Subject: plasma chemistry round-robin test call

Dear Colleagues,

The need for a community-wide activity on validation of plasma chemical kinetics in commonly used gases has been clearly identified. As you might know, this need was again expressed in the discussion about developing a COST Action on plasma chemistry at a workshop held in Eindhoven earlier in the year. Miles Turner is coordinating this work.

As a preliminary to the eventual COST action, we would like to propose a round-robin to assess the consistency in results of calculations from different participants in a simplified system. The main purpose is to get an idea of the variation in results from different groups for the same simple system.

We are very interested in hearing your comments to this proposal and on your suggestions for how to make it more worthwhile. Here is our specific proposal (to be refined after hearing your thoughts):

What is a round-robin? A set of conditions and parameters will be identified and anyone interested in participating is welcome. Participants will be asked to calculate specific species concentrations using a zero-dimensional model of their choice for a given set of parameters (gas composition, pressure, electrical power input, etc.). One person will collect the results and distribute them anonymously to all participants. Thus, everyone will see all results but no names will be attached. In light of this comparison, some participants may choose to refine or correct their results. This is perfectly acceptable and the round robin will continue until everyone is satisfied that they have done the best calculation possible – or until the deadline has been reached.

What comparisons should be made? We propose to perform a first round of calculations in a simplified, zero-dimensional system in dry synthetic air (N2:O2 = 4:1), at atmospheric pressure at ambient temperature for a given electrical input power. There are two aspects to this comparison – one is the choice of the plasma chemistry model and the other is the choice of the software used to solve the rate equations. As a prelude, it would probably be useful compare results for a given, and extremely simplified plasma chemistry so as to identify differences due only to the solver used. Then we would move on to synthetic air where all participants would define themselves the plasma chemistry and rates to be used in their calculations.

What should be the calendar?
October 6, 2016: collection of replies to the announcement with comments on the exact definition of the problem to be solved by the participants.
October 12, 2016: LXCat discussion session at the GEC in Bochum (19h-21h). We will aim to close the session with a brief discussion of the round-robin, hopefully having defined the exact problem by that time.
March 1, 2017: completion of first round.
October 1, 2017: completion of second and following rounds and presentation of results (anonymously) at the GEC. All round-robin participants so desiring will be co-authors of the GEC presentation. Decision about publication.

Looking forward to hearing from you!
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