PM2.5 Speciation in MOVES2013

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PM Speciation

- **Background**
- **New Methodology**
  - New PM2.5 species
  - New Speciation Calculator
  - New Sulfate Calculator
  - New Crankcase Emission Calculator
- **New data**
  - New speciation profiles
  - Data on fuel and lubricating oil sulfur on sulfate emissions
  - Data on updated crankcase emissions

Background

- **PM2.5 speciation data**
  - Shows differences in profiles according to:
    - Technology, Model year
    - Fuel Type
    - Emission process (running, start, extended idle)
- **PM Speciation in MOVES2013**
  - Allows differentiation in PM speciation profiles by:
    - Technology/Regulatory class (e.g. pre-2007/2007+ diesel)
    - Model year
    - Fuel Type
    - Emission process (running, start, extended idle)
- **Additional PM species needed for air quality models**

$PM_{2.5}$ Species in MOVES 2013

Revised definition in MOVES 2013 to be consistent with CMAQ5.0

In MOVES 2010

New PM species in MOVES2013

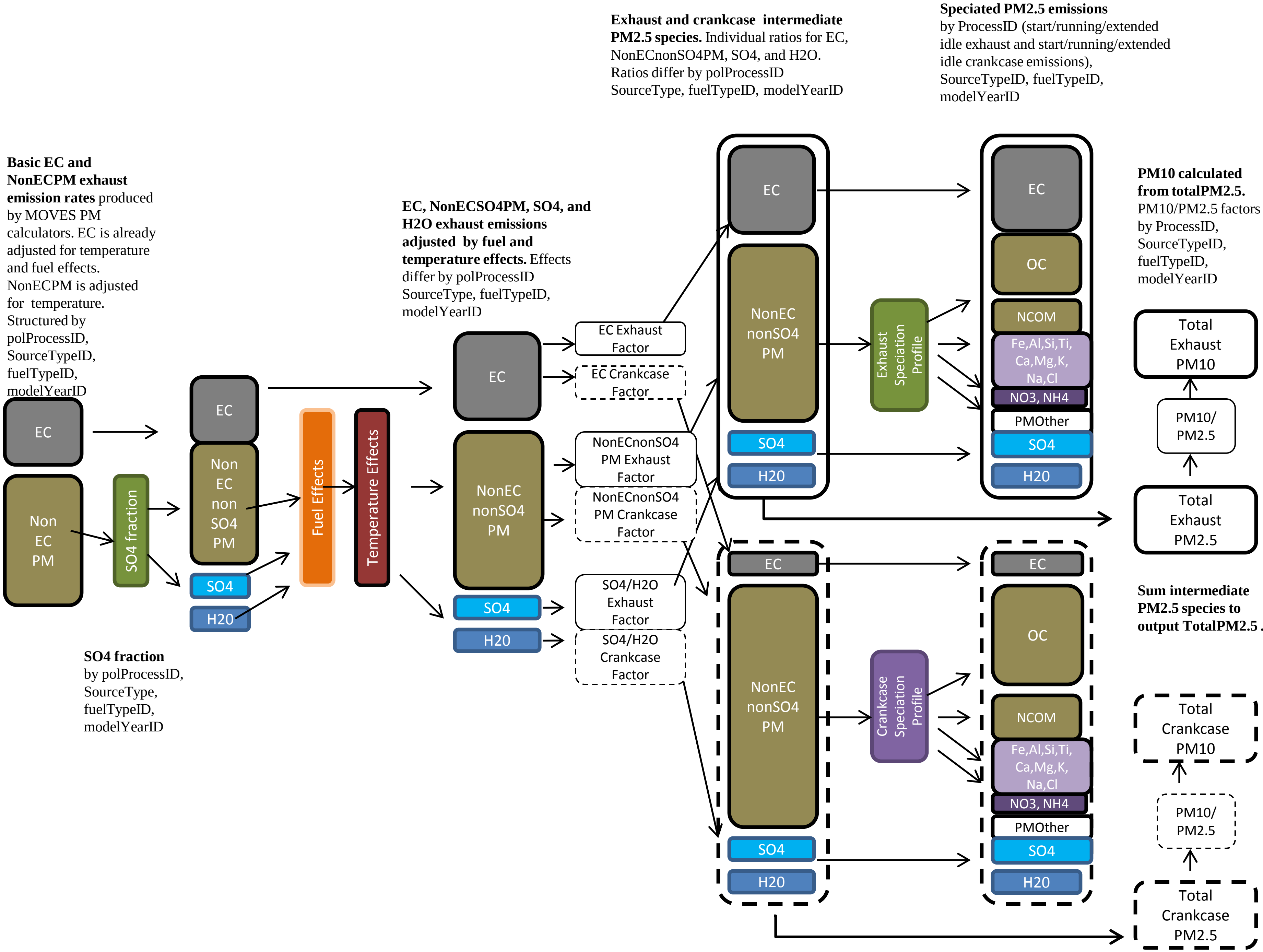
New CMAQv5.0 species included to improve modeling of organic mass, atmospheric chemistry, anthropogenic sources, and model validations with receptor measurements[1]

PM2.5 Species	CMAQv5.0 Species Name	Required in CMAQv4.7.1	Required in CAMx5.4
Primary organic carbon	POC	x	x
Elemental carbon	PEC	x	x
Sulfate	PSO4	x	x
Nitrate	PNO3	x	x
Ammonium	PNH4	x	x
Non-carbon organic matter	PNCOM		x
Iron	PFE		
Aluminum	PAL		
Silica	PSI		
Titanium	PTI		
Calcium	PCA		
Magnesium	PMG		
Potassium	PK		
Manganese	PMN		
Sodium	PNA		x
Chloride	PCL		x
Water	PH2O		x
Primary unspeciated PM2.5	PMOTHR	x	x

1. Simon, H.; CMAQv5.0 PM other speciation. http://www.airqualitymodeling.org/cmaqwiki/index.php?title=CMAQv5.0_PMother_speciation

PM Speciation Overview

1. Intermediate Speciation
   - Individual and composite species used to simplify/facilitate PM2.5 emission rate adjustments and calculations
   - Intermediate species:
     - EC: Elemental carbon
     - NonECPM: Non-elemental carbon
     - NonECnonSO4PM: Non-elemental carbon, non-sulfate particulate matter
     - SO4: Sulfate
     - H2O (aerosol): Sulfate-bound water
   - Fuel & temperature effects applied to the intermediate species
2. Full Speciation
   - Produces all 18 PM2.5 species needed air quality models



Basic EC and NonECPM exhaust emission rates produced by MOVES PM calculators. EC is already adjusted for temperature and fuel effects. NonECPM is adjusted for temperature. Structured by polProcessID, SourceTypeID, fuelTypeID, modelYearID
EC
Non EC PM
SO4 fraction
SO4 fraction by polProcessID, SourceType, fuelTypeID, modelYearID
EC
Non EC non SO4 PM
SO4
H20
Fuel Effects
Temperature Effects
EC, NonECSO4PM, SO4, and H2O exhaust emissions adjusted by fuel and temperature effects. Effects differ by polProcessID SourceType, fuelTypeID, modelYearID
EC
NonEC nonSO4 PM
SO4
H20
EC Exhaust Factor
EC Crankcase Factor
NonECnonSO4 PM Exhaust Factor
NonECnonSO4 PM Crankcase Factor
SO4/H2O Exhaust Factor
SO4/H2O Crankcase Factor
Exhaust and crankcase intermediate PM2.5 species. Individual ratios for EC, NonECnonSO4PM, SO4, and H2O. Ratios differ by polProcessID SourceType, fuelTypeID, modelYearID
EC
NonEC nonSO4 PM
SO4
H20
Exhaust Speciation Profile
Crankcase Speciation Profile
Speciated PM2.5 emissions by ProcessID (start/running/extended idle exhaust and start/running/extended idle crankcase emissions), SourceTypeID, fuelTypeID, modelYearID
EC
OC
NCOM
Fe,Al,Si,Ti, Ca,Mg,K, Na,Cl
NO3, NH4
PMOther
SO4
H20
PM10 calculated from totalPM2.5. PM10/PM2.5 factors by ProcessID, SourceTypeID, fuelTypeID, modelYearID
Total Exhaust PM10
PM10/ PM2.5
Total Exhaust PM2.5
Sum intermediate PM2.5 species to output TotalPM2.5 .
Total Crankcase PM10
PM10/ PM2.5
Total Crankcase PM2.5

PM Speciation Steps

- **Intermediate Speciation**

1. Use EC and NonECPM emission rates
   - EC already adjusted for fuel effects
   - Both already adjusted for temperature effects
   - Stored at the operating mode level to model EC/PM differences by operating mode
2. Calculate SO4, H2O (aerosol), and nonECnonSO4 from the nonECPM
3. Adjust SO4, H2O (aerosol) for fuel effects:
   - Sulfate Calculator: SO4/H2O
   - Fuel effects: nonECnonSO4
4. Adjust SO4, H2O, nonECnonSO4 for temperature effects
   - (Not used at this time because general temperature effects applied previous to step 1)
   - Coded such that different temperature effects can be applied

PM Speciation Steps

5. Calculate exhaust and crankcase emissions
6. Sum intermediate species (EC, nonECnonSO4, SO4, H2O (aerosol)) to calculate total PM2.5 emissions
7. Calculate PM10 emissions using $PM_{10}/PM_{2.5}$ ratios

	$PM_{10}/PM_{2.5}$
gasoline	1.130
diesel	1.087

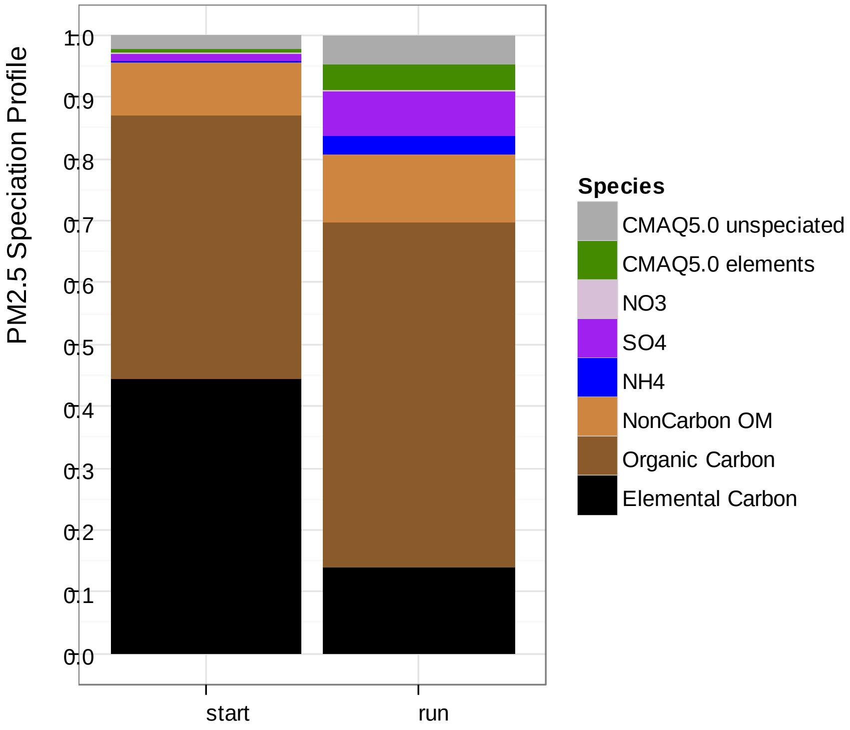
8. **Full Speciation:** Apply speciation profiles to nonECnonSO4 to calculate PM2.5 species needed for CMAQ
9. Calculate additional particle-phase metal compounds required for the national emissions inventory, not included in the PM speciation calculator
   – Discussed in “Additional Toxics Presentations”

$PM_{2.5}$ Profiles in MOVES 2013

- **Kansas City Light-duty Gasoline Vehicle Study (CRC E-69)**
  - Stratified random sample of vehicles in Kansas City Area
  - Conducted in Summer/Winter of 2004-2005
  - Source of $PM_{2.5}$ emission rates in MOVES
  - Speciated $PM_{2.5}$ data
    - 99 vehicles tested for speciation of total 496 tested vehicles
    - Included Summer/Winter testing
    - In-use vehicles ranging from 1976 to 2004 model year
- **HD Vehicle Chassis Dyno Testing for Emissions Inventory (CRC E-55/E59)**
  - Conducted 2001-2005
  - Source of PM Emission rates in MOVES
  - Speciated $PM_{2.5}$ data
    - Available by driving schedule (idle, cruise, transient)
    - 9 trucks tested for speciation of 75 total vehicles
    - In-use vehicles ranging from 1985 to 2004 model year
- **Phase 1 of the HEI & CRC Advanced Collaborative Emissions Study**
  - 2007+ Technology
    - Four 2007 heavy-duty diesel engines
  - Includes exhaust and crankcase speciation measurements
  - Source of updated 2007+ Diesel crankcase emission factors

Kansas City Light-Duty Gasoline $PM_{2.5}$

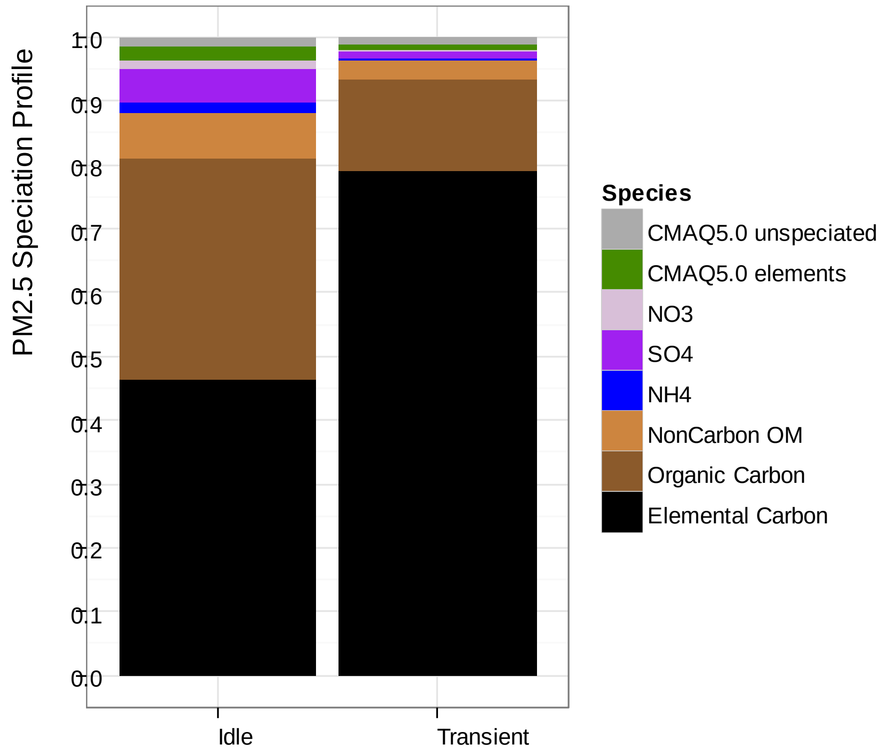
- **Weighted Mean by Start and Running Emissions**
  - Weighted according to PM emissions and vehicle-miles traveled of each vehicle class
- **Elemental Carbon**
  - Used to update EC rates in MOVES2013
- **Organic Matter**
  - Organic matter (OM) scaled down to achieve mass balance and correct for positive artifact (Reff et al. 2009)
  - OM ~ 1.2 * OC
- **Elements, Sulfate, other Ions**
  - Larger contribution to running
- **PM sampling artifact removed from profile and emission rates**
  - Silicone sampling lines contributed to PM measurements
  - PM2.5 LDGV running rates reduced ~ 13 - 14% compared to MOVES2010



CRC E-55/E59 Heavy-Duty Diesel $PM_{2.5}$

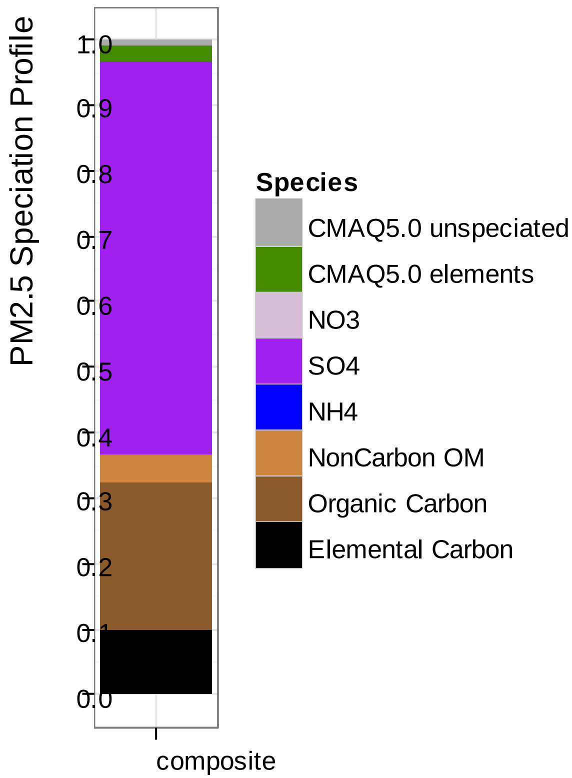
- **Median profile by idle and transient cycles**
  - Median used due to small sample size
  - Idle cycle for extended idle and start
  - Transient cycle for running emission
- **MOVES2013 maintains load-based EC/PM fractions developed for conventional diesel in MOVES**
  - EC/PM fractions compare well between load based rates and speciation profiles
  - Use updated profile fraction to estimate non-EC species:
  - Larger % of inorganic species on the idle cycle

	Extended Idle	Start	Running
MOVES2013 EC/PM Rates	26.6%	33.2%	79.4%
E55/59 $PM_{2.5}$ Speciation profile	46.4%	46.4%	79.0%



Phase 1 ACES 2007+ Heavy-Duty Diesel $PM_{2.5}$

- **Contains tailpipe exhaust + crankcase emissions**
  - Four 2007 heavy-duty diesel engines
  - 16-hour cycle
    - Contains FTP and CARB 5-Modes
    - Captures diesel particulate filter regeneration events
    - Gains sufficient PM mass for speciation analysis
- **Large SO4 contribution**
- **Used to inform EC and SO4 speciation rates in MOVES2010**
- **Updated in MOVES2013 to include additional CMAQ PM2.5 species**



MOVES2013 Sulfate Calculator

1. **Sulfate emissions based on PM2.5 speciation profiles**
   - MOVES can replicate PM profiles measured in exhaust test-programs
   - Sulfate contribution to base PM2.5 rates is accounted for
   - Total PM = Sum of PM species
2. **Accounts for fuel and lube oil contributions**
   - Adjusted to the fuel sulfur level
   - Accounts for contribution from lubricating oil

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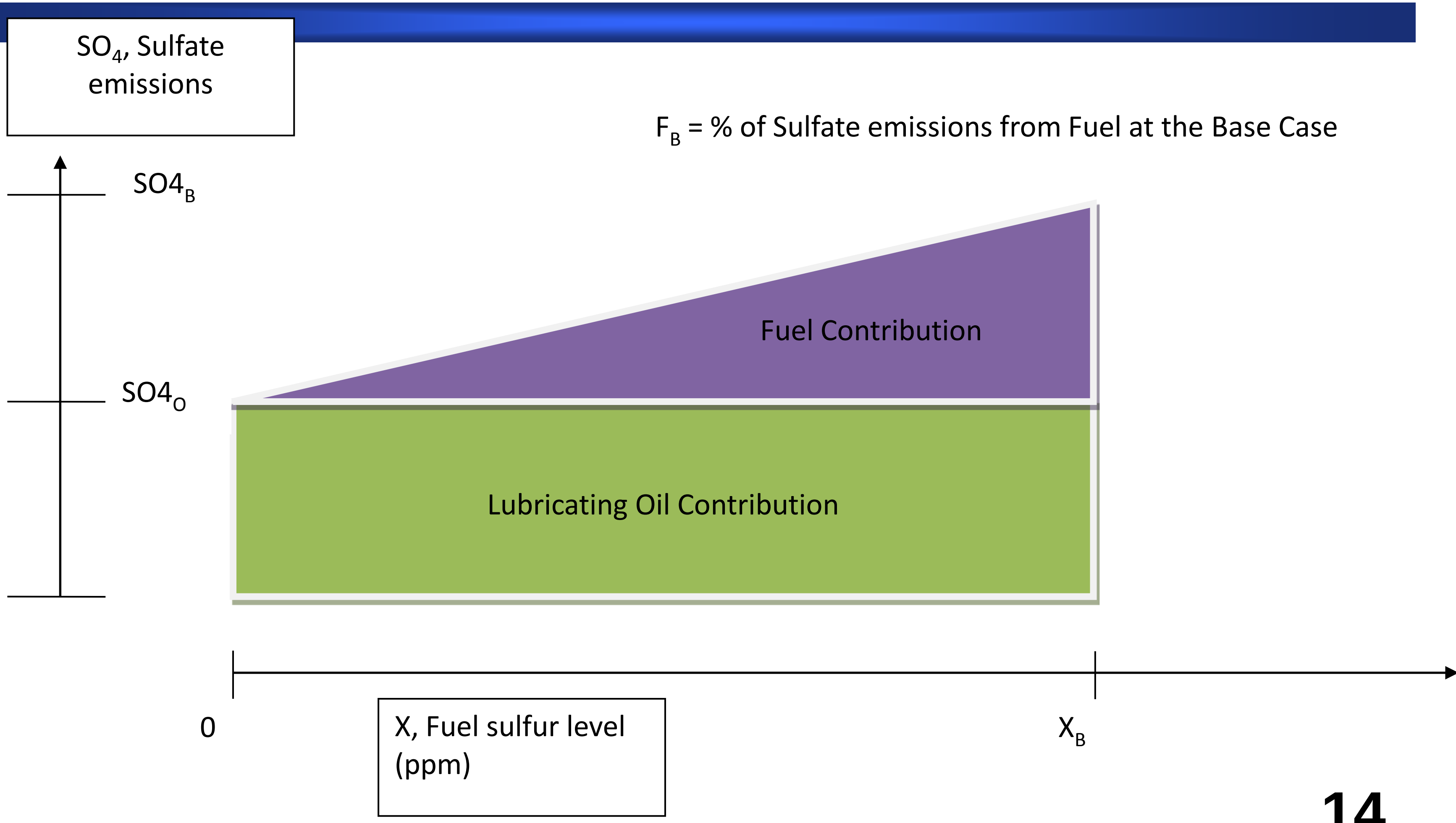
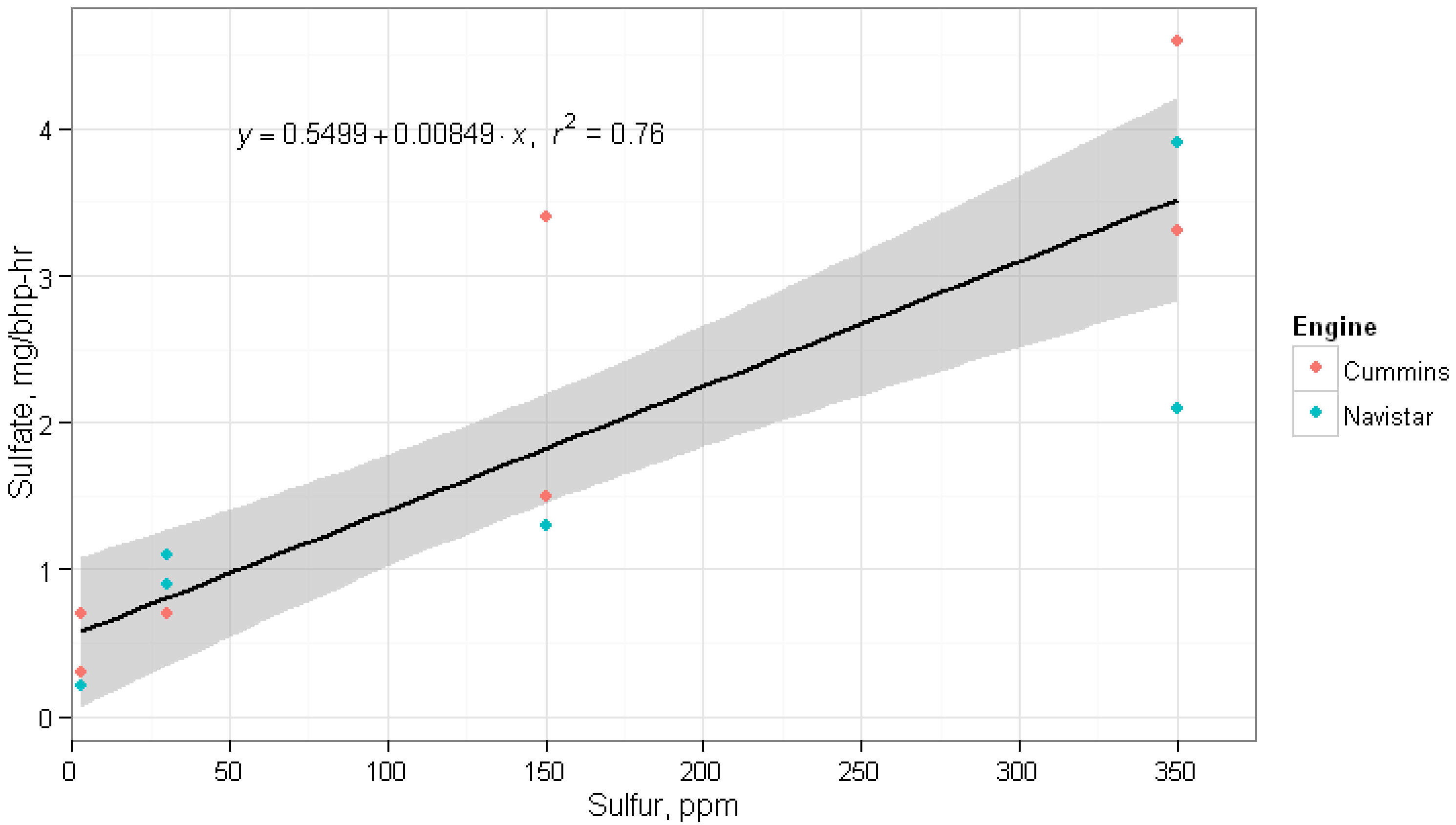
MOVES2013 Sulfate Calculator



Sulfate Calculator Values for Conventional Diesel



Data from the DECSE (2001) project

MOVES2013 Sulfate Calculator

- **Gasoline vehicles**
  - Coefficients estimated from sulfate measurements made with high sulfur fuel (Kansas City Light-duty Vehicle Emissions Study) and EPA in-house testing at low sulfur fuel, (Sobotowski,2013)
- **Conventional Diesel (pre-2007)**
  - Regression of sulfate vs. fuel sulfur measurements from the Diesel Emissions Control- Sulfur Effects Project (DECSE 2001)
- **2007+ Diesel**
  - Coefficients from model estimated by Kittelson et al. (2008) *Effect of fuel and lube oil sulfur on the performance of a diesel exhaust gas Continuously Regenerating Trap.*

MOVES2013 Sulfate Calculator

Source	Process	$SO_4/PM_{2.5}$ fraction	SO_4/NonEC PM fraction (S_B)	Fuel sulfur Level, ppm (x_B)	Estimated fraction from fuel sulfur (F_B)
Gasoline	running exhaust	7.2%	8.4%	161.2	68.7%
	start exhaust	0.9%	1.7%		
Pre-2007 diesel	running exhaust	1.0%	4.9%	172.0	72.6%
	extended idle and start	5.3%	9.8%		
Post-2007 diesel	running, extended idle, start	67.6%	73.6%	11.0	48.3%

$$SO4_x = NonECPM \times S_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1\right)\right]$$

S_B = reference sulfate fraction
x = the user- supplied or default fuel sulfur level for the MOVES run
x_B = reference fuel sulfur level
F_B =the percentage of sulfate originating from the fuel sulfur in the reference case, and
$SO4_x$ = sulfate emissions at the fuel sulfur content for the MOVES run

MOVES2013 Sulfate Calculator: Example

1. ***Calculate sulfate emissions from 100 grams of gasoline PM from a passenger car at 5 ppm fuel sulfur content***

MOVES2013 Sulfate Calculator: Example

1. ***Calculate sulfate emissions from 100 grams of gasoline PM from a passenger car at 5 ppm fuel sulfur content***
   - *EC=14, NonECPM = 86*
   - *Fraction of sulfate in NonECPM, S_B = 8.4%*
   - *Fuel contribution to sulfate, F_B = 68.7%*
   - *Reference fuel sulfur level from Kansas City, x_B = 161.2*
   - *Fuel sulfur content, x = 5*

Source	Process	$SO_4/PM_{2.5}$ fraction	SO_4/NonEC PM fraction (S_B)	Fuel sulfur Level, ppm (x_B)	Estimated fraction from fuel sulfur (F_B)
Gasoline	running exhaust	7.2%	8.4%	161.2	68.7%

MOVES2013 Sulfate Calculator: Example

1. ***Calculate sulfate emissions from 100 grams of gasoline PM from a passenger car at 5 ppm fuel sulfur content***
   - *EC=14, NonECPM = 86*
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   - *Fuel contribution to sulfate, F_B = 68.7%*
   - *Reference fuel sulfur level from Kansas City, x_B = 161.2*
   - *Fuel sulfur content, x = 5*

$$SO4_x = NonECPM \times S_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1\right)\right]$$

$$SO4_x = 86 \times 0.084 \times \left[1 + 0.687 \times \left(\frac{5}{161.2} - 1\right)\right]$$

$$SO4_x = 7.2 \times [0.33] = 2.4$$

Answer: By reducing the sulfur level from 161.2 to 5 ppm, the sulfate is reduced by 2/3 to 2.4 grams SO4

Updates to SO_2 Calculator

Source	MOVES2010b SO2 conversion values (%)	MOVES2013 SO2 conversion values (%)
Gasoline	99.84%	99.69%
Pre-2007 Diesel	98.00%	97.48%
2007 Diesel	54.16%	88.15%

Large increase in SO2 conversion, because lube oil contribution large fraction of the diesel 2007+ sulfate emissions

SO2 fractions updated to be consistent with SO4 updates

MOVES2013 Crankcase Calculator

1. Speciation different between crankcase and exhaust emissions
2. Crankcase emissions for 2007+ diesel engines are included with the exhaust measurements for certification

Background: Diesel Crankcase Emissions

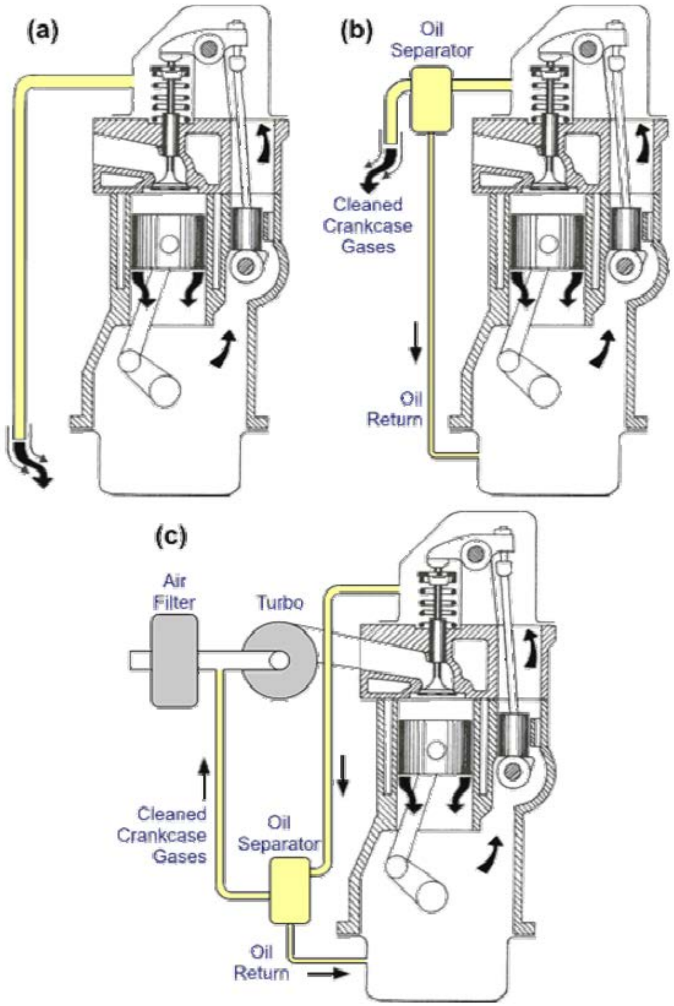


Figure 6. Crankcase Ventilation Systems
(a) Open unfiltered crankcase ("road draft tube"); (b) Open crankcase filtration system; (c) Closed crankcase ventilation (CCV)

a) **Open unfiltered crankcase**
   - 'Road draft tube'
   - Used on pre-2007 turbocharged diesel engines

b) **Open crankcase filtration system**
   - Most 2007+ heavy-duty diesel engines
   - Crankcase emissions included in certification measurement
   - DPFs lower emissions substantially, such that engines can meet the standard with filtered crankcase emissions.

c) **Closed system**
   - Degrades turbocharger performance

d) **Routing the crankcase to the DPF (not shown)**
   - Poisons the DPF
   - Requires a pump in the crankcase to overcome pressure differential in DPF

Source: Dieselnet, ACES program

Speciation Differences

- **Conventional Diesel Crankcase Emissions**
  - Blow-by gases + oil droplets
  - Large OC/PM fraction
- **Conventional Diesel Exhaust**
  - Large EC/PM fraction

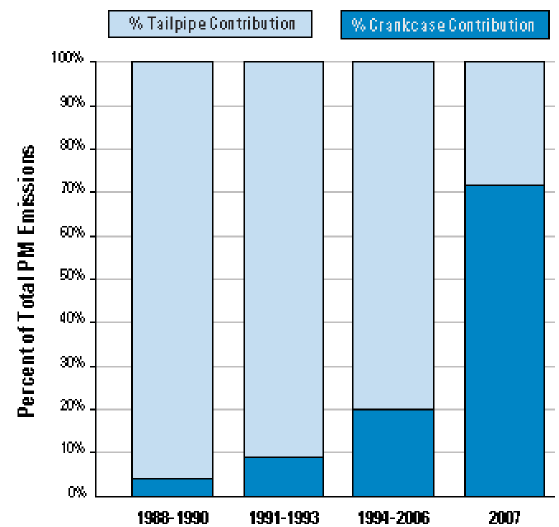
Measurements made on two conventional diesel transit buses (Zielinska et al. 2008)

	Crankcase	Tailpipe Exhaust
EC/PM2.5	1.57%	81.05%

Large Crankcase Contribution

- Crankcase contributes a larger fraction of the total emissions
- Crankcase emissions included in the regulatory measurements of 2007+ diesel engine

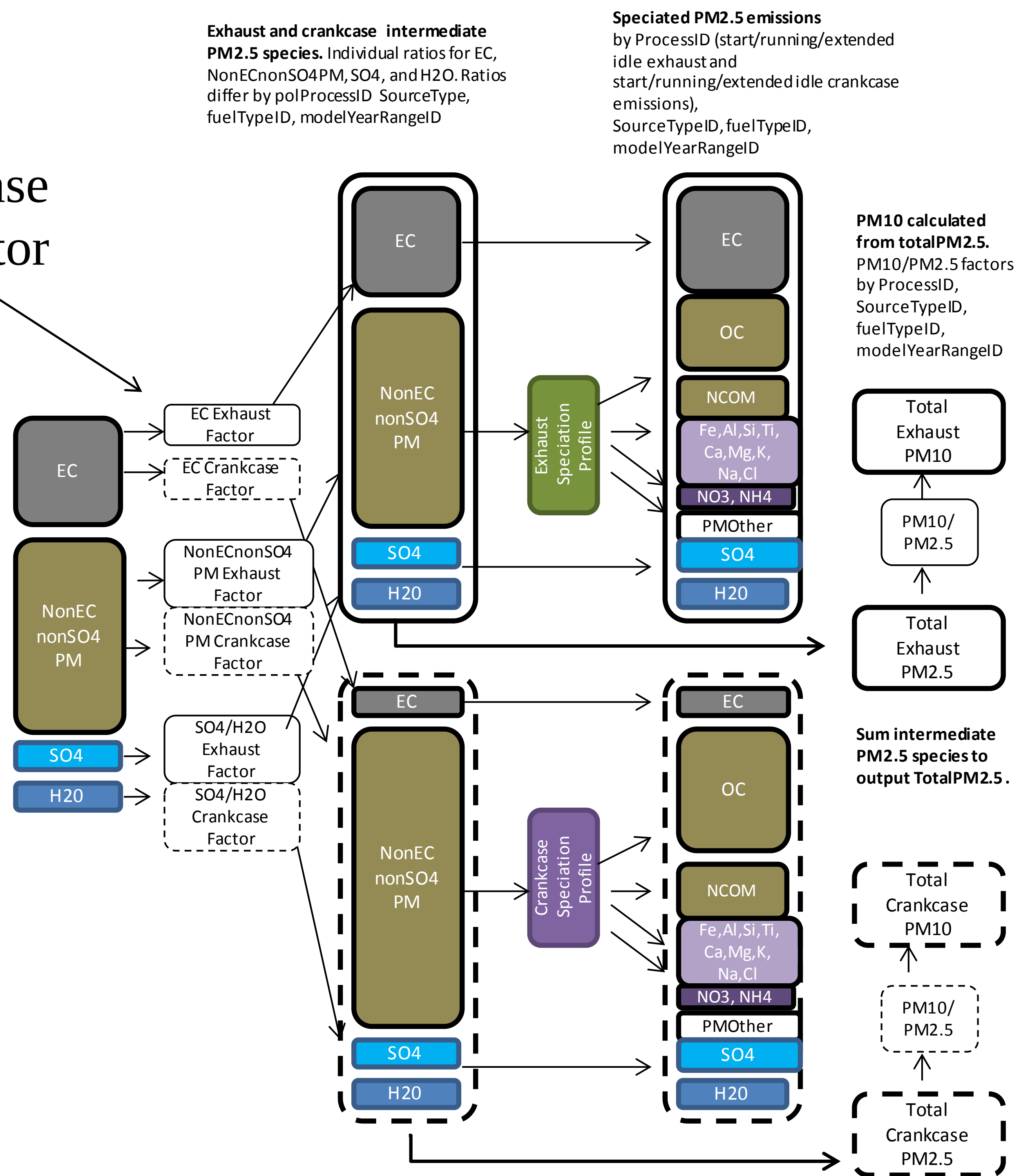
FIGURE 1
EMISSIONS CONTRIBUTIONS TAILPIPE & CRANKCASE



Crankcase emissions levels in diesel engines have remained relatively low compared to tailpipe emissions until 2006. On newer engines, as emissions from tailpipes reduce, crankcase emissions become a greater share of total allowable particulate matter (PM) emissions.

Source: Donaldson Filtration Solutions

Crankcase Calculator



MOVES2013 Crankcase Values for Diesel PM2.5

		Pre-2007 Diesel			2007+ Diesel
Pollutant	Process	Start	Running	Extended Idle	All processes
EC	Exhaust	1	1	1	0.62
nonECnonSO4PM		1	1	1	0.62
SO4		1	1	1	0.62
H2O		1	1	1	0.62
EC	Crankcase	0.009	0.004	0.012	0.38
nonECnonSO4PM		0.295	0.954	0.268	0.38
SO4		0.295	0.954	0.268	0.38
H2O		0.295	0.954	0.268	0.38

Splits 2007+ diesel emissions into exhaust and crankcase emissions

The pre-2007 diesel crankcase emission factors shown are derived such that the crankcase PM2.5 emissions are 20% of the PM2.5 exhaust measurements, and have an EC/PM split of 1.57%.

MOVES2013 Crankcase Calculator: Example

1. ***Calculate Crankcase emissions from 100 grams of conventional diesel running PM. What is the EC/PM fraction?***

MOVES2013 Crankcase Calculator: Example

1. ***Calculate Crankcase emissions from 100 grams of conventional diesel running PM. What is the EC/PM fraction?***

	Running Emissions				
EC	79				
nonECnonSO4PM	20				
SO4	1				
H2O	0				
Sum =	100				
EC/PM =	79.4%				

MOVES2013 Crankcase Calculator: Example

1. ***Calculate Crankcase emissions from 100 grams of conventional diesel running PM. What is the EC/PM fraction?***

	Running Emissions		Crankcase Emissions Factor		Crankcase Emissions
EC	79	x	0.004	=	0.31
nonECnonSO4PM	20	x	0.954	=	18.72
SO4	1	x	0.954	=	0.96
H2O	0	x	0.954	=	0
Sum =	100				
EC/PM =	79.4%				

MOVES2013 Crankcase Calculator: Example

1. ***Calculate Crankcase emissions from 100 grams of conventional diesel running PM. What is the EC/PM fraction?***

	Running Emissions		Crankcase Emissions Factor		Crankcase Emissions
EC	79	x	0.004	=	0.31
nonECnonSO4PM	20	x	0.954	=	18.72
SO4	1	x	0.954	=	0.96
H2O	0	x	0.954	=	0
Sum =	100				20
EC/PM =	79.4%				1.6%

Answer: Crankcase PM2.5 = 20 grams

EC/PM = 1.6% (same as measured by Zielinska et al. 2008)

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MOVES2013
2007+ Diesel Crankcase Emissions

- **PM2.5 Speciation**
  - Speciation measurements in ACES combined exhaust + crankcase emissions
  - Same speciation applied to exhaust and crankcase emissions
- **Crankcase emissions**
  - Included in the base PM rates for 2007 diesel which are estimated on certification standards
  - 38% of total emissions (tailpipe+ crankcase)
    - CRC ACES Phase 1 Program
- **MOVES2013**
  - Splits 2007+ diesel emissions into exhaust and crankcase emissions

		2007+ Diesel
Pollutant	Process	All processes
EC	Exhaust	0.62
nonECnonSO4PM		0.62
SO4		0.62
H2O		0.62
EC	Crank-case	0.38
nonECnonSO4PM		0.38
SO4		0.38
H2O		0.38

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Summary

- **Calculates PM2.5 species needed for air quality modeling**
- **Incorporates differences in PM2.5 speciation by:**
  - Source Type
  - Fuel type
  - Temperature
  - Model year/technology
  - Emission process
- **New sulfate calculator**
  - Based on PM2.5 speciation
  - Accounts for sulfate contribution from lubricating oil and fuel
- **New crankcase calculator**
  - Accounts for crankcase emissions in the exhaust measurements
  - Calculates separate PM2.5 speciation for tailpipe and crankcase

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PM Speciation

Reductions to PM2.5 in MOVES2013 compared to MOVES2010b due to silicone contamination.

Strata	Vehicle Type	Model group	Start	Running
1	Truck	pre-1981	0%	35.3%
2		1981-1990	0%	25.3%
3		1991-1995	0%	34.5%
4		1996-2005	0%	19.1%
5	Car	pre-1981	0%	14.6%
6		1981-1990	0%	3.5%
7		1991-1995	0%	6.1%
8		1996-2005	0%	8.5%

Updated Light-duty EC/PM2.5 ratios

Updated EC/PM2.5 ratios by start and running in MOVES2013

	Start EC/PM		Running EC/PM	
Vehicle Type	MOVES2010	MOVES2013	MOVES2010	MOVES2013
Car	35.0%	44.4%	18.0%	14.0%
Truck	33.0%		7.0%	

MOVES2013 Crankcase Values

		Pre-2007 Diesel			2007+ Diesel	1969-2050 Gasoline/CNG	1960-1968 Gasoline Vehicles	Gasoline Motor-cycles
Pollutant	Process	Start	Running	Extended Idle	All processes	All processes	All processes	All processes
EC	Exhaust	1	1	1	0.62	1	1	1
nonECnonSO4PM		1	1	1	0.62	1	1	1
SO4		1	1	1	0.62	1	1	1
H2O		1	1	1	0.62	1	1	1
EC	Crankcase	0.009	0.004	0.012	0.38	0.008	0.2	0
nonECnonSO4PM		0.295	0.954	0.268	0.38	0.008	0.2	0
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