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Interactive comment on "Accelerating simulations using Direct Relation Graphs for atmospheric chemistry mechanism reduction" *by* Zacharias M. Nikolaou et al.

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This paper presents an interesting approach to chemical mechanism reduction. The series of mechanisms used for air quality modeling include the Regional Atmospheric Chemistry Mechanism (RACM), the Carbon Bond Mechanism and the Statewide Air Pollution Research Center Mechanism (SAPRC) and these are reduced mechanisms. The reduction process used by the mechanism developers has not been a formal process like the one discussed by the authors. Mechanism developers have used a process based on chemical knowledge and the simulation of many environmental chamber experiments to develop their reduced mechanisms. Sometimes mechanism develop-

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ers used their mechanisms to simulate results of simulations made with highly detailed, very explicit mechanisms or to make simulations of field observations. Most often box models are used in these simulations to eliminate (or ignore) the impact of meteorology on the chemistry. Developers add and subtract species, reactions and entire chemical reactions schemes from their reduced mechanisms until the simulations adequately fit the results of environmental chamber experiments, simulations made by very explicit mechanisms or field observations. The aggregated species used in the reduced mechanisms, such as those in RADM, are used to simplify the representation of atmospheric chemistry. The selection of the model species and their corresponding reactions can affect the mechanism's ability to simulate particular domains. For example, early versions of Carbon Bond and SAPRC were designed to simulate highly polluted urban regions and they would not have been accurate for regional or global atmospheric simulations. The design goals of the developers could be considered to be a source of bias in the reduced mechanisms. However, possible design bias is not limited to the developers of RACM, Carbon Bond or SAPEC. The authors should point out clearly that there is no single skeletal mechanism. There are in fact, many possible skeletal mechanisms that may be generated from a larger atmospheric chemistry mechanism. A skeletal mechanism for ozone simulation will be very different than one for the modeling of acid deposition. A skeletal mechanism for acid deposition would be based on the mechanism's ability to simulate sulfate, nitric acid, organic acids and aqueous phase oxidants (H2O2 and organic peroxides). The two skeletal mechanisms would be expected to be very different even if the two skeletal mechanisms were derived from the same source mechanism. The same could be said about a skeletal mechanism for the simulation of secondary particulate matter formation. A potential user must realize the dangers in using a skeletal mechanism for ozone as a general propose atmospheric mechanism in a global or regional model. I believe that the authors' overall approach is valid to produce an ozone skeletal mechanism. But I recommend that a wider variety of conditions that range from relatively clean to the highly polluted be used for the box modeling. Also, in the WRF-Chem modeling, a range of

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altitudes (layers) from the surface to the upper troposphere should be considered in the authors analysis and evaluation because RACM was designed to be valid over this range too. The authors might write something about applying their methods to highly explicit chemical mechanisms. A. Kaduwela, D. Luecken, W. Carter and R. Derwent. New Directions: Atmospheric Chemical Mechanisms for the Future. Atmospheric Environment, 122, 609-610, (2015), propose that very explicit chemical mechanisms be developed first and then objectively reduced to develop new reduced mechanisms for regulatory modeling. The authors approach could be useful in providing a suite of skeletal mechanisms for ozone, PM and other pollutants. I must note that there has been much research from combustion that has been applied to the reduction of atmospheric chemical mechanisms. For example, Michael J. Pilling and his colleagues have been particularly active. For example, see the paper: A.C. Heard, M.J. Pilling and A. S. Tomlin, Mechanism Reduction Techniques Applied to Tropospheric Chemistry, Atmospheric Environment, 32, 1059-1073 (1998). The authors should improve their discussion of prior research. Finally, J is not a photolysis rate rather it is a photolysis rate coefficient (or photolysis frequency and its units are reciprocal time). A photolysis rate is the product of J and the chemical species that photolyzes. Please correct this in the paper.

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