General comments:

The work conducts comprehensive comparison of different cluster dynamics-based parameterizations for SA-DMA nucleation by integrating box-model simulations, 3-D modeling, and in-situ observations. It is found that ACDC_DB performs well in modeling 3-D NPF for both winter and summer in Beijing and shows promise for application in various atmospheric environments. Furthermore, ACDC_RM_SF0.5 exhibits effective applicability at ~280 K, but has limitations in predicting $J_{1.4}$ at elevated T. While Dynamic_Sim is applicable for simulating NPF in polluted atmospheres but makes significant overestimation of $J_{1.4}$ under conditions of high T and low CS.

The topic discussed in this paper is highly meaningful for developing parameterizations for various nucleation systems. The reported results are clearly presented and are relevant to the scope of *Atmos. Chem. Phys.* I recommend publication of this manuscript after consideration of the following comments.

Specific comments:

1) Lines 94-95: Please explain briefly the reason for considering such three simplifications within Dynamics_Sim.
2) Line 281: To make a clear understanding among readers, it would be better to provide the concept of the chemical initial and boundary conditions in WRF-Chem/R2D-VBS simulations.
3) Figure 6C: It can be noted that ACDC_DB and Dynamic_Sim also exhibit an underestimation of averaged PNSDs in the 2-100 nm range in comparison to observation. Can the authors account for the cause of this phenomenon?

Technical corrections:

1) Lines 143-144: "*n* and *m* represent the number of SA and DMA molecules in a cluster" should be "*m* and *n* represent the number of SA and DMA molecules in a cluster".
2) Lines 465 and 482: "ACDC_RM" should be "ACDC_RM_SF0.5".
3) Supporting Information, lines 37 and 38: "A: ΔG = 13.5 kcal/mol; B: ΔG = 12.9 kcal/mol" should be "A: ΔG = -13.5 kcal/mol; B: ΔG = -12.9 kcal/mol".