



UNIVERSITY OF
BIRMINGHAM

Soot Formation and Particulate Characteristics in the Cylinder and Exhaust Pipe of a Gasoline Direct Injection Engine

Aawishkar Dharmadhikari, Yusong Yu, Haoye Liu and Hongming Xu

**Department of Mechanical Engineering
University of Birmingham**

Cambridge Particle Meeting 2018
15th June, 2018



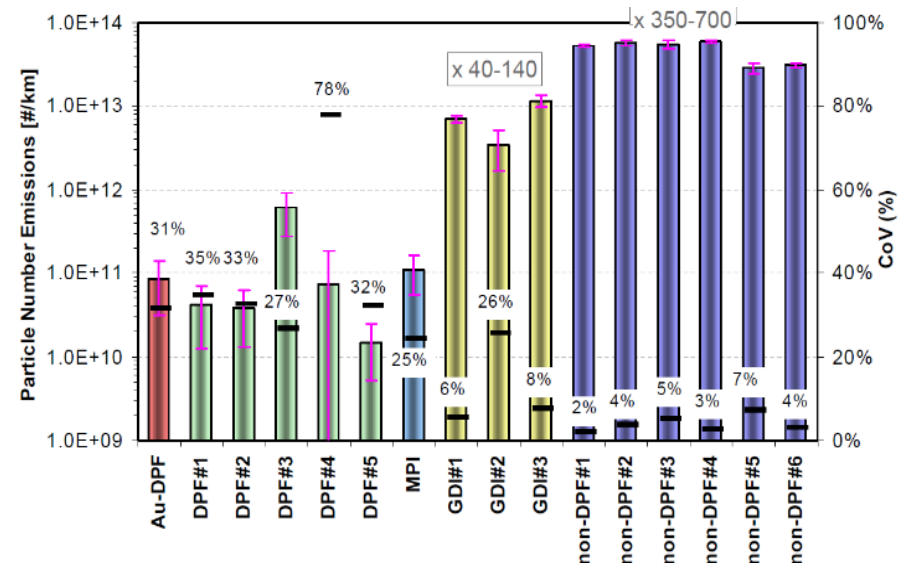
Outline

- **Introduction**
- **Objectives**
- **Engine and Experimental System**
- **Simulation Models**
 - Stochastic Reactor Model (SRM)
 - Particle Growth Model (PGM)
- **Experiment Results and Discussion**
 - Particulate Matter Results
 - Gas Emissions Results
- **Modeling Results and Discussion**
 - Particle Growth Model Results
- **Conclusions and Future Plan**

Introduction



- The research evidence reported by the **European Particle Measurement Programme (PMP)** shows that, the measurement of PM emissions from gasoline engines varies significantly during vehicle tests and its variation is several times higher than those from diesel vehicles.
- **Strict gasoline emission legislations** imposed on light and heavy-duty vehicles have been of prime consideration in automotive industry.
- Importance of investigating the evolution of particle formation and growth in both **engine cylinder and the exhaust system.**



Objectives

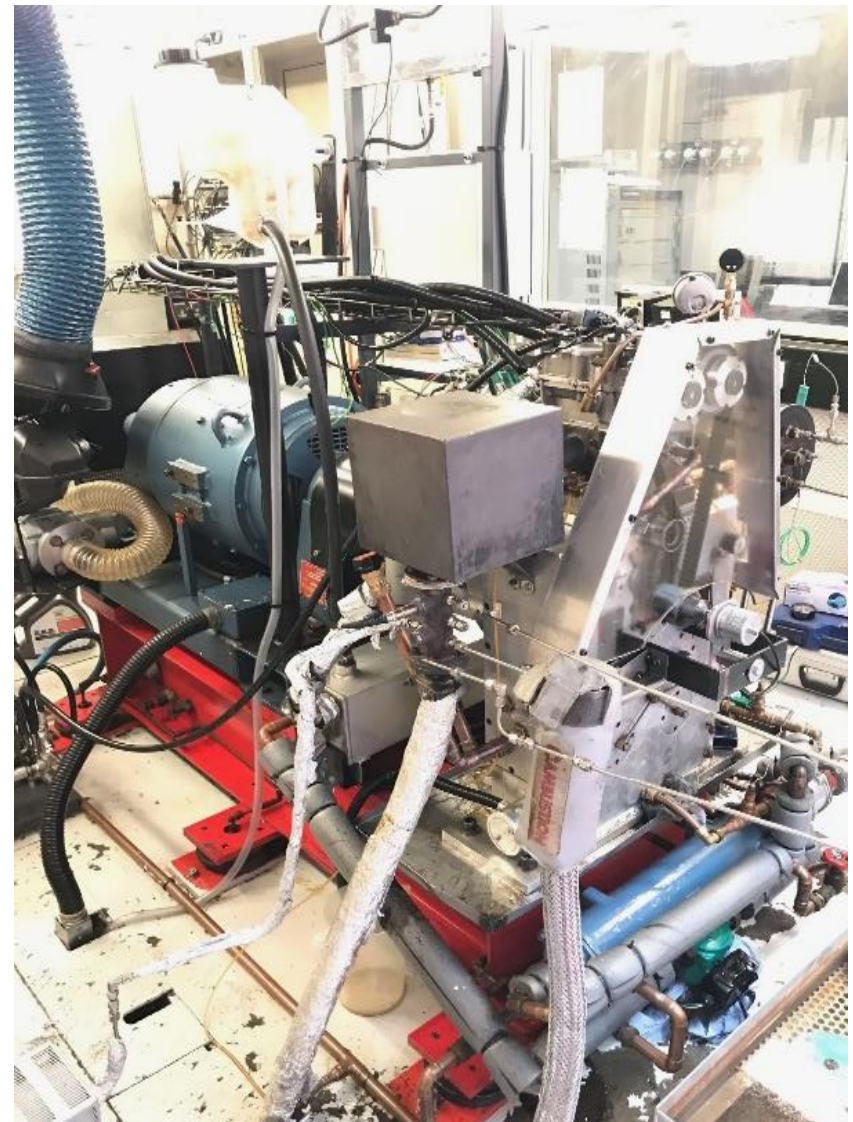


- **To investigate soot formation in the cylinder of a Gasoline Direct Injection (GDI) engine using modelling and experimental approaches**
- **To develop a combined mathematical model to investigate surface growth and particulate trends along an exhaust pipe**
- **To study particulate characteristics in the gasoline exhaust pipe, including particle evolution, particle inception, coagulation, and volatile species condensation**

GDI Experimental Setup



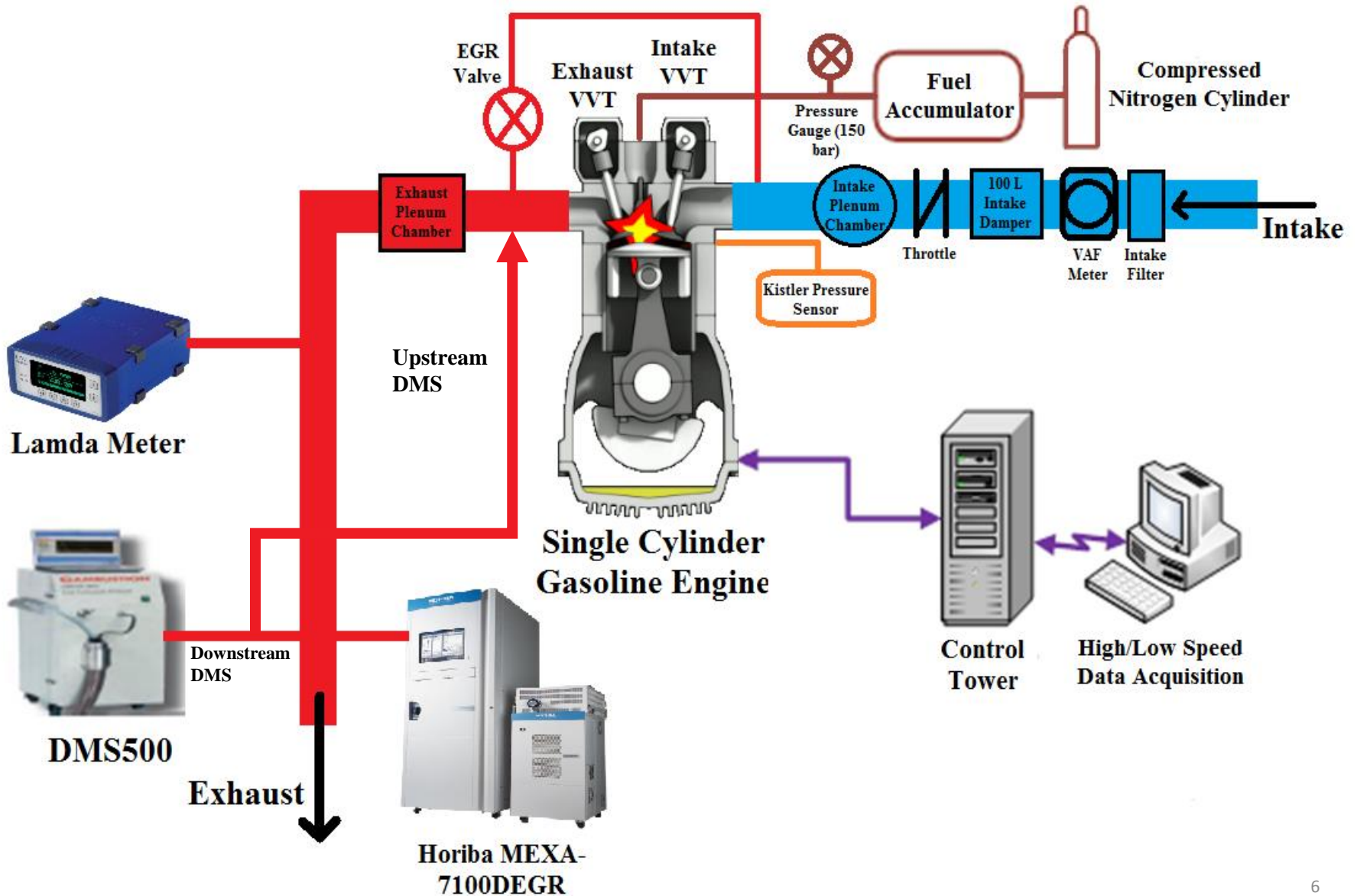
Speed (r/min)	1500
Fuel	ULG
Displacement Volume (cc)	500
Equivalence ratio	1
Injection pressure (MPa)	15
Spark timing (CA BTDC)	25
IMEP (bar)	5.5
Injection timing(CA BTDC)	100-360
Testing position	Upstream/ Downstream exhaust plenum chamber
Corresponding exhaust temperature (C deg)	650/300



GDI Experimental Setup



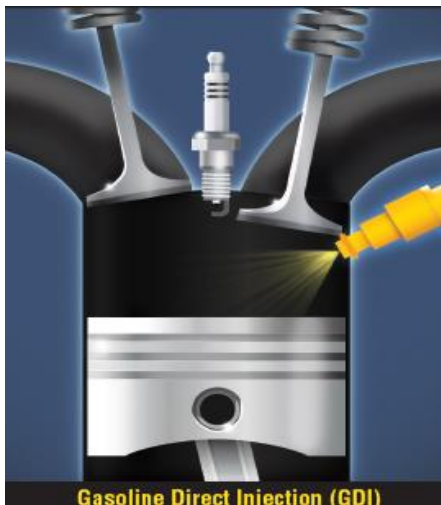
UNIVERSITY OF BIRMINGHAM



Stochastic Reactor Model (SRM) Setup

Model in-cylinder soot formation and morphology (fuel to agglomerates) using SRM Engine Suite

- **Stochastic Reaction Model (SRM Engine Suite):** spatially zero-dimensional, based on Probability Density Function (PDF)
- Detailed information on the **soot morphology** and **bulk quantities** (number concentration, mass concentration, particle size distribution)



Simulate for internal combustion engine performance and exhaust emissions.

Model heat transfer, DI, SI, Soot formation inclusive of chemical mechanisms.

Precise Particulate Matter (PM) Estimation for variant fuels and engine operating conditions

Particle Growth Model (PGM) Construction

Particulate Matter modelling to investigate

- **Nucleation** and **condensation** of volatile species, **coagulation** and particles **deposition** processes are considered and modelled.

(1) Nucleation model (CNT formulation, Becker-Döring et al., 1935)

$$R_n = \frac{(\rho_g \xi_i)^2}{\rho_i w_i} \sqrt{\frac{2\sigma_i}{\pi w_i}} \exp\left(-\frac{\Delta G^*}{k_B T}\right) \left(\frac{m_p^*}{w_i}\right)^{2/3}$$

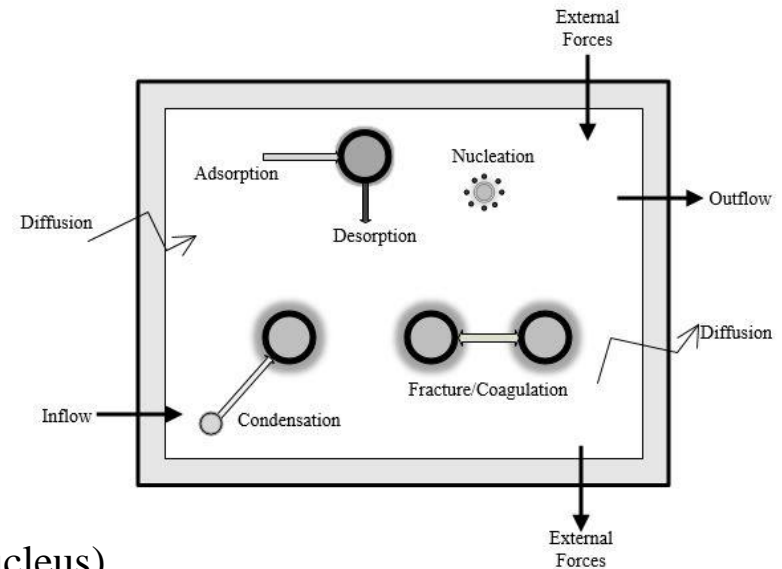
(The nucleation rate)

$$\Delta G^* = \frac{4}{3} \pi r^{*2} \sigma$$

(The nucleation barrier)

$$r^* = \frac{2\sigma}{k_B T \ln S}$$

(The radius of critical nucleus)



- Where 'i' is the nucleating species; ξ represents the mass fraction of each gaseous species;
- ρ_g is the gas density; ρ_i is the liquid density of 'i' species; w_i is the molecular weight;
- σ is the surface tension coefficient; k_B is the Boltzmann constant; T is gas temperature;
- m_p^* is the mass of the critical cluster; S is the vapor super saturation ratio ($S = p/p^*$).

Particle Growth Model (PGM) Construction

(2) Condensation model (Kulmala et al., 1998)

$$R_c = 2\pi\bar{D}_{pj}\beta_{M,ij}D_i \left[N_i - \Gamma_{ij}N_{ie} \exp\left(\frac{4\sigma_i\mu_i}{k_B T_{pj}\rho_j\bar{D}_{pj}}\right) \right] N_j$$

$$\beta_{M,ij} = \frac{0.75(1 + Kn_{ij})}{Kn_{ij}^2 + Kn_{ij} + 0.283Kn_{ij} + 0.75} \quad \text{Fuchs-Sutugin expression}$$

- Where N_{ie} is the equilibrium molecular concentration over a flat surface;
- $\beta_{M,ij}$ is the correction factors; Kn_{ij} is the Knudsen number; D_i is the i-vapor diffusion coefficient.
- \bar{D}_{pj} is the mean diameter of each particle zone; Γ is the activity coefficients.

(3) Deposition model (Williams and Loyalka, 1991)

$$k = 0.042Re \left(\frac{0.0791}{Re^{1/4}} \right)^{1/2} Sc^{1/3} \frac{D}{d}$$

- Where Re is the Reynolds number for the conditions in the exhaust pipe;
- Sc is the Schmidt number; D is the pipe diameter; d is the mean droplet diameter.

Particle Growth Model (PGM) Construction

(4) Coagulation model (Fuchs interpolation formula, Seinfeld, 1986) The rate of change of particle concentration

$$\frac{dN}{dt} = -\frac{1}{2}\beta(v_1, v_2)N^2$$

- Where β the collision frequency by Fuchs interpolation formula:

$$\beta = 2\pi (d_{p_i} + d_{p_j}) (D_i + D_j) \left[\frac{d_{p_i} + d_{p_j}}{d_{p_i} + d_{p_j} + 2g_{ij}} + \frac{8(D_i + D_j)}{c_{ij} (d_{p_i} + d_{p_j})} \right]^{-1}$$

$$c_{ij} = \sqrt{\bar{c}_i^2 + \bar{c}_j^2} \quad g_{ij} = \sqrt{g_i^2 + g_j^2}$$

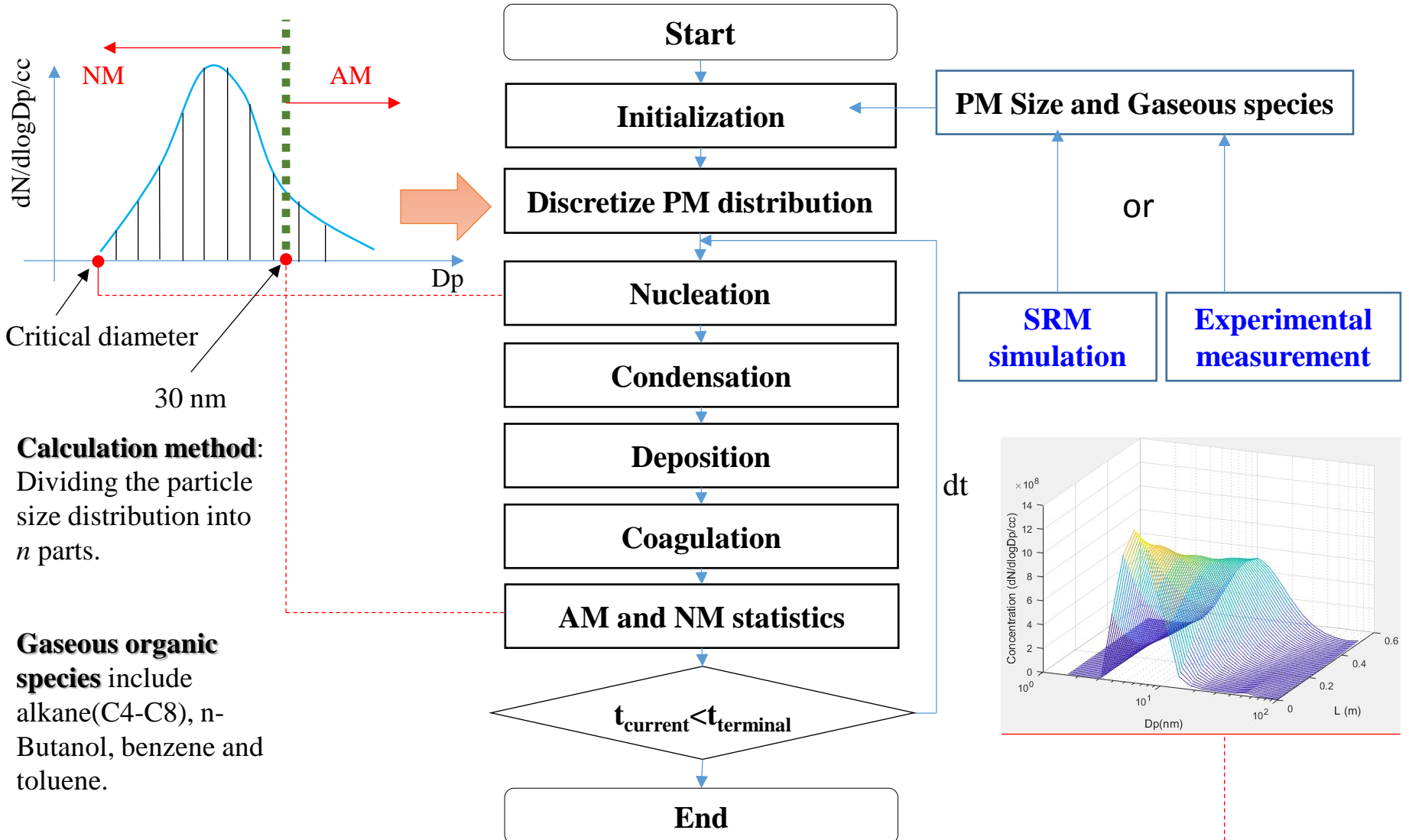
$$g_i = \frac{1}{3d_{p_i}\lambda_{p_i}} \left[(d_{p_i} + \lambda_{p_i})^3 - (d_{p_i}^2 + \lambda_{p_i}^2)^{3/2} \right] - d_{p_i}$$

Particle velocity: $\bar{c}_i = \sqrt{\frac{8k_B T}{\pi m_i}}$ Particle mean free path: $\lambda_{p_i} = \frac{8D_i}{\pi \bar{c}_i}$

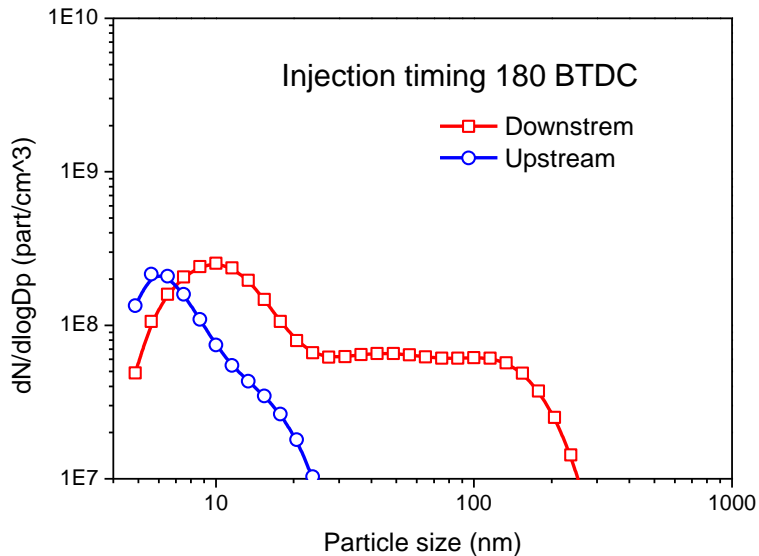
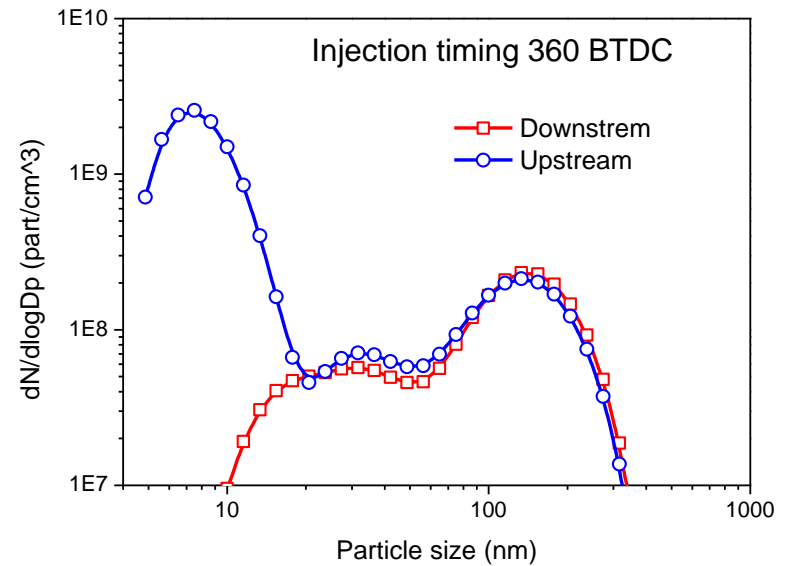
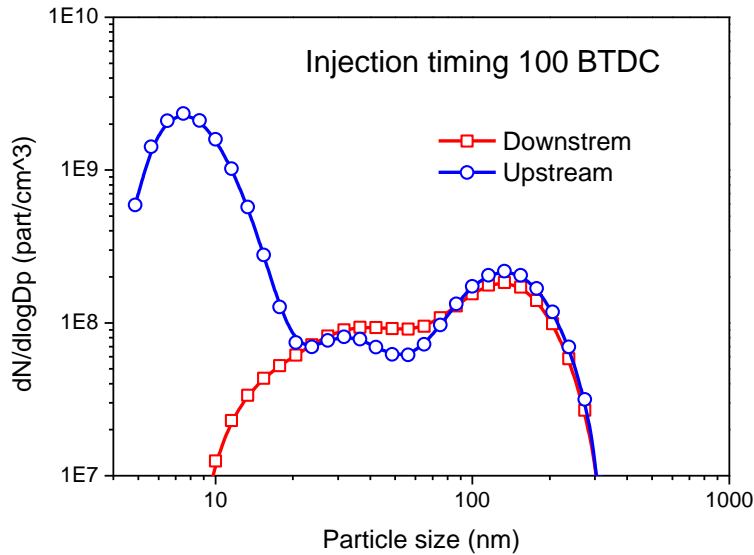
Particle diffusivity: $D_i = \frac{k_B T}{3\pi\mu d_{p_i}} C_{ci} = \frac{k_B T}{3\pi\mu d_{p_i}} \left[1 + \frac{2\lambda_{p_i}}{d_{p_i}} \left(A_1 + A_2 \exp\left(-\frac{A_3 d_{p_i}}{\lambda_{p_i}}\right) \right) \right]$

Particle Growth Model (PGM) Setup

- Calculation procedure of the PM evolution in the exhaust pipe:

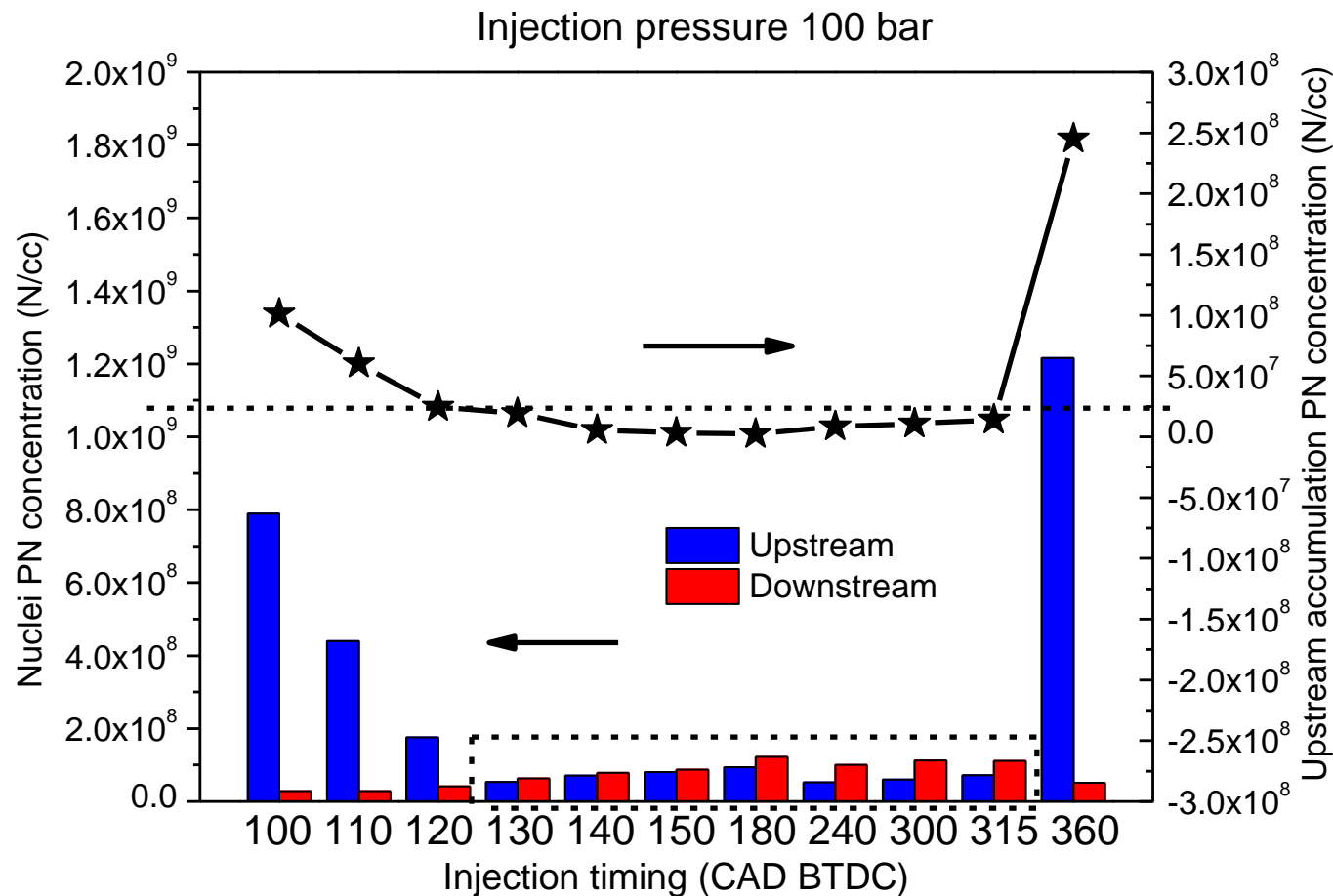


GDI Experiment Results



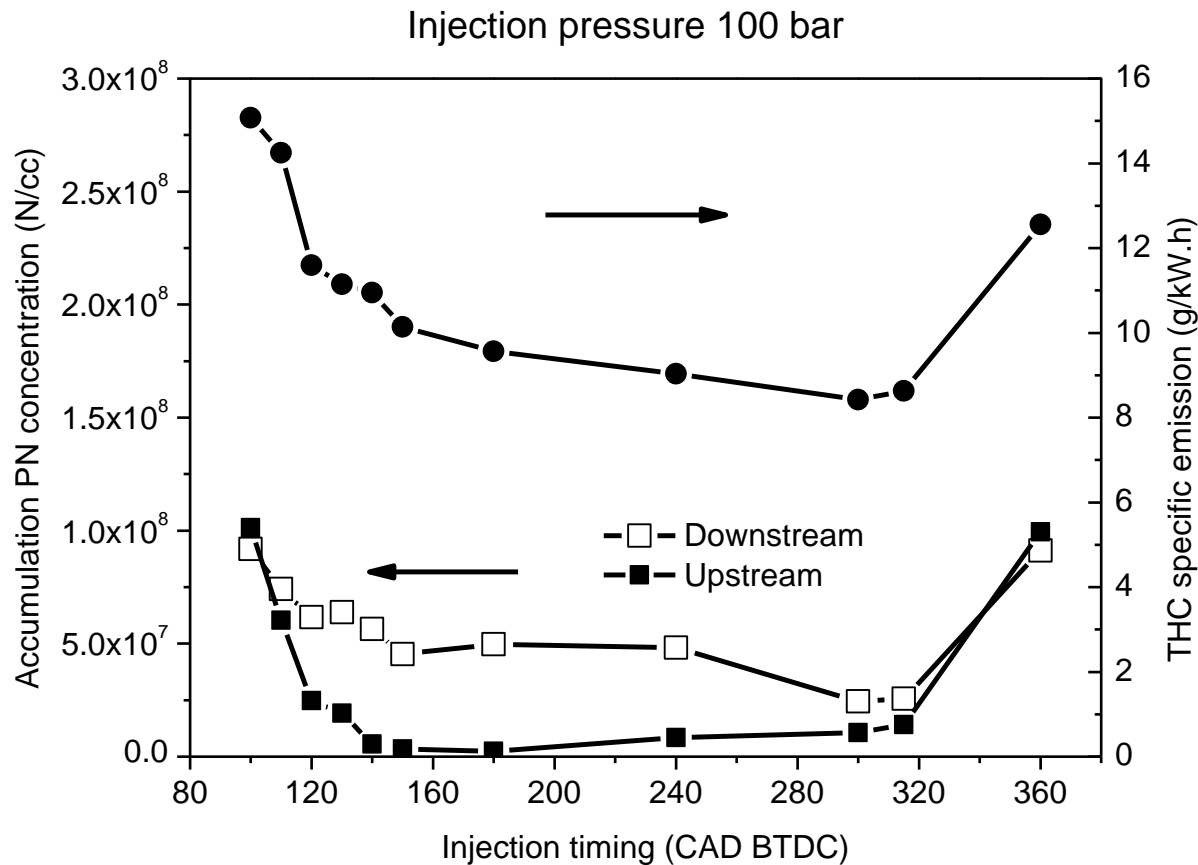
- Late injection (under-mixing) or too early injection (pool fire) result in high accumulation PN emissions.
- The nuclei PN decreases downstream the exhaust plenum chamber both late or too early injection.
- PN increases downstream for middle injection (130-315 CAD BTDC).

GDI Experiment Results



- When accumulation PN concentration is higher than $2.5 \times 10^7 / \text{cc}$, nuclei PN concentration downstream is lower than that upstream.
- This indicates nuclei PM is absorbed by accumulation PM along the exhaust system.

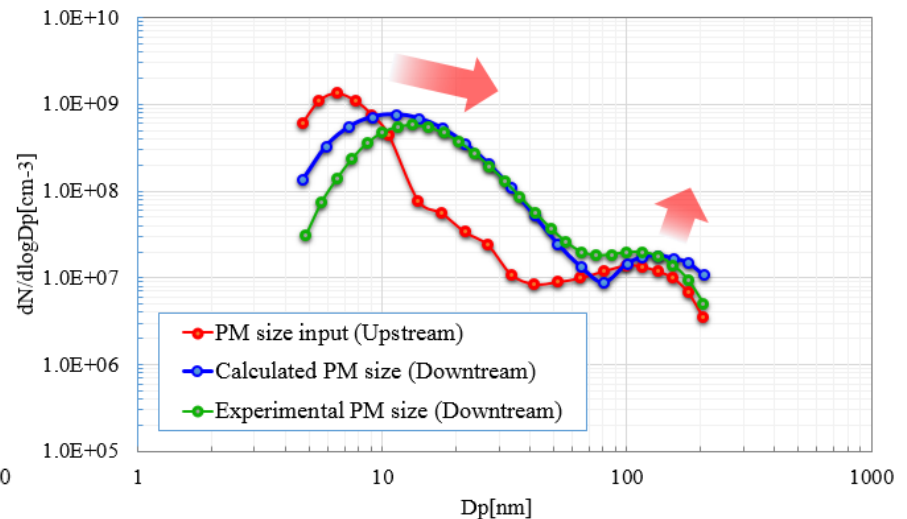
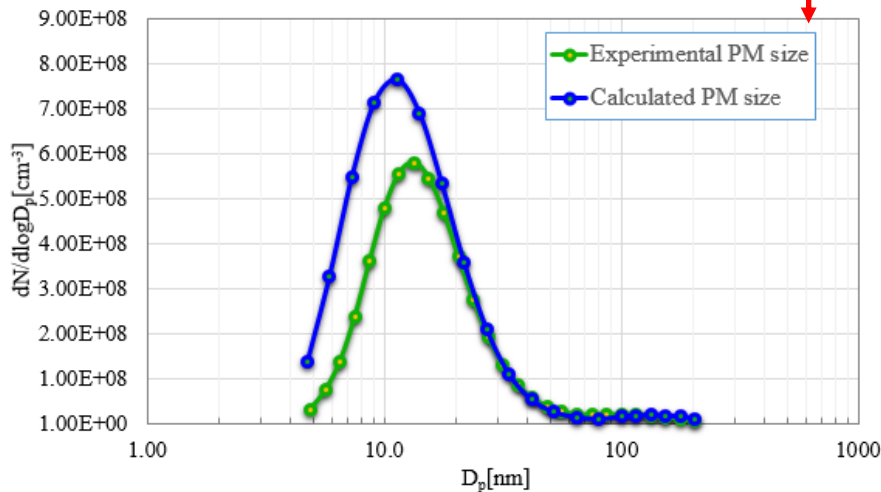
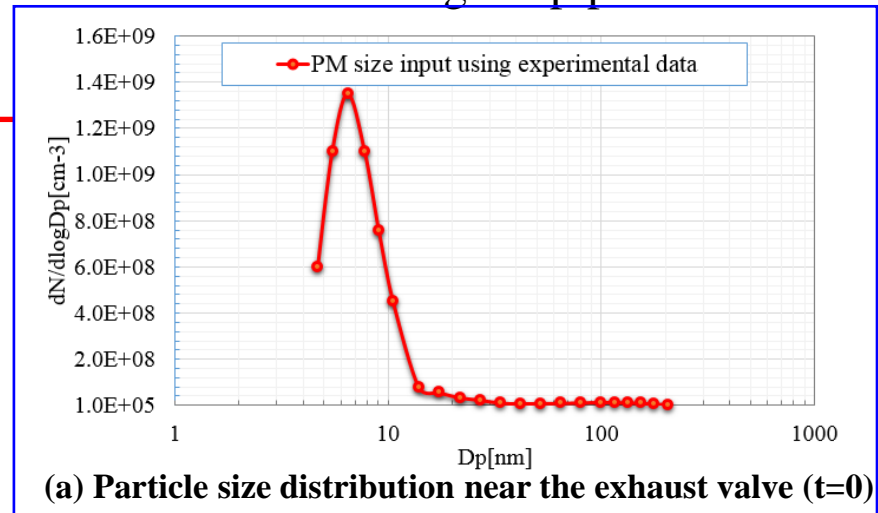
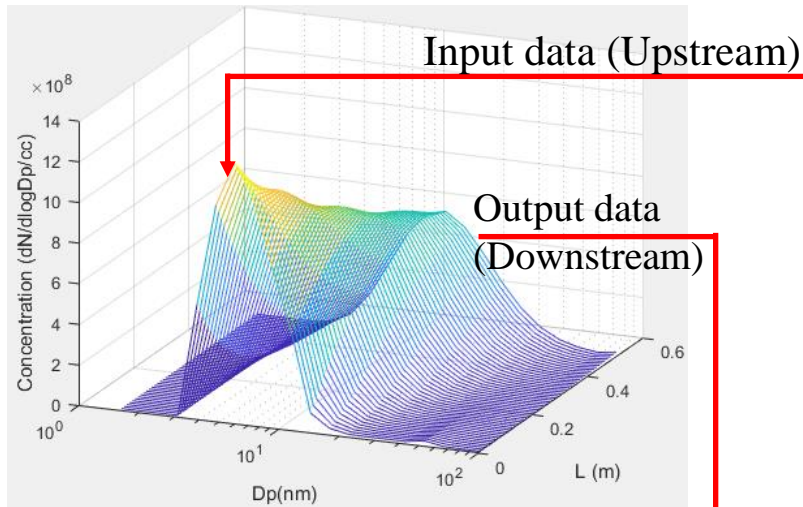
GDI Experiment Results



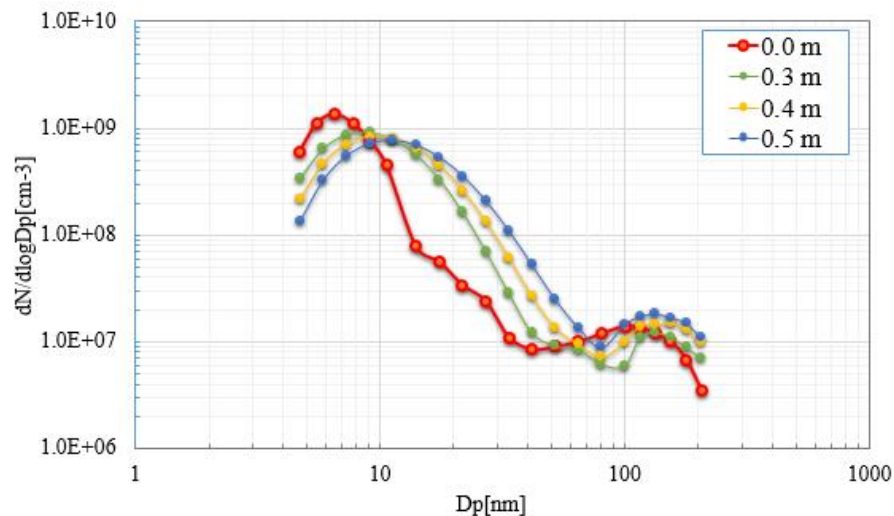
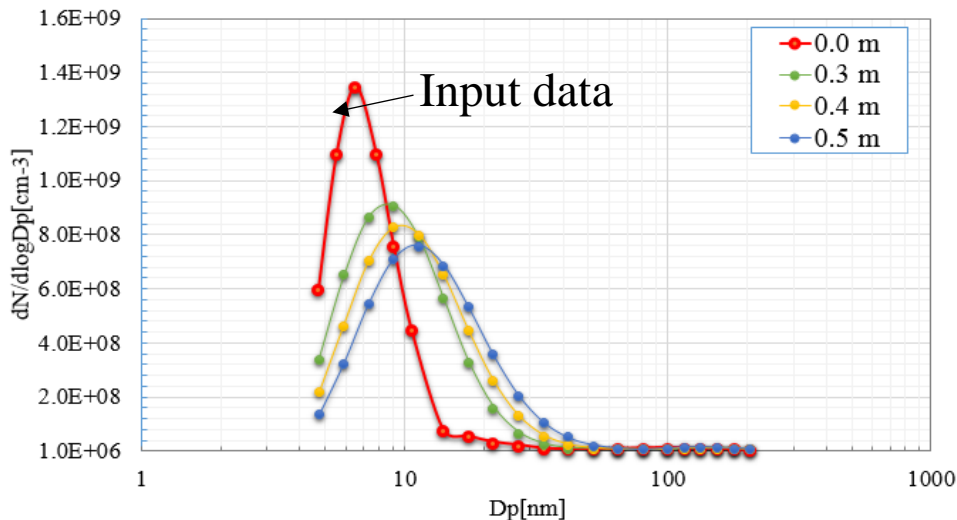
- THC emission has high relevance with accumulation PN.
- The newly-formed PM along the exhaust system may come from the condensation of hydrocarbon.

Particle Growth Model (PGM) Results

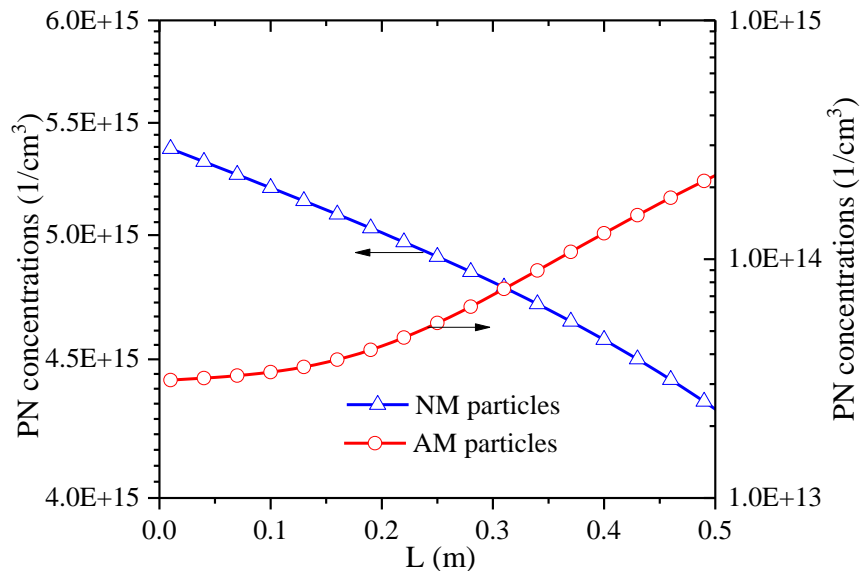
- To compare with experimental results, FPM simulation starts at the position near the exhaust valve and ends at the position 0.5 m downstream along the pipe.



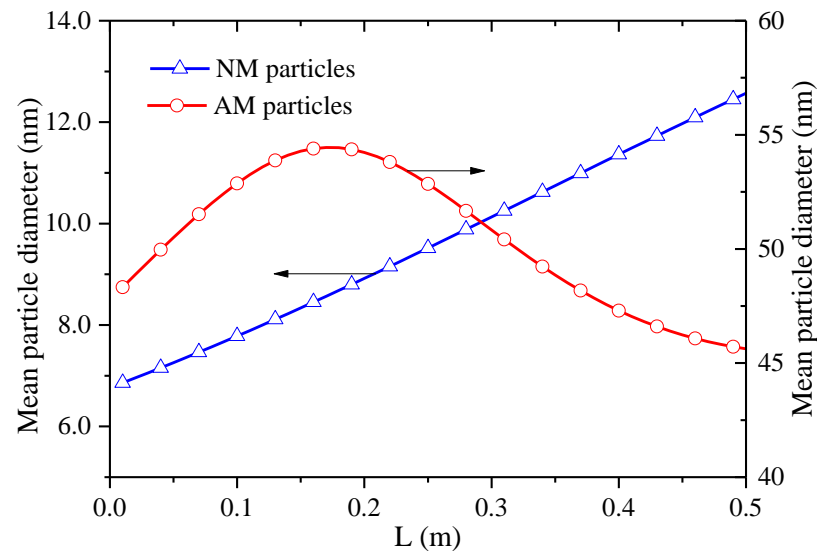
Particle Growth Model (PGM) Results



(a) Calculated particle size distributions at the different position



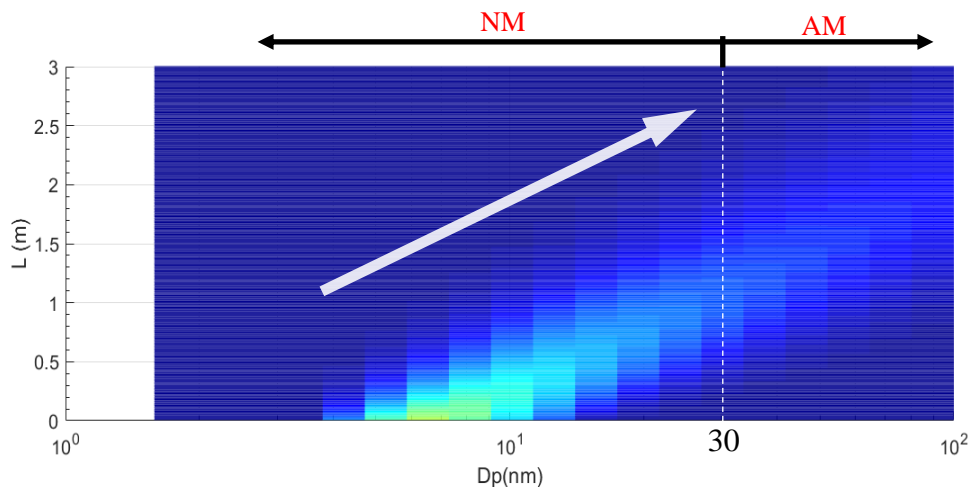
(b) Particle number concentrations



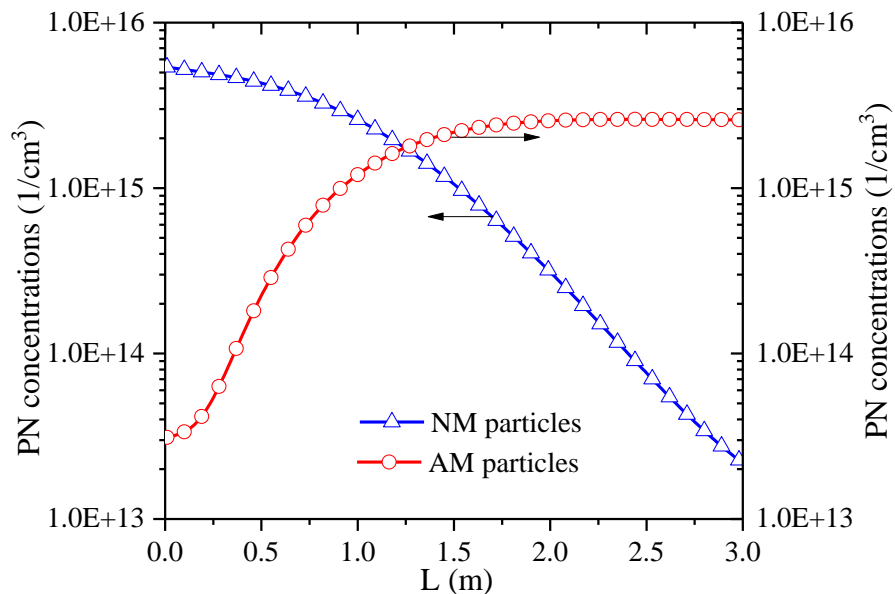
(c) Mean particle diameter

Particle Growth Model (PGM) Results

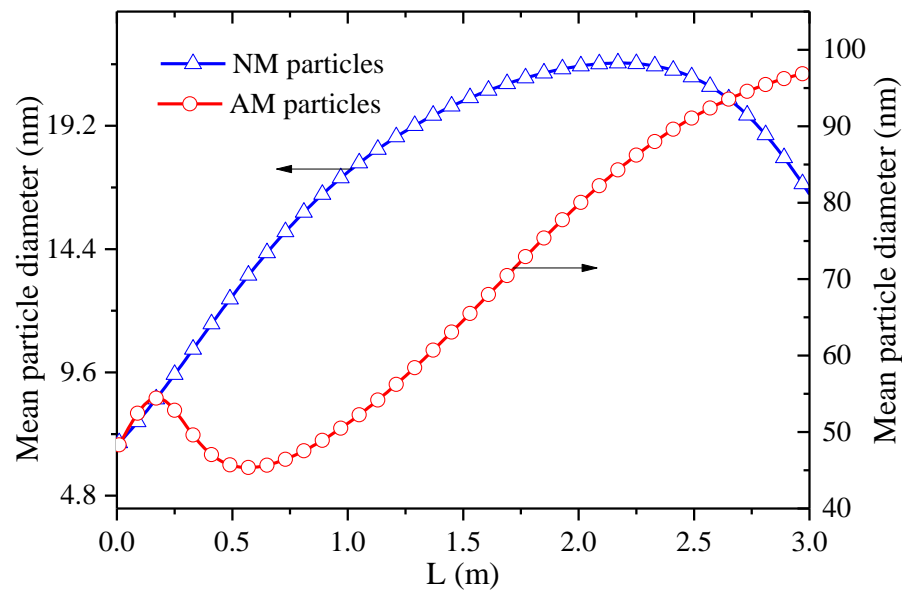
- PM Evolutions inside the exhaust pipe (3.0 m length)



- Number concentration of the NM Particles greatly decreases when the position is greater than approx. 1.0 m downstream from the exhaust valve.
- Size and number of the AM particles increases as the distance increases due to coagulation.



(a) Particle number concentrations



(b) Mean particle diameter



Conclusions & Future Plan

- Late injection (under-mixing) or too early injection (pool fire) result in high accumulation PN emissions. Nuclei PM is absorbed by accumulation PM along the exhaust system.
- THC emission has high relevance with downstream accumulation PN. THC emission has high relevance with accumulation PN. The newly-formed PM along the exhaust system may come from the condensation of hydrocarbon.
- The SRM and PGM simulations show precise PM results based on variant boundary conditions and experimental results. The next stage of research is to use these models to investigate the impact of injection timing on soot formation and PM characteristics and investigate variant fuel performance for gas and particulate emissions for in-cylinder and exhaust pipe.

Thank you