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Interactive comment on "Assessment of the reduction methods used to develop chemical schemes: building of a new chemical scheme for VOC oxidation suited to three-dimensional multiscale HO_x-NO_x-VOC chemistry simulations" *by* S. Szopa et al.

Anonymous Referee #1

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The paper discusses reduction methods for the organic part of reaction mechanisms for the gas-phase of the troposphere. The reduction is based on a reference reaction scheme that describes the chemistry in all details, if possible on the level of elementary reactions. The paper presents a rule-based approach for the reduction which is then automatically done by a computer program. Despite increasing computing power the

size of the chemical reaction mechanism is still a limiting factor for 3d chemistry and transport models (CTM). Therefore reduction of a large mechanism is always necessary. The paper presents a substantial contribution towards a clearer and more objective approach to implement chemistry in CTMs. The paper fits well within the scope of ACP.

There a number of points that requires clarification. a) abstract, l(ine)3: What is meant by " different scales" b) The abstract should already make reference to the preceeding article by Aumont et al., where the method is presented, by which the detailed mechanism (reference mechanism) is generated. c) p 758,l 5; "..at different scales" To be useful in CTMs the reaction mechanism must be applicable to ALL chemical regimes encountered in the model domain (in space and time). d) p 758,l 7:"No attempt" This is a very severe limitation, which is often simply forgotten by the users of the reduced model. Since the latter contains reaction of aldehydes, ketones peroxides, etc, model results for these compounds are interpreted as meaningful output of the model simulation. It would be helpful in this matter, to clarify with help of the simulations for the scenarios of the paper to what extend mixing ratios of those compounds are quantitatively modelled. Without such a statement the reduced scheme has a very limited range of application. e)p 759,l 22: "Modifications.." Please, be more specific. How does the program decide what a " closest structure " is. f)p 759,l 25: "Mass conservation"? Does this imply "C-conservation" g)p 760,l 14: " Correlation" Here one needs a statement about agreement or discrepancy in absolute terms (for example slope, correlation, and offset) The description of the pre-reduction is rather brief and needs to be extended in order to be understandable. h)p 761,l 26: In the presence of long-lived compounds like methane, CO and small alkanes the system cannot reach a stationary state within several days. i)p 762,section 4: Comparison of simulations with the full and the reduced scheme are necessary to assess the validity of the reduction. Comparison with field data are questionable, because disagreement can always be attributed to the use of an inadequate meteorological model. It is not clear to me what one can learn about the reduction of reaction mechanisms from such a comparison. j) p 764,l 10-20:

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Does the grouping into classes conserve carbon? If not, how large is the violation? k)p 765,l 12: What is the inorganic imbalance? l)p 766,l 5-p 767,l 14: I have difficulties to understand what has be done. m)p 771,section 6: Before comparing simulations with the full and the reduced scheme, one would like to learn more about the impact of the inorganic chemistry including the reactions of CO, methane, and HCHO. These compounds are not directly influenced by the reduction. What is their influence on the OH-reactivity, the burden of ROx, the formation of ozone In other words, how large is the remaining contribution of the other organic chemistry that underwent reduction? This information for all scenarios would set the frame with respect to which the deviations between full and reduced scheme should be assessed. For example, I presume that for the clean air cases (relaxation scenarios) the contributions of the latter are only minor and negligible differences between the full and reduced scheme are to be expected independent of the reduction method.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 755, 2005.