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Interactive comment on "CFD modeling of a vehicle exhaust laboratory sampling system: sulfur driven nucleation and growth in diluting diesel exhaust" *by* M. Olin et al.

Anonymous Referee #1

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Olin et al. study nucleation in diesel exhaust using CFD tools. It's a nice piece of work but the presentation could be significantly better. Findings should be discussed more in-depths, underlying reasoning explained, most of the figures need to be re-done since they are so tiny, and the manuscript's Finglish needs some serious work. In the following, I will give detailed comments on contents and presentation issues BUT I feel that bringing the language up to par is far beyond any reasonable review demand.

p. 2908, l. 23f "Two versions of the model code, an Eulerian and a Lagrangian model, are presented."

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Why two models? What's the motivation?

p. 2910, l. 23f "A steadystate simulation is performed, where all time derivatives are zero, which provides shorter computation time."

I don't think it's necessary to define what steady-state means. I would expect readers to know. Instead it would be nice to have a sentence like "the nature of the setup (no time-dependence) allows for a steady-state approach which saves time" that motivates why steady-state is possible and desirable.

p. 2911, l. 8f "but the influence of nucleation and condensation on the properties on the fluid side is negligible."

Is it? Has it been tested? How large is the effect? With sulfuric acid between 10^9 and 10^{11} and J 10^7 it doesn't seem all that clear-cut even if the residence time is very short. Given that you have the other model that includes feedback it would be quite easy to qualify and quantify this statement. Readers cannot be expected to take it on faith, can they?

p. 2911, l. 16ff "Due to fewer dimensions in Lagrangian model compared to the Eulerian model, a very high temporal resolution can be simulated. That can be used to ensure the suffciency of spatial resolution of the computational grid of the Eulerian model by comparing the results from both models."

Well, how exactly? When the high-res model uses input from the low-res model, how does it work as quality control?

p. 2911, l. 24f ""Nucleation" is a key process controlling particle number concentration in diluting exhaust is particle formation, which is generally considered sulfur-driven."

Too many verbs in the first part of this sentence. Please re-write. I would also take issue with the word sulfur-driven. It's really sulfuric acid, isn't it?

p. 2912, l. 10f "Nucleation exponents 1 and 2 are found to fit to atmospheric measure-

ment results better than the values from CNT (Sihto et al., 2009),"

That may be true in Finland, but not, for example, in China. Never mind if CNT works there, but values well above 2 have been observed. www.atmos-chem-phys.net/11/12663/2011/ www.atmos-chem-phys.net/14/2169/2014/

p. 2912, l. 28f "until recently"

One could argue that this is a rather liberal use of the word "recently". Various instruments and techniques to go below 3nm have been around for quite some years already. In fact, given the size ranges in the manuscript, a PSM could really provide some valuable additional insight.

p. 2913, l. 3ff "Particle dynamics, such as condensation and coagulation, alter the particle distribution during the time, when newly formed clusters grow to measurable sizes. Therefore, the actual and the observed nucleation rates are unequal and their nucleation exponents can be different too."

This is rather trivial, so why write it? There seems to be something missing to make this an actual thought.

p. 2914, l. 2 "in this case"

Do you mean "in this study"?

p. 2914, l. 2f "In this case, the following nucleation scheme is used:"

Why this scheme and not some other? I mean, there is plenty to choose from. It would be nice to hear reasons as surely there must be some.

p. 2917, l. 8f "slightly higher sulfuric acid concentrations"

What does slightly mean here? Fuel sulfur content is 6-fold, to what difference in sulfuric acid concentrations does that translate?

p. 2917, l. 10ff "Volatile nucleation mode concentration increased in both measure-

ments, when sulfuric acid concentration increased over the time, though all the operation parameters remained constant."

What exactly is the point of this sentence? In itself it seems rather trivial: more sulfuric acid leads to more nucleation. Is this supposed to me a summary of the experiments? If so, something more and less obvious could be nice.

p. 2917, l. 14ff

The whole paragraph is written in a funny way. First you say what the domain consists of. Then you go on describing some part that is not included without stating explicitly that this part has been left out. This could be re-written to be clearer.

The corresponding picture needs a serious makeover. There should really be two figures, one with the experimental setup, and one just showing the computational domain. And the figure needs to be way clearer. Thin lines, tiny letters, it's really not a pleasure to look at. You might also want to reconsider if making it to scale is such a great idea. I would prefer clarity.

p. 2917, l. 27 "gaseous sulfuric acid"

Say vapor instead. Sulfuric acid vapor. It is a gas, yes, but in the context of this work it is much clearer to use gas for air and vapor for the stuff that condenses (water, sulfuric acid, ...). I would change this throughout the text. Generally, in aerosol physics, one speaks of condensable vapors. It's merely a convention but it is useful to distinguish what role a compound plays in a system (carrier gas, condensable vapor, or whatever). It makes everything much clearer.

p. 2918, l. 12 "lambda value"

Would be nice to have a definition here.

p. 2918, l. 13f "RH was not measured, but RH = 10% can be considered an upper limit"

And the reason for this is?

p. 2918, l. 14f "Total hydrocarbon mole fraction (except for volatile hydrocarbons) was fitted to obtain the measured volatile nucleation mode particle sizes."

This needs some explanation. What was fitted to what and why?

p. 2918, l. 21 "but the cooling is not simulated here"

Why not? Given that it actually makes a difference. . .

p. 2919, l. 8 "onto which liquids condense and coagulate"

This sounds a bit funny. I thought vapors condense and particles coagulate.

p. 2919, l. 11f "the assumption that soot particles do not grow by condensation but gases condense into empty spaces of the fractal particles"

That would imply that residence times are too short for condensation to fill all the gaps and the particle to grow beyond its initial size. Is that so?

p. 2920, l. 22 "relevant size of a particle from which atmospheric aerosol formation starts"

Can this atmospherically relevant size simply be transferred to the largely different conditions (temperature, vapor concentrations etc) in diesel exhaust?

p. 2921, l. 7f "Figures 4 and 5 show that nucleation begins at the boundary of hot exhaust and cold dilution air."

Well, actually, those figures show very little because they are very, very small. The same applies to the following figures. Also, we don't really see that nucleation begins at the boundary of hot and cold air. There is no temperature information in the figure, so how could we possible see that? In general, these nice, colorful figures show very little detail. I would like to see some T and J profiles along the radius to actually be able to observe the difference between the nucleation exponents.

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p. 2921, l. 16f "In R cases, volatile nucleation mode number concentration was decreased 3–9% due to coagulation, depending on the case. Cases with smallest particles had the highest coagulation losses due to increased coagulation coefficient. Coagulation to soot mode contributed over 70% of the total coagulation loss."

Is the assumption that soot doesn't grow still used here? Is it justified with all that coagulation going on?

p. 2922, l. 6ff "CMDvol at the outlet in R cases was obtained by fitting simulated and measured diameters of average volume with the amount of hydrocarbons in raw exhaust."

This could be clearer. What was fitted to what and which parameter was adjusted?

p. 2922, l. 16ff "However, CMDvol would increase then, but not with as fast growth rate as CMDcore, due to smaller particle size."

Really? In atmospheric observations, the growth rate often decreases with particle size which is intuitively quite simple: in the case of bigger particles, the same growth rate requires much more condensable vapor. What's working against that in this case? Kelvin? Collision rate?

p. 2924, l. 6ff "The time domain was divided to 106 time steps, which corresponds to a higher resolution compared to the Eulerian simulation, where the paths pass through 6000–8000 computational cells."

What exactly is the benefit of this? If I understood correctly, the model is fed with output from the CFD domain which has much poorer resolution.

p. 2924, l. 23f "However, the difference of the concentrations can also be partially accounted for numerical error caused by the lower resolution in the Eulerian simulation."

This of course needs some explanation. By what mechanism is the difference produced?

p. 2925, l. 1 "some numerical error exists"

That sounds like a euphemism. It seems like a bit of a mess. Can you explain what exactly is happening there? "Numerical error" is rather vague.

p. 2925, l. 13 "It can be executed with very high time resolution"

Again: what is the point of high time resolution if the input data doesn't have the same resolution?

p. 2925, l. 21 "too low"

Too low for what?

p. 2926, l. 4f "which is the cut-size D50 of used particle counter TSI CPC 3025"

Well, cut sizes differ from unit to unit, even if it's the same model. One also has to keep in mind that the detection efficiency curve is not a step function. So while this is the best thing that can be done in this situation, it is not more than a rough estimation.

p. 2953, figure 10

It would be MUCH better to include those lines in one of the improved figures 4-8. That would provide some context. In any case, the figure in its current form is not very enlightening and needs some thinking about.

p. 2954, figure 11

Where does all the noise between 0.02 and 0.03 come from? Also those jumps for the right curves seem somewhat unphysical. What's happening there?

p. 2955, figure 12

With all the noise it's kinda hard to determine what the actual message of the figure is. I can't offer any good ideas but it would be nice to present this in a clearer way.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 2905, 2015.