**Atmospheric
Chemistry
and Physics
Discussions**

Interactive
Comment

Interactive comment on "On the influence of fuel sulfur induced stable negative ion formation on the total concentration of ions emitted by an aircraft gas turbine engine: comparison of model and experiment" *by* A. Sorokin et al.

A. Sorokin et al.

Received and published: 30 June 2004

On the Influence of Fuel Sulfur Induced Stable Negative Ion Formation on the Total Concentration of Ions Emitted by an Aircraft Gas Turbine Engine: Comparison of Model and Experiment By A. Sorokin, F. Arnold and P. Mirabel

Answer to referees

General comment: It seems that some of the referees have not seen the detailed description of the model used here. We recall that this model was given in the article : Emission of ions and charged soot particles by aircraft engines by Sorokin et al., Atmospheric Chemistry and Physics, Vol. 3, pp 325-334, 2003. The experimental

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

results to which this article refers and which were not yet published at the time we submitted this article are now published: H. Haverkamp et al., Positive and negative ion measurements in jet aircraft engine exhaust: concentrations, sizes and implications for aerosol formation , Atmospheric Environment, 38, 2879-2884 , 2004. Additional information on the Partemis measurements campaign ca be found in: Wilson et al., Measurement and prediction of emissions of aerosols and gaseous precursors from gas turbine engines (PartEmis): an overview, Aerospace science and technology, 8, 131-143, 2004.

We do agree with the referees that the development of a detailed model of chemiions and charged soot particles formation in an aircraft engine combustor is an important but difficult task since the output of the model depends on many kinetic processes occurring in the combustor.

However, we did not intent to present such a detailed model in this article. The development of such a model which should include detailed hydrodynamic flow, kinetics of combustion and ion-molecule interactions, soot formation processes etc., is for the moment out of scope, because of the high complexity of the processes involved, of the absence of completely documented database for ion-molecular rate coefficients. In addition, very few experimental measurements are available to validate the models.

To our knowledge, the only relevant publications dealing with ion formation and evolution in an aircraft engine are those of Starik et al. (Aerospace Sci. Tech., 2002, mentioned by one referee) and Sorokin et al., (2003) on which our simulation was based. The article by Starik et al. uses a large number of reactions (over 400 for ionic species), however for most of the reactions of ionic species, only the forward reactions are considered and the reverse reactions, which are clearly important at the high temperatures encountered in a combustor, are not taken into account. In addition, soot thermo-emission was not considered, although it is a very important process at these temperatures. On another side, the model by Sorokin et al. uses only a very simplified chemistry, but includes detailed description of electron thermo-emission, electron

attachment to soot particles and to neutral molecules, electron-ion and ion-ion recombination, ion-soot interaction.

Referee # 1 raised the question of the comparison between Starik's results and our model results. Starik's et al model computes a total ion emission index EI of 2.1015 ions per kg of fuel burned at cruise altitude. To our knowledge, this value has never been validated since no measurements are available under these conditions.

Our model predicts, for a well identified engine on the ground, emission index EIi of (1 - 3)x1016 ions per kg of fuel, value which compares very favorably with the measurements made on the same engine, on the ground, leading to an emission index of (2 - 8) x 1016 ions/kg(fuel) (Arnold et al., 2000 ; Sorokin and Mirabel, 2001). Our model results are also in very good agreement with the recent measurements made during the Partemis campaign: EI = (1.2 - 2) x 1016.

Referee # 2 notes that "the formation is not modeled at all, Three different values of ion production are evaluated as inputs to the model". Referee 3 expresses approximately the same concern.

In spite of its apparent simplicity, our model is able to accurately predict emission indexes for the total amount of ions. Starik's model uses hundreds of reactions, but the initial chemiionization step reduces to a single reaction (formation of CHO+ and electrons from CH radicals). This is quite equivalent to the situation in our model where the ion production rate is parameterized by Q(t), the number of chemiions produced in cubic centimeter per second, which is time dependant in the combustor. Sensitivity studies given in our previous publication (Sorokin et al., 2003) have clearly shown that any increase of Q over a value of approximately 1015 ions cm-3s-1 do not lead to any change of the ion concentration at the combustor exit due to the self-limiting effect of ion-ion recombination. Therefore, the output of the model is quite insensitive to the value of the ion production rate (as long as Q(t) $>$ 1015 ions cm-3s-1 for the given engine) and a simple parametrization leads to very satisfactory results.

We cannot agree with the argument of referee # 4 that the "model was set up to yield agreement with the experimental observations". The model was published in 2003 (and therefore developed before), prior its use in the Partemis project. In fact it was first used to model the ion measurements reported by Arnold et al. (2000), in complement to the work done in the plume (Sorokin and Mirabel, 2001). Furthermore, in our model, only the rate of ion production is parameterized, the other processes (electron thermo-emission, electron attachment to soot particles etc.) are fully taken into account : see a description of these processes and formulas used in Sorokin et al., (2003). Since our model consists of four coupled differential equations, each equation having several terms, it would be surprising that this model was developed only to yield agreement with some specific experimental observations. The discussion about the "over parameterized model input" has been given above.

Referees # 2 and 3 state that the conclusion of this paper is almost trivial: increasing the amount of sulfur in the fuel will increase the amount of sulfur bearing ions.

First of all, it is still nice that the model can reproduce trivial things. What is less trivial is that all the processes modeled (ion-electron, ion-ion interaction etc.), are highly non linear. Figures 3 and 4 shows that the electron detachment efficiency has an impact not only on the negative ions, but also on the positive ions.

In conclusion, some modifications will be made to the article. The abstract will be refocused, the description of the model slightly modified and the reference list will be actualized.

Interactive comment on Atmos. Chem. Phys. Discuss., 3, 6001, 2003.

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper