



**Knowledge brief**

## **Modelling Ultrafine particle dynamics using SALSA**

### **Introduction**

Ultrafine particles (UFP) are particles with a size smaller than 0.1  $\mu\text{m}$  that can have substantial negative effects on human health. Exposure to ultrafine particles can cause pulmonary inflammation and cardiovascular diseases. It is also linked to diabetes and cancer (Schraufnagel, 2020). The particles usually form with sizes of only a few nanometers and quickly increase in size due to a number of processes. According to some publications, the degree of toxicity is greater for smaller particles (Moreno-Ríos et al., 2022). It is therefore important to understand the processes leading to different size distributions of ultrafine particles.

This knowledge brief describes calculations using the "Sectional Aerosol module for Large Scale Applications" (SALSA). Our goal is to investigate the importance of particle dynamics, specifically coagulation, near a road when compared with dispersion. On the road a lot of ultrafine particles are expected, since traffic is one of its most important sources. However, ultrafine particles can quickly grow to larger particles, changing their behavior. It is important to know to what extent the particle dynamics should be taken into account when modelling ultrafine particles, or if dispersion has a much larger influence on the concentration of UFP than the particle dynamics. Taking into account particle dynamics makes the model more complicated and increases the modelling time.

### **SALSA 2.0**

SALSA2.0 is an aerosol microphysics module that describes the interaction between particles (Kokkola et al., 2018). SALSA2.0 can be used as a stand-alone box model, but can also be implemented as a submodule in Large Eddy Simulations and chemical transport models (Kurppa et al., 2019; Kokkola et al., 2018).

SALSA2.0 works with particle size classes, as illustrated in Figure 1. Particles are divided in bins for each size class and two subranges are defined. Different aerosol types are concentrated over different particle size classes, therefore different chemical components are included in the two subranges (Kokkola et al, 2008). Subrange 1 includes the smaller particles and contains only sulfate and organic carbon. Subrange 2 includes the larger ultrafine particles. The components present in subrange 2 are Sulfate, organic Carbon, sea salt, black Carbon and mineral dust. For subrange 2, a distinction is made between soluble and insoluble particles (Kokkola et al., 2018).

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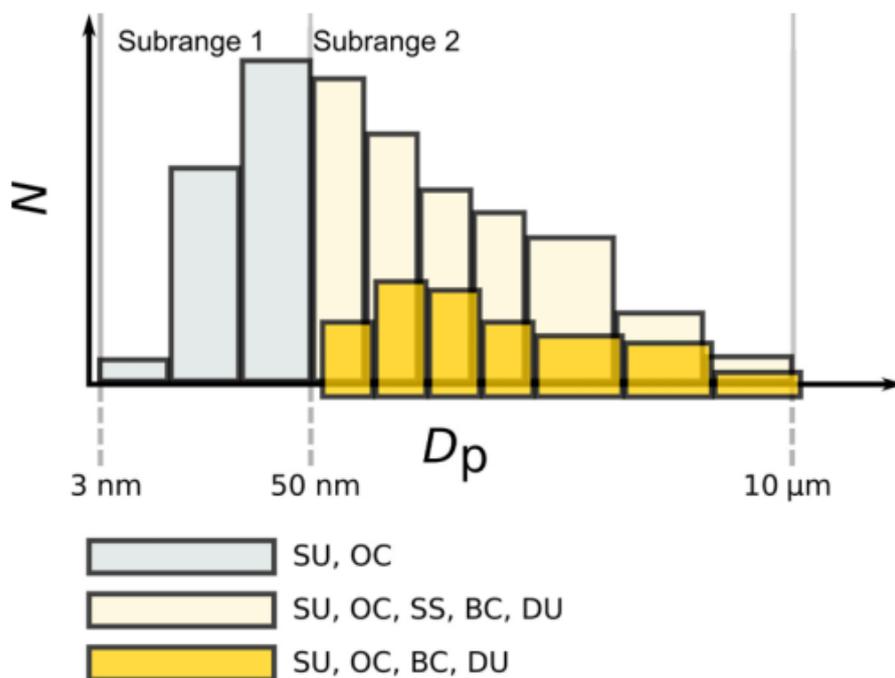
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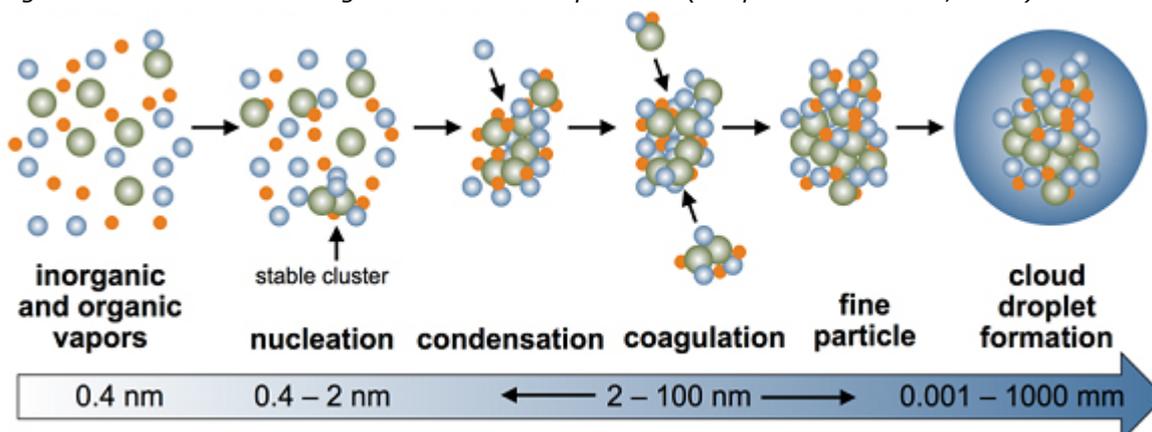
Figure 1 The number size distribution as a function of particle diameter. The colors show the components present in the subranges. For subrange 2 a distinction is made between soluble and insoluble particles. The components that can be included in the model are: sulfate (SU), organic carbon (OC), sea salt (SS), black carbon (BC) and mineral dust (DU) (Adapted from Kokkola et al., 2018).



The microphysical processes implemented in SALSA are nucleation, condensation, cloud activation, sulfate production, coagulation and hydration. (Kokkola et al., 2008).

In Figure 2 the most important processes for ultrafine particles are shown. Ultrafine particles can form from the gas phase; this is called nucleation (Curtius, 2006). Ultrafine particles can grow by coagulation and condensation. Coagulation is the collision of particles resulting in the formation of a new, larger particle. Condensation is the transfer of gas-phase molecules to existing particles (Holmes, 2007).

Figure 2 The formation and growth of ultrafine particles (Adapted from: PNNL, 2016) .



## Method

For the experiments discussed here, the SALSA2.0 module implemented in the HAM model version 2.3 (Tegen et al., 2019) is used. However, only one cell is studied, so it is used as a box model. SALSA2.0 implemented in the HAM model needs several input parameters. The temperature, specific humidity and atmospheric pressure are always given as parameters. An option to use a dilution rate was implemented in the box model to simulate dispersion. The dilution rate is a fraction of the particles that leaves the cell every timestep. The dilution rate can be set to zero if no dispersion should take place.

Two cases were studied here:

1. Case without dispersion, only coagulation. Calculations were performed for three different initial particle number concentrations.
2. Case with dispersion. The cell is ventilated with clean air. Calculations were performed for two different initial particle number concentrations.

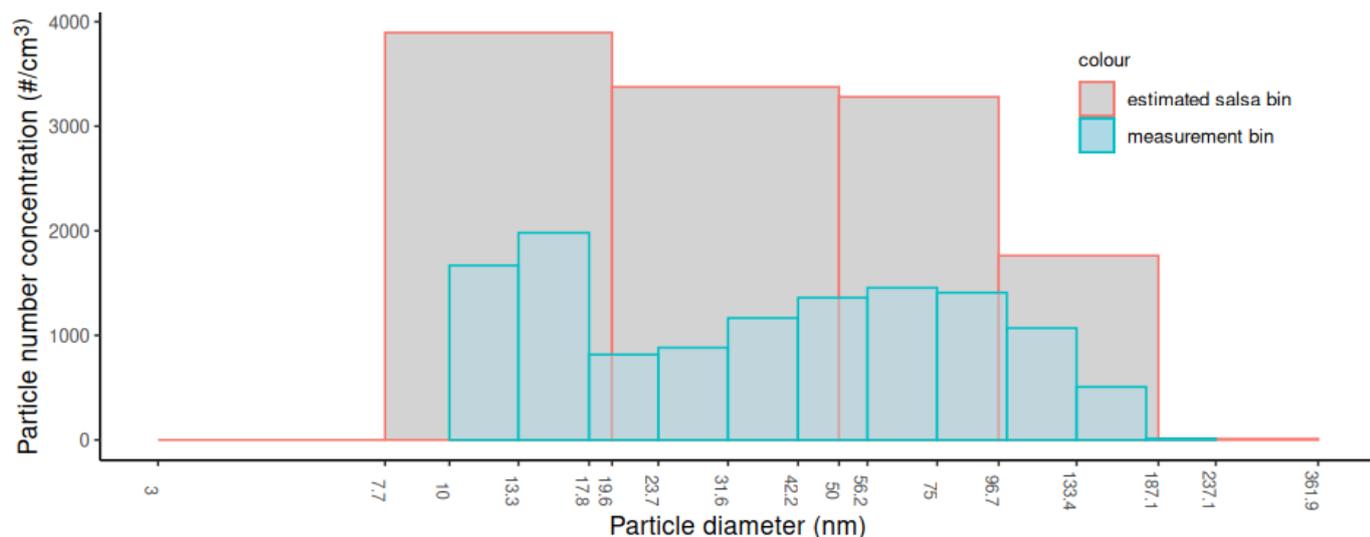
The temperature for all runs is set to 293 K, the specific humidity to 0.009661 kg/kg and the atmospheric pressure to 99890 Pa. Processes such as nucleation, aerosol radiation, hydration, wet and dry deposition, condensation of H<sub>2</sub>SO<sub>4</sub> and ionization due to galactic cosmic rays are switched off in the model runs we performed. Only coagulation is taken into account. We modelled the time-evolution of the size distribution of the particles for a number of intervals.

### *Initial concentration and particle distribution*

In May of 2024 measurements of ultrafine particle number concentrations and size distributions were performed with a NanoScan SMPS Nanoparticle Sizer 3910 device (manufactured by TSI) close to the highway A2, at the gas station Haarrijn, in the Netherlands. The measurements were collected at four different distances downwind from the middle of the road: roughly 60, 200, 220 and 320 m. At each distance the measurements were performed for about 30 minutes. The wind direction was perpendicular to the highway, with a maximum wind speed of around 2.5 m/s. The initial particle number concentration and size distribution as input for the model runs presented here are based on the measurement location closest to the highway, which is at 60 meters from the middle of the highway. The measured time-averaged particle number concentration and size distribution of the UFP are shown in Figure 3, along with the initial size distribution chosen as input for the SALSA model.

The ranges of the bins from the NanoScan are different from the ranges of the bins used in SALSA. The particle number concentration for each SALSA bin is calculated by summing the bins from the measurements overlapping with the SALSA bins. If a measurement bin overlaps with multiple SALSA bins, the particle number concentration is distributed over the SALSA bins taking into account the amount of overlap with each bin. The first SALSA bin does not contain any particles, as the NanoScan cannot detect particles with a diameter below 10 nm. The number of particles in the smallest bin is therefore unknown. Particles with a diameter below 10 nm have most likely been present, but we do not know how many.

Figure 3 Particle number concentration and size distribution of UFPs. In blue the particle number concentration for the measurement bins is shown. The grey bins (outlined with red) show particle number concentrations for the SALSA bins calculated using the contents of the measurement bins.



Apart from the particle number concentration in each bin, the model input also requires information about the type of particles (soluble/insoluble) and chemical components, this is shown in Table 1. We used the composition that was provided as default in the model.

Table 1 Overview of the chemical components present in the two subranges.

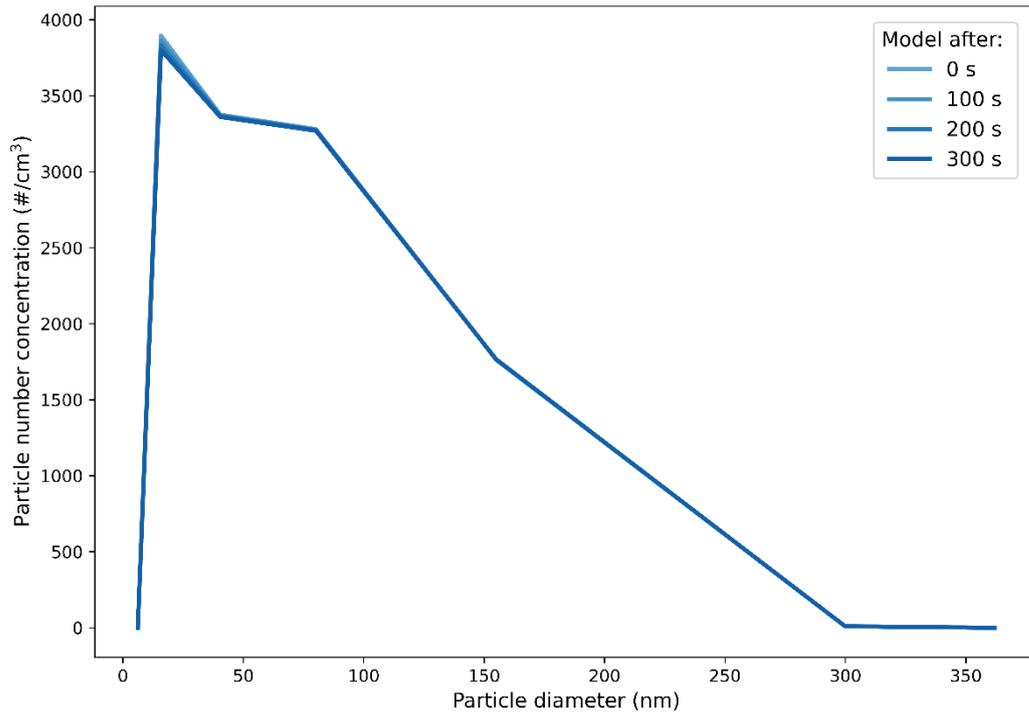
Chemical component	Subrange 1 (3- 50 nm)	Subrange 2 (50 nm- 10 µm)	
		Soluble	Insoluble
Sulfate	20%	50%	1%
Organic carbon	80%	5%	1%
Black carbon		5%	1%
Sea salt		10 %	
Mineral dust		30%	97%

## Results and discussion

### Evolution without dispersion

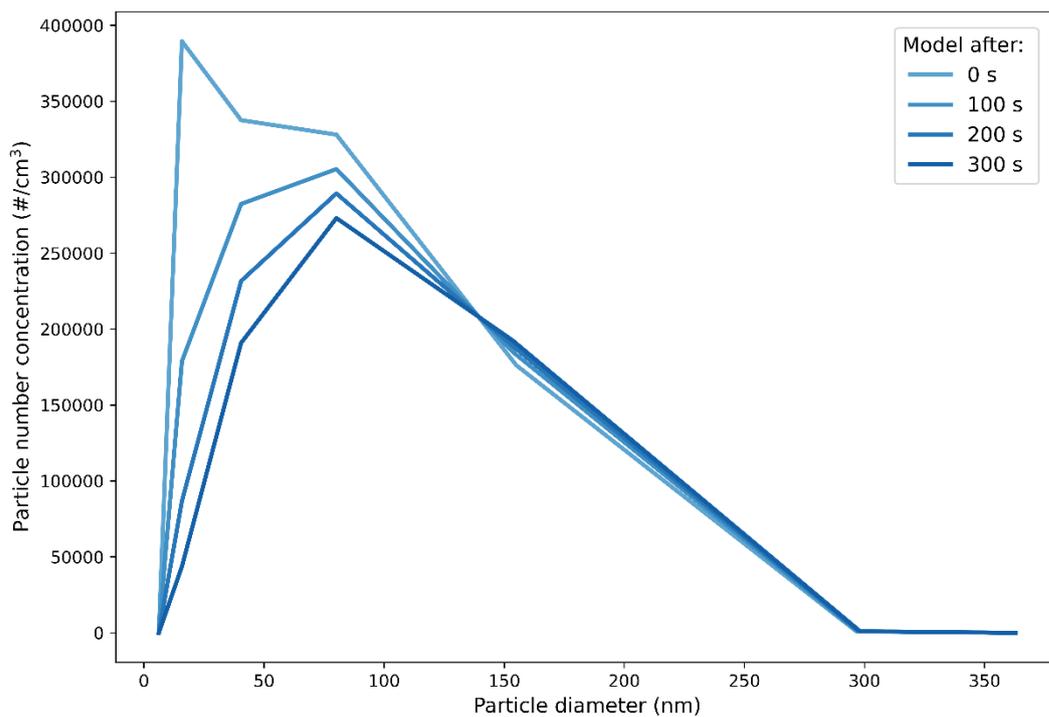
In Figure 4 the modeled particle number concentrations per particle size class after 0, 100, 200 and 300 seconds are shown for a cell without ventilation. The particle number concentration in the second bin decreases (just) a little bit. This decrease happens because the smallest particles cluster together and form larger particles (coagulation).

Figure 4 Particle number concentration as a function of the particle diameters. The initial size distribution is shown in light blue, the darker colors show the distribution at 100, 200 and 300 seconds (see legend).



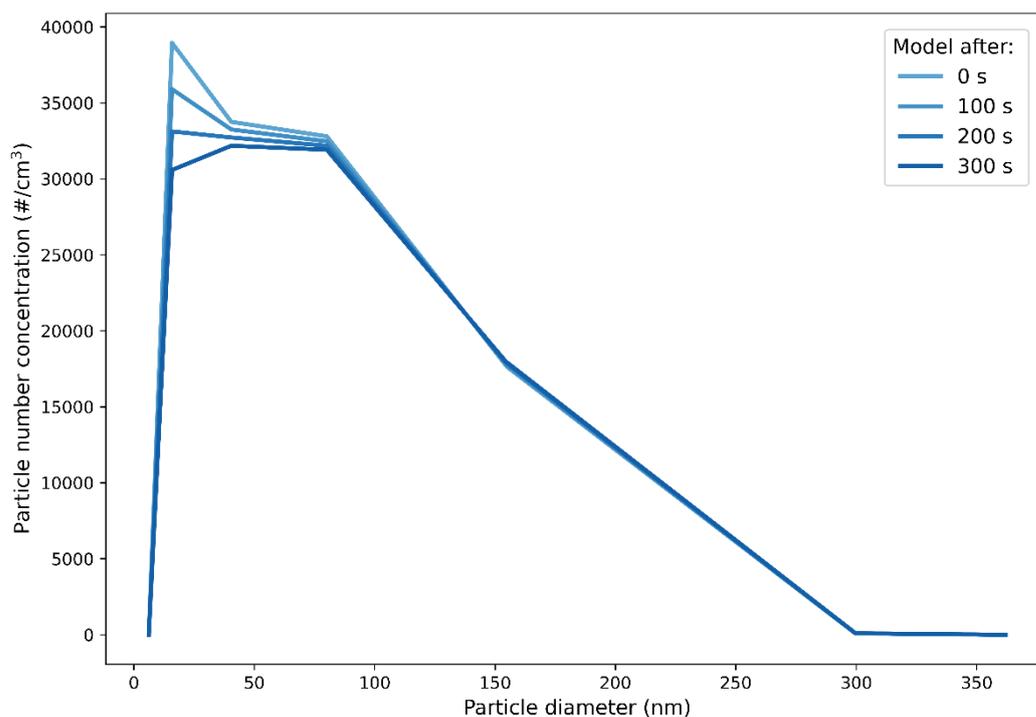
It is expected that coagulation effects are more prominent when the particle number concentration increases. To verify this mechanism, the initial particle number concentration is increased by a factor of 100. In Figure 5 particle number concentration and size distribution for several time steps are shown. The particle number concentration in the second, third and fourth bin clearly decreases over time, whereas the particle number concentration in the fifth bin increases. The increase in larger particles is much smaller than the decrease in smallest particles as many small particles cluster into relatively few bigger particles. So, indeed the effect of coagulation is increased when the initial number of particles is increased.

Figure 5 Particle number concentration as a function of the particle diameters. The initial size distribution is shown in light blue, the darker colors show the distribution at 100, 200 and 300 seconds (see legend). The numbers of particles in the initial size distribution considered here are increased by a factor 100 compared to that shown in Figure 4.



When the initial particle number concentration is increased by a factor of 10, a decrease of the particle number concentration in the second and third size bin can still be observed for the first 300 seconds (see in Figure 6).

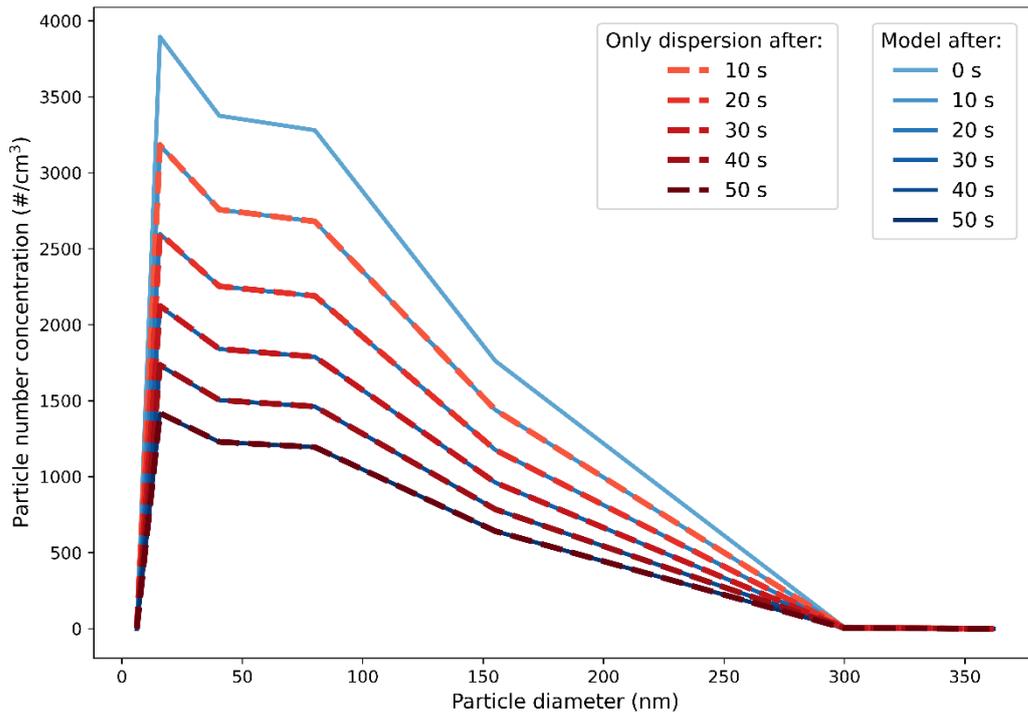
Figure 6 Particle number concentration as a function of the particle diameters. The initial size distribution is shown in light blue, the darker colors show the distribution at 100, 200 and 300 seconds (see legend). The numbers of particles in the initial size distribution considered here are increased by a factor 10 compared to that shown in Figure 4.



### Evolution with dispersion

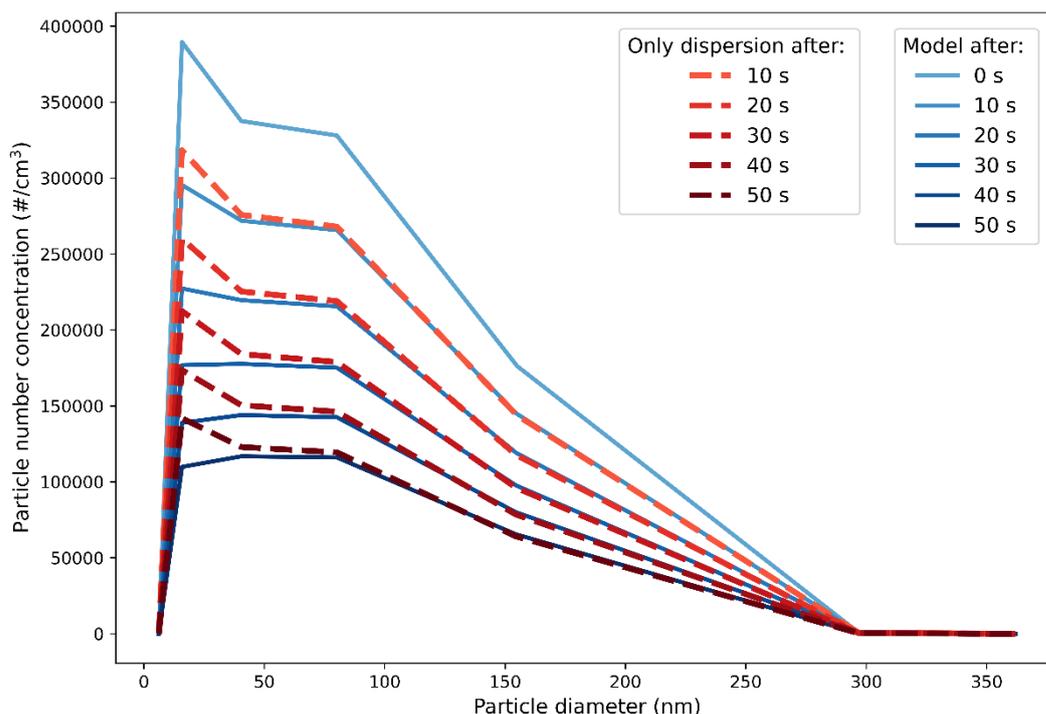
For the particle number concentration levels measured close to highways, the particle dynamics of the UFPs already seem to have little effect at short time scales. We now investigate how ventilation of the cell with clean air will affect our results. A dilution rate ( $r$ ) of  $0.02 \text{ s}^{-1}$  is used. This effectively means that every second, the particle number concentration in the cell is decreased by 2%. Figure 7 shows the particle number concentration versus the particle diameter for the first 50 seconds of the simulation. This decrease in concentration due to dispersion is shown by the dashed lines. It is evident that, under these conditions, the dispersion has a larger effect on the decrease of the particle number concentration than the particle dynamics. There is almost no difference between the solid lines showing the effect of both coagulation and dispersion and the dashed lines showing only the effect of dispersion. So, the effect of dispersion (i.e. dilution) is much larger than that of coagulation. The effect of only dispersion is calculated by reducing the particle number concentration by 2% for every timestep. The shape of the distribution of particle sizes does not really change.

Figure 7 Particle number concentration as a function of the particle diameter. The initial size distribution is shown in light blue and the distribution is also shown after 10, 20, 30, 40 and 50 seconds. The dilution rate is set to  $0.02 \text{ s}^{-1}$ . The decrease in concentration due to dispersion only is shown by the dashed line. Note that the time steps shown here are smaller than the time steps shown for the case without dispersion.



When the initial particle number concentration is increased by a factor 100, as shown in Figure 8, a difference is observed between the results from the model taking into account dispersion and coagulation and the dashed line showing only the effect of dispersion. The particle number concentration in the second bin decreases when coagulation is taken into account. We also look at initial particle concentrations higher than the measured value to see for what initial particle concentration the effect of coagulation is observed. The measurements used for the initial particle number concentration are an average of 30 minutes, so it is possible that sometimes a higher particle number concentration is observed.

Figure 8 Particle number concentration as a function of the particle diameters. The initial size distribution is shown in blue and the distribution is also shown after 10, 20, 30, 40 and 50 seconds. The dilution rate is set to  $0.02 \text{ s}^{-1}$ . The decrease in particle number concentration due to dispersion only is shown by the dashed line. The number of particles in the initial size distribution considered here are increased by a factor 100.



## Conclusion

We measured particle size resolved UFP concentrations close to a highway to set a realistic initial size distribution for a box model using the coagulation module of SALSA2.0. Two cases were studied. The first case only studied the effect of coagulation on the particle number concentration. The second case also included dispersion.

The following observations were made:

- The first calculation showed very low reaction rates due to particle dynamics, with only a small change of number of the smallest particles and hardly any effect on concentrations in the other size bins. When the measured particle number concentration is multiplied by a factor 100, the coagulation reaction rate becomes much higher and particle dynamics shows a significant effect on time evolution of the size distribution.
- When ventilation of the box with clean air is considered with a dilution rate of  $0.02 \text{ s}^{-1}$ , the dilution causes the total number of particles to reduce quickly. The results from a model run containing both coagulation and dispersion versus a situation with dispersion only, yield similar outcomes when based on the measured concentration levels. So, the effect of dispersion (i.e dilution) is much larger than that of coagulation.
- When the initial particle concentration in the distribution is multiplied by a factor of 100, the number of particles in the second bin (with a particle diameter of 7.7-

19.6 nm) are reduced due to coagulation and dispersion, but the effect of coagulation is very small (if at all) for particle diameters greater than 19.6 nm.

- We conclude that, within the measurement and modelling set-up, particle dynamics is not important/relevant from a distance of 60 meter from the road until minutes after release and the dispersion of concentrations of particles of different size classes can be assumed as if inert. 60 meter is the minimum distance of the measurements to the middle of the highway.
- For further research it is important to validate the results from SALSA with more measurements, which should be performed for a longer period of at least several weeks. Also, it would be interesting to investigate if the chemical composition used in the simulation is representative of the chemical composition near a road.

## References

Curtius, M., *Nucleation of atmospheric aerosol particles*, Comptes Rendus Physique, Volume 7, 2006, 1027-1045, <https://doi.org/10.1016/j.crhy.2006.10.018>

Holmes, N.S., *A review of particle formation events and growth in the atmosphere in the various environments and discussion of mechanistic implications*, Atmospheric Environment, Volume 41, Issue 10, 2007, 2183-2201, ISSN 1352-2310, <https://doi.org/10.1016/j.atmosenv.2006.10.058>

Kokkola, H. , Korhonen, H. , Lehtinen, K. E. J. , Makkonen, R. , Asmi, A. , Järvenoja, S. , Anttila, T. , Partanen, A.-I. , Kulmala, M. , Järvinen, H. , Laaksonen, A. and Kerminen, V.-M. , *SALSA – a Sectional Aerosol module for Large Scale Applications*, Atmospheric Chemistry and Physics, 2008, 8 (9), pp.2469-2483.

Kokkola, H. and Kühn, T. and Laakso, A. and Bergman, T. and Lehtinen, K. E. J. and Mielonen, T. and Arola, A. and Stadtler, S. and Korhonen, H. and Ferrachat, S. and Lohmann, U. and Neubauer, D. and Tegen, I. and Siegenthaler-Le Drian, C. and Schultz, M. G. and Bey, I. and Stier, P. and Daskalakis, N. and Heald, C. L. and Romakkaniemi, S., *SALSA2.0: The sectional aerosol module of the aerosol--chemistry--climate model ECHAM6.3.0-HAM2.3-MOZ1.0*, Geoscientific Model Development, Volume 11, 2018, 3833--3863

Kurppa, M. and Hellsten, A. and Roldin, P. and Kokkola, H. and Tonttila, J. and Auvinen, M. and Kent, C. and Kumar, P. and Maronga, B. and Järvi, L., *Implementation of the sectional aerosol module SALSA2.0 into the PALM model system 6.0: model development and first evaluation*, Geoscientific Model Development ,2019

Moreno-Ríos, A.L., Tejeda-Benítez, L.P., Bustillo-Lecompte, C. F. *Sources, characteristics, toxicity, and control of ultrafine particles: An overview*, Geoscience Frontiers, Volume 13, Issue 1, 2022, 101147, ISSN 1674-9871, <https://doi.org/10.1016/j.gsf.2021.101147>.  
(<https://www.sciencedirect.com/science/article/pii/S1674987121000116>)

PNNL (Pacific Northwest National Library), *Scientists more accurately model the formation and growth of tiny particles that influence clouds and climate*, <https://phys.org/news/2016-03-scientists-accurately-formation-growth-tiny.html>, March 2016. [Retrieved at: 09-09-2025]

Schraufnagel, Dean E., *The health effects of ultrafine particles*, *Experimental & Molecular Medicine* (2020) 52:311–317

Tegen, I. and Neubauer, D. and Ferrachat, S. and Siegenthaler-Le Drian, C. and Bey, I. and Schutgens, N. and Stier, P. and Watson-Parris, D. and Stanelle, T. and Schmidt, H. and Rast, S. and Kokkola, H. and Schultz, M. and Schroeder, S. and Daskalakis, N. and Barthel, S. and Heinold, B. and Lohmann, U., *The global aerosol--climate model ECHAM6.3--HAM2.3 -- Part 1: Aerosol evaluation*, Geoscientific Model Development, Volume 12, 2019, 1643--1677