Interactive comment on “Modelling the contribution of biogenic VOCs to new particle formation in the Jülich plant atmosphere chamber” by L. Liao et al.

Anonymous Referee #2

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In this paper Liao et al. present results from real plant BVOC emission and SO2 oxidation followed by new particle formation and growth. Gas phase reactions are represented with high level of details using Master Chemical Mechanism. However, quite heavy approximations are needed to simulate the condensational growth of particles. In order to achieve agreement between measurement and modelling results, some assumptions are made. The topic of the manuscript fits the scope of ACP and is timely important and the results presented might have some importance, although I do not see too much new information. Because the measurement setup is described in other manuscript (Dal Maso et al, 2014), I concentrate here on modelling part of the study.
where I have some serious criticism. Major revisions are needed before the manuscript can be accepted for publication.

Abstract: If SO2 measurements are missing, how can it be a merit that measured and modelled H2SO4 concentrations agree as it is only based on guessing the input concentration?

Abstract: “The modelled total monoterpene concentration was in line with PTR-MS observations, and we provided the distributions of individual isomers of terpenes, when no measurements were available.” To whom and for what purpose these there provided?

Abstract: “The aerosol dynamic results supported the hypothesis that H2SO4 is one of the critical compounds in the nucleation process.” This is not a new result, and I do not see how this is supported by the results presented. Did you test some nucleation mechanisms without H2SO4?

Abstract: “We classified the VOC oxidation products into two sub-groups including extremely low-volatility organic compounds (ELVOCs) and semi-volatile organic compounds (SVOCs)”. This sounds like everything is classified, but what actually is done based on the page 27981, some oxidated compounds are chosen to represent ELVOCs and SVOCs. This should be rephrased.

Overall, I would like to see more clearly in the abstract what is the main result of this study. Is it that after some assumption made the model skill to simulate particle formation is highest when ELVOCs are taken into account, or is it that wall losses are actually the critical point in chamber measurements. In the case of the first one, all assumptions should be explained and their effect on modelling results should be discussed. If the case of wall losses, then a more careful analysis of previous studies is needed. Also clear difference between this and Dal Maso et al. (2014) should be made.

Page 27976, lines 9-10: At the moment there is too much speculation in the modelling setup to really quantify the role of ELVOCs and SVOSs on SOA formation. So this
should be rephrased.

Page 27982: Is the choice of saturation vapor pressures of ELVOC and SVOC affecting the results and on what are the chosen values based on?

Page 27982, lines 2-4: “In order to not systematically underestimate the total particle volume concentration, the formation of the five condensable compounds were multiplied with a fixed correction factor of two.” Where is this factor of two coming from? Based on figures 10 and 11, the modelled aerosol size distributions look totally different than the measured ones. Could it be that the factor should be different for ELVOC than for SVOC? It would change how Figure 14 looks like and based on this it would be impossible to say how different compounds contribute to SOA formation. I see this as a major weakness of this study. Although MCM provides good chemistry, it does not produce compounds with low enough volatility. So why to use such a mechanism to study SOA formation?

Page 27983, lines 1-2: Is sulfuric acid condensing on the walls?

Page 27983, lines 24-26: I cannot see a clear diurnal pattern in Figure 3. Was there a period with lights totally off?

Page 27984: Why is the measured condensation sink used to calculate the condensation of sulfuric acid and nitric acid if modelled total number and volume distributions agree with measured ones? If the shape of particle size distributions totally differs, does it mean that properties of condensing compounds are not representative of actual compounds? If there is no ammonia, is nitric acid even condensing?

Page 27985, lines 14-15: What does this UV intensity correction mean? Is the correction 80% within every day so that correction is 0% when UV-lights are turned on every day, and growing linearly to 80%, or is it 0% in the day1 and grows to 80% on day4?

Page 27986: If SO2 concentration measurements are missing, why to speculate reasons for differences between modelled and measured sulfuric acid concentrations?
Page 27989: There is discussion on “Sub-3 nm particles”, but in the text and figures it is stated that concentrations are total for particles larger than 1.6nm. It should be made clear what is meant here.

Page 27991: What makes such a big difference between modelled total aerosol particle volumes when only nucleation method is changed? Still the total SOA should be approximately the same.

Page 287992: Why is SVOC contribution to aerosol total volume much lower on day 4 than on day 3?

Figures: Figures 8 and 13 are difficult to read and all information is actually in Figures 7 and 11, so these could be removed.

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