2.5}$ deposition rate under variable speed and ventilation modes

[a]Ventilation	Speed (km/h)	Hyundai Verna	Peugeot 307	Peugeot 206
W1/2	**0**	9.6	3.0	5.4
	40	3	2.4	4.2
	60	1.2	4.2	1.2
	80	0.6	4.2	0.6
AC FA	**0**	12.6	8.4	6.6
	40	9.6	6.6	3.6
	60	0.6	2.4	2.4
	80	0.6	0.6	0.6
AC Rec	**0**	12	12.6	8.4
	40	6.6	7.2	4.8
	60	7.8	3.6	2.4
	80	7.2	2.4	0.6

[a] W1/2: Window half opened; AC FA: AC on fresh air mode; AC Rec: AC on recirculation mode

3.2. In-vehicle Air Quality Simulations and ER Estimations

Simulated results for all vehicles under various ventilation modes and speed conditions during moving tests are illustrated in Figure 6 with additional details presented in Figures B-3.3 – B-3.4 (Appendix B.3). While the models captured the main patterns of the data variations, a tendency of slight under-prediction (2% for CONTAM and 5% for MBE) of measured concentrations can be discerned. Similarly, $PM_{2.5}$ concentrations were underestimated by ~15% in CONTAM and 19% using the MBE. This negative bias can be attributed to potential in-vehicle sources. Taking into account the accuracy of monitoring equipment, between 89 and 100% of the cases confirm the existence of a source element.

Equivalent emission rates (ER) to improve the match between measured in-vehicle concentrations with simulated results ranged from 0 to 1842 mg/h for CO and 0 to 20 mg/h for $PM_{2.5}$ (refer to Appendix B.4 for more details). Near zero values are indicative of no sources/self pollution potential or sources below the detection limit of the analyzers.

An average of 1 minute time shift was observed between in and out-vehicle measurements. Thus by examining the ERs while taking into account this shift in time, the results obtained still revealed the presence of an in-vehicle source of pollution. The change of ERs fluctuated between a 4% decrease and a 27% increase. Therefore the observed ERs are not an artifact of the time shift.

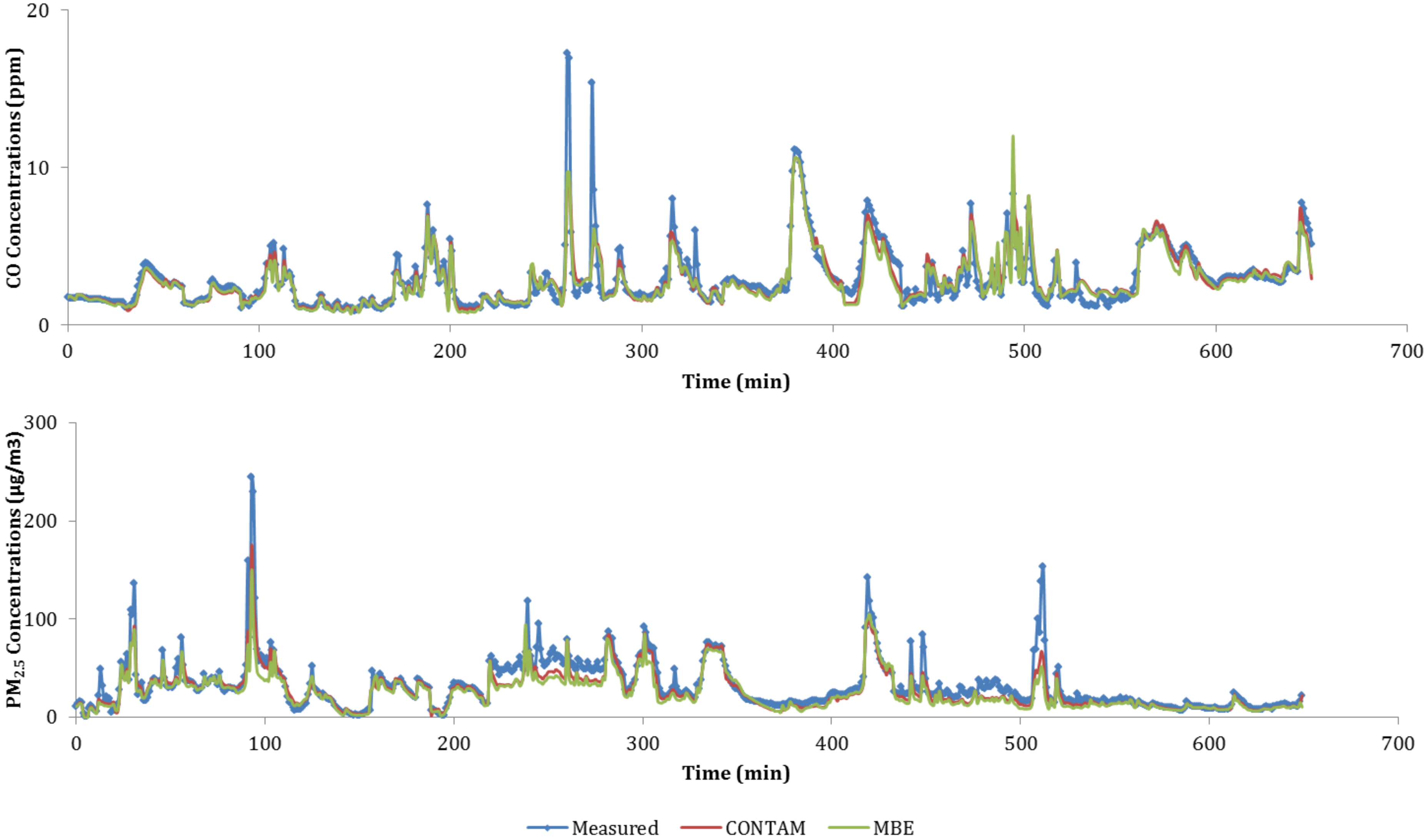


Figure 6 Measured and simulated in-vehicle CO and $PM_{2.5}$ concentrations (Detailed in Appendix B.3)

A stepwise regression analysis was applied on the significant ERs (non-zero) to track changes with vehicle type, speed, and ventilation mode. The resulting model (Equation 11) was considered with no interactions between variables since a vif test reported values close to unity showing no co-linearity.

$$\text{Log(ER)} = 2.1 + 0.85\ \text{P206} + 0.76\ \text{P307} - 0.38\ \text{REC} + 0.45\ \text{W1/2} + 0.01\ \text{Speed} + \varepsilon \qquad (11)$$

Where ER is the source Emission Rate, P206: Peugeot 206, P307: Peugeot 307, REC: AC on recirculation mode and W1/2: Window half-opened.

The model is significant with low p-values (< 2.2e-16) and an R-squared indicating that 22% of the source variability can be explained by the models. The low R-squared value is due to the existence of other parameters affecting the ERs that were not considered in this study like weather and traffic conditions. The model show an increase in the ERs from AC on recirculation to AC on Fresh air to window half opened. The rate of source increase is 1% with speed irrespective of the car and ventilation mode (i.e. an increase of 10km/h increases the source ERs by 10%). Older vehicles were equally associated with an increase in ER values with the highest ERs recorded for the Peugeot 206 (model year 2006) followed by the Peugeot 307 (model year 2007), and then the Hyundai Verna (model year 2011).

Similarly, a linear regression model was developed on the significant $PM_{2.5}$ Emission Rates (p-value< 2.2e-16; R-squared: 0.34) to assess their change with vehicle type, speed, and ventilation mode (Equation 12). The vif test returned values close to unity indicating no co-linearity between the different parameters.

$$\text{Log(ER)} = -1.82 + 0.197\ \text{HV} + 0.189\ \text{P206} + 1.05\ \text{FA} + 1.6\ \text{W1/2} + 0.006\ \text{Speed} + \varepsilon \qquad (12)$$

Where ER is the source Emission Rate, HV: Hyundai Verna, P206: Peugeot 206, FA: AC on fresh air mode and W1/2: Window half-opened.

The $PM_{2.5}$ ERs for the three vehicles increased from AC on recirculation to AC on fresh air to window half opened. While a 10 km/h increase in speed depicted a 6% increase in ERs, but the effect vehicle age was not as clear as in the case of CO. Instead, $PM_{2.5}$ ERs increased from the Peugeot 307 (model 2007) to Hyundai Verna (model 2011) and the Peugeot 206 (model 2006) at approximately the same rate. This may be attributed to the engine power of the vehicles since the two similar ERs correspond to the Hyundai Verna (66kW; 89hp) and Peugeot 206 (65kW; 87hp) with similar engine power. The Peugeot 307 has a higher engine power (81kW; 108hp). In this case, a conclusion about engine power and self-pollution cannot be ascertained due to the limited number of vehicles tested.

In-vehicle self-pollution rates are reported by the best fitted and average source ERs (Table 5). The best fitted source emission rates do not match the average rate due to the high temporal fluctuations in the ERs, but they both change similarly with speed and ventilation conditions. A 41 and 82% improvement could be accomplished by adding respectively the average and best fitted source emission rates (Figure 7).

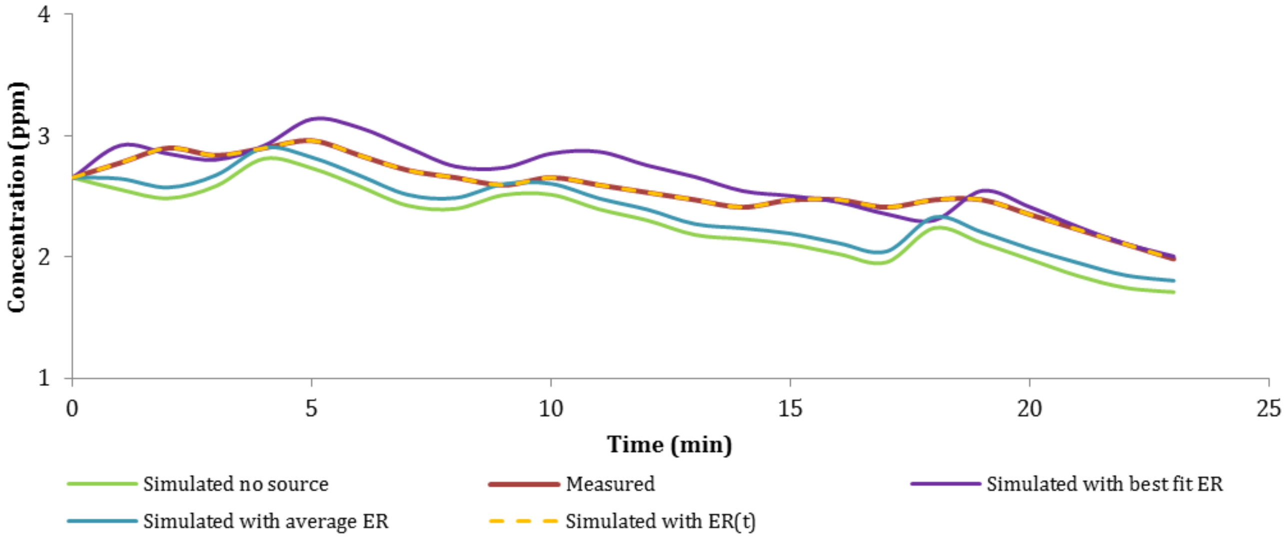


Figure 7 In-vehicle concentration improvement after adding source ERs (Peugeot 307- Rec- 40 km/h)

Table 5 Average and best fitted Source emission rates

Car Type	[a]Ventilation-Speed	CO source			$PM_{2.5}$ source		
		Best fitted ER (mg/h)	Average of ER(t) (mg/h)	Average of ER(t) (mg/h)	Best fitted ER (mg/h)	Average of ER(t) (mg/h)	Average of ER(t) (mg/h)
		MBE	MBE	CONTAM	MBE	MBE	CONTAM
Peugeot 307	W1/2-0	2.24	4.23	3.71	0.18	0.16	0.19
	W1/2-40	4.24	6.19	5.61	0.22	0.55	0.43
	W1/2-60	4.48	7.19	8.55	0.08	2.09	1.89
	W1/2-80	307.76	238.29	234.5	0.22	1.13	0.71
	AC FA-0	12.43	13.49	15.71	0.04	0.04	0.04
	AC FA-40	17.95	19.56	21.20	0.11	0.11	0.09
	AC FA-60	50.99	38.88	42.73	0.22	2.44	1.91
	AC FA-80	43.29	46.95	47.68	0.2	0.21	0.13
	AC Rec-0	2.21	7.21	8.01	0.04	0.01	0.01
	AC Rec-40	49.85	14.50	15.90	0.04	0.07	0.06
	AC Rec-60	17.92	26.72	25.20	0.22	0.27	0.27
	AC Rec-80	22.40	44.91	45.56	0.18	0.20	0.19
Peugeot 206	W1/2-0	8.60	9.99	7.52	1.11	1.12	1.27
	W1/2-40	11.54	12.55	12.69	1.52	1.79	1.59
	W1/2-60	15.67	17.53	16.57	2.40	1.49	1.63
	W1/2-80	66.40	38.57	44.68	3.61	2.06	1.76
	AC FA-0	9.34	10.95	9.00	0.40	0.55	0.29
	AC FA-40	9.10	10.46	8.15	0.48	0.67	0.28
	AC FA-60	7.02	15.45	15.15	1.96	1.31	1.03
	AC FA-80	26.42	20.45	20.21	0.20	0.35	0.29
	AC Rec-0	6.44	7.58	7.54	0.17	0.19	0.12
	AC Rec-40	16.46	10.00	10.70	0.01	0.01	0.01
	AC Rec-60	14.90	9.99	8.46	0.1	0.13	0.12
	AC Rec-80	16.74	22.42	19.37	0.6	0.93	0.56
Hyundai Verna	W1/2-0	7.65	8.67	8.31	1.28	1.29	1.74
	W1/2-40	8.25	14.95	9.24	1.28	1.63	1.63
	W1/2-60	35.86	28.61	22.22	1.95	1.20	1.02
	W1/2-80	45.89	33.36	22.34	3.91	2.03	1.68
	AC FA-0	7.65	8.68	9.29	1.93	2.01	1.73
	AC FA-40	20.85	16.77	17.93	2.74	2.50	1.82
	AC FA-60	3.83	3.67	2.86	0.69	0.68	0.54
	AC FA-80	5.26	3.07	3.27	0.46	0.49	0.34
	AC Rec-0	2.55	3.57	3.75	1.28	0.12	0.07
	AC Rec-40	5.10	5.03	4.22	1.28	0.06	0.03
	AC Rec-60	4.26	6.54	5.51	0.26	0.11	0.07
	AC Rec-80	5.61	6.39	5.35	0.13	0.39	0.22

[a] W1/2: Window half opened; AC FA: AC on fresh air mode; AC Rec: AC on recirculation mode

3.3. Models Comparison and Assessment

Both modeling approaches (MBE and CONTAM) simulated well the measured data albeit minor differences between them that were assessed using the RMSE comparison between the measured and simulated data. The RMSEs illustrate the similarity between the two models $RMSE_{CONTAM}$ = 0.860; $RMSE_{MBE}$ = 0.862. The minor difference can be attributed to additional terms included in CONTAM but not the MBE such as in- and out-vehicle temperature. The mass balance in MBE and CONTAM (Equations 9 and 10) can be simplified to Equations (13) and (14), respectively.

$$V\frac{dC}{dt} = QC_0 - QC + ER \qquad (13)$$

$$\rho_{in} V\frac{dC}{dt}(m) = Q(m)C_0(m) - Q(m)C(m) + ER \qquad (14)$$

Where ρ_{in} is the in-vehicle air density (kg/m^3), Q(m) the mass flow (kg/h) and C(m) the mass concentration of contaminant (kg/kg air).

The concentrations (C) are expressed in mg/m^3 and the air flow as a volumetric flow (Q) expressed in m^3/h. The two equations are matched by transforming the flows and concentrations to the same units through the density of in- and out-vehicle air. Note that CONTAM uses a constant mass flow between ambient and in-cabin conditions, using the ambient air density for the flow conversion. Additionally, it uses in-vehicle air density for the conversion of concentrations. Therefore $C(m) = \frac{1}{\rho_{in}} C$ and $Q(m) = \rho_{out} Q$. Consequently the source ERs of MBE and CONTAM can be compared using equations (15) and (16).

$$ER_{MBE} = V\frac{dC}{dt} - QC_0 + QC \qquad (15)$$

$$ER_{CONTAM} = V\frac{dC}{dt} - \rho_{out} Q\frac{1}{\rho_{in}} C_0 + \rho_{out} Q\frac{1}{\rho_{in}} C \qquad (16)$$

Flow and concentration adjustments can be carried out between the two approaches reducing the differences by approximately 96%. Figure 8 shows a typical result after flow and concentration adjustments. Consequently a simple mass balance equation can be used for in-vehicle air quality simulations without having to rely on more advanced models such as CONTAM.

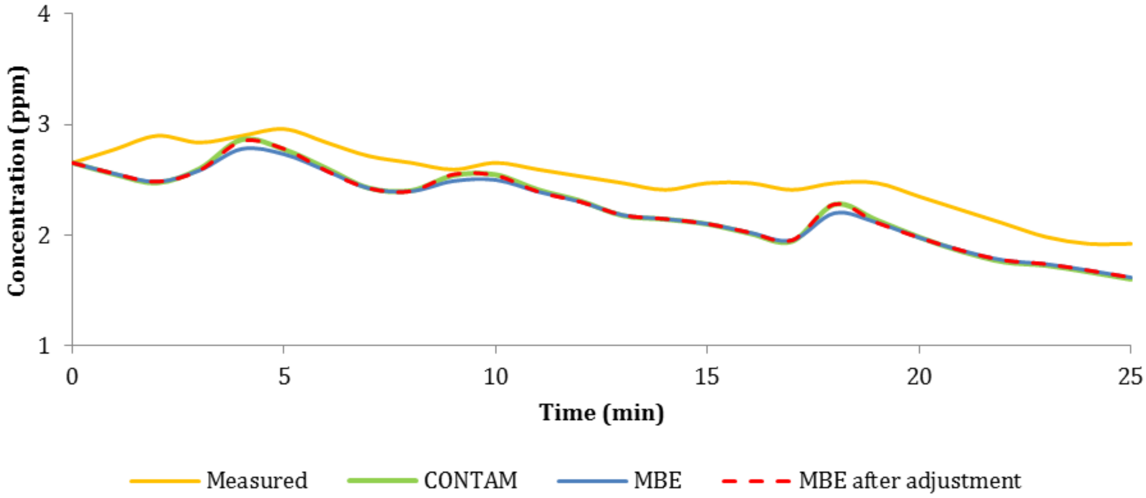


Figure 8 Change in CO concentration after adjustment (Peugeot 307- Rec- 40 km/h)

3.4. Idle tests: Validation of Self pollution

Previous studies (Abi-Esber el al., 2013; Delfino *et al.*, 2012) have observed in-vehicle self-pollution in urban areas but with a lack of certain physical parameters (AER, DR) that are essential for the validation of self-pollution results. In this study self-pollution was assessed in a rural area and relying on real time determination of the AERs and DRs. It should be noted that tests in rural areas reduce the effect of ambient pollution on the ERs results. Tests under idle conditions highlight the effect of in-vehicle self-pollution potential particularly from infiltration through firewalls under AC on recirculation mode. Under this type of ventilation, the inside air is presumably isolated from the outdoor environment corresponding to a state of closure of all possible inlets between the inside and the ambient air. As for AC on fresh air and window half opened ventilation modes, equivalent in-vehicle emission rates represent the sum of the exhaust return and infiltration through firewalls. Naturally, the difference between the two AC modes represents the infiltration associated with the exhaust return (assuming a constant infiltration rate through firewalls which is reasonable given that the overall intrusion into the passenger's compartment increases from AC on recirculation to AC on fresh air intake to widow half-opened).

While assuming a zero fresh air intake (zero exhaust return) under AC on recirculation mode, the ERs obtained under idle conditions would represent the maximum infiltration through firewalls. And since some system may provide up to 20% fresh air intake when the AC is on recirculation mode (Ausgabe, 2006), an upper and lower limit for each case of self-pollution could be set.

Table 6 In-vehicle self-pollution obtained from ERs under idle conditions

[a]Car type /Contaminant		ER from infiltration through firewalls (mg/h)	Total ER from the vehicle itself (mg/h)	ER exhaust return (total ER - ER infiltration through firewalls) (mg/h)
P307	CO	6.40-8.01	15.71	7.7-9.3
	$PM_{2.5}$	0.008-0.010	0.04	0.03-0.032
P206	CO	6.03-7.54	9.00	1.460-2.968
	$PM_{2.5}$	0.096-0.120	0.29	0.170-0.194
HV	CO	3.00-3.75	9.29	5.54-6.29
	$PM_{2.5}$	0.056-0.070	1.73	1.660-1.674

[a] P307: Peugeot 307; P206: Peugeot 206; HV: Hyundai Verna

CHAPTER 4 CONCLUSION

This study confirms the occurrence of in-vehicle self-pollution, which is affected mostly by ventilation and speed conditions. The equivalent in-vehicle emission rates (ERs) of CO and $PM_{2.5}$ varied consistently with speed and ventilation conditions. They decreased from window half opened, to AC on fresh air, to AC on recirculation mode, and increased with speed. Additionally the vehicle age exhibited a correlation with CO ERs, whereby a noticeable increase was recorded with age. In contrast, $PM_{2.5}$ ERs were possibly more affected by the power of the engine. These observations can be generalized by increasing the sample size tested with emphasis the effect of car make, engine power and age. The Inter-model validation applied between CONTAM and the MBE revealed high correspondence between the two, emphasizing the adequacy of using the simple mass balance model to represent the in-vehicle compartment.

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APPENDIX A SUPPLEMENTARY MATERIAL

A.1. CONTAM model description

CONTAM simulates the microenvironment on a macroscopic scale considering each zone as well mixed. It generates a set of nodal equations for the different zones that are subjected to numerical analysis for accomplishing the simulations. Simulations can be conducted under steady, transient or cyclical states. It has mainly been used for building ventilation and smoke management analyses, and assessing occupant exposure to indoor contaminants (Walton *et al.*, 2013). Zone properties, contaminant characteristics, weather and ambient concentration records along with airflow data, contaminants removal and generation are used to determine indoor contaminant concentrations, flows and relative pressure.

The vehicle is considered as one single node with uniform temperature and contaminant concentration. Contaminant properties ranging from molecular weight to particulate mean diameter were introduced in the model. The average zone and ambient temperature ranges respectively between 19-27^{0}C, and 16-31^{0}C. The barometric pressure is directly calculated by CONTAMW after introducing the average elevation of each trajectory.

Airflow paths are the components that connect two zones or a zone to the ambient environment. These features can be cracks, openings like windows and doors, fans, etc. Airflow paths and their properties should be included in the fan system and their function, as constant mass or volume flow (Walton *et al.*, 2013).The AER rate previously determined is introduced in CONTAM under a constant volume flow path and the $PM_{2.5}$ deposition rate is represented by a deposition sink model.

A.2. Analysis of the AER and the $PM_{2.5}$ DR

A. Estimation of the Air Exchange Rate (AER)

Temporal in and out-vehicle CO concentrations were measured during the tests and used to estimate the AER for each car under the different speed and ventilation conditions. The AERs increased invariably with speed, car age (Hyundai Verna: 2011; Peugeot 307: 2007 Peugeot 206: 2006), and across the different ventilation modes (from AC on recirculation to AC on fresh air to window half opened) (Figure A-2.1). For these ventilation modes, the CO concentrations initially introduced were flushed out relatively quickly within minutes (5-30 min) in comparison to more than 100 minutes when the AC is on recirculation mode (30-100 min) (Figure A-2.2). This can be attributed to flow dynamics that produce large differences in pressure around the vehicle with higher speed (turbulence) causing in and out-vehicle conditions to reach faster equilibrium particularly under window half opened. In all cases, an exponential decay pattern (Figure A-2.2) can be discerned across all vehicles, ventilation and speed conditions. A Kruskal Wallis test resulted in low p-values (1.47e-12, 2.19e-12, 1.47e-12) confirming the significant effect of ventilation, vehicle speed and age respectively on the AER.

A previous study has proposed statistical models for the AERs estimation under AC on fresh air and recirculation modes (Hudda *et al.*, 2011). The following models applied to the considered cars and different conditions of this study indicate high difference in the AER results therefore these models are case specific.

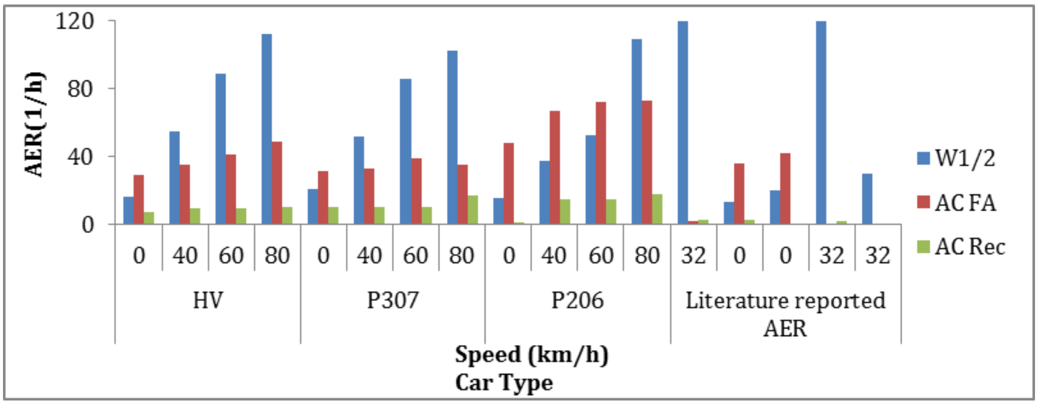
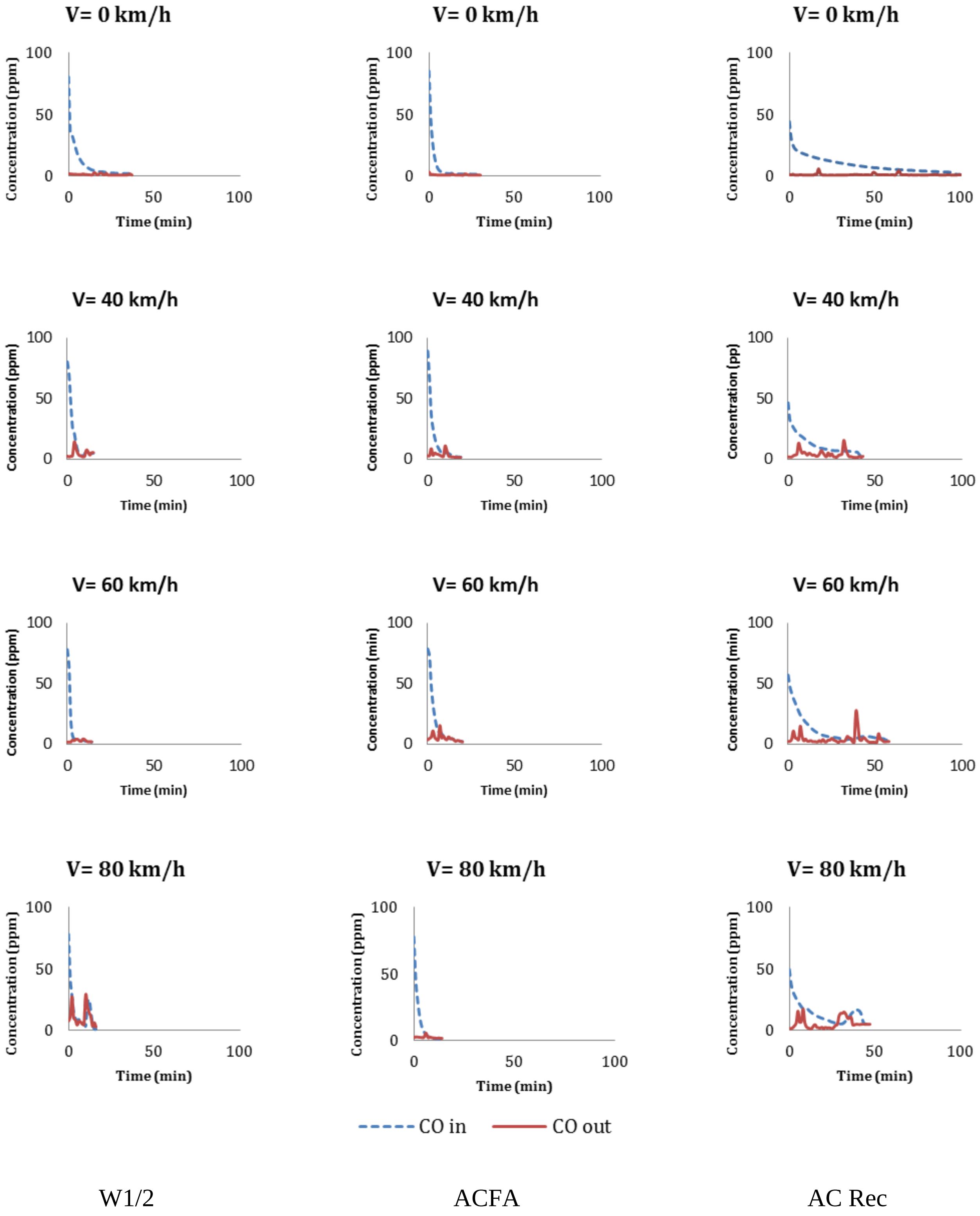
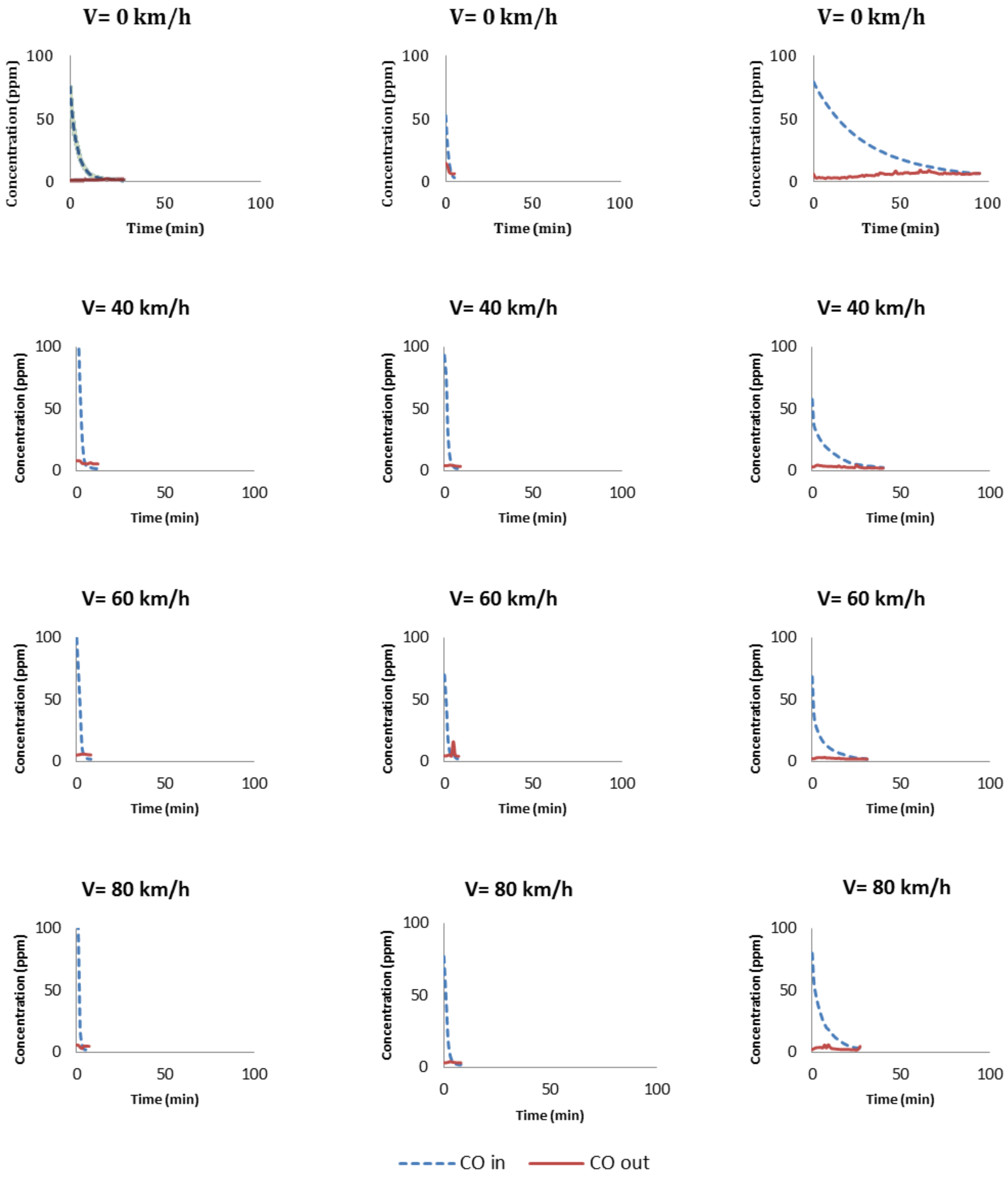


Figure A-2.1 AER results compared to the Literature reported values

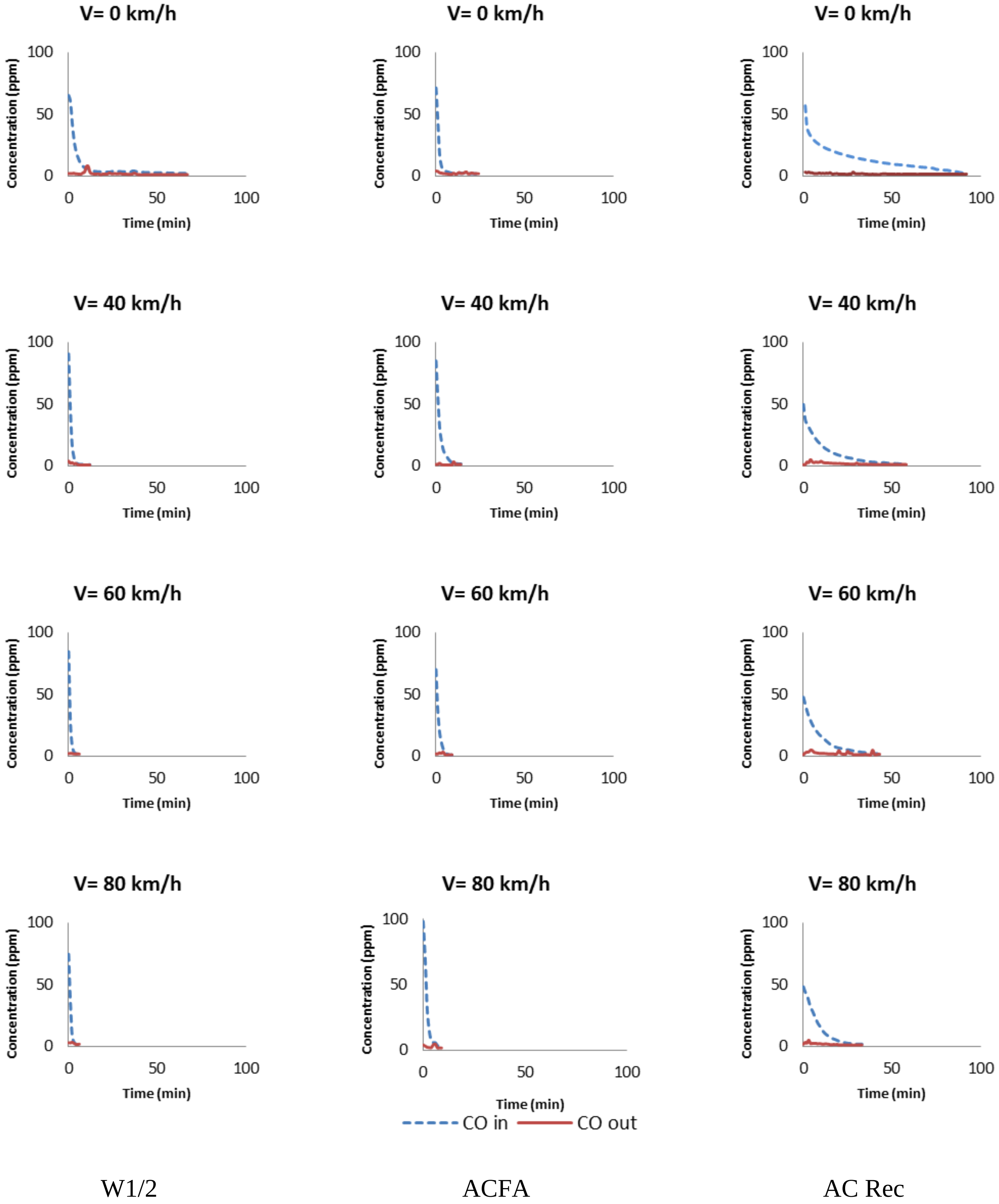


(a) Peugeot 307 CO concentrations



W1/2 ACFA AC Rec

(b) Peugeot 206 CO concentrations



(c) Hyundai Verna CO concentrations
Figure A-2.2 In and Out-Vehicle CO concentrations

B. Estimation of the $PM_{2.5}$ deposition rate (DR)

The measurements of in and out-vehicle $PM_{2.5}$ concentrations were used to estimate the $PM_{2.5}$ DR. The resultant DRs tend to increase with speed decrease and have the highest values under AC on recirculation mode compared respectively to AC on fresh air and window half opened (Figure A-2.3). The $PM_{2.5}$ concentrations initially introduced were flushed out within few minutes (5-20 min) under window half opened and AC on fresh air mode and taking more time under AC on recirculation (20-50 min) (Figure A-2.4). This can be attributed to the AER that increase the DRs for lower AERs. An exponential decay pattern is noticed across all vehicles under all ventilation and speed conditions. A Kruskal Wallis test returned low p-values (0.019, 0.0017, 0.0017) considering the effect of each parameter alone confirming the hypothesis that the deposition rate significantly change with, speed, ventilation and car type respectively. A moderately strong correlation between the AER and DRs (55%) was found. This relation is not consistent between different studies; some reported a negative correlation, some reported a positive correlation while others revealed no effect of the AER on the DRs (Wan-Chen *et al.*, 2014; Kanaani *et al.*, 2008; He *et al.*, 2005; Gong *et al.*, 2009). This strong correlation may be an artifact of the fitting process since the DR was obtained based on the estimated AER.

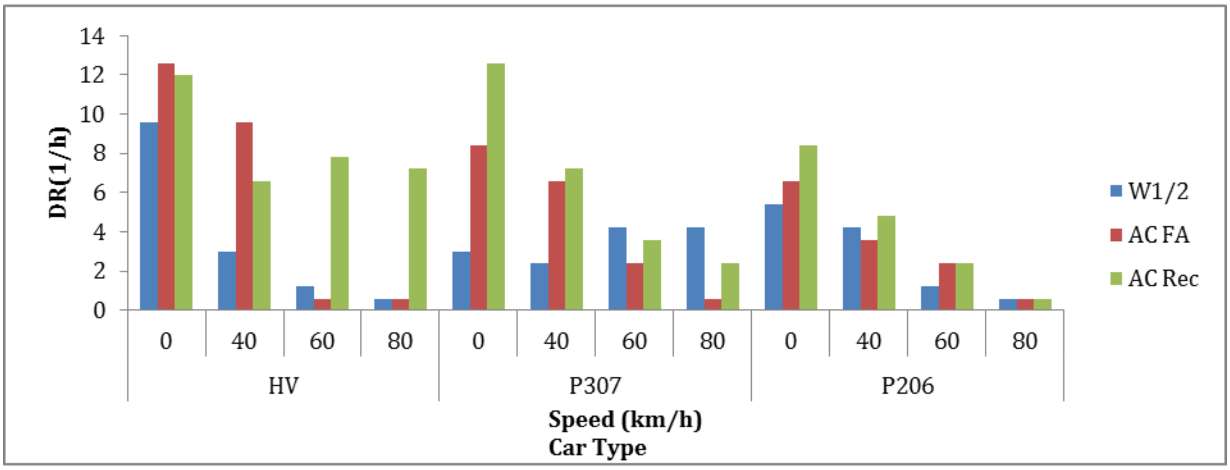
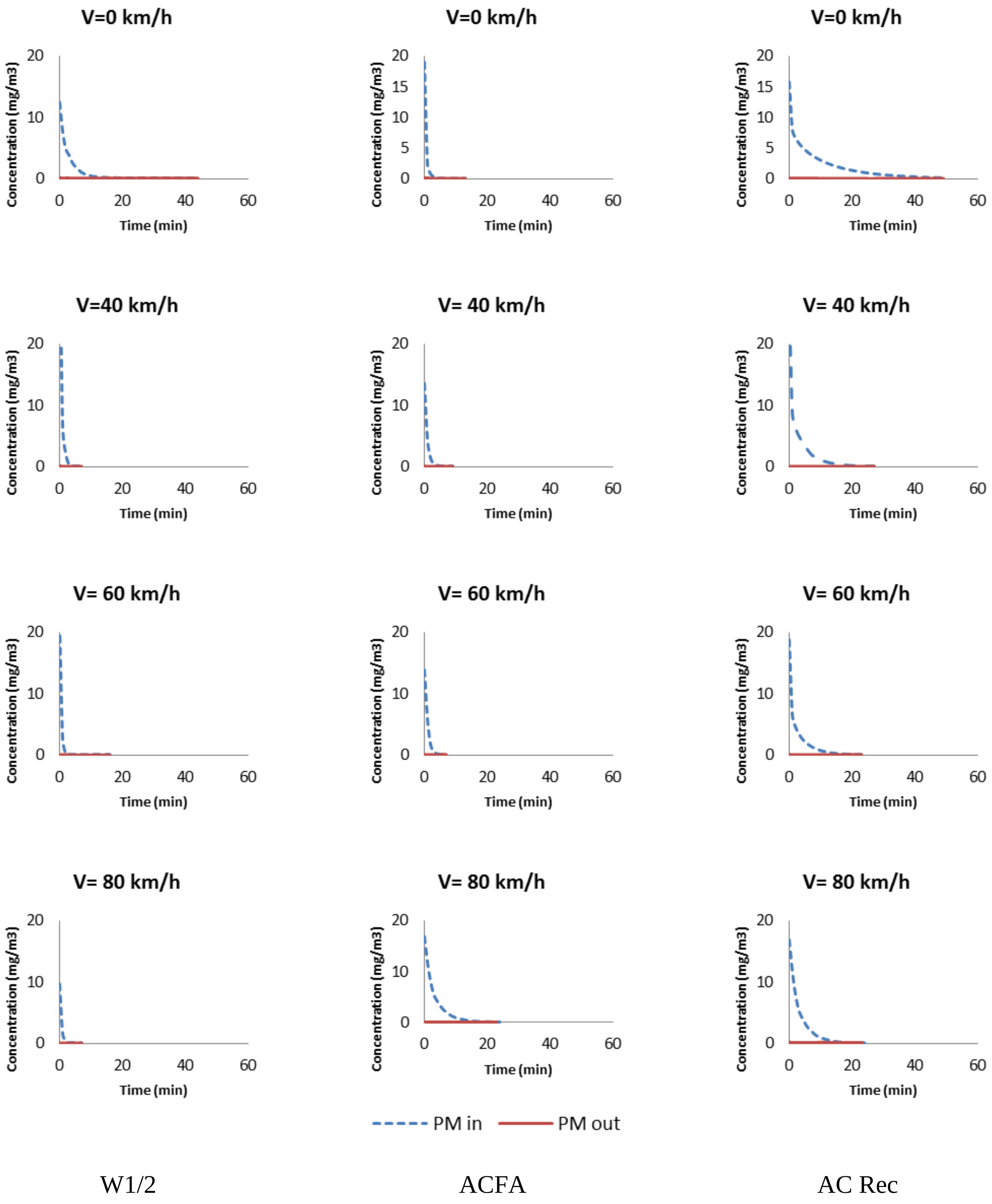
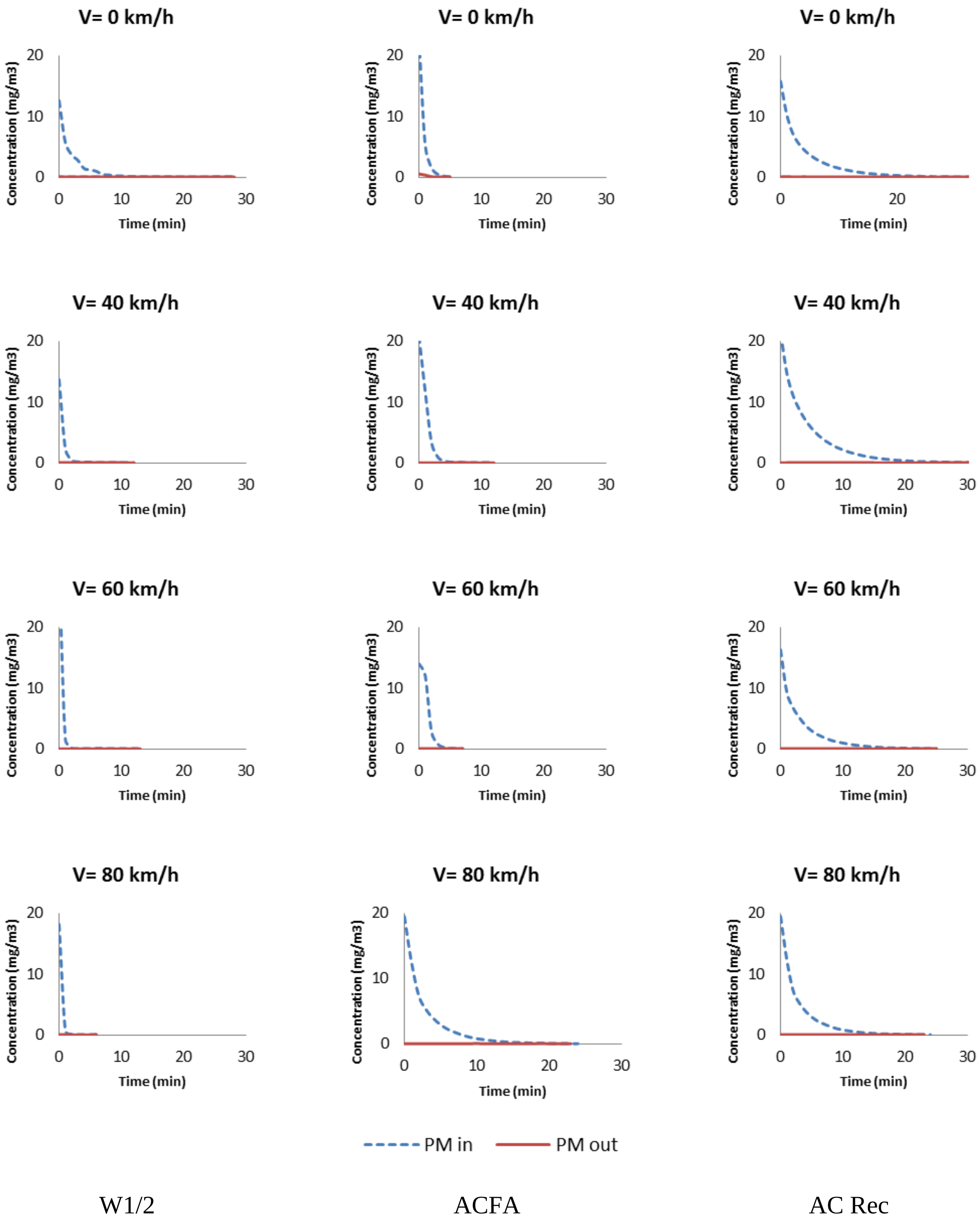


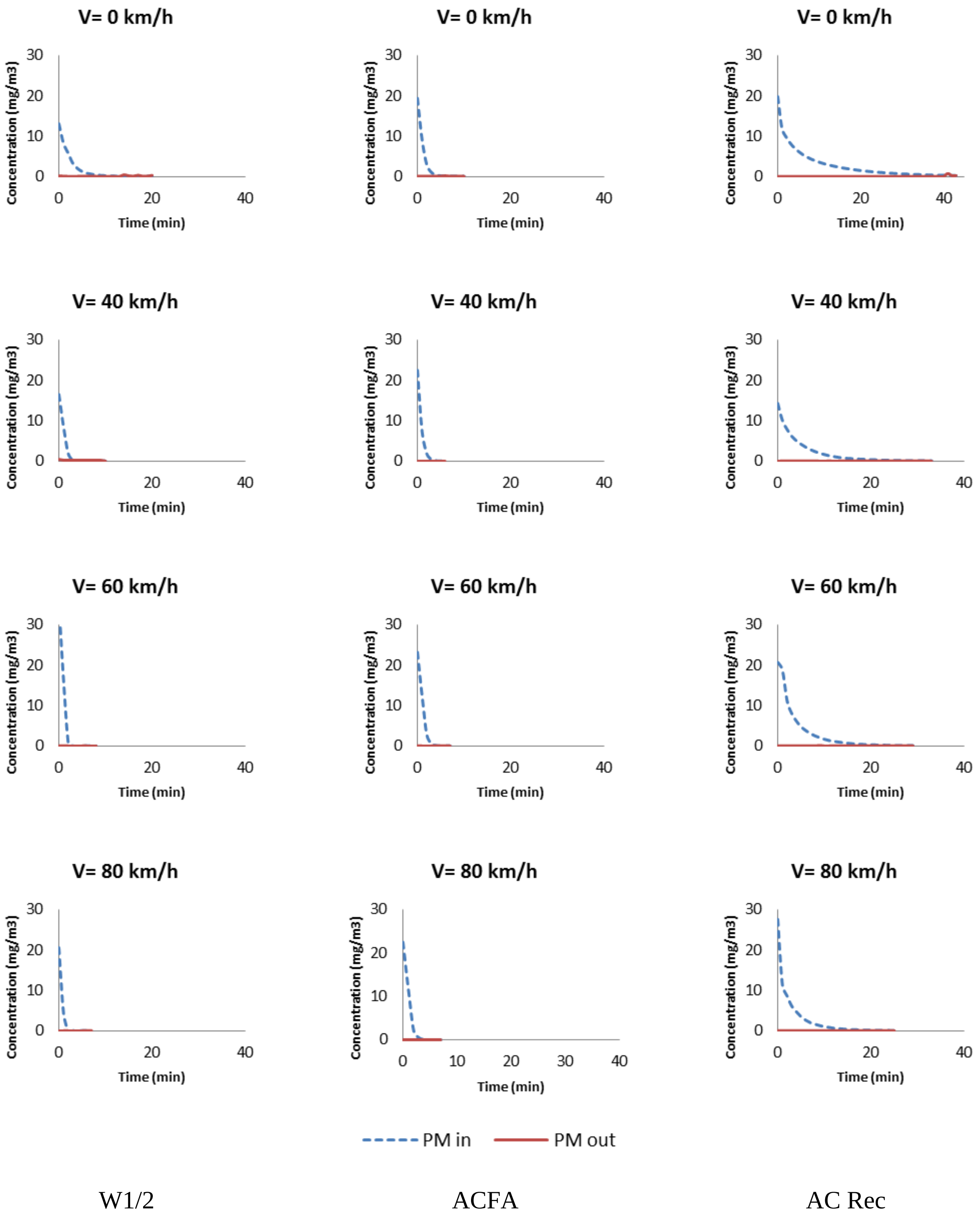
Figure A-2.3 DR results



(a) Peugeot 307 $PM_{2.5}$ concentrations

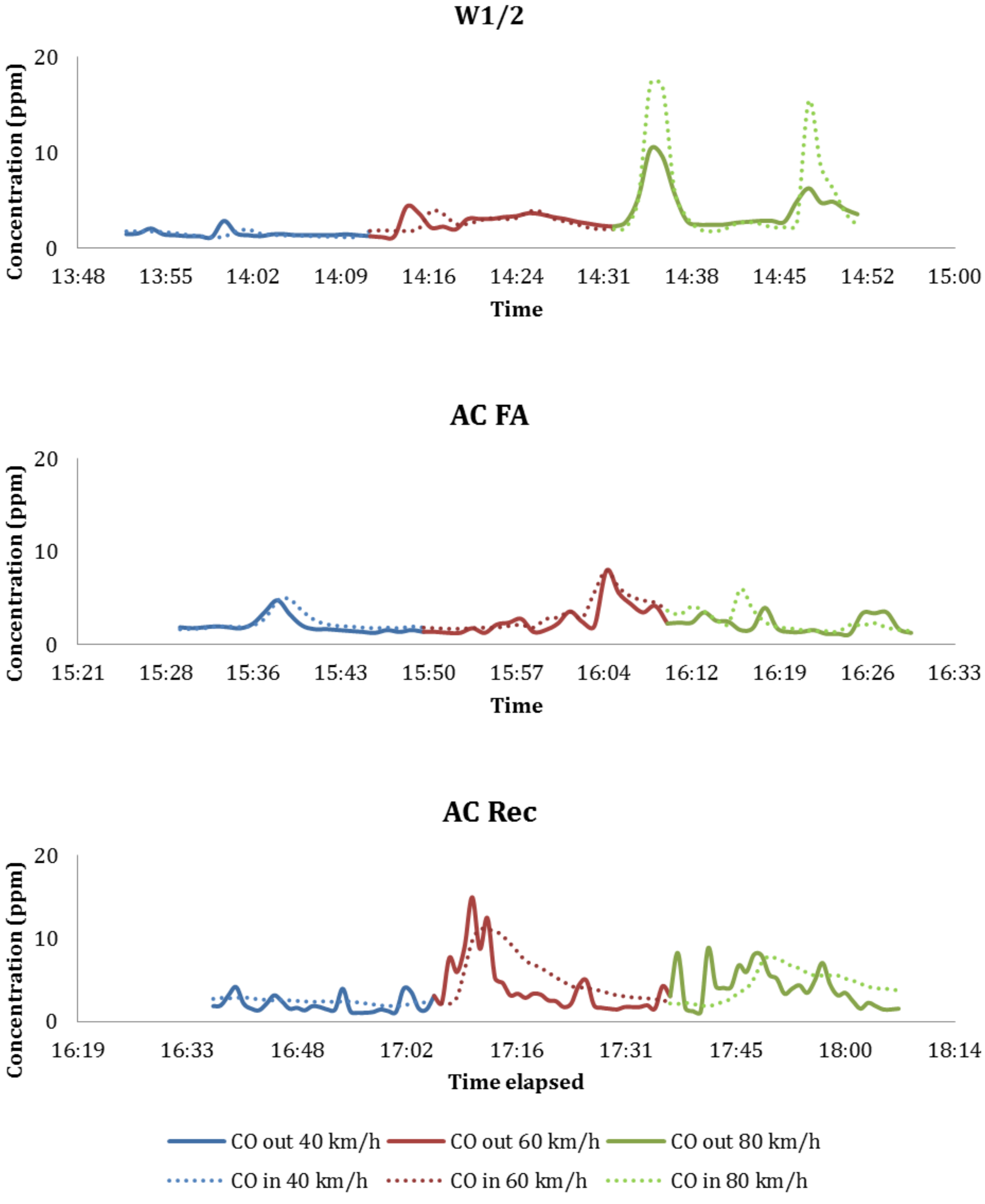


(b) Peugeot 206 $PM_{2.5}$ concentrations

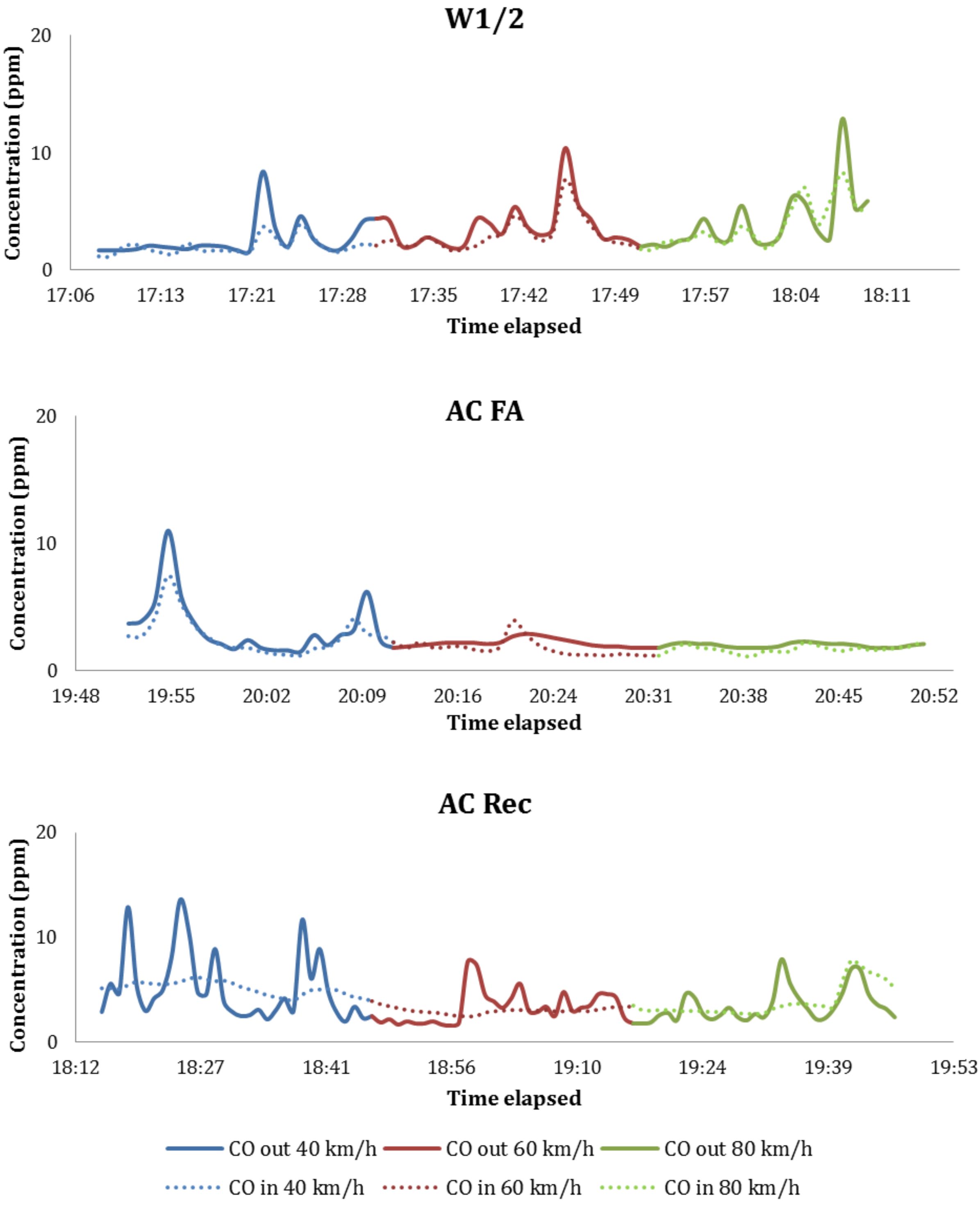


(c) Hyundai Verna $PM_{2.5}$ concentrations
Figure A-2.4 In and Out-Vehicle $PM_{2.5}$ Concentrations

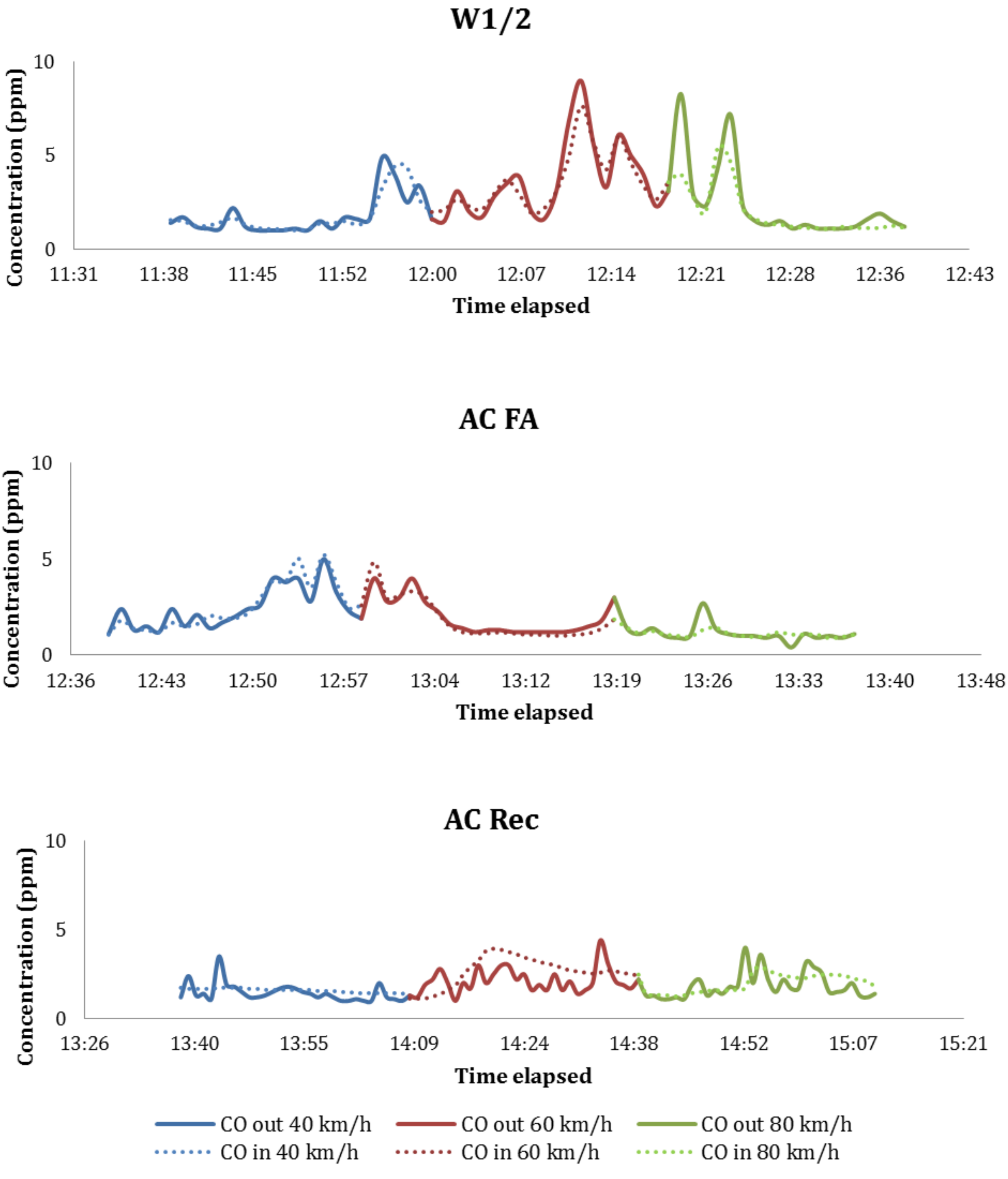
A.3. Field testing trips and simulations results



(a) Peugeot 307 CO concentrations

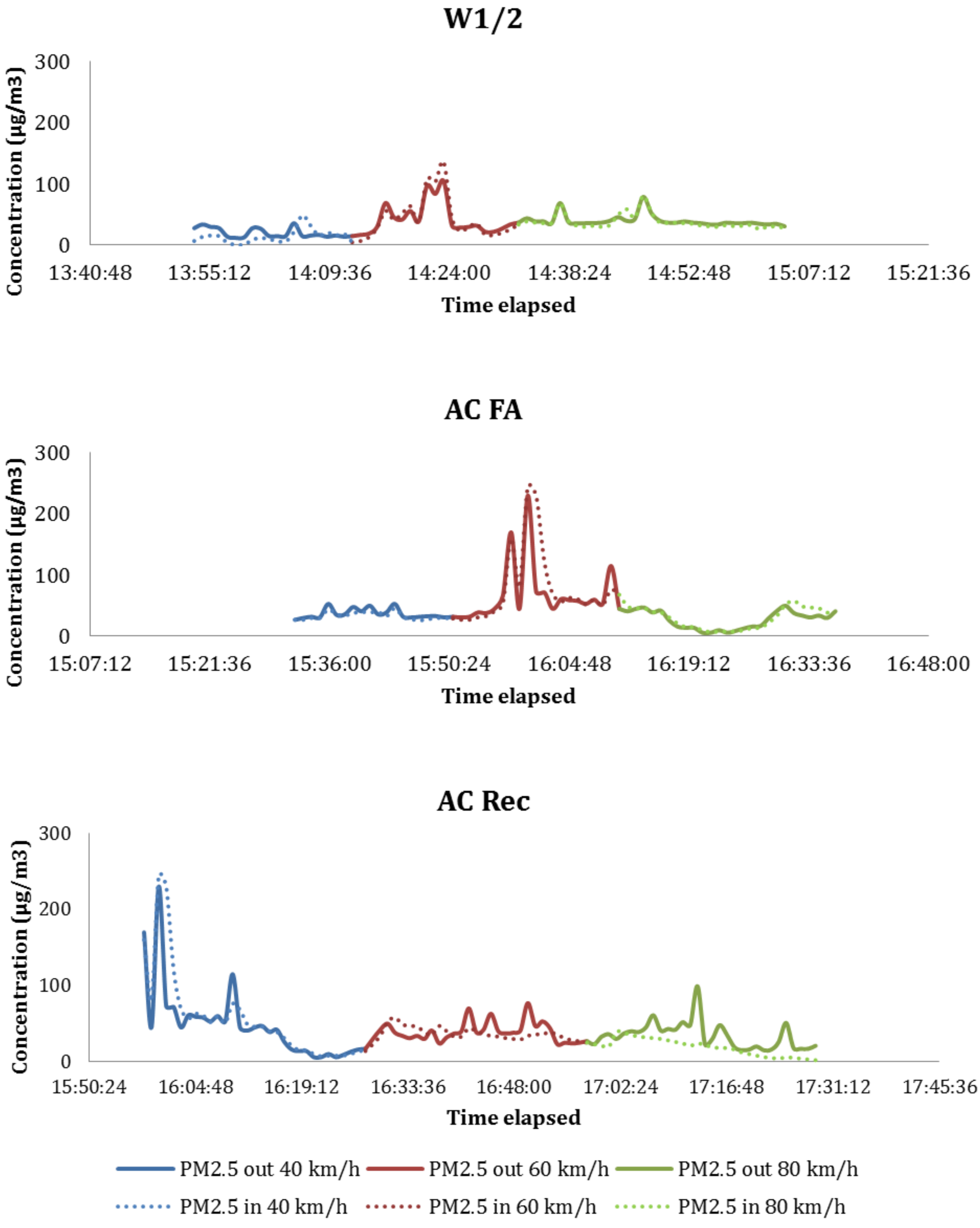


(b) Peugeot 206 CO concentrations

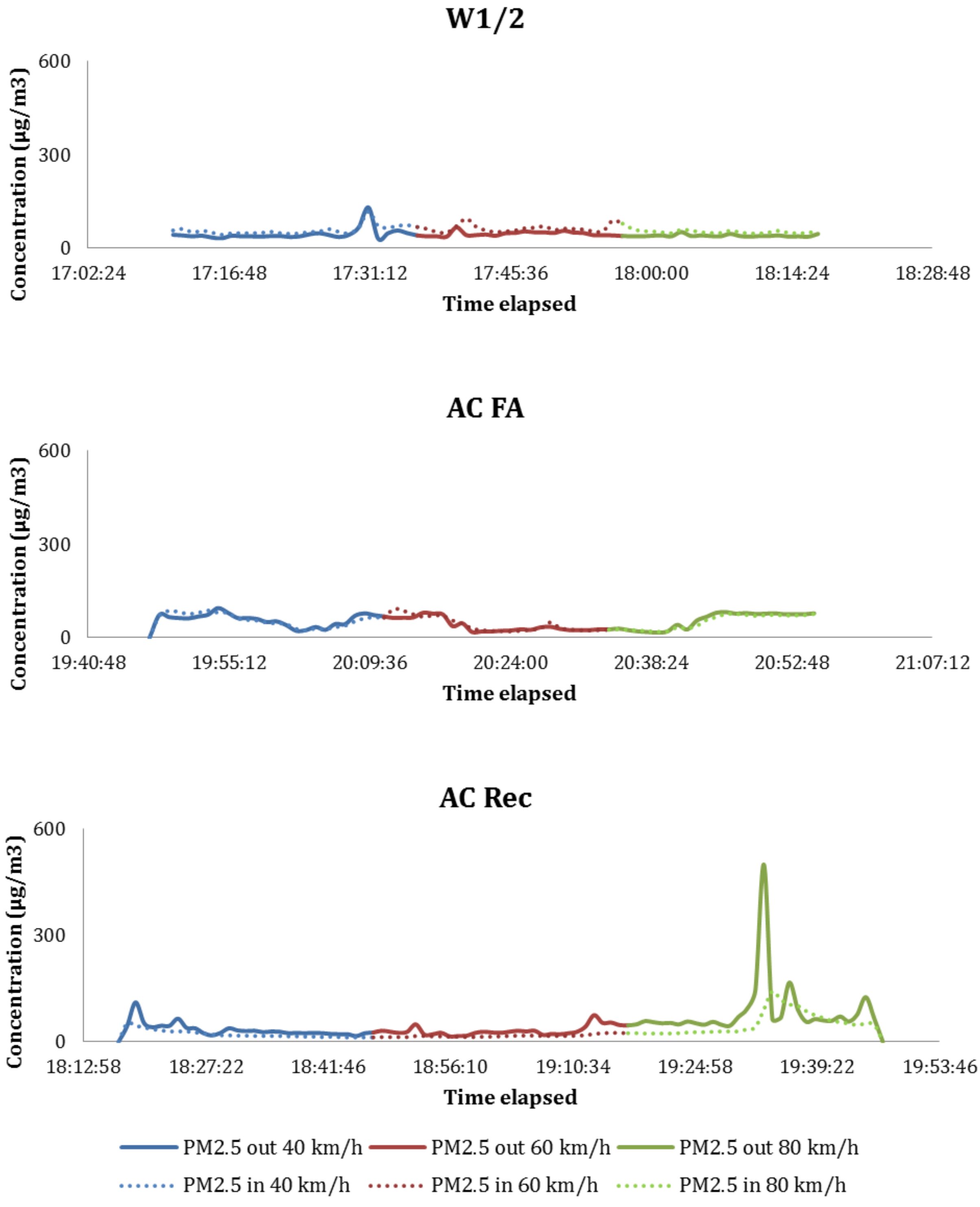


(c) Hyundai Verna CO concentrations

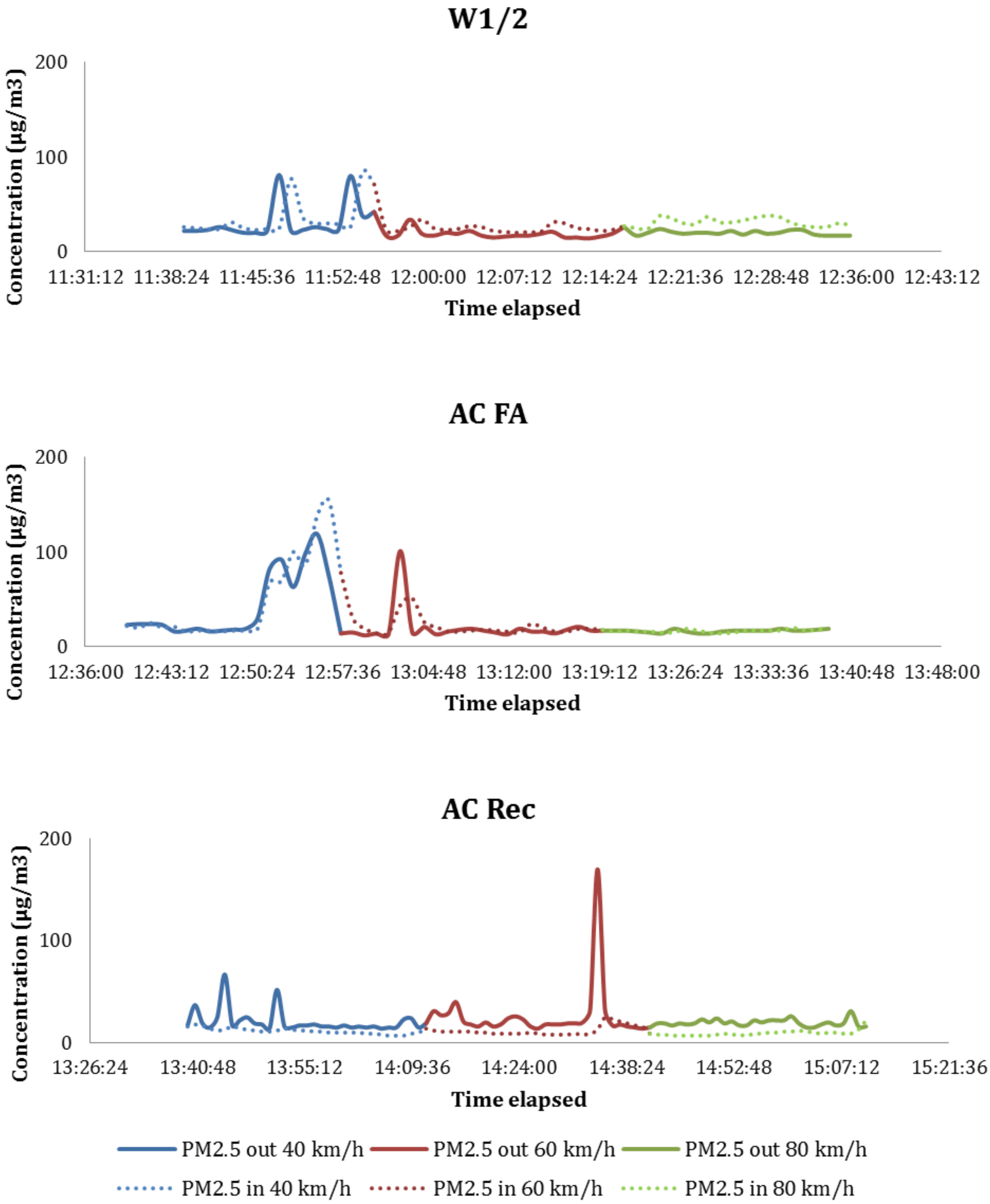
Figure A-3.1 In and out-vehicle CO concentrations during moving tests



(a) Peugeot 307 $PM_{2.5}$ concentrations

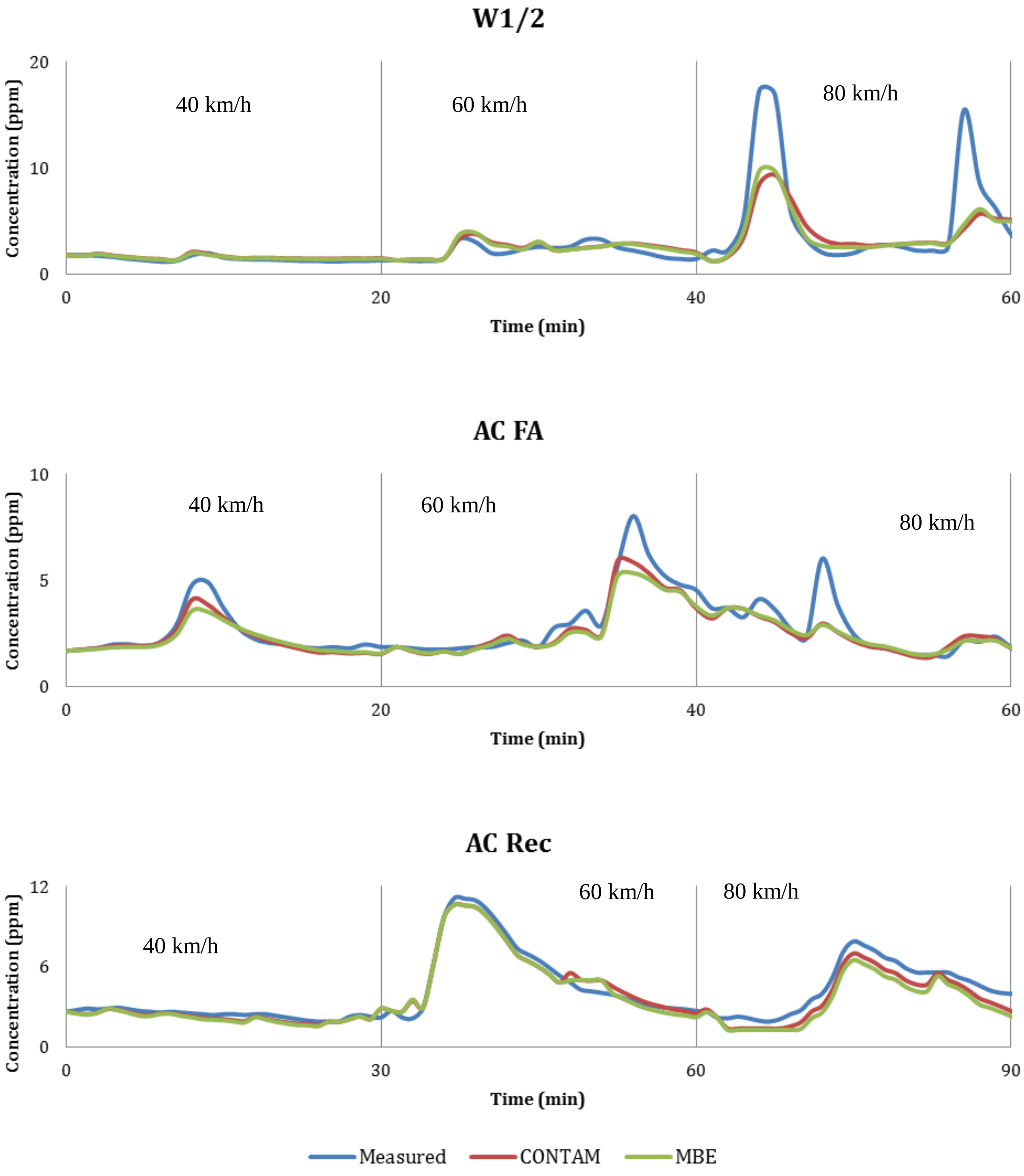


(b) Peugeot 206 $PM_{2.5}$ concentrations

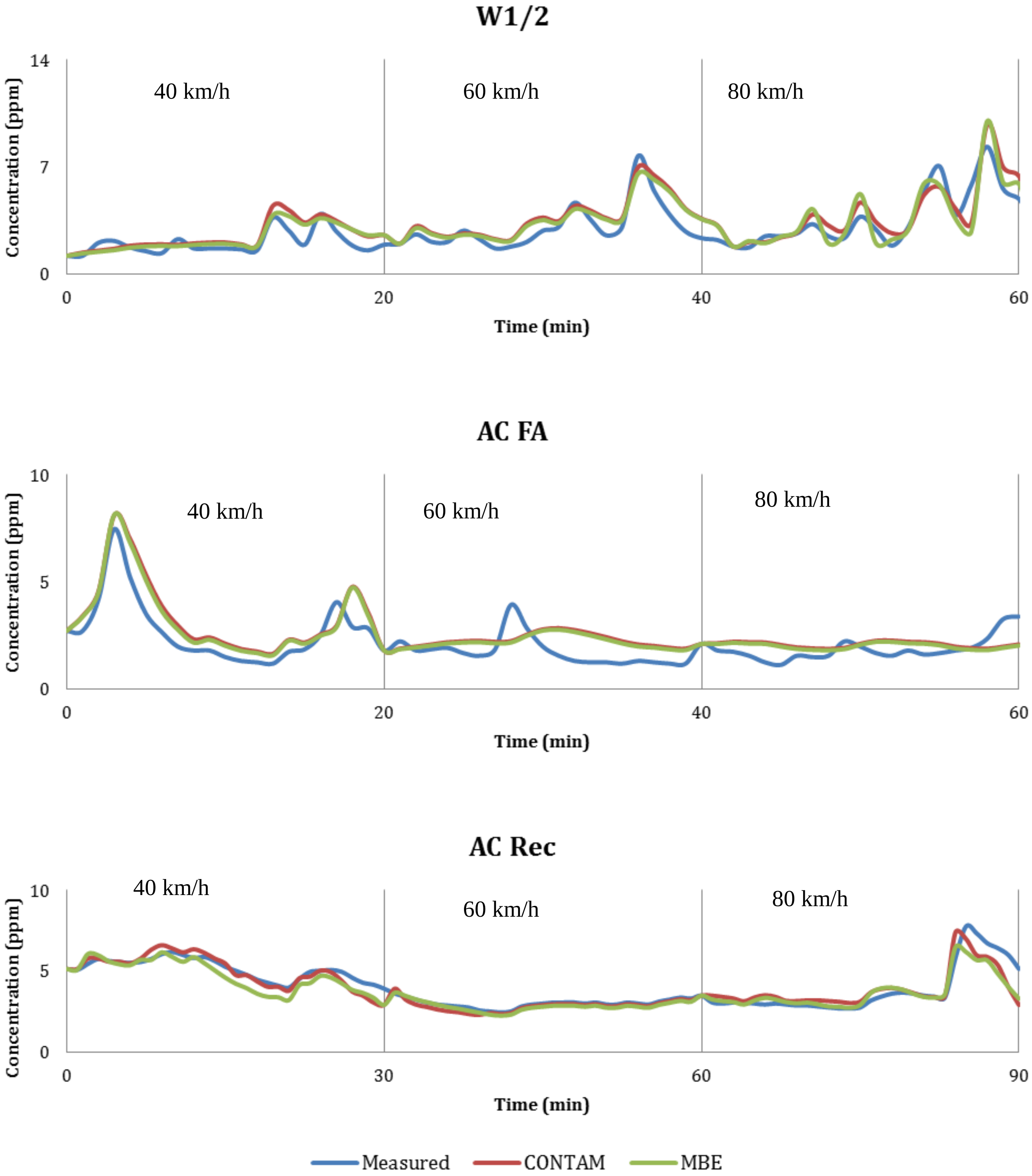


(c) Hyundai Verna $PM_{2.5}$ concentrations

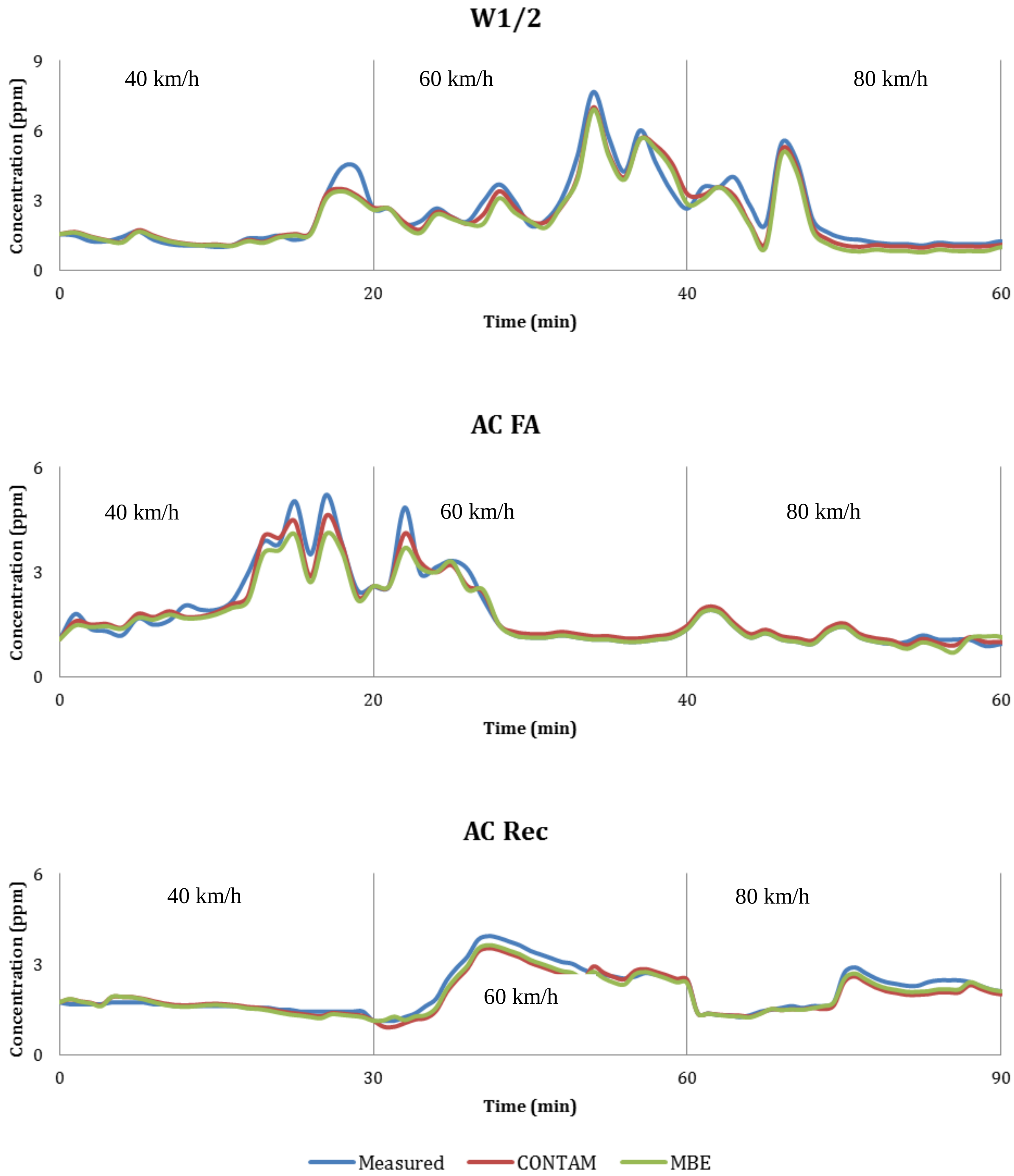
Figure A-3.2 In and out-vehicle $PM_{2.5}$ concentrations during moving tests



(a) Peugeot 307 CO concentrations

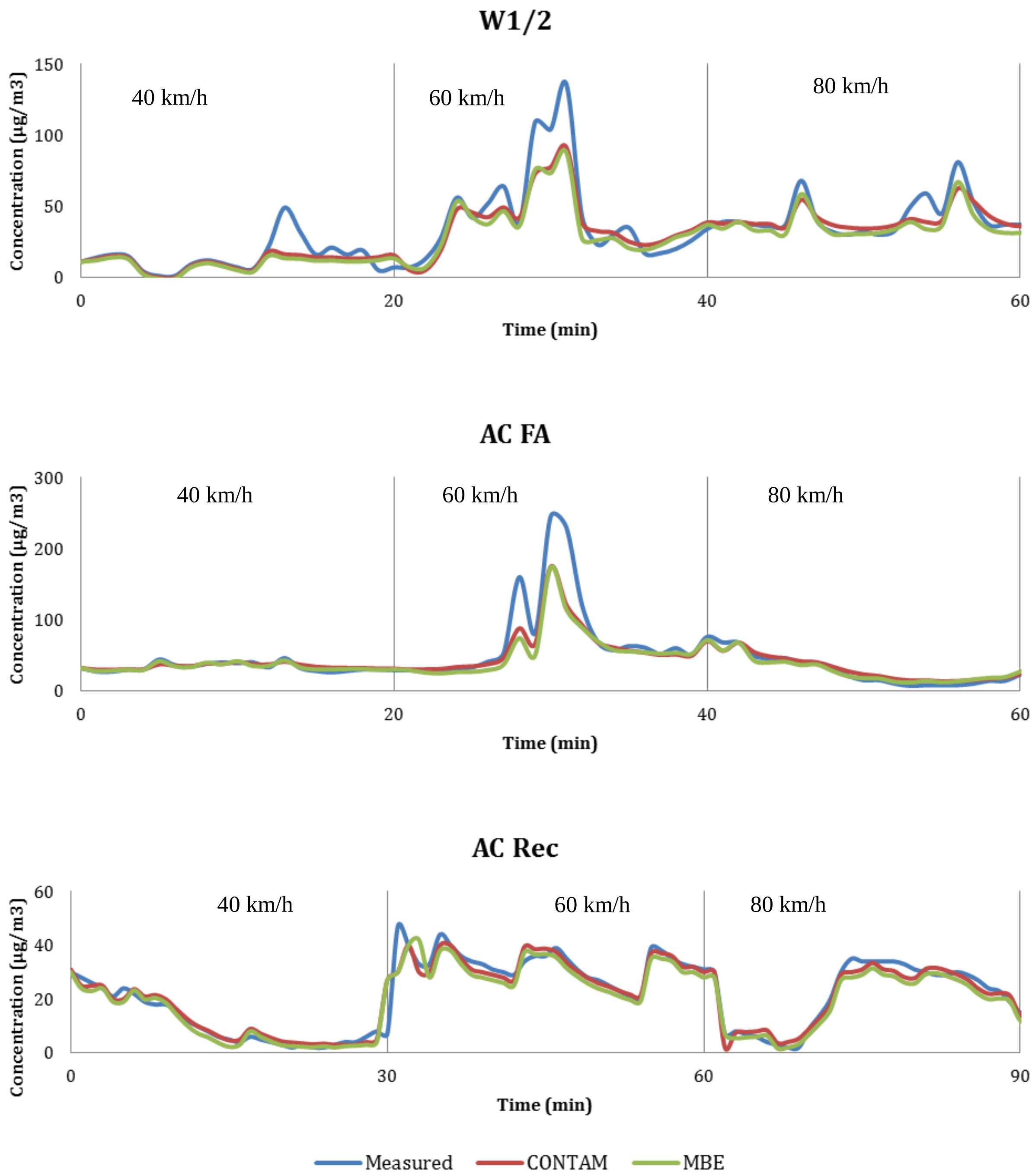


(b) Peugeot 206 CO concentrations

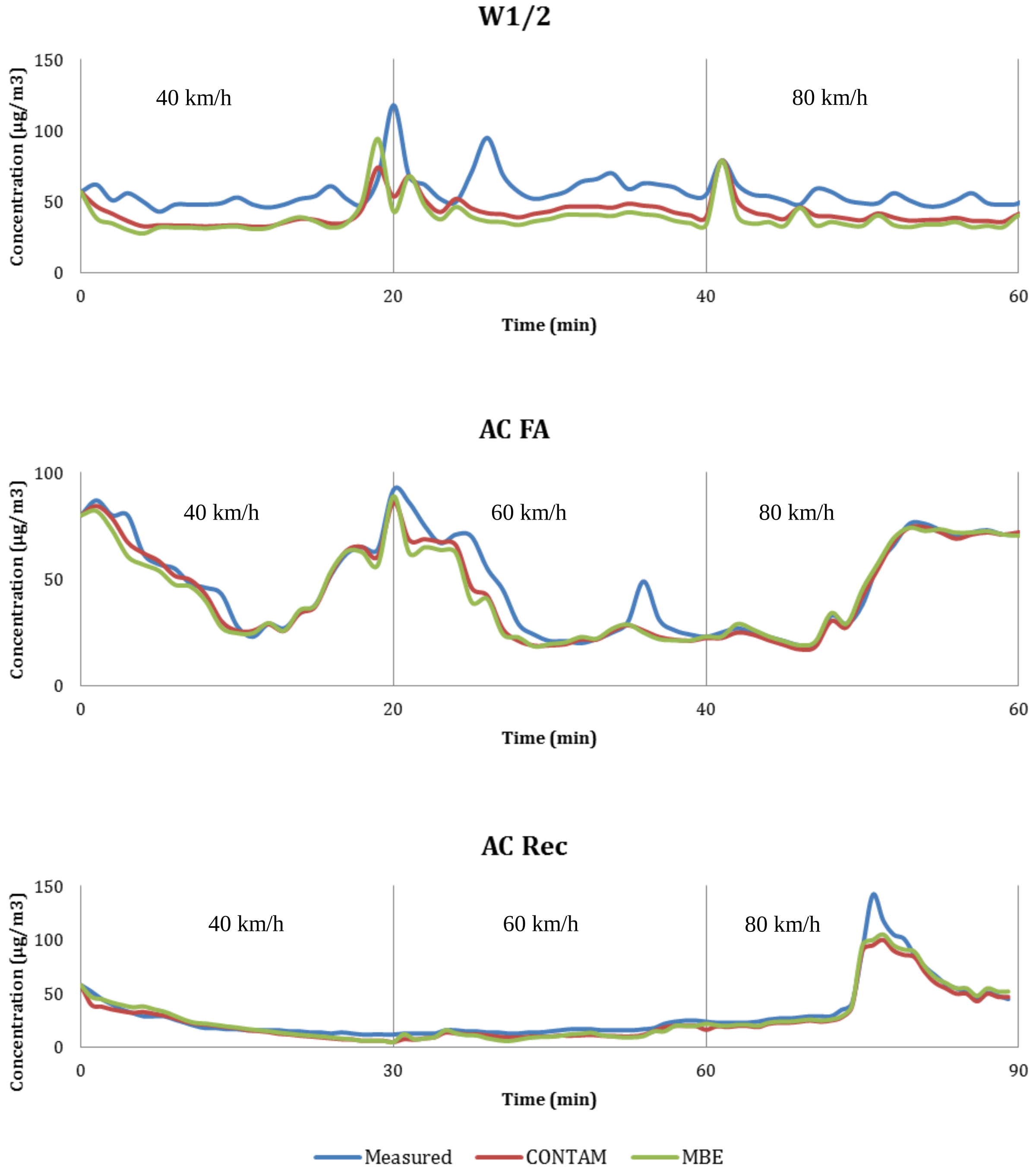


(c) Hyundai Verna CO concentrations

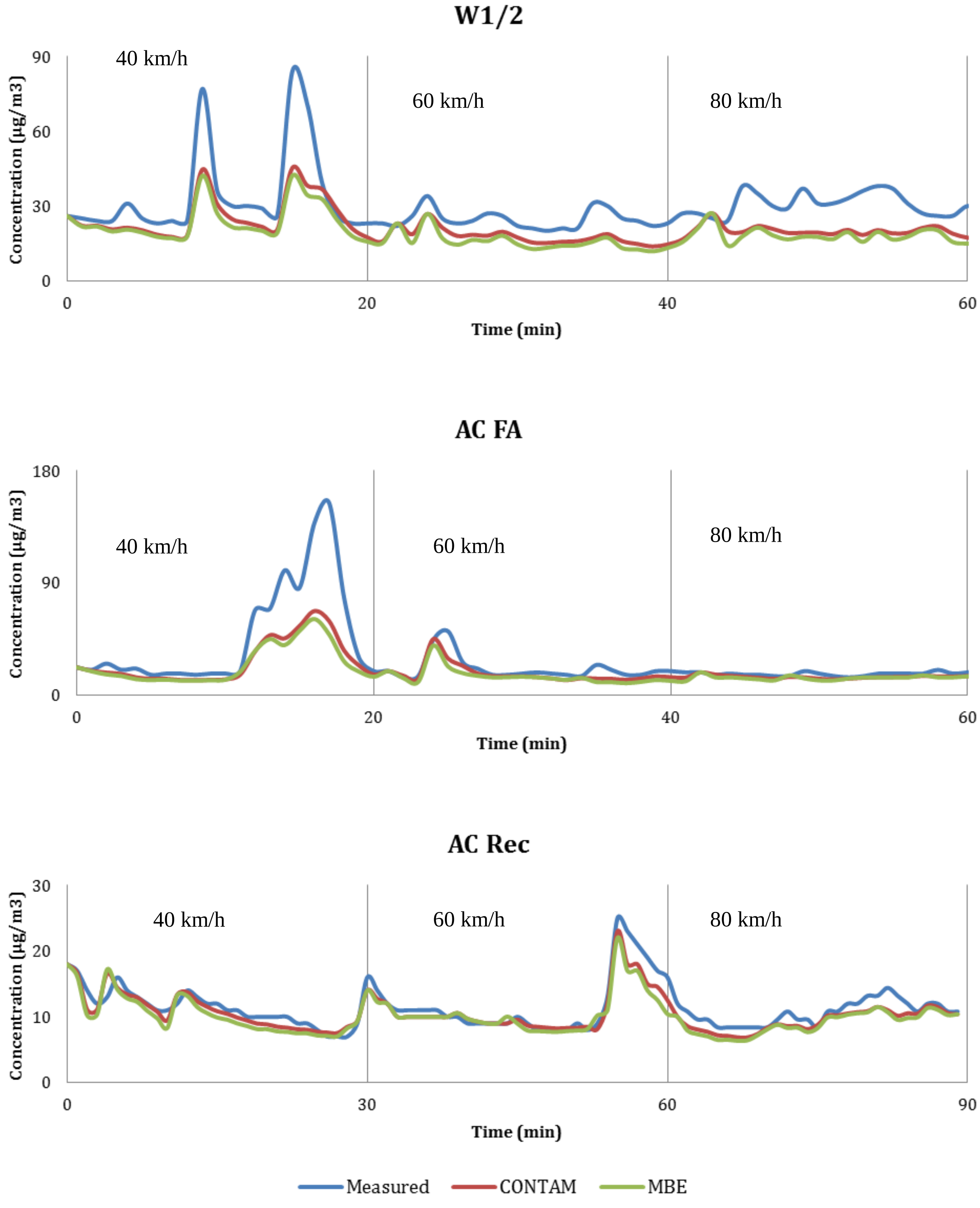
Figure A-3.3 Simulated and measured in vehicle CO concentrations during moving tests



(a) Peugeot 307 $PM_{2.5}$ concentrations



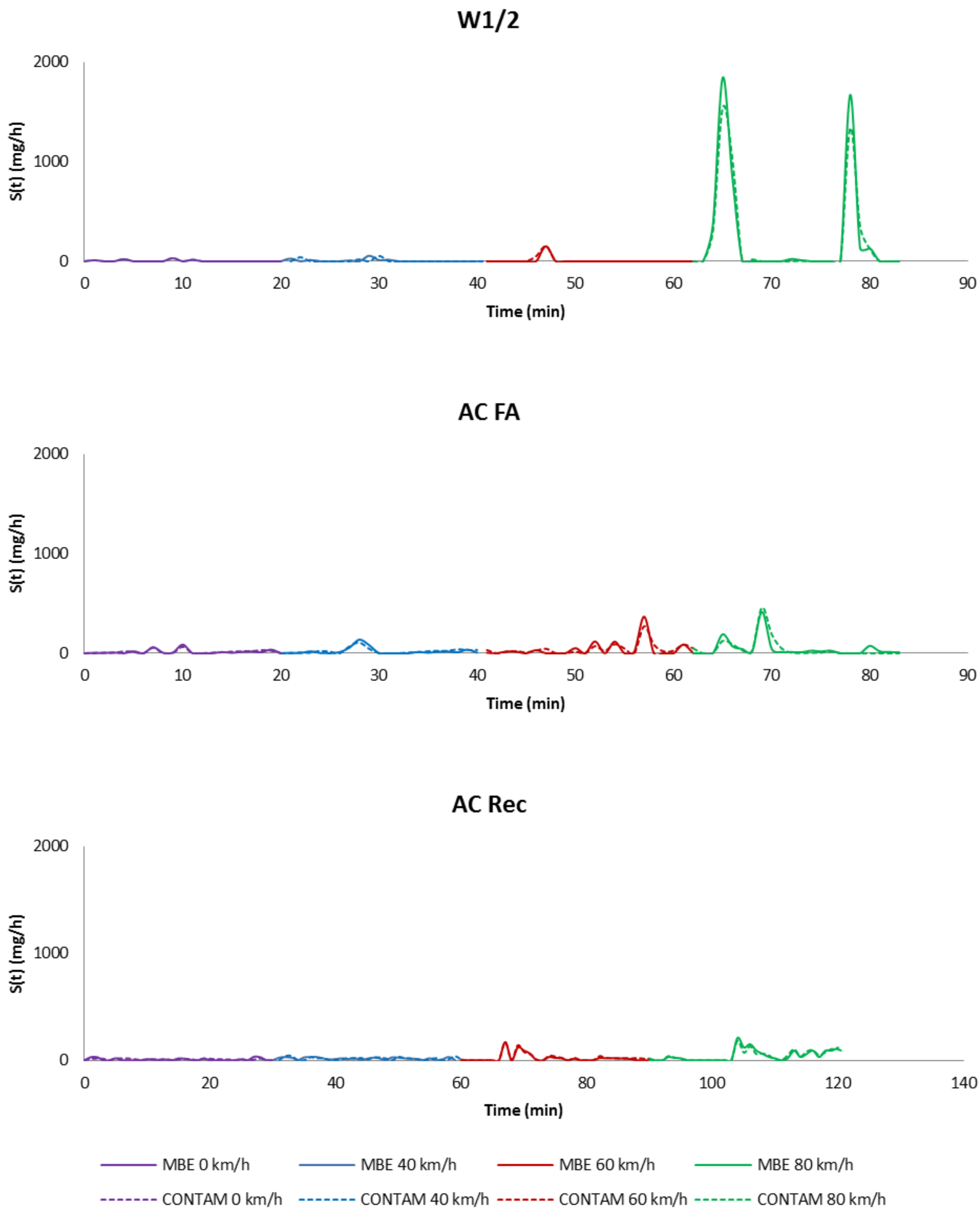
(b) Peugeot 206 $PM_{2.5}$ concentrations



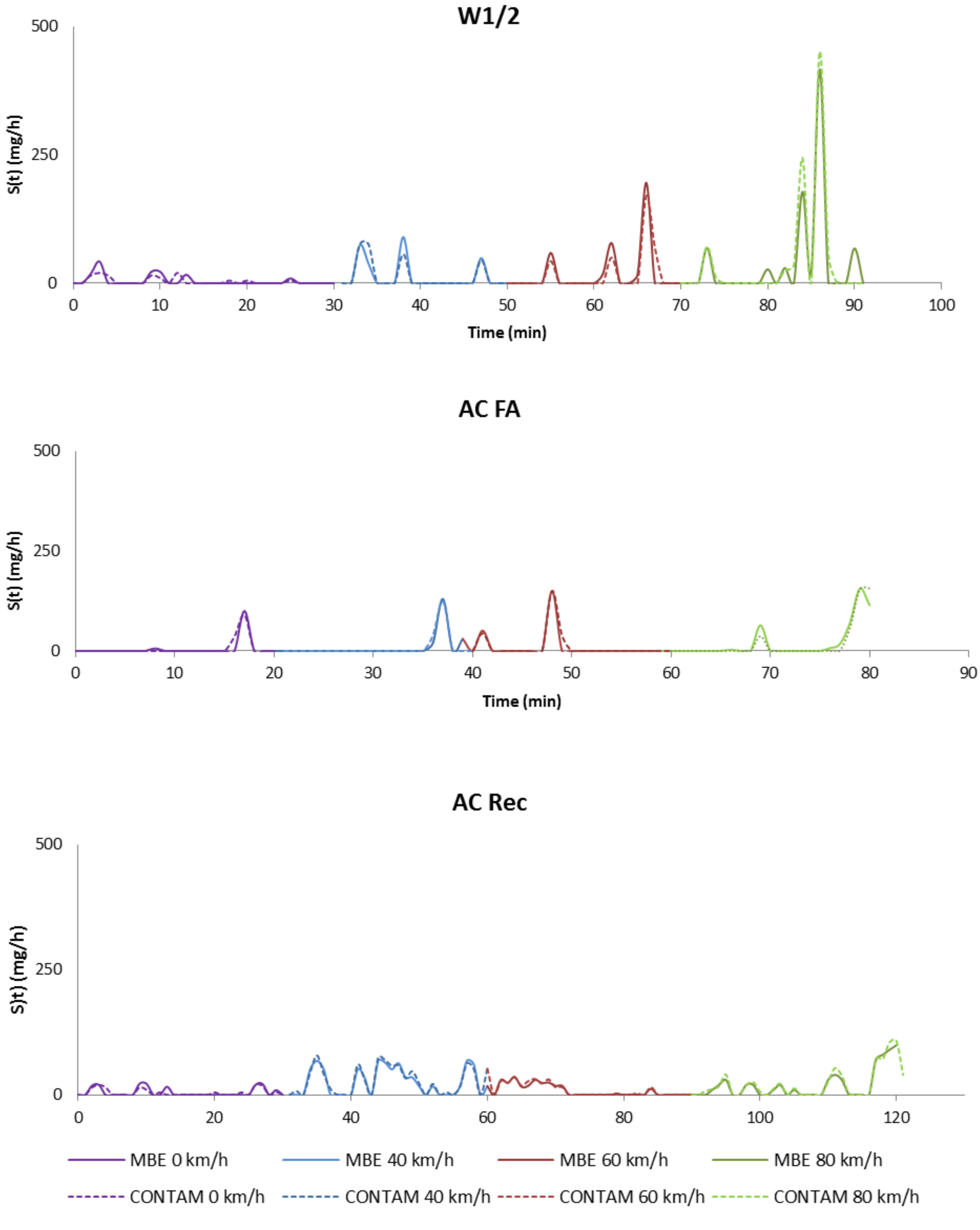
(C) Hyundai Verna $PM_{2.5}$ concentrations

Figure A-3.4 Simulated and measured in vehicle $PM_{2.5}$ concentrations during moving tests

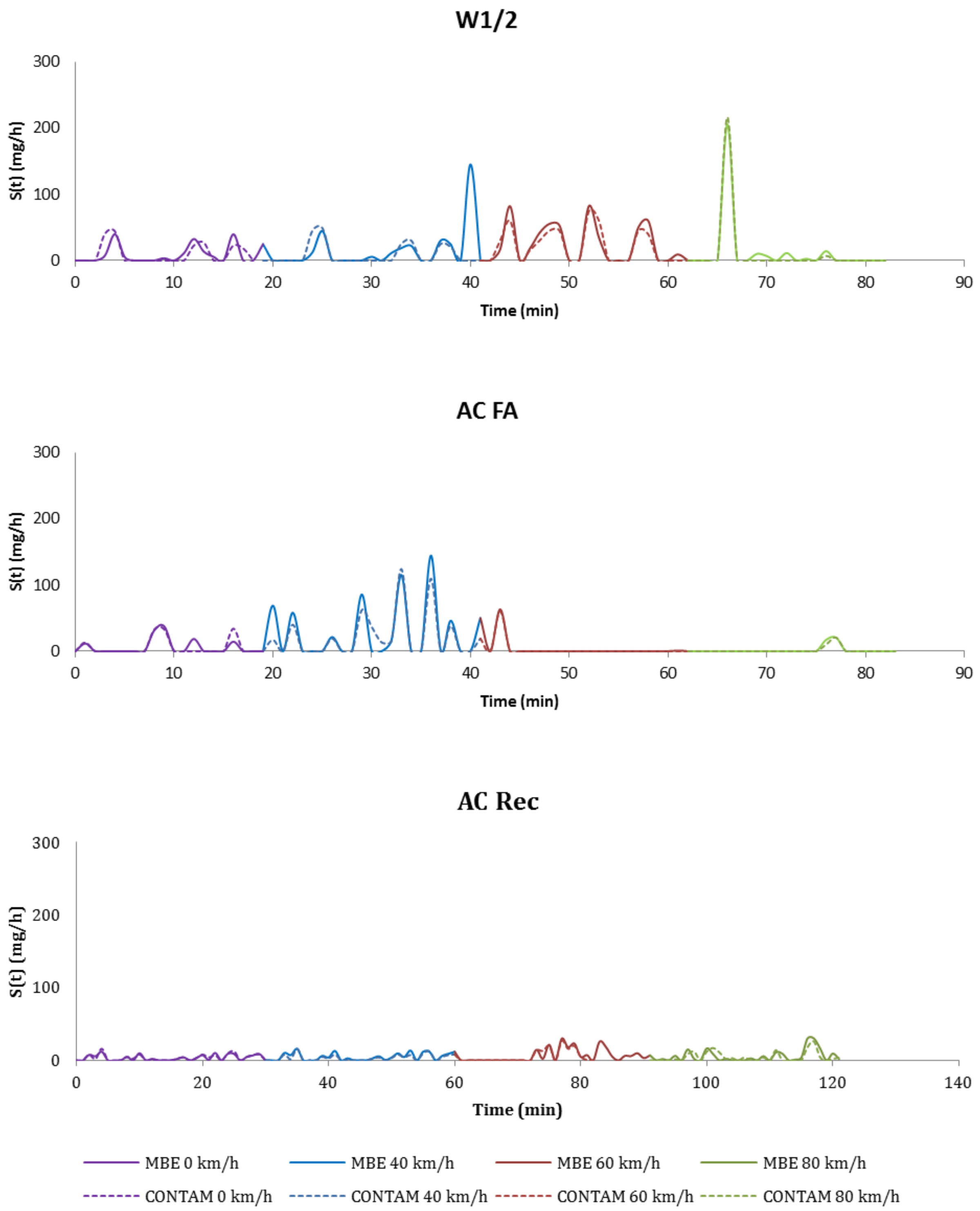
A.4. Source Emission Rate Results



(a) Peugeot 307 CO

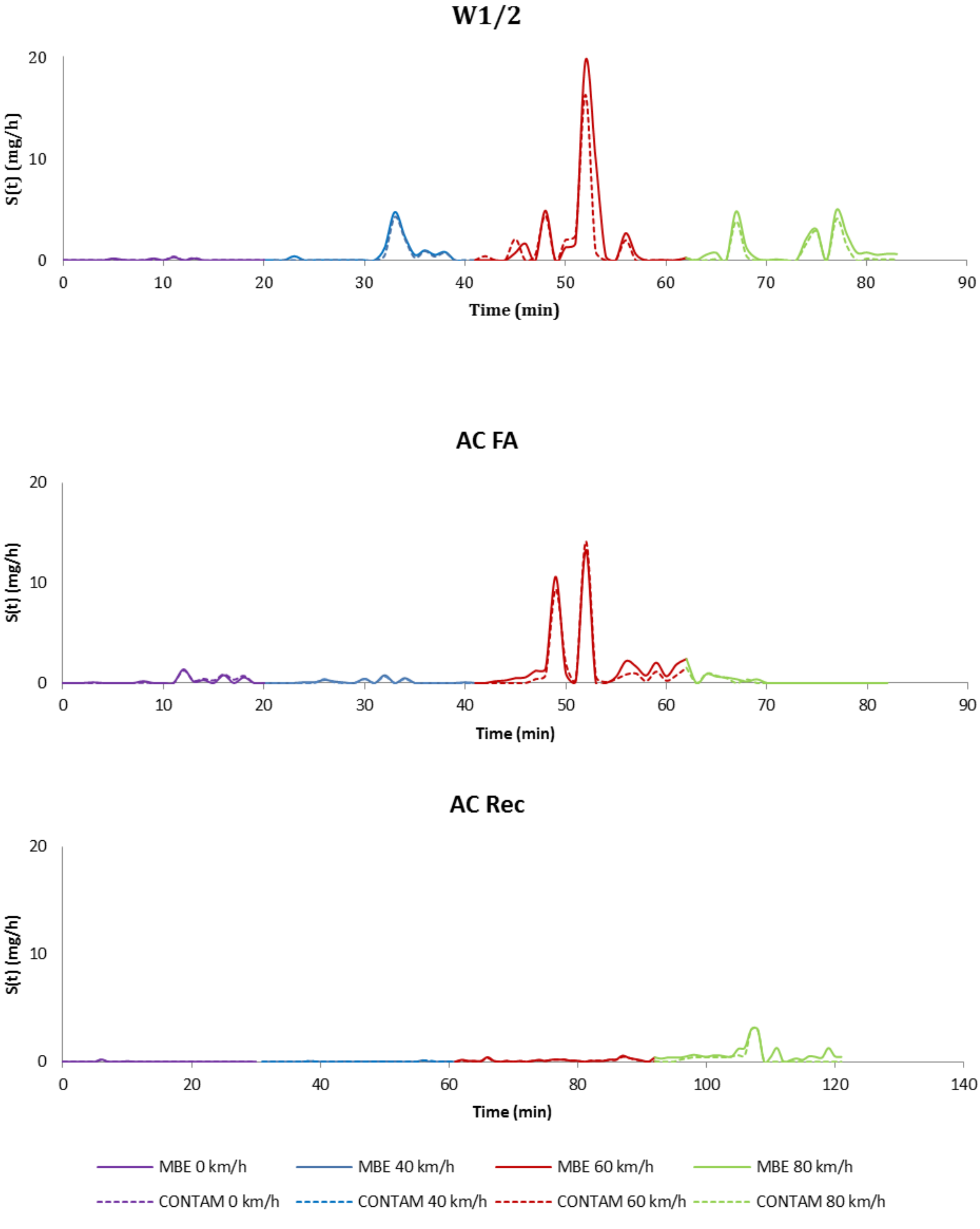


(b) Peugeot 206 CO

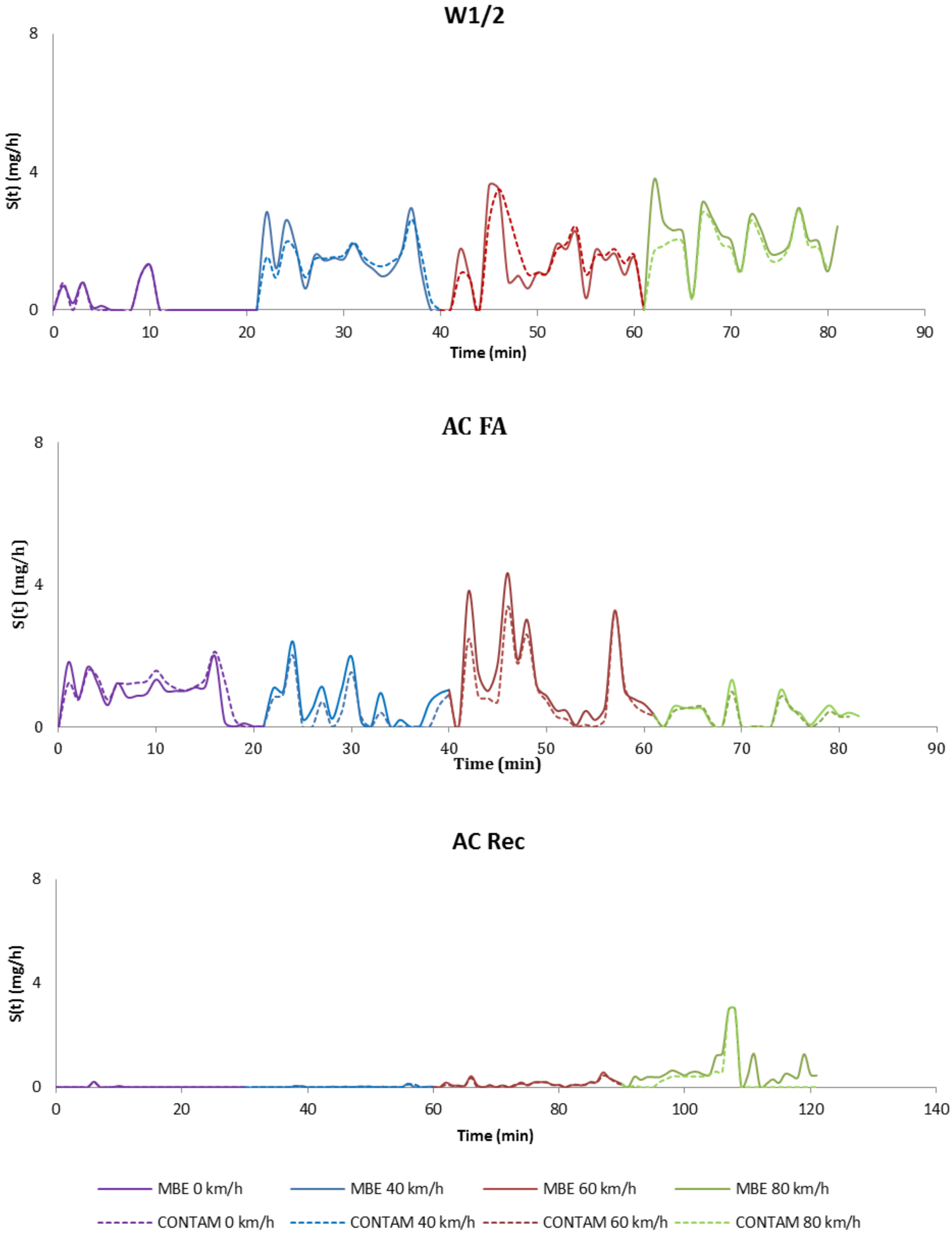


(c) Hyundai Verna CO

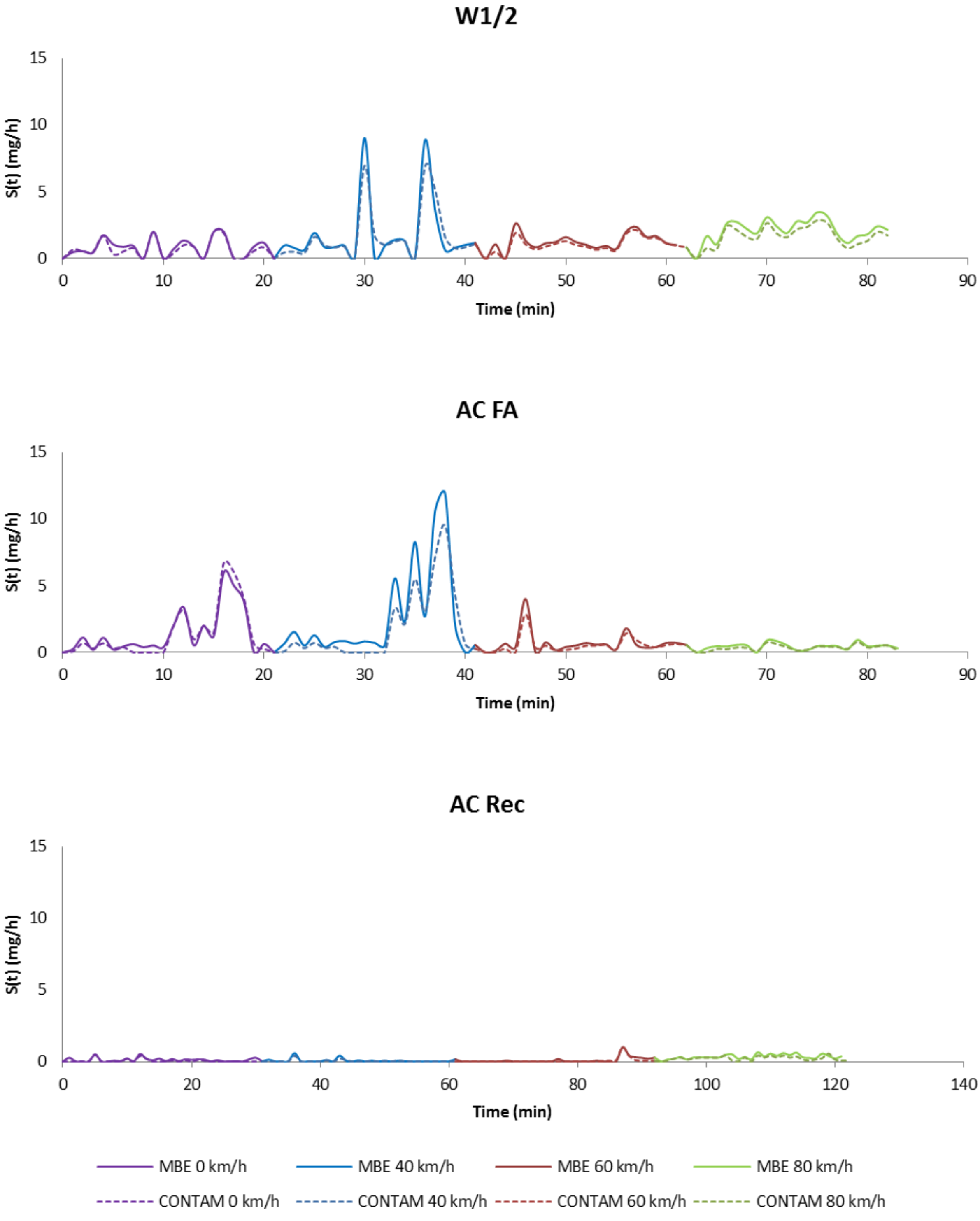
Figure A-4.1 CO source emission rate over time



(a) Peugeot 307 $PM_{2.5}$



(b) Peugeot 206 $PM_{2.5}$



(c) Hyundai Verna $PM_{2.5}$

Figure A-4.2 $PM_{2.5}$ source emission rate over time

A.5. R coding

Emission rates considering the equipment's accuracy

```
#P307-PM2.5-W1/2
AER=21
V=2.24
error=0.001
DR=3
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-0.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))
```

```
AER=51.6
V=2.24
error=0.001
DR=2.4
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-40.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=85.8
V=2.24
```

```
error=0.001
DR=4.2
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-60.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=102
V=2.24
error=0.001
DR=4.2
```

```
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-
80.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
a
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S
S<-na.omit(S)
S

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))
```

#P307-PM2.5-FA

```
AER=31.8
V=2.24
error=0.001
```

```
DR=8.4
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-
0.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
a
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S
S<-na.omit(S)
S

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=33
V=2.24
```

```
error=0.001
DR=6.6
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-
40.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
a
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S
S<-na.omit(S)
S

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=39
```

```
V=2.24
error=0.001
DR=2.4
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-
60.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
a
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S
S<-na.omit(S)
S

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))
```

```
AER=35.4
V=2.24
error=0.001
DR=0.6
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-w-
80.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)


M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))
```

#P307-PM2.5-Rec

```
AER=10.8
```

```
V=2.24
error=0.001
DR=12.6
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-
rec-0.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=10.8
V=2.24
error=0.001
DR=7.2
```

```
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-
rec-40.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=10.8
V=2.24
error=0.001
DR=3.6
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-
rec-60.csv",header=T)
```

```
colnames(y)
Cin<-y$Cin/1000
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))


AER=17.4
V=2.24
error=0.001
DR=2.4
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/pm-p307-rec-80.csv",header=T)
colnames(y)
Cin<-y$Cin/1000
```

```
Cin
Cout<-y$Cout/1000
Cout

a.in<-matrix(NA,19,100)
a.in
for(j in 1:20){
  for(i in 1:100){
    a.in[j,i]<-rnorm(1,y$Cin[j],error)
  }
}
a.in

a.out<-matrix(NA,19,100)
a.out
for(j in 1:19){
  for(i in 1:100){
    a.out[j,i]<-rnorm(1,y$Cout[j],error)
  }
}
a.out

a<-matrix(NA,19,100)
a
for(j in 1:18){
  for(i in 1:100){
    a[j,i]<-(a.in[j+1,i]-a.in[j,i])
  }}
S=V*a*60-AER*V*a.out+AER*V*a.in+DR*a.in*V
S
S<-na.omit(S)

M1<-matrix(NA,1,100)
M2<-matrix(NA,1,100)
M1
for(i in 1:100){
  M1[,i]<-mean(S[,i], na.rm = FALSE)
  M2[,i]<-median(S[,i], na.rm = FALSE)
}
M1
M2
table(sign(M1))
table(sign(M2))
```

CONTAM and MBE comparison

```
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/report/Thesis report/contam-mbe-measured.csv",header=T)
colnames(y)
cor(y$Measured,y$CONTAM)
cor(y$Measured,y$MBE)
```

ANOVA deposition rates – source emission rates

```
x<-data.frame(speed=factor(rep(c("0","40","60","80"),9)),car=rep(c("HV","Peugeot
307","Peugeot 206"),c(12,12,12)),ventilation=rep(c("W1/2","AC FA","AC Rec"),c(4,4,4)),
k=c(9.6,3,1.2,0.6,12.6,9.6,0.6,0.6,12.,6.6,7.8,7.2,3,2.4,4.2,4.2,8.4,6.6,2.4,0.6,12.6,7.2,3.6,2.4,5.4
,4.2,1.2,0.6,6.6,3.6,2.4,0.6,8.4,4.8,2.4,0.6))
boxplot(k~speed,data=x)
boxplot(k~car,data=x)
boxplot(k~ventilation,ylab="Deposition rate",data=x)
fit<-aov(k~speed*ventilation, data=x) #p>0.05 k are not significatly different with speed and
ventilation
summary(fit)
plot(fit)

#peugeot 307
y.PM1<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC
FA","AC Rec"),c(4,4,4)), s=c(0.16,0.55,2.09,1.13,0.04,0.11,2.44,0.21,0.01,0.07,0.27,0.2))
boxplot(s~speed,data=y.PM1)
boxplot(s~ventilation,ylab="PM2.5 emission rates",data=y.PM1)
fit.s<-aov(s~speed, data=y.PM1)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.PM1)
summary(fit.v)
plot(fit.v)
fit<-aov(s~ventilation*speed, data=y.PM1)
summary(fit)

y.CO1<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC
FA","AC Rec"),c(4,4,4)),
s=c(4.23,6.19,7.19,238.29,13.49,19.56,38.88,46.95,7.21,14.5,26.72,44.91))
boxplot(s~speed,data=y.CO1)
boxplot(s~ventilation,ylab="CO emission rates",data=y.CO1)
fit.s<-aov(s~speed, data=y.CO1)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.CO1)
summary(fit.v)
plot(fit.v)

#peugeot 206
y.PM<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC
FA","AC Rec"),c(4,4,4)), s=c(1.12,1.79,1.49,2.06,0.55,0.67,1.31,0.35,0.19,0.01,0.13,0.93))
y.PM
boxplot(s~speed,data=y.PM)
boxplot(s~ventilation,ylab="PM2.5 emission rates",data=y.PM)
fit.s<-aov(s~speed, data=y.PM)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.PM)
summary(fit.v)
plot(fit.v)
fit<-aov(s~ventilation*speed, data=y.PM)
summary(fit)
```

```
y.CO2<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC FA","AC Rec"),c(4,4,4)),
s=c(9.99,12.55,17.53,38.57,10.95,10.46,15.45,20.45,7.58,10,9.99,22.42))
y.CO2
boxplot(s~speed,data=y.CO2)
boxplot(s~ventilation,ylab="CO emission rates",data=y.CO2)
fit.s<-aov(s~speed, data=y.CO2)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.CO2)
summary(fit.v)
plot(fit.v)

#Hyundai verna
y.PM<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC FA","AC Rec"),c(4,4,4)), s=c(1.29,1.63,1.2,2.03,2.09,2.5,0.68,0.49,0.12,0.06,0.11,0.39))
y.PM
boxplot(s~speed,data=y.PM,main="Hyundai verna PM2.5 emission rates (mg/h)")
boxplot(s~ventilation,ylab="PM2.5 emission rates",data=y.PM)
fit.s<-aov(s~speed, data=y.PM)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.PM)
summary(fit.v)
plot(fit.v)

y.CO3<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC FA","AC Rec"),c(4,4,4)), s=c(8.67,14.95,28.61,33.36,8.68,16.77,3.67,3.07,3.57,5.03,6.54,6.39))
boxplot(s~speed,data=y.CO3,main="Hyundai verna CO emission rates (mg/h)")
mean(y.CO3$s)
boxplot(s~ventilation,ylab="CO emission rates",data=y.CO3)
fit.s<-aov(s~speed, data=y.CO3)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.CO3)
summary(fit.v)
plot(fit.v)

#HV CONTAM
y.CO<-data.frame(speed=factor(rep(c("0","40","60","80"),3)),ventilation=rep(c("W1/2","AC FA","AC Rec"),c(4,4,4)), s=c(8.31,9.24,22.22,22.34,9.29,17.93,2.86,3.27,3.75,4.22,5.51,5.35))
y.CO
boxplot(s~speed,data=y.CO)
boxplot(s~ventilation,ylab="CO emission rates",data=y.CO)
fit.s<-aov(s~speed, data=y.CO)
summary(fit.s)
plot(fit.s)
fit.v<-aov(s~ventilation, data=y.CO)
summary(fit.v)
plot(fit.v)
```

Source emission rates

```
##CO
```

```
x<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/CONTAM vs MBE/MBE/cte
AER/CO.csv",header=T)
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/CONTAM vs MBE/MBE/cte
AER/COno0.csv",header=T)
require(car)
hist(as.numeric(log(y$CO)),xlab="log(CO source)",main="CO emission rates")
colnames(x)
length(x$CO[x$CO==0])/length(x$CO)
length(x$CO[x$CO==0 &x$Car=="P206"
&x$Ventilation=="W1/2"])/length(x$CO[x$Car=="P206"])
length(x$CO[x$CO==0
&x$Car=="P307"&x$Ventilation=="REC"])/length(x$CO[x$Car=="P307"])
length(x$CO[x$CO==0 &x$Car=="HV"
&x$Ventilation=="FA"])/length(x$CO[x$Car=="HV"])
length(x$CO[x$CO==0 &x$Car=="P206"])/length(x$CO[x$Car=="P206"])
length(x$CO[x$CO==0 &x$Car=="P307"])/length(x$CO[x$Car=="P307"])
length(x$CO[x$CO==0 &x$Car=="HV"])/length(x$CO[x$Car=="HV"])
length(x$CO[x$CO==0 &x$Ventilation=="W1/2"])/length(x$CO[x$Ventilation=="W1/2"])
length(x$CO[x$CO==0 &x$Ventilation=="REC"])/length(x$CO[x$Ventilation=="REC"])
length(x$CO[x$CO==0 &x$Ventilation=="FA"])/length(x$CO[x$Ventilation=="FA"])
max(x$CO)

hist(as.numeric(x$CO[x$CO!=0]))
hist(as.numeric(log(x$CO[log(x$CO)>-0.31])),xlab="log(CO source)",main="CO emission
rates above detection")
shapiro.test(log(x$CO[log(x$CO)>-0.31]))
require(car)
v<-x$Ventilation[log(x$CO)>- 0.31]
c<-x$Car[log(x$CO)>- 0.31]
s<-x$Speed[log(x$CO)>-0.31]
CO<-x$CO[log(x$CO)>- 0.31]
vif(lm(log(CO)~v+c+s))
a<-data.frame(CO,v,c,s)
null<-lm(log(CO)~1,data=a)
full<-lm(log(CO)~.,data=a)
step(null,scope=list(upper=full),direction="both")
full<-lm(log(CO)~.^2,data=a)
step(null,scope=list(upper=full),direction="both")

boxplot(log(CO)~v,data=a)
boxplot(log(CO)[a$v=="FA" &a$c=="HV"]~s[a$v=="FA" &a$c=="HV"],data=a)
boxplot(log(CO)[a$c=="HV"]~v[a$c=="HV"],data=a)
boxplot(log(CO)[a$v=="FA"]~c[a$v=="FA"],data=a)

##PM2.5
x<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/CONTAM vs MBE/MBE/cte
AER/PM.csv",header=T)
colnames(x)
y<-read.csv("C:/Users/Ghinwa/Documents/Documents/Thesis/CONTAM vs MBE/MBE/cte
AER/PMno0.csv",header=T)
hist(as.numeric(log(y$PM2.5)),xlab="log(PM2.5 source)",main="PM2.5 emission rates")
max(x$PM2.5)

length(x$PM2.5[x$PM2.5==0])/length(x$PM2.5)
```

```
length(x$PM2.5[x$PM2.5==0 &x$Car=="P206"
&x$Ventilation=="W1/2"])/length(x$PM2.5[x$Car=="P206"])
length(x$PM2.5[x$PM2.5==0
&x$Car=="P307"&x$Ventilation=="REC"])/length(x$PM2.5[x$Car=="P307"])
length(x$PM2.5[x$PM2.5==0 &x$Car=="HV"
&x$Ventilation=="FA"])/length(x$PM2.5[x$Car=="HV"])
length(x$PM2.5[x$PM2.5==0 &x$Car=="P206"])/length(x$PM2.5[x$Car=="P206"])
length(x$PM2.5[x$PM2.5==0 &x$Car=="P307"])/length(x$PM2.5[x$Car=="P307"])
length(x$PM2.5[x$PM2.5==0 &x$Car=="HV"])/length(x$PM2.5[x$Car=="HV"])

hist(as.numeric(x$PM2.5[x$PM2.5!=0]))
hist(as.numeric((x$PM2.5)))
shapiro.test(log(x$PM2.5[x$PM2.5!=0]))
hist(as.numeric(log(x$PM2.5[log(x$PM2.5)>-3.4])),xlab="log(PM2.5 source)",main="PM2.5
emission rates above detection")
shapiro.test(log(x$PM2.5[log(x$PM2.5)>- 3.4]))

v<-x$Ventilation[log(x$PM2.5)>- 3.4]
c<-x$Car[log(x$PM2.5)>- 3.4]
s<-x$Speed[log(x$PM2.5)>- 3.4]
PM2.5<-x$PM2.5[log(x$PM2.5)>- 3.4]
vif(lm(log(PM2.5)~v+c+s))
a<-data.frame(PM2.5,v,c,s)

null<-lm(log(PM2.5)~1,data=a)
full<-lm(log(PM2.5)~.,data=a)
step(null,scope=list(upper=full),direction="both")
full<-lm(log(PM2.5)~.^2,data=a)
step(null,scope=list(upper=full),direction="both")

boxplot(log(PM2.5)~v,data=a)
boxplot(log(PM2.5)[a$v=="FA" &a$c=="HV"]~s[a$v=="FA" &a$c=="HV"],data=a)
boxplot(log(PM2.5)[a$c=="HV"]~v[a$c=="HV"],data=a)
boxplot(log(PM2.5)[a$v=="FA"]~c[a$v=="FA"],data=a)
```